A Mathematical Analysis of Reaction Diffusion Systems in Chemical and Biological Reactors with Macro and Micro Structures

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by

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To my parents Kanti and Olga Parshotam and to my loving wife Kavita

Declaration

This thesis is submitted to Massey University and has not been submitted for a higher degree to any other University or Institution.

Aroon Parshotam

Aroon Parshotam

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Abstract

This thesis is concerned with generalised models for biological and chemical reactors such as the tubular, fluidised, fixed, packed, continuously stirred and trickle bed reactors.

Suppose n chemical components at concentrations C_i ($i = 1,2,..,n$) are "diffusing" and reacting in a homogeneous incompressible fluid with a known velocity profile $u(z)$ independent of C_i so that in the reactor region Λ, $div\ u$ is zero. Immersed in the fluid may be a uniformly distributed population of particles which absorb these chemicals and act as local sites for reaction-diffusion phenomena. The particles are sources and sinks for the chemicals C_i in the fluid and these fluid concentrations govern the boundary conditions for the particle or local behaviour.

A system of equations is set up as a general model for these complex interactions. The principle limitations of this model are firstly that $u(t, z)$, the velocity profile in Λ is known and not coupled with the concentrations C_i in any way, and secondly the particles are assumed to be fixed relative to the coordinate system of z in Λ and sufficiently small so that a representative sample of them can be taken to be in a spatially constant concentration environment in Λ.

The objectives of this thesis are generalised comparison theorems for these systems which are used to prove uniqueness, existence, stability and other general qualitative features of such models. A number of examples from literature are examined.

Models conforming to the system described in this thesis have applications in biological wastewater treatment, biochemical manufacture, urea removal by the compact artificial kidney and industrial fermentation processes. Other potential modelling areas concern fertiliser or pollutants diffusing in soil moisture and reacting with soils, oxidation with product formation in waste deposits and industrial ore reduction processes. There are many other industrial and environmental problems with similar interacting macro and micro structures. These include the catalytic cracking and synthesis processes in chemical industries ranging from the making of synthesis gas from coal to oil refining.

1

General Introduction

1.0 Introduction

This chapter introduces the physical problem. In section 1.1, we give some examples of chemical, microbiological and biochemical reactors, briefly discussing how and where they may be utilised and giving some details of their dynamical biochemical, microbiological and chemical aspects. Many of these reactors have in common macro and micro structures. This is an important theme of this thesis. Our principal motivating example in this study is the fluidised bed biofilm reactor (FBBR). In section 1.2, we introduce the plan of this thesis and in section 1.3, discuss some of the new contributions presented. In section 1.4, we discuss some other potential modelling areas and in section 1.5, survey some relevant literature.

1.1 The Physical Problem

This thesis is concerned with generalised models for systems of reaction-diffusion equations based on the dynamics and structure of biological and chemical reactors. Typical of these reactors are: (a) the tubular reactor, within which homogeneous reactions are often conducted; (b) the packed bed reactor, often used to conduct heterogeneous catalyzed reactions; (c) the stirred vessel, operated batchwise, semibatchwise, or continuously (CSTR); (d) the fluidised-bed reactor (FBR), and (e) the trickle bed reactor. These are schematized in FIG. 1.1 and are described in detail by CARBERRY [45].

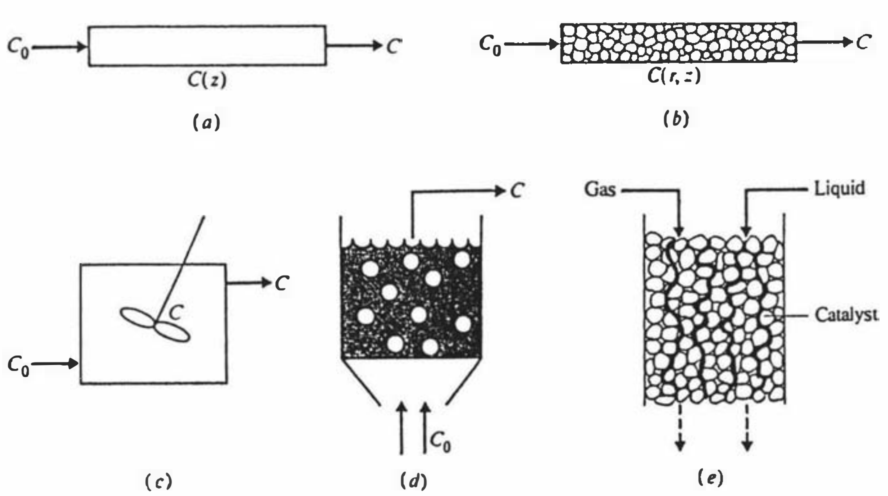


FIG. 1.1 Diverse reactor types: (a) tubular (b) packed bed (c) CSTR (d) fluidised bed (e) trickle bed.

The problem of heat and mass transfer in packed and fixed bed reactors with irregularly shaped porous catalyst particles was studied extensively by ARIS [19]. In fact, much of this work in chemical reactor theory has contributed significantly to the mathematical theory of diffusion, reaction, heat transfer and mass transfer.

An analysis of diffusion in biological particles using this chemical reactor theory was first proposed by ATKINSON and DAOUD [25], where immobilised cell particles were treated as catalytic slabs. Other authors extended this chemical reactor analogy to microbiological and biochemical reactors such as the fluidised bed biofilm reactor (FBBR) (SHIEH *et al.* [261-266]). Many of the well established procedures for heterogeneous chemical catalytic reactor modelling can be adopted to reactors such as the FBBR (RAO BHAMIDIMARRI *et al.* [242]). This is because there are analogies between chemical reactions and properties of certain biological systems. One such analogy is rather obvious: we may consider living organisms to be a dynamic structure built of molecules and ions, many of which react and diffuse. However, unlike most chemical reactions, enzymic reactions in microbiological and biochemical reactors are mainly isothermal (CHANG [68]). In general however, many concepts such as the effectiveness factors for general reaction rate forms have analogous definitions for chemical, microbiological and biochemical systems (SHIEH *et al.* [261-266]). The effectiveness factor (defined as the rate of reaction divided by the rate which would occur with no resistance to component transfer inside or outside the particles) is an important parameter in reactor designing. It has been useful as a rough estimate of intraparticle diffusion effects in particles such as porous catalysts, flocs, solid spherical supports and adsorbent particles. The effectiveness factor is also used in lieu of extensive numerical calculations in these particles. There are many other such analogies and it is now acceptable to consider microbiological and biochemical reactors with procedures and concepts developed for heterogeneous chemical catalytic reactor modelling (ATKINSON [26], BAILY and OLLIS [30]). Since this thesis is concerned with generalised models for such reactors, we do not specify in great detail the parameters for every special system. However we do go into detail with the fluidised bed biofilm reactor (FBBR) as a motivating example in order to get an understanding of the physical problem.

The Fluidised Bed Biofilm Reactor (FBBR)

The fluidised bed biofilm reactor (FBBR) is a biochemical processing system with applications to biological wastewater treatment and biochemical manufacture (JERIS *et. al.* [134] and ATKINSON [26]). It is a high energy, high efficiency system in which the liquid to be treated is passed upwards through a bed of small particles such as activated carbon granules at velocities sufficient to fluidise the bed. Each particle of support material (activated carbon or otherwise) provides surface area for biological growth, resulting in a biomass for the whole bed, an order of magnitude greater than conventional dispersed growth systems. This growth is initiated by seeding the bed with microorganisms to form what is known as a biofilm around the support particles which establishes a miniature reaction-diffusion controlled chemical microsystem. The very high growth support surface afforded by these bioparticles results in denitrification of volatile solid concentrations as high as 30,000 mg l^{-1} and a bed detention time as low as 6 minutes for 99% nitrate removal.

It has been demonstrated in numerous pilot studies to be cost effective and has also been investigated at least to pilot scale for all of the basic treatment processes, including carbon oxidation, nitrification and denitrification for a variety of domestic and industrial wastewaters. A photo of a fluidised bed biofilm reactor (FBBR) is given in FIG. 1.2.

Models for all the reactors (except for the tubular reactor) discussed in this section have a system of reaction-diffusion equations appropriate to a microsystem coupled via boundary conditions to a system modelling a macrosystem composed of convection reaction-diffusion equations with additional source terms accounting for outputs from the particles. These convection reaction-diffusion equations provide the boundary conditions for the microsystem associated with the particles.

Such models for one system or another have appeared in the literature frequently during the last decade (MULCAHY *et al.* [199-202]; LIN [170]; LIAPUS and RIPPIN [169]).

They generally assume, as we do here that the fluid velocity distribution is divergence free, fixed and not coupled with the diffusion and chemical or biochemical processes.

FIG. 1.2 The Fluidised Bed Biofilm Reactor (FBBR)

In this thesis, an attempt is made to model such reactors both for the interpretation of performance characteristics and for successful process design. Mathematical models for such reactors are needed for the description of steady-state and dynamic behaviour for process design, optimisation and control. While insufficient detail can lead to a model incapable of accurately representing the reactor's response to changes in operating variables, too much detail can lead to a model that may be computationally impractical. From a purely analytical point of view, there is no more difficulty in increasing the number of model equations. However this may lead to an impractical model in that there may be too many parameters to identify from the operating data. The type of model and its level of complexity in representing the physical system, will depend on the use for which the model is being developed. We are simply presenting a generalised model for such reactors. These models turn out to have interesting and useful structural and mathematical properties.

The mass-heat analogy provides a useful basis for transferring mass transport results to heat flow problems. Structurally, the heat transport aspects are mathematically equivalent to another chemical component. Since our generalised models consider an arbitrary number of interacting chemical components, we may assume that one of these components is temperature. The theory developed in this thesis does not therefore exclude heat transfer considerations which are relevant to fluidised bed combustors and to mass transfer in nonisothermal reactors (see ARIS [20]) or even the fluidsed bed gasifier (MA [176]). Therefore, without loss of generality, we will only consider mass transfer models.

For convenience, we call reactors with the macro and micro structures described in this section, "Particle Reactors".

1.2 The Plan of this Thesis

In Chapter 2 we set up the coordinate systems and equations representing a generalised model for such a particle reactor. A system of equations is presented as a general model for these complex interactions. The principle limitations of this model are firstly that $u(t, z)$, the velocity profile in A is assumed to be known and not coupled with the bulk concentrations C_i in any way, and secondly the particles are fixed relative to the coordinate system of z in A and sufficiently small so that a representative sample of them can be taken to be in a spatially constant concentration environment in A.

In Chapter 3, we look at the unsteady state or time dependent problem. Generalised comparison theorems are developed and used to study questions of uniqueness, existence and other qualitative features of our models. We examine the stability of both the steady state and the unsteady state solutions and study links between stability behaviour and uniqueness of steady state solutions. The question of existence of solutions is examined by using some recently developed imbedding techniques (MCNABB [186]).

In Chapter 4, we look at the steady state or time independent problem. Here we study the question of existence of solutions by using the new techniques referred to in Chapter 3. We also study relationships between unsteady state or time dependent solutions and steady state or time independent solutions.

In Chapter 5, we show that linear models for particle reactors treated in this thesis are amenable to various algebraic and geometrical factorization transformations which dramatically reduce their dimensionality.

Linear systems of convection reaction-diffusion equations for these reactors have a structure which allows a geometric factorization of steady state problems giving a significant reduction in their dimensionality. Moreover, convection dominated linear systems with quasisymmetric reaction terms may be further simplified by matrix transformations which uncouple the differential equations. The boundary conditions are also uncoupled when the diagonal diffusivity matrix D governing diffusion in the particle is a scalar multiple of the corresponding matrix H describing the diffusivity characteristic of the fluid boundary layers around the particles. The dominant transient behaviour of the systems may be handled by establishing an analogous system of time independent equations for mean action time variables and higher moments. These equations have the same amenable structure. Outputs, time lags and various mean residence and first passage times associated with establishing steady outputs from a concentration free initial state, can be expressed in terms of the steady state solutions and mean action time variables.

In Chapter 6, a number of reactor models from literature are examined as examples of the theory developed in this thesis. Since some of these sections are taken from completed published papers without a lot of change, there may be repetition in the model development and problem description.

At the end of each chapter is a section on notes and comments where relevant literature is reviewed and where future mathematical work and ideas are discussed. At the end of this thesis is a references and bibliography section which includes papers which have been referred to in this thesis and papers which are not referred to but are still relevant to the subject matter.

1.3 New Contributions of this Thesis

The model structure presented in this thesis is novel in the way systems of reaction-diffusion equations appropriate to the microsystem are coupled via boundary conditions to systems modelling the macrosystem composed of convection reaction-diffusion equations with additional source terms accounting for outputs from the particles. Despite the complexity of this coupling, it is shown that many standard and classic methods for obtaining stability, uniqueness and existence of unsteady state and steady state problems can be extended to this problem. The principal result which makes these extensions possible is a generalised comparison theorem similar in type to those for weakly coupled parabolic and elliptic systems. In addition we develop some new techniques for our problem which can also be applied to elliptic and parabolic systems coupled in other ways.

Major results of this thesis are uniqueness, existence and stability theorems for solutions to the unsteady state and steady state problems. It can be shown that such results may be obtained by imbedding the general system which may obey no monotone property into a system of twice the order which does possess a monotone property. The monotone properties of these imbedded systems suggest the use of monotone iterative methods in obtaining existence of solutions and this in turn suggests new methods for numerical computation of solutions. It can fortunately be shown that stability, uniqueness and existence may be implied in the original system. As a result, our computed solution in the imbedded system also gives rise to a numerical solution of the original system. This imbedding idea is relatively new and is also useful in generalising many qualitative features such as the relationships between parabolic and elliptic equations to parabolic and elliptic systems of equations. This idea is even shown to be useful in solving algebraic equations by monotone iteration.

We show that linear systems of convection reaction-diffusion equations for these reactors have a structure which allows a geometric factorization of steady state problems giving a significant reduction in their dimensionality. These equations are also amenable to algebraic uncoupling transformations which reduce the dimensionality of the problem and which simplify the tasks of obtaining analytic and numerical solutions or estimates.

The recent concept of mean action times (MCNABB and WAKE [190]) for scalar equations is generalised to systems of equations and factorization and uncoupling techniques may be also applied to an associated linear system for vectors composed of the mean action time variable for each chemical component. These vector functions give the time lags for the various chemical outputs of the system during its transition from one steady output mode to another and the mean first passage times, mean particle residence times and higher moments associated with tracer pulse inputs of the chemicals.

Such results also apply to systems of reaction-diffusion equations where there may be no coupling in the boundary conditions and also provides us with ways of uncoupling parabolic and elliptic systems.

Our comparison theory is also shown to be useful in developing some techniques for obtaining upper and lower pointwise bounds to solutions. These prove to be favourable compared to results obtained by orthogonal collocation and standard finite difference methods. The bounds provide us with some qualitative features of solutions of such equations and also prove to be excellent as approximate solutions.

1.4 Other Potential Modelling Areas

There are a myriad of applications for such macro micro structure models in different disciplines as diverse as geology and mining, medicine, agriculture, chemical and biochemical industries and environmental technology. We give a brief description and references of some of these that have come to our attention.

Our first example concerns industrial fermentation processes which may be both aerobic and anaerobic. Such processes involve a general class of chemical changes produced in organic compounds (substrates) through the activity of micro-organisms and include various alcohol fermentations and the production of acetic acid (vinegar), lactic acid, citric acid and gluconic acid, as well as acetone, butanol and glycerol. Microorganisms have the potential to achieve almost any conversion, involving water soluble organic compounds by means of complex sequences of enzyme catalysed reactions.

The basic fermenter types are usually discussed using terminology establised for chemical reactor theory, namely: (a) the batch fermenter (BF); (b) the continuous stirred-tank fermenter (CSTF); (c) the tubular fermenter (TF) and (d) the fluidised bed fermenter (FBF).

Many biochemical conversions are not achieveable in the absence of microorganisms and continuous fermenters which use suspended organisms suffer from the fact that these organisms can simply be 'washed out'. Continuous stirred-tank fermenters (CSTF) are limited in throughput as a result of this phenomena and tubular fermenters (TF) with suspended flocs, become an impossible arrangement without a constant resupply of microorganisms at the inlet. An alternative answer to the last problem is the fluidised bed fermenter (FBF) (ANDREWS and PRZEZDZIECKI [17], ATKINSON [26], PARSHOTAM *et al.* [224]) which is a hybrid between the stirred tank fermenter and the tubular fermenter, in which the microbial particles are suspended by the upflowing liquid stream and gravitational forces prevent them from being swept away (elutriated).

The end products of industrial processes involving microorganisms are more microbial mass and various biochemicals, one or several of which may be recovered. The main classes of biochemical products from industrial fermentation processes are antibiotics, steroids, vitamins, enzymes and organic acids (AIBA *et al.*[2]). The microbial mass produced concurrently with the biochemicals is largely a waste product but may be used as an animal feed supplement in view of its protein content (LOEWY and SIEKEVITZ [172]). Occasionally, the production of microbial mass is a major objective, as with baker's yeast and the removal of organic impurities from polluted water.

There are other potential modelling areas which are similar in principle to the FBBR and have a similar interacting structures as particle reactors. An example of such a system is the Rotating Cylinder (RC). This is a biological system where a cylinder is covered by layers of microorganisms held in place by extracellular material around a support rotating cylinder. As with the FBBR, the biological rotating cylinder is also an ingeneous method of removing non-settleable organic contents of wastewater. It is however more ideal on a small scale. The system involves lowering a rotating cylinder into a stream of wastewater which is being pumped through the rotating cylinder bath. The cylinder acts as a medium that provides a large surface area for microbial growth and if it is not fully submerged, it gets well aerated. Substrate diffuses through this biofilm and the organic content is converted into growth of these organisms which can be separated more easily. There are also gases, such as CO_2 being produced by these organisms in aerobic respiration which escapes to the atmosphere. As with the FBBR, the cylinder may be temporarily removed and cleaned and the separated biomass wasted as excess sludge. The Rotating Biological Disk Contactor Plant is similar to the rotating cylinder but where slabs are covered by a thin biofilm consisting of layers of microorganisms held in place by extracellular material. This provides more surface area for biological film growth (see FIG. 1.3). Both these reactors involve reaction diffusion systems within the biofilms with boundary conditions given by concentrations in the bulk fluid.

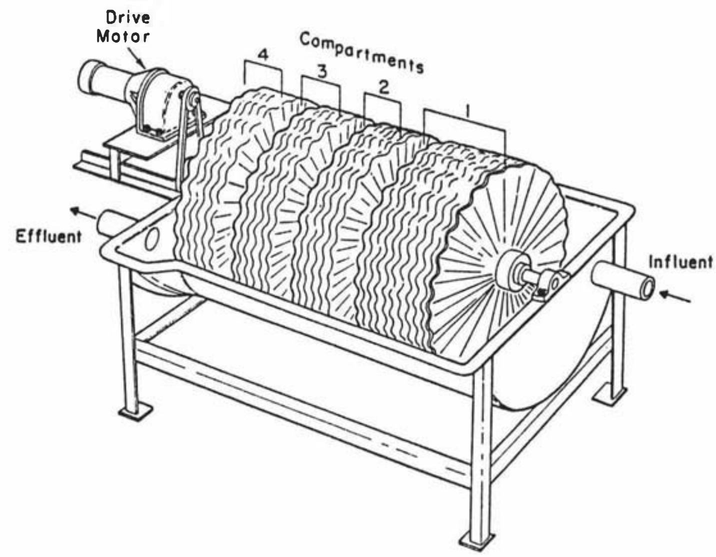


FIG. 1.3 The Rotating Biological Contactor Plant

A medical application concerns modelling urea removal by the compact artificial kidney (LIN [170]) and an example of this system will be seen in Chapter 6. There are perfusion models of chemicals and tracers through various organs such as the liver and muscle tissue. These sometimes involve a hierachy of structures for instance in the muscle tissue model, chemicals in the blood are transferred from the capillary system by diffusion into the interstitial fluid and then into the muscle cells. Each of these systems introduces a new dimension in the model.

For petrochemical industry applications see ARIS [20, 21]. Here the use of catalytic reactors and the consequent availability of many inexpensive chemicals, makes the synthesis of a variety of organic acids and solvents commercially attractive. By contrast to the petrochemical industry, we find that studies into aternative fuel sources from agricultural products such as in the production of the solvents acetone, butanol and ethanol (ABE fermentation) in immobilised cell packed bed reactors from whey permeate also involve models with similar interacting macro and micro structures (QURESHI [236]).

Other potential modelling areas concern fertiliser or pollutants diffusing in soil moisture and reacting with soils. Interest in the transport of chemicals in soils is motivated by the potential of agricultural and other chemicals (fertilizers, pesticides, industrial wastes) to move from the soil surface through the unsaturated zone toward the groundwater table. Studies of solute transport in soil adsorption columns (VAN GENUCHTEN and PARKER [288]) also result in model equations with interacting macro and micro structures which are coupled in the boundary conditions.

Solute transport studies involving layered media are also important for investigating how restricting layers affect rates of solute migration in the soil profile and, more generally, for examining the influence of soil heterogeneity on solute transport. The leaching of solutes in the unsaturated zone may be affected greatly by the presence of soil layers. Soil stratification is a natural phemenon that is common to many soils. Also, artificial barriers (e.g., clay liners) are often used to slow down or prevent the movement of certain chemicals. There has been considerable attention focused on solute transport through homogeneous soils and some work on heterogenous or multiple layered soil profiles which are approximated by a series of homogeneous soil layers (SELIM *et al.*[259] and LEIJ *et al.*[165]) each having its unique physical and chemical characteristics. The resulting mathematical models in literature usually involve one dimensional dispersion advection equations involving single chemicals such as a herbicide diffusing in up to three layers

(LEIJ *et al.*[165]). Boundary conditions are necessary in order to maintain the solute concentration continuity at the boundary between any two soil layers and there is much discussion about the boundary conditions (VAN GENUCHTEN and PARKER [288], LEIJ *et al.* [165]) . Usually the boundary condition at the interface of one layer is given by the solution to the dispersion advection equation in the adjacent layer. Such equations are also found in models of fluid flow through multiple porosity, multiple permeability media that do not necessarily have to be layered (LIU [171]). This problem is interesting because it does not involve interacting macro and micro structures found in this thesis but it still involves the coupling of reaction diffusion equations in the boundary conditions. We can apply our theory without difficulty to systems of reaction advection dispersion equations in multilayered soils, multiple porosity and multiple permeability media. These may all include solute adsorption and desorption.

There are many industrial, geological and environmental problems concerned with interacting macro and micro structures. These include catalytic cracking and synthesis processes in chemical industries, ore reduction (MCNABB [184, 185]), groundwater and geothermal modelling, the making of synthesis gas from coal (KATO and WEN [136]), the mining of methane gas from coal beds, the oxidation with product formation in waste deposits, combustion theory and various oil refining processes.

1.5 Notes and Comments

There is considerable literature on the fluidised bed biofilm reactor (FBBR). A history of its development, its design and operating conditions is given by RAO BHAMIDIMARRI [241]. Some other examples of fluidised bed reactors from literature are given by ANDREWS [16, 17], BOSMAN [42], CHUNG and WEN [71], COOPER and ATKINSON [77], DENAC *et al.* [82], FOSTER [92], HANCHER *et al.* [113], JERIS and OWENS [134], KORNEGAY and ANDREWS [147], MULCAHY *et al.* [199-202] and SHIEH *et al.* [261-266].

There is considerable literature on the effectiveness factor for particles in chemical and bichemical reactors. Some examples are given by ANDREWS [18], ARIS [21], BISCHOFF [38], CHANG [67], CHURCHILL [72], GOTO [107], LEE and TSAO [163], MOO-YOUNG and KOBAYASHI [198], ROBERTS and SATTERFIELD [249], SHIEH *et al.* [261-266], STEWART and VILLADSEN [275] and WADIAK and CARBONELL [300].

It should be noted that such mechanistic models described in this section are not the only models available and that control models that treat such particle reactors as a black box also prove to be very useful (KHANNA and SEINFELD [144]).

Our results on reaction diffusion systems in this thesis may also be applied to population dynamics (LADDE *et al.* [153, p. 181], ZHENG [311, 312], PAO [214]) and bacteriology (PAO [218]).

2

Model Development

2.0 Introduction

In section 2.1, we shall set up the coordinate system, the spaces and the notation for our generalised particle reactor model that will be required for our model development. These shall be used throughout this thesis.

A system of equations together with their initial and boundary conditions is set up as a generalised particle reactor model for the complex interactions in a particle reactor. The various types of equations and their various boundary conditions will be examined and the assumptions and limitations of this model will also be discussed.

Finally, in section 2.2 we shall discuss some relevant literature.

2.1 Generalised Particle Reactor Model Development

A reactor occupies a fixed region Λ in R^3 space and z denotes the coordinates of a point in Λ. Fluid flows through Λ with a solenoidal fluid velocity distribution $u(z)$ which in general may vary with time. The boundary $\partial\Lambda$ of Λ is subdivided into three surfaces $\partial\Lambda_1$, $\partial\Lambda_2$ and $\partial\Lambda_3$ where fluid flows into Λ through $\partial\Lambda_1$ and out through $\partial\Lambda_3$, while $\partial\Lambda_2$ is impervious to fluid. If n_i denotes the outward normal to $\partial\Lambda_i$ and $\upsilon_i=|u\cdot n_i|$, then for all time

$$-\upsilon_1=u\cdot n_1 \leq 0 \text{ on } \partial\Lambda_1,\ \upsilon_2=u\cdot n_2 = 0 \text{ on } \partial\Lambda_2 \text{ and } \upsilon_3=u\cdot n_3 \geq 0 \text{ on } \partial\Lambda_3. \quad \textbf{(2.1.1)}$$

The reactive particles are fixed relative to the z-coordinate system at all time t and Ω is a representative active region per unit volume occupied by the particles at a point z in Λ. In this sense, the region Ω is multiply connected and it represents the shape of this biomass around the various particles one would find in a small neighbourhood around z, i.e., it represents the region occupied by N particles of various sizes and shapes, where N is the number of particles in unit volume of fluid. The particles and this region Ω are assumed to be small enough so that bulk fluid concentrations are constant spatially about Ω. We also assume Ω is independent of z (the particles are uniformly mixed and distributed) and the particles do not change position significantly with time. This is not an unrealistic assumption for fluidised beds with a stratified structure and is obviously justified for packed bed reactors. This active region is assumed to have an inner boundary $\partial\Omega_1$ enclosing inert cores and on which

$$\frac{\partial c_i}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda, \quad \textbf{(2.1.2)}$$

where c_i is the concentration per unit volume in Ω, of the ith chemical component. These concentrations are assumed to be governed by a system of weakly coupled reaction-diffusion equations

$$\frac{\partial c_i}{\partial t} - D_i \nabla_x^2 c_i = f_i(t, x, c_j) \text{ in } (0, T] \times \Omega \times \Lambda, \tag{2.1.3}$$

where x denotes points in Ω relative to a suitable coordinate system, ∇_x^2 denotes the Laplacian operator in Ω space, D_i is the appropriate diffusion coefficient for the ith component and $f_i(t, x, c_j)$ are Lipschitz continuous functions in c_j. On the outer boundary $\partial\Omega_2$ of Ω, the concentrations interact with the fluid concentrations $C_i(t, z)$ according to boundary conditions

$$D_i \frac{\partial c_i}{\partial n} = H_i(C_i - c_i) \text{ on } (0, T] \times \partial\Omega_2 \times \Lambda, \tag{2.1.4}$$

where $\frac{\partial c_i}{\partial n}$ denotes the gradient of c_i on $\partial\Omega_2$ along the outward normal and the positive constants H_i are mass transfer coefficients associated with boundary layer transport. The units for c_i and C_i are assumed to be compatible so that when $c_i = C_i$ on $\partial\Omega_2$, there is no flux across the boundary layer. We see that the concentrations c_i depend not only on x and t, but also on z from the functions $C_i(t, z)$ appearing in (2.1.4). There may be some chemical components which are immobile in Ω and for these D_i and H_i are zero. Such components can only interact with the fluid concentrations C_i in Λ through the reaction term f_i via interacting mobile ingredients. The boundary conditions (2.1.2) and (2.1.4) have no relevance for these immobile components. The consideration of the boundary condition (2.1.4) includes the Dirichlet type ($D_i/H_i \equiv 0$), the Neumann type ($D_i \not\equiv 0$, $H_i \equiv 0$), and the Robin type ($D_i \not\equiv 0$, $H_i \not\equiv 0$). The boundary conditions (2.1.2) and (2.1.4) therefore includes various mixed type of boundary conditions. The initial conditions are of the form

$$c_i = c_{i,0} \text{ in } \Omega \times \Lambda, \text{ at } t = 0. \tag{2.1.5}$$

In the fluid region Λ, the concentrations C_i are assumed to satisfy the system of weakly coupled convection reaction-diffusion equations

$$\frac{\partial C_i}{\partial t} - \mathscr{D}_i \nabla^2 C_i + u \cdot \nabla C_i + \int_{\partial\Omega_2} D_i \frac{\partial c_i}{\partial n} = F_i(t, z, C_j) \text{ in } (0, T] \times \Lambda, \tag{2.1.6}$$

where the "diffusion" constant $\mathscr{D}_i$ is assumed to incorporate dispersion effects, ∇^2 is the Laplacian operator in Λ, involving z-coordinates, the fourth term accounts for the flux of chemical i into Ω representing the N particles in unit volume of fluid and the fluid reaction term F_i is the source of C_i due to reactions in the fluid itself. The functions F_i like the functions f_i above are assumed to be Lipschitz continuous functions in the dependent variables C_j.

The surface integral in equation (2.1.6) which is a measure of the total flux of C_i through $\partial\Omega_2$ into Ω is only a function of t and z, and can from (2.1.4), be expressed in the form $H_i\mathscr{A}C_i - H_i\int_{\partial\Omega_2} c_i$, where $\mathscr{A}$ is the area of $\partial\Omega_2$ (see ARIS [21, p.24]).

There is no transport of fluid over $\partial\Lambda_2$ and fluid concentrations C_i at $\partial\Lambda_1$ and $\partial\Lambda_3$ are subject to boundary conditions as discussed by WEHNER and WILHELM [306] and DANCKWERTS [79], respectively. These boundary conditions are of the form

$$\upsilon_1 C_i + \mathscr{D}_i \frac{\partial C_i}{\partial n_1} = \upsilon_1 C_{i,1} \text{ on } (0, T] \times \partial\Lambda_1, \tag{2.1.7}$$

$$\frac{\partial C_i}{\partial n_\alpha} = 0 \text{ on } (0, T] \times \partial\Lambda_\alpha, \ \alpha = 2, 3, \tag{2.1.8}$$

where $C_{i,1}$ is the inlet fluid concentration.

There may be some chemical components where there is no dispersion in Λ and for these $\mathscr{D}_i$ are zero. The boundary condition (2.1.8) has no relevance for these components. Furthermore, if $u \cdot \nabla C_i \equiv 0$ for some of these chemical components , then the boundary conditions (2.1.7) has no relevance as well.

The consideration of the boundary condition (2.1.7) thus includes the Dirichlet type ($\mathscr{D}_i/\upsilon_1 \equiv 0$), the Neumann type ($\mathscr{D}_i \neq 0, \upsilon_1 \equiv 0$), and the Robin type ($\mathscr{D}_i \neq 0, \upsilon_1 \neq 0$). The boundary conditions (2.1.7) and (2.1.8) therefore includes various mixed type of boundary conditions. The initial conditions are of the form:

$$C_i = C_{i,0} \text{ in } \Lambda, \text{ at } t = 0. \tag{2.1.9}$$

We now have a system of reaction-diffusion equations (2.1.3) coupled with convection reaction-diffusion equations (2.1.6) via the boundary conditions (2.1.4) and the source term in (2.1.6) accounting for the flux of chemical component i through $\partial\Omega_2$. These equations which we label S_n involve the dependent variables $c_i(t, x, z)$ defined in $[0, T] \times \overline{\Omega} \times \Lambda$ and $C_i(t, z)$ defined in $[0, T] \times \overline{\Lambda}$ and the subscript n denotes the maximum number of chemical components in either the macro or the microsystem. Associated with this system are the boundary conditions and initial conditions B_n given by the equations (2.1.2), (2.1.5), (2.1.7)-(2.1.9). This coupled system S_n, B_n of reaction-diffusion equations is degenerate in $(0, T] \times \Omega \times \Lambda$ space in the sense that the Laplacian operators of equations (2.1.3) and (2.1.6) involve only the x in Ω and z in Λ respectively. The steady state or time independent system will be denoted as $\hat{S}_n$, $\hat{B}_n$.

Our generalised particle reactor equations S_n, B_n form a system of up to $2n$ weakly coupled equations which may be a combination of ordinary differential equations, first order partial differential equations and parabolic equations. At steady state, these equations may be a combination of algebraic equations, first order partial differential equations and elliptic equations. In many of these cases, the boundary conditions may be irrelevant for the same reasons given above.

Let I be the set of integers corresponding to up to n chemical components in Ω and J be the set of integers corresponding to up to n chemical components in Λ. If for example $i \in I$ and $D_i = H_i = 0$, then we assume that $i \notin J$, i.e., there is no corresponding chemical component in Λ. If, on the other hand $i \in I$ and $D_i, H_i > 0$, we may assume that there is a corresponding chemical component in Λ and the components c_i are coupled to components C_i by the boundary condition (2.1.4). If $i \in J$, there may not necessarily be a corresponding component in I, unless $D_i, H_i > 0$ for some $i \in I$ and for this, the components c_i are also coupled to components C_i by the boundary condition (2.1.4). All the other possibilities are similar.

We denote by $n(I)$ and $n(J)$ the number of elements in I and J, respectively and the solutions of the system S_n, B_n are denoted by the ordered pair $(c_i, C_i) \equiv (c_1, c_2, \ldots, c_{n(I)}, C_1, C_2, \ldots, C_{n(J)})$.

The boundaries of $\partial\Omega$ and $\partial\Lambda$ are assumed to be of finite curvature so that each point can be found on a closed ball of finite radius contained in $\overline{\Omega}$ or $\overline{\Lambda}$. This is known as the inner sphere property.

2.2 Notes and Comments

The physical basis of the boundary condtions (2.1.7) and (2.1.8) has been discussed at length in the literature (e.g. DANCKWERTS [79], WEHNER and WILHELM [306], PEARSON [231], KREFT and ZUBER [148] and SMITH [270]).

The dispersion coefficient $\mathscr{D}_i$ in (2.1.6) reflects two mechanisms for solute spreading, molecular diffusion and mechanical dispersion. Much work has been published on this dispersion phenomena, in particular to investigate the dispersion tensor. In cylindrical reactors the dispersion in the direction of flow (longitudinal or axial dispersion) is noticeably different from the dispersion perpendicular to the direction of flow (transverse or radial dispersion).

Compared to the work published on the longitudinal dispersion coefficient $\mathcal{D}_{iL}$, relatively few results have been reported on the transverse dispersion $\mathcal{D}_{iT}$. The mechanisms causing transverse or radial dispersion are molecular diffusion and "wandering" from the flow path (SIMPSON [267], LEIJ and DANE [164]) and in some instances it may be considered equal to the coefficient of molecular diffusion (CARBERRY [45]). Values for $\mathcal{D}_{iT}$ are more difficult to obtain than values for $\mathcal{D}_{iL}$, because the concentration distribution needs to be measured in a direction perpendicular to the flow. Studies of longitudinal or axial dispersion are reported by BABCOCK *et al.*[29], BRITTAN [43] CHUNG and WEN [71], RASMUSON and NERETNICKS [243], RASMUSON [244], MECKLENBURGH and HARTLAND [195-197] and in some instances researchers have developed criteria based on the reactor length for conditions where axial dispersion can safely be neglected.

There has been considerable interest in the chemical engineering literature on the transport equation (2.1.6) neglecting the functional and reaction terms. This equation is commonly known as a convection-dispersion equation (CDE) or an advection-dispersion equation (ADE). HARLEMAN and RUMER [116] presented an analytical solution for the two dimensional ADE for steady state conditions, assuming that longitudinal dispersion could be neglected. Analytical solutions for the steady state problem, which accounted for longitudinal dispersion were provided by GRANE and GARDNER [109] and VERRUIJT [291]. BEAR [34] discusses methods to obtain analytical solutions for some specific problems and LEIJ and DANE [164] provide an analytical solution for the two dimensional transport problem which accounts for both longitudinal and transverse dispersion. This solution can also be adapted to three dimensional dispersion.

Approximate solutions for the equation (2.1.6) for a one-dimensional time independent reactor with arbitrary kinetics is given by GROTCH [112]. An exact solution to the equation (2.1.6) for arbitrary shapes and first order kinetics without the additional contribution from the particles is given by VRENTAS and VRENTAS [297] with the fluid velocity field zero and by VRENTAS and VRENTAS [298] with a linear source term with fluid velocity distribution u as a function of z and t and with $div\ u = 0$. These solutions are given in terms of a Greens's function formulation.

There is very little literature on the coupled system (2.1.3) and (2.1.6). This set of equations for one component without reaction and simpler boundary conditions goes back to the work of DEISLER and WILHELM [81]. For the case with no dispersion ($\mathcal{D} = 0$), a classical solution of the coupled system (2.1.3) and (2.1.6) was given by ROSEN [251] in terms of an infinite integral. BABCOCK *et al.* [29] and PELLETT [232] have presented analytical solutions for this case including dispersion. Approximate solutions have also been given by RASUMSON and NERETNIEKS [243] and improved by RASMUSON [244]. These are also given as an infinite integral which has to determined numerically.

This thesis suggests that many of these exact analytical solutions may be used as bounds for our true solution with arbitrary reaction kinetics. However, we will not be demonstrating this in this work.

3

The Unsteady State Problem

3.0 Introduction

This chapter considers the unsteady state or time dependent problem. The objectives are generalised comparison theorems, uniqueness, stability and existence theorems for solutions.

In section 3.1, we shall collect some notational conventions and basic definitions and give some general results and relationships of the spaces that are needed in order to obtain the exact result on the solvability of linear parabolic equations. The maximum principle for parabolic equations which will be used throughout this thesis will also be defined.

In section 3.2 we shall show that although our system is nonstandard, it is governed by generalised comparison theorems similar in type to those for weakly coupled parabolic systems. These comparison theorems are a useful tool for proving uniqueness, existence and stability of solutions.

In section 3.3, we use the strong comparison theorem to show that solutions of system S_n, B_n are uniquely specified by the functions $c_{i,0}$, $C_{i,0}$ and $C_{i,1}$.

In section 3.4, we see that for the purposes of uniqueness, stability and existence theorems, we may assume at the outset that the system S_n, B_n is a quasimonotone system, i.e. f_i and F_i are monotone nondecreasing in c_j and C_j respectively for $j \neq i$. This is not a restriction on these theorems, since if this monotone property is not satisfied, then S_n, B_n with general functions f_i and F_i can be imbedded in a system S_{2n}, B_{2n} of the same form. It can be shown that solutions of this new system generate solutions of the original system and therefore uniqueness, stability and existence can be implied in the original system.

In section 3.5, we establish some useful sufficient conditions for the global stability of all solutions of the general system S_n, B_n. It is shown that such stability implies the uniqueness of the solutions to the steady state or time independent problem.

In section 3.6, we show that solutions of problem S_n, B_n specified by $c_{i,0}$, $C_{i,0}$ and $C_{i,1}$ exist. This is done by constructing a sequence of approximate solutions which converges monotonically and uniformly (in appropriate function spaces) to a limit function which is shown to be a solution of the system S_n, B_n.

Finally, in section 3.7, we discuss some relevant literature and future work.

3.1 Definitions, Notation and General Results for Linear Parabolic Equations

It is important in the theory of nonlinear differential equations to obtain theorems on *a priori* estimates and existence of linear differential equations in order to derive estimates for nonlinear differential equations. In this section, we shall collect some notational conventions and basic defintions.

We shall also give some general results and relationships of the spaces that are needed in order to obtain the exact result on the solvability of linear parabolic equations. The Maximum Principle for parabolic equations which will be used throughout this thesis will also be defined.

3.1.1 Definitions and Notation

The following notation will be used throughout this section

$x = (x_1, x_2, ..., x_m)$ denotes a point in R^m,
$T > 0$, where T denotes a point in R,
$t \in [0, T]$,
$\mathcal{G}$ is a bounded, open, connected domain in R^m,
$\partial\mathcal{G}$ denotes the boundary of $\mathcal{G}$,
$\overline{\mathcal{G}}$ denotes the closure of $\mathcal{G}$,
$Q_T = (0, T]\times\mathcal{G}$ is regarded as a subset of R^{m+1},
$\Gamma_T = (0, T]\times\partial\mathcal{G}$,
$\overline{Q}_T = [0, T]\times\overline{\mathcal{G}}$,
$\overline{\Gamma}_T = [0, T]\times\partial\mathcal{G}$,
$u \in R$,
$D_x u = (\partial u/\partial x_1, ..., \partial u/\partial x_m)$.

Definition 3.1.1.
A vector field $\boldsymbol{v}(t, x) = (\boldsymbol{v}_1(t, x), ..., \boldsymbol{v}_m(t, x))$ is said to be a *unit outerward normal* (outward normal or outernormal) at $(t, x) \in \Gamma_T$ if $(t, x-h\boldsymbol{v}) \in Q_T$ for small $h > 0$. The *outernormal derivative* is then given by
and $v(t,x)$ is a unit vector normal to Γ_T

$$\frac{\partial u}{\partial \boldsymbol{v}} = \lim_{h\to 0} \frac{u(t, x) - u(t, x - h\boldsymbol{v})}{h}.$$

3.1.2 General Results and Relationships between Hölder, $L^{r,q}$ and Sobolev Spaces Spaces

The following definitions of Hölder, $L^{r,q}$ and Sobolev Spaces are adapted from LADYZHENSKAYA [155, pp.4-9].

Hölder Spaces

For a positive real number, l, say, let $[l]$ denote the greatest integer not exceeding l. For $A \subseteq Q_T$, we shall say that $f \in C^{l/2,l}[A, R]$ if f: $A \to R$ is continuous, the partial derivatives of f, with respect to x, up to order $[l]$ are continuous on A and its $[l]$th order partial derivatives with respect to x are Hölder continuous on A with exponent $l - [l]$, and further the partial derivatives of f, with respect to t, up to order $[l/2]$ are continuous on A and its $[l/2]$th order partial derivative with respect to t is Hölder continuous on A with exponent $l/2-[l/2]$. For $0 < l < 1$ and $f \in C^{l/2,l}[A, R]$, we shall use the following notation:

$$\|f\|_l^A = \|f\|_0^A + \langle f\rangle_l^A,$$

where

$$\|f\|_0^A = \sup_{(t,x)\in A} |f(t,x)|,$$

$$\langle f\rangle_l^A = H_{x,l}^A(f) + H_{t,l/2}^A(f),$$

$$H^A_{x,l}(f) = \sup_{\substack{(t,x),(t,y)\in A \\ \|x-y\|\le\rho}} \frac{|f(t,x)-f(t,y)|}{\|x-y\|^l},$$

$$H^A_{t,l/2}(f) = \sup_{\substack{(t,x),(t',x)\in A \\ |t-t'|\le\rho}} \frac{|f(t,x)-f(t',x)|}{|t-t'|^{l/2}}.$$

For any $l > 0$ and $f \in C^{l/2,l}[A, R]$, we shall use the folowing notation:

$$\|f\|_l^A = \sum_{j=0}^{[l]} \sum_{2r+s=j} \|D_t^r D_x^s f\|_0^A + \langle f\rangle_l^A,$$

where $D_t^r D_x^s f$ denotes the partial derivative of f with respect to x and t of order s and r, respectively, for all r and s such that $2r+s < l$;

$$\langle f\rangle_l^A = \sum_{2r+s=[l]} H^A_{x,l-[l]}(D_t^r D_x^s f) + \sum_{0<\beta<1} H^A_{t,\beta}(D_t^r D_x^s f),$$

for $\beta = (l-2r-s)/2$.

Since $\overline{Q}_T$ is closed, it is required that the derivatives of order $\le l$ can be continuously continued from the interior of Q_T to all of $\overline{Q}_T$. If $\alpha = 1$, we also say that f is Lipschitz continuous.

$L^{r,q}$ Spaces

$L^{r,q}[\overline{Q}_T, R]$ is the Banach space consisting of all equivalent clases of Lebesgue measurable functions u defined on $\overline{Q}_T$ into R with a finite norm

$$\|u\|_{L^{r,q}[\overline{Q}_T, R]} = \left(\int_0^T \left[\int_{\mathcal{G}} |u(t,x)|^q \, dx\right]^{r/q}\right)^{1/r},$$

where $q \ge 1$ and $r \ge 1$.

If $r = q$, then $L^{q,q}[\overline{Q}_T, R]$ is denoted by $L^q[\overline{Q}_T, R]$ and the norm

$$\|u\|_{L^{q,q}[\overline{Q}_T, R]},$$

by

$$\|u\|_{L^q[\overline{Q}_T, R]}.$$

Sobolev Spaces

For nonnegative integer l, $W_q^{l,2l}[\overline{Q}_T, R]$ is the Banach space consisting of the elements $L^q[\overline{Q}_T, R]$ having generalised (weak or distributional) derivatives of the form $D_t^r D_x^s$ with any r and s satisfying the inequality $2r+s \le 2l$. The norm in it is defined by

$$\|u\|_{W_q^{l,2l}[\overline{Q}_T, R]} = \sum_{j=0}^{2l} \sum_{2r+s=j} \|D_t^r D_x^s u\|_{L^q[\overline{Q}_T, R]},$$

where the summation $\sum_{2r+s=j}$ is taken over all nonnegative integers r and s satisfying the condition $2r+s \le 2l$.

For nonintegral l, $W_q^l[\overline{Q}_T, R]$ is a Banach space consisting of the elements u of $W_q^{[l]}[\overline{Q}_T, R]$ with finite norm

$$\|u\|_{W_q^l[\overline{\mathcal{G}}, R]} = \|u\|_{W_q^{[l]}[\overline{\mathcal{G}}, R]} + \|u\|_{L_q^{l-[l]}[\overline{\mathcal{G}}, R]},$$

where

$$\|u\|_{W_q^{[l]}[\overline{\mathcal{G}}, R]} = \sum_{j=0}^{[l]} \sum_j \|D_x^j u\|_{L^q[\overline{\mathcal{G}}, R]},$$

$$\|u\|_{L_q^{l-[l]}[\overline{\mathcal{G}}, R]} = \sum_{j=[l]} \left(\int_{\overline{\mathcal{G}}} \mathrm{d}x \int_{\overline{\mathcal{G}}} |D_x^j u(x) - D_y^j u(y)|^q \frac{\mathrm{d}y}{\|x-y\|^{m+q(l-[l])}} \right)^{1/q},$$

and

$\sum_j$ denotes summation over all possible derivatives of u of order j satisfying the condition $j \leq [l]$;
$\sum_{j=[l]}$ denotes the summation over all possible derivatives of u of order $j = [l]$.

For nonintegral l, the Banach space $W_q^{l/2,l}[\overline{\Gamma}_T, R]$ is defined analogously (LADYZHENSKAYA [155, p.81]).

General Results in Hölder, $L^{r,q}$ and Sobolev Spaces

We now prove some general results in Hölder, $L^{r,q}$ and Sobolev spaces.

Lemma 3.1.1
If $f, g \in C^{\alpha/2,\alpha}[A,R]$, then $f+g \in C^{\alpha/2,\alpha}[A,R]$ and $\|f+g\|_\alpha^A \leq \|f\|_\alpha^A + \|g\|_\alpha^A$.

Proof

$$\begin{aligned}
\|f+g\|_\alpha^A &= \sup_{(t,x)\in A} |f(t,x)+g(t,x)| + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\leq\rho}} \frac{|[f(t,x)+g(t,x)]-[f(t,y)+g(t,y)]|}{\|x-y\|^\alpha} \\
&\quad + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\leq\rho}} \frac{|[f(t,x)+g(t,x)]-[f(t',x)+g(t',x)]|}{|t-t'|^{\alpha/2}} \\
&\leq \sup_{(t,x)\in A} |f(t,x)| + \sup_{(t,x)\in A} |g(t,x)| + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\leq\rho}} \frac{|f(t,x)-f(t,y)|}{\|x-y\|^\alpha} + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\leq\rho}} \frac{|g(t,x)+g(t,y)|}{\|x-y\|^\alpha} \\
&\quad + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\leq\rho}} \frac{|f(t,x)-f(t',x)|}{|t-t'|^{\alpha/2}} + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\leq\rho}} \frac{|g(t,x)-g(t',x)]|}{|t-t'|^{\alpha/2}} \\
&\leq \|f\|_\alpha^A + \|g\|_\alpha^A,
\end{aligned}$$

as required.❑

Lemma 3.1.2
If $f, g \in C^{\alpha/2,\alpha}[A, R]$, then $fg \in C^{\alpha/2,\alpha}[A, R]$ and $\|fg\|_\alpha^A \leq \|f\|_\alpha^A \; \|g\|_\alpha^A$.

Proof

$$\begin{aligned}
\|fg\|_\alpha^A &= \sup_{(t,x)\in A} |f(t,x)g(t,x)| + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\leq\rho}} \frac{|f(t,x)g(t,x)-f(t,y)g(t,y)|}{\|x-y\|^\alpha} \\
&\quad + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\leq\rho}} \frac{|f(t,x)g(t,x)-f(t',x)g(t',x)|}{|t-t'|^{\alpha/2}}
\end{aligned}$$

$$\le \sup_{(t,x)\in A} |f(t,x)| \sup_{(t,x)\in A} |g(t,x)|$$
$$+ \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\le\rho}} \frac{|f(t,x)g(t,x)-f(t,x)g(t,y)+f(t,x)g(t,y)-f(t,y)g(t,y)|}{\|x-y\|^{\alpha}}$$
$$+ \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\le\rho}} \frac{|f(t,x)g(t,x)-f(t,x)g(t',x)+f(t,x)g(t',x)-f(t',x)g(t',x)|}{|t-t'|^{\alpha/2}}$$

$$\le \sup_{(t,x)\in A} |f(t,x)| \, [\, \sup_{(t,x)\in A} |g(t,x)| + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\le\rho}} \frac{|g(t,x)+g(t,y)|}{\|x-y\|^{\alpha}} + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\le\rho}} \frac{|g(t,x)-g(t',x)]|}{|t-t'|^{\alpha/2}}]$$
$$+ \sup_{(t,x)\in A} |g(t,x)| \, [\, \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\le\rho}} \frac{|f(t,x)+f(t,y)|}{\|x-y\|^{\alpha}} + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\le\rho}} \frac{|f(t,x)-f(t',x)]|}{|t-t'|^{\alpha/2}}]$$

$$\le \|f\|_{\alpha}^{A} \, \|g\|_{\alpha}^{A},$$

as required.❑

The next three lemmas and their corollaries that follow are analogous in Hölder, L^q and Sobolev spaces.

Lemma 3.1.3

Suppose $0<\beta\le\alpha\le 1$. *Then* $C^{\alpha/2,\alpha}(A)\subseteq C^{\beta/2,\beta}(A)$.

Proof

Suppose $f\in C^{\alpha/2,\alpha}[A, R]$. We are required to show that

$$\|f\|_{\beta}^{A} = \|f\|_{0}^{A} + H_{x,\beta}^{A}(f) + H_{t,\beta/2}^{A}(f)$$
$$= \sup_{(t,x)\in A} |f(t,x)| + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\le\rho}} \frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\beta}} + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\le\rho}} \frac{|f(t,x)-f(t',x)|}{|t-t'|^{\beta/2}},$$

is finite, given that

$$\|f\|_{\alpha}^{A} = \|f\|_{0}^{A} + H_{x,\alpha}^{A}(f) + H_{t,\alpha/2}^{A}(f)$$
$$= \sup_{(t,x)\in A} |f(t,x)| + \sup_{\substack{(t,x),(t,y)\in A\\ \|x-y\|\le\rho}} \frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\alpha}} + \sup_{\substack{(t,x),(t',x)\in A\\ |t-t'|\le\rho}} \frac{|f(t,x)-f(t',x)|}{|t-t'|^{\alpha/2}},$$

is finite.

Suppose that (t, x), $(t, y)\in A$ and $0<\|x-y\|<1$. Then

$$\frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\beta}} = \frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\alpha}} \|x-y\|^{\alpha-\beta} \le \frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\alpha}},$$

since $\alpha-\beta\ge 0$. On the other hand, if (t, x), $(t, y)\in A$ and $\|x-y\|\ge 1$,

$$\frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\beta}} = \frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\alpha}} \|x-y\|^{\alpha-\beta} \le k^{\alpha-\beta} \frac{|f(t,x)-f(t,y)|}{\|x-y\|^{\alpha}}.$$

where

$$k = \sup\{\|x-y\| : x, y\in \mathcal{G}\}.$$

A similar argument holds if we have to show that

$$\sup_{\substack{(t,x),(t',x)\in A \\ |t-t'|\le\rho}} \frac{|f(t,x)-f(t',x)|}{|t-t'|^{\beta/2}},$$

is finite and the result follows by combining these arguments.❑

A trivial consequent of this result is the following corollary:

Corollary 3.1.1
Suppose $0<\alpha,\beta\le 1$. *Then* $C^{\alpha/2,\alpha}(A)\cap C^{\beta/2,\beta}(A)=C^{\gamma/2,\gamma}(A)$ *where* $\gamma=\min\{\alpha,\beta\}$.

The following lemma is stated without proof in BURKILL [44]

Lemma 3.1.4
Suppose $1\le p_1\le p_2$. *Then* $L^{p_2}[A,R]\subseteq L^{p_1}[A,R]$.

Corollary 3.1.2
Suppose $1\le p_1,p_2$. *Then* $L^{p_2}[A,R]\cap L^{p_1}[A,R]=L^{p}[A,R]$ *where* $p=\min\{p_1,p_2\}$.

The following lemma and its corollary follows from Lemma 3.1.4 and the definition of Sobolev spaces.

Lemma 3.1.5
Suppose $1\le p_1\le p_2$. *Then* $W^{l,2l}_{p_2}[A,R]\subseteq W^{l,2l}_{p_1}[A,R]$.

Corollary 3.1.3
Suppose $1\le p_1,p_2$. *Then* $W^{l,2l}_{p_2}[A,R]\cap W^{l,2l}_{p_1}[A,R]=W^{l,2l}_{p}[A,R]$ *where* $p=\min\{p_1,p_2\}$.

We define the following operator which takes a space into itself

Definition 3.1.2
The Nemytskii operator $\mathcal{N}(u)$ is defined by

$$\mathcal{N}(u)(t,x)=h(t,x,u),\ (t,x)\in\overline{Q}_T$$

for $u\in C^{(1+\alpha)/2,1+\alpha}[\overline{Q}_T,R]$.

We now present a result concerning the Nemytskii operator $\mathcal{N}(u)$. The proof is found in LADDE *et al.*[153, p.221] and TEMME [282, p.65].

Lemma 3.1.6
Let $h\in C^{\alpha/2,\alpha}[[0,T]\times\mathcal{G}\times R,R]$, *and let* $\mathcal{N}(u)$ *be the Nemytskii operator* $\mathcal{N}(u)$. *Then*

(i) $\mathcal{N}\in C[C^{(1+\alpha)/2,1+\alpha}[\overline{Q}_T,R],C^{\alpha/2,\alpha}[\overline{Q}_T,R]]$;

(ii) $\mathcal{N}$ *takes bounded sets in* $C^{(1+\alpha)/2,1+\alpha}[\overline{Q}_T,R]$ *into bounded sets in* $C^{\alpha/2,\alpha}[\overline{Q}_T,R]$.

Remark 3.1.1
From the fact that the space $C^{(1+\alpha)/2,1+\alpha}[\overline{Q}_T,R]$ is compactly imbedded in $C^{0,1}[\overline{Q}_T,R]$, the Nemytskii operator belongs to $C[C^{0,1}[\overline{Q}_T,R],C[\overline{Q}_T,R]]$.

We present another result concerning the Nemytskii operator $\mathcal{N}(u)$.

Lemma 3.1.7
Let $h \in C^{\alpha/2,\alpha}[[0, T]\times\overline{\mathcal{G}} \times R, R]$, and let $\mathcal{N}(u)$ be the Nemytskii operator $\mathcal{N}(u)$. Then
(i) $\mathcal{N} \in C[L^{r,q}[\overline{Q}_T, R], L^{r,q}[\overline{Q}_T, R]]$;
(ii) *$\mathcal{N}$ takes bounded sets in $L^{r,q}[\overline{Q}_T, R]$ into bounded sets in $L^{r,q}[\overline{Q}_T, R]$.*

Proof
$\mathcal{N}$ maps all of $L^{r,q}[\overline{Q}_T, R]$ into $L^{r,q}[\overline{Q}_T, R]$ since $\overline{Q}_T$ is bounded and $h \in C^{\alpha/2,\alpha}[[0, T]\times\overline{\mathcal{G}} \times R, R]$. Therefore $\mathcal{N}$ is a continuous and bounded operator.□

The Relationships between these Spaces
The spaces defined in this section are needed to obtain the exact result on the solvability of boundary value problems for linear parabolic equations in spaces $W_q^{1,2}[\overline{Q}_T, R]$. This is related with the fact that the differential properties of the boundary values of functions from the classes $W_q^{1,2}[\overline{Q}_T, R]$ and of their derivatives can be exactly described in terms of the spaces $W_q^{l/2,l}[\overline{\Gamma}_T, R]$ with nonintegral l: $l = k-1/q$, where k is an integer. This relationship is given in the following result. For details, see LADYZHENSKAYA [155, pp. 79-82] or LADDE *et al.* [153, p.218].

Lemma 3.1.8
If $u \in W_q^{1,2}[\overline{Q}_T, R]$, then for all nonnegative integers r and *s,*

$$2r + s < 2 - 2/q,$$

$$D_t^r D_x^s u|_{t=0} \in W_q^{2-2r-s-2/q}[\overline{\mathcal{G}}, R],$$

and

$$\|u\|_{W_q^{2-2r-s-2/q}[\overline{\mathcal{G}}, R]} \le C\|u\|_{W_q^{1,2}[\overline{Q}_T, R]}.$$

Moreover, for $2r + s < 2 - 1/q$,

$$D_t^r D_x^s u|_{\overline{\Gamma}_T} \in W_q^{1-r-s/2-1/2q,2-2r-s-1/q}[\overline{\Gamma}_T, R],$$

$$\|u\|_{W_q^{1-r-s/2-1/2q,2-2r-s-1/q}[\overline{\Gamma}_T, R]} \le C\|u\|_{W_q^{1,2}[\overline{Q}_T, R]}.$$

We say how smooth functions in a Sobolev space are, by imbedding Sobolev spaces continuously into Hölder spaces. This is called the Sobolev Lemma or the Imbedding Theorem. We shall firstly require the following defintion:

Definition 3.1.3
Let X and Y be normed spaces. We say that the normed space X is *imbedded* in the normed space Y iff
(i) X is a vector subspace of Y;
(ii) the identity operator e defined on X into Y by $ex = x$ for all $x \in X$ is continuous.

Also required is the following definition which gives the smoothness properties of the boundary $\partial\mathcal{G}$ that is required in the Sobolev Lemma.

Definition 3.1.4
Let $\mathcal{G}$ be an m-dimensional domain with boundary $\partial\mathcal{G}$. We say that $\partial\mathcal{G}$ belongs to class $C^{2+\alpha}$, if for every $x \in \partial\mathcal{G}$, there exists a neighbourhood U of x such that $\partial\mathcal{G} \cap U$ can be represented in the form

$$x_i = h(x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_m),$$

for some i, $1 \le i \le m$, where $h \in C^{2+\alpha}[\partial\mathcal{G}, R]$.

We now state the following imbedding theorem. For proof, see LADYZHENSKAYA [155, p.60].

Theorem 3.1.1 *(Imbedding Theorem or Sobolev Lemma)*
Let $\mathcal{G} \subseteq R^m$ and let $\partial\mathcal{G}$ be of class $C^{2+\alpha}$. Suppose that $q = (m+2)/(1-\alpha)$ for $0 < \alpha < 1$. Then $W_q^{1,2}[\overline{Q}_T, R]$ is imbedded in $C^{(1+\alpha)/2,1+\alpha}[\overline{Q}_T, R]$.

3.1.3 Solvability of Linear Parabolic Equations

We will discuss in this section a specific example of a parabolic equation that occurs in this thesis. For the definitions of more general linear and quasilinear second order equations of parabolic type, as well as their uniformly parabolic conditions, see LADYZHENSKAYA [155, p. 11].

Let a_{ij}, b_i and c belong to $C^{\alpha/2,\alpha}[\overline{Q}_T, R]$ and let $c \le 0$ in $\overline{Q}_T$. Let $\mathcal{L}$ be a second order differential operator defined by

$$\mathcal{L} = \frac{\partial}{\partial t} - L, \tag{3.1.1}$$

where

$$L = \sum_{i,j=1}^{m} a_{ij}(t, x)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{m} b_i(t, x)\frac{\partial}{\partial x_i} + c(t, x). \tag{3.1.2}$$

Definition 3.1.5
The differential operator $\mathcal{L}$ defined by (3.1.1) is said to be *parabolic* at a point $(t, x) \in Q_T$, if the coefficient matrix $a_{ij}(t, x)$ is positive definite, that is there exist two functions $\underline{\lambda}$ and $\overline{\lambda}$ such that

$$0 < \underline{\lambda}(t, x)\|\xi\|^2 \le \sum_{i,j=1}^{m} a_{ij}(t, x)\xi_i\xi_j \le \overline{\lambda}(t, x)\|\xi\|^2, \tag{3.1.3}$$

for all $\xi \in R^m - \{0\}$. If

$$\underline{\lambda}(t, x) > 0 \text{ in } Q_T,$$

then $\mathcal{L}$ is called *parabolic* in Q_T. If

$$\underline{\lambda}(t, x) \ge \lambda_0 > 0,$$

for a positive number λ_0 then $\mathcal{L}$ is called *almost strictly parabolic* in Q_T. If

$$\frac{\overline{\lambda}(t, x)}{\underline{\lambda}(t, x)} \le K,$$

for some positive number K, then $\mathcal{L}$ is called *strictly uniformly parabolic* in Q_T, that is (3.1.3) can be written as

$$\frac{1}{K}\|\xi\|^2 \le \sum_{i,j=1}^{m} a_{ij}(t,x)\xi_i\xi_j \le K\|\xi\|^2,$$

for all $\xi \in R^m$, $(t,x) \in Q_T$.

Let $\mathcal{G}$ be a bounded domain in R^m, $Q_T = (0,T] \times \mathcal{G}$ for $T > 0$ and $\Gamma_T = (0,T] \times \partial\mathcal{G}$. Let $p, q \in C^{(1+\alpha)/2, 1+\alpha}[\overline{\Gamma}_T, R]$ be nonnegative functions and let $\nu(t,x)$ be the unit outward normal vector field on $\partial\mathcal{G}$ (which belongs to the class $C^{2+\alpha}$) for $t \in [0,T]$.

Consider the nonlinear second order parabolic initial boundary value problem (*IBVP* for short):

$$\left.\begin{aligned} \mathcal{L}u &= h(t,x,u) \text{ in } Q_T, \\ \mathcal{B}u &= \phi(t,x) \text{ on } \Gamma_T, \\ u(0,x) &= \phi_0(x) \text{ in } \overline{\mathcal{G}}, \end{aligned}\right\} \tag{3.1.4}$$

where

$$\phi \in C^{(1+\alpha)/2, 1+\alpha}[\overline{\Gamma}_T, R], \tag{3.1.5}$$

$$\phi_0 \in C^{2+\alpha}[\overline{\mathcal{G}}, R], \tag{3.1.6}$$

$$h \in C^{\alpha/2,\alpha}[[0,T] \times \overline{\mathcal{G}} \times R, R], \tag{3.1.7}$$

and

$$\mathcal{B}u = p(t,x)u + q(t,x)\frac{du}{d\nu} \; . \tag{3.1.8}$$

Definition 3.1.6
We shall say that the *compatibility conditions* of order $k \ge 0$ are fulfilled for the *IBVP* (3.1.4)-(3.1.8) if

$$\sum_{i=0}^{j}\binom{j}{i}(p^{(j-i)}(x)u^{(j)}(x) + q^{(j-i)}(x)\frac{du^{(j)}(x)}{d\nu}) = \phi^{(j)}(x)$$

on $\partial\mathcal{G}$ for $j = 0, 1, \ldots, k$, where,

$$u^{(j)}(j) = u^{(j)}(0,x) = \frac{\partial^j u(t,x)}{\partial t^j}\Big|_{t=0},$$

$$\phi^{(j)}(j) = \phi^{(j)}(0,x) = \frac{\partial^j \phi(t,x)}{\partial t^j}\Big|_{t=0},$$

and

$$\sum_{i=0}^{j}\binom{j}{i}(p^{(j-i)}(0,x)u^{(j)}(0,x) + q^{(j-i)}(0,x)\frac{du^{(j)}(0,x)}{d\nu}) = \frac{\partial^j}{\partial t^j}(p(t,x)u(t,x) + q(t,x)\frac{du(t,x)}{d\nu})\Big|_{t=0}.$$

We now consider the linear second order parabolic initial boundary value problem (*IBVP* for short)

$$\left.\begin{aligned} \mathcal{L}u &= h(t,x) \text{ in } Q_T, \\ \mathcal{B}u &= \phi(t,x) \text{ on } \Gamma_T, \\ u(0,x) &= \phi_0(x) \text{ in } \overline{\mathcal{G}}. \end{aligned}\right\} \tag{3.1.9}$$

Let us now state the classical existence and uniqueness theorem whose proof can be found in LADYZHENSKAYA [155, p.320] and FRIEDMAN [94, p.144].

Theorem 3.1.2. *Assume that*

(i) $a_{ij}, b_i, c \in C^{\alpha/2,\alpha}[\overline{Q}_T, R]$, $c(t,x) \le 0$ *and* $\mathcal{L}$ *is strictly uniformly parabolic in* Q_T;

(ii) $p, q \in C^{(1+\alpha)/2,1+\alpha}[\overline{\Gamma}_T, R]$ *for p and q nonnegative functions and there exists* $\mu_1 > 0$ *such that* $p \ge \mu_1$;

(iii) $\partial\mathcal{G}$ *belongs to class* $C^{2+\alpha}$;

(iv) $h \in C^{\alpha/2,\alpha}[\overline{Q}_T, R]$;

(v) $\phi \in C^{(1+\alpha)/2,1+\alpha}[\overline{\Gamma}_T, R]$ and $\phi_0 \in C^{2+\alpha}[\overline{\mathcal{G}}, R]$;

(vi) *the IBVP* (3.1.9) *satisfies the compatibility condition of order* $[(1+\alpha)/2]$.

Then the linear parabolic IBVP (3.1.9) *has a unique solution u such that* $u \in C^{1+\alpha/2,2+\alpha}[\overline{Q}_T, R]$.

The following result provides the global *a priori* Schauder-type estimates for classical solutions of *IBVP* (3.1.9).

Theorem 3.1.3.
Assume that the hypotheses of Theorem 3.1.2 hold. Then for any $u \in C^{1+\alpha/2,2+\alpha}[\overline{Q}_T, R]$, *there exists a positive constant C which is independent of u such that*

$$\|u\|_{2+\alpha}^{\overline{Q}_T} \le C(\|\mathcal{L}u\|_{\alpha}^{\overline{Q}_T} + \|\mathcal{B}u\|_{1+\alpha}^{\overline{\Gamma}_T} + \|\phi_0\|_{2+\alpha}^{\overline{\mathcal{G}}}). \tag{3.1.10}$$

Moreover, if u is the classical solution of the IBVP (3.1.9), *then* (3.1.10) *reduces to*

$$\|u\|_{2+\alpha}^{\overline{Q}_T} \le C(\|h\|_{\alpha}^{\overline{Q}_T} + \|\phi\|_{1+\alpha}^{\overline{\Gamma}_T} + \|\phi_0\|_{2+\alpha}^{\overline{\mathcal{G}}}). \tag{3.1.11}$$

Remark 3.1.2
Analogous theorems to Theorem 3.1.2 and Theorem 3.1.3 hold for the *IBVP* (3.1.9) with Dirichlet boundary conditions. In this case it is required that $\phi \in C^{1+\alpha/2,2+\alpha}[\overline{\Gamma}_T, R]$ with the compatibility conditions of order $1+\alpha/2$ (see LADYZHENSKAYA [155, p.320]).

We shall state some results for solutions in the Sobolev spaces $W_q^{1,2}[\overline{Q}_T, R]$, $q > 1$ analogous to the Schauder results in the Hölder spaces $C^{1+\alpha/2,2+\alpha}[\overline{Q}_T, R]$. Let us state the following uniqueness and existence theorem that provides us with generalised (weak) solutions of (3.1.9). Its proof can be found in LADYZHENSKAYA [155, p.341].

Theorem 3.1.4 *Assume that*

(i) $a_{ij}, b_i, c \in C^{\alpha/2,\alpha}[\overline{Q}_T, R]$, $c(t,x) \le 0$ *and* $\mathcal{L}$ *is strictly uniformly parabolic in* Q_T;

(ii) $p, q \in C^{(1+\alpha)/2,1+\alpha}[\overline{\Gamma}_T, R]$, *for p and q nonnegative functions and there exists* $\mu_1 > 0$ *such that* $p \ge \mu_1$;

(iii) $\partial\mathcal{G}$ *belongs to class* $C^{2+\alpha}$;

(iv) $h \in L^q[\overline{\mathcal{G}}, R]$ for $q > 1$;

(v) $\phi \in W_q^{1/2-1/2q,1-1/q}[\overline{\Gamma}_T, R]$ *and* $\phi_0 \in W_q^{2-2/q}[\overline{\mathcal{G}}, R]$;

(vi) *the IBVP* (3.1.9) *satisfies the compatibility condition of order* $[(q-3)/2q]$.

Then the linear parabolic IBVP (3.1.9) *has a unique solution u such that* $u \in W_q^{1,2}[\overline{Q}_T, R]$.

The following theorem provides global *a priori* Agmon-Douglis-Nirenberg type of estimates for generalised (weak) solutions of the *IBVP* (3.1.9). Its proof can be found in LADYZHENSKAYA [155, p.342].

Theorem 3.1.5
Assume that the hypotheses of Theorem 3.1.4 hold. Then for any $u \in W_q^{1,2}[\overline{Q}_T, R]$, *there is a constant* C *which is independent of* u *such that*

$$\|u\|_{W_q^{1,2}[\overline{\mathcal{Q}}, R]} \leq C(\|\mathcal{L}u\|_{L^q[\overline{\mathcal{Q}}, R]} + \|\mathcal{B}u\|_{W_q^{1/2-1/2q, 1-1/q}[\overline{\Gamma}_T, R]} + \|\phi_0\|_{W_q^{2-2/q}[\overline{\mathcal{G}}, R]}). \tag{3.1.12}$$

Moreover, if u *is a generalized solution belonging to* $W_q^{1,2}[\overline{Q}_T, R]$, *then*

$$\|u\|_{W_q^{1,2}[\overline{Q}_T, R]} \leq C(\|F\|_{L^q[\overline{Q}_T, R]} + \|\phi\|_{W_q^{1/2-1/2q, 1-1/q}[\overline{\Gamma}_T, R]} + \|\phi_0\|_{W_q^{2-2/q}[\overline{\mathcal{G}}, R]}). \tag{3.1.13}$$

Remark 3.1.3
Analogous theorems to Theorem 3.1.2 and Theorem 3.1.3 hold for the *IBVP* (3.1.9) with Dirichlet boundary conditions (LADYZHENSKAYA [155, p.341]).

3.1.5 The Maximum Principle for Parabolic Equations

Throughout this thesis, we will use various forms of the maximum principle for the parabolic operator to obtain information about the solutions of our equations. A simple form of the maximum principle that we will find useful is the following

Lemma 3.1.8 (Maximum Principle)
Let $\psi \in C^{1,2}[\overline{Q}_T, R]$ *be such that* $\mathcal{L}\psi \leq 0$ in Q_T, $\mathcal{B}\psi \leq 0$ *on* Γ_T *and* $\psi(0, x) \leq 0$ in $\mathcal{G}$. *Then* $\psi \leq 0$ *on* $\overline{Q}_T$.

Other forms of the maximum principle for the parabolic operator are given by PROTTER and WEINBERGER [234] and SPERB [271]. In section 3.2 we shall develop some Generalised Comparison Theorems which are also useful in obtaining information about solutions of our equations.

3.2 Generalised Comparison Theorems

There are important techniques in the theory of differential equations which are concerned with estimating a function satisfying a differential equation by extremal solutions of an associated differential inequality. One technique is available when the solution of the differential equation satisfy certain comparison theorems. A tremendous advantage offered by theorems of this type arises from the relative ease with which one can find solutions of inequalities as opposed to equations and the useful feature that each solution of the inequality is a constraint on a whole class of perhaps unknown solutions. These comparison theorems are a useful tool for proving uniqueness, existence and stability theorems for solutions. The maximum principle for parabolic and elliptic equations is an example of such a theorem.

Our generalised particle reactor equations S_n, B_n form a system of up to $2n$ weakly coupled, degenerate equations which may be a combination of ordinary differential equations, first order partial differential equations and parabolic equations. The degeneracy is is not only concerned with the possibility of D_i or $\mathcal{D}_i$ being zero for some i but is also associated with the fact that in the case that D_i is nonzero, the Laplacian for the c_i equations involves only the x dependent variables whereas for the C_i equations it involves only the z dependent variables. The weak coupling is also non standard in that through equation (2.1.6) the C_i equations have a functional connection to the c_i variables via $\int_{\partial\Omega_2} D_i \frac{\partial c_i}{\partial n}$. Despite these features we are able to show in this section that this system is governed by generalised comparison theorems similar in type to those for weakly coupled parabolic systems in MCNABB [182, 186]. However, additional smoothness properties such as the inner sphere property is used for comparison theorems and this smoothness hypothesis together with some Lipschitz continuity conditions on f_i and F_i are required for our generalised strong comparison theorem. We are also able to show by a counterexample that only in some cases are there analogous theorems for the corresponding time independent or steady state system.

3.2.1 Some Basic Comparison Theorems

We first require some weak and strong comparison theorems for ordinary differential equations, first order partial differential equations and parabolic equations. These weak comparison theorems are similar in that they assume at the outset that a solution is bounded by comparison functions and rules out the existence of a contact point for these functions for all time. There are no restrictions on the nonlinear functions. The strong comparison theorems are similar in that they provide stronger results for a solution bounded by comparison functions and spells out the consequences of the existence of contact points of these comparison functions. There are however restrictions on the nonlinear functions for such strong comparison theorems.

Weak and Strong Comparison Theorems for Ordinary Differential Equations

We shall firstly look at weak and strong comparison theorems for ordinary differential equations. The first two theorems are from MCNABB [186] and are only included here for the sake of completeness.

Theorem 3.2.1 (Weak Comparison Theorem) *Suppose that*

(i) *The functions c_1 and c_2 are defined and are continuous in* $[0, T]$, *their first order t derivatives exist and are uniformly bounded and continuous in the region* $(0, T]$;

(ii) $c_1(0) < c_2(0)$;

(iii) $\dfrac{dc_1}{dt} - h(t, c_1) < \dfrac{dc_2}{dt} - h(t, c_2)$ *on* $(0, T]$.

Then

$c_1(t) < c_2(t)$ *on* $[0, T]$.

Proof

Let us suppose that $c_1 \geq c_2$ somewhere in $[0, T]$. Then, since $c_1 - c_2$ is continuous in $[0, T]$, and $c_1(0) - c_2(0) < 0$, there is a point t^* in $(0, T]$ such that $c_1(t^*) = c_2(t^*)$ and $c_1 < c_2$ on $[0, t^*)$. But then $\dfrac{\partial c_1}{\partial t}(t^*) \geq \dfrac{\partial c_2}{\partial t}(t^*)$, and $h(t^*, c_1) = h(t^*, c_2)$. Since this violates (iii), at t^*, no such t^* exists in $[0, T]$ and therefore $c_1(t) < c_2(t)$ on $[0, T]$.❑

If $h(t, c)$ satisfies a Lipschitz condition then a stronger result can be stated.

Theorem 3.2.2 (Strong Comparison Theorem) *Suppose that*

(i) *The functions c_1 and c_2 are defined and are continuous in* $[0, T]$, *their first order t derivatives exist and are uniformly bounded and continuous in the region* $(0, T]$;

(ii) $c_1(0) < c_2(0)$;

(iii) $\frac{dc_1}{dt} - h(t, c_1) \leq \frac{dc_2}{dt} - h(t, c_2)$ *on* $(0, T]$;

(iv) *The function h is Lipschitz continuous in c so that there is a finite constant* $K > 0$ *for which*

$|h(t, c_1) - h(t, c_2)| \leq K|c_1 - c_2|$ *in* $[0, T]$.

Then

$c_1(t) < c_2(t)$ *on* $[0, T]$.

Proof

Let us suppose that $c_2(0) - c_1(0) = A > 0$, and let

$$w = c_1 + \frac{A}{2}e^{-2Kt}.$$

Then

$$\begin{aligned}\frac{dw}{dt} - h(t, w) &= \frac{dc_1}{dt} - KAe^{-2Kt} - h(t, c_1) - [h(t, w) - h(t, c_1)]\\ &\leq [\frac{dc_1}{dt} - h(t, c_1)] + K|w - c_1| - KAe^{-2Kt}\\ &\leq [\frac{dc_2}{dt} - h(t, c_2)] + \frac{KA}{2}e^{-2Kt} - KAe^{-2Kt}\\ &< \frac{dc_2}{dt} - h(t, c_2).\end{aligned}$$

Now $w(0) < c_2(0)$ and so by Theorem 3.2.1 (Weak Comparison Theorem), $w < c_2$ on $[0, T]$ and $c_1 < w < c_2$ on $[0, T]$.❑

The following theorem is also a strong comparison theorem

Theorem 3.2.3 (Strong Comparison Theorem) *Suppose that*

(i) *The functions* c_1 *and* c_2 *are defined and are continuous in* $[0, T]$, *their first order t derivatives exist and are uniformly bounded and continuous in the region* $(0, T]$;

(ii) $c_1(0) \leq c_2(0)$;

(iii) $\frac{dc_1}{dt} - h(t, c_1) \leq \frac{dc_2}{dt} - h(t, c_2)$ *on* $(0, T]$;

(iv) *The function h is Lipschitz continuous in c so that there is a finite constant* $K > 0$ *for which*

$|h(t, c_1) - h(t, c_2)| \leq K|c_1 - c_2|$ *in* $[0, T]$.

Then

$c_1(t) \leq c_2(t)$ *on* $[0, T]$.

Proof

Let

$$w = c_2 + \lambda e^{2Kt}.$$

Then

$$\begin{aligned}
\frac{dw}{dt} - h(t, w) &= \frac{dc_2}{dt} - h(t, w) + 2K\lambda e^{2Kt} + h(t, c_2) - h(t, c_2) \\
&\le \frac{dc_1}{dt} - h(t, c_1) + 2K\lambda e^{2Kt} - [h(t, w) - h(t, c_2)] \\
&\le \frac{dc_1}{dt} - h(t, c_1) + 2K\lambda e^{2Kt} - K|w - c_2| \\
&\le \frac{dc_1}{dt} - h(t, c_1) + 2K\lambda e^{2Kt} - K\lambda e^{2Kt} \\
&\le \frac{dc_1}{dt} - h(t, c_1) + K\lambda e^{2Kt} \\
&< \frac{dc_1}{dt} - h(t, c_1).
\end{aligned}$$

Now $w(0) < c_1(0)$ and so by Theorem 3.2.1 (Weak Comparison Theorem), $w < c_1$ on $[0, T]$ for all λ which implies that $c_1 \le c_2$.❑

The following theorem provides a stronger result and spells out the consequences of the existence of contact points of these comparison functions.

Theorem 3.2.4 (Strong Comparison (Contact) Theorem) *Suppose that*

(i) *The functions c_1 and c_2 are defined and are continuous in $[0, T]$, their first order t derivatives exist and are uniformly bounded and continuous in the region $(0, T]$;*

(ii) *$c_1 \le c_2$ in $[0, T]$;*

(iii) $\dfrac{dc_1}{dt} - h(t, c_1) \le \dfrac{dc_2}{dt} - h(t, c_2)$ *on $(0, T]$;*

(iv) *The function h is Lipschitz continuous in c so that there is a finite constant $K > 0$ for which*

$$|h(t, c_1) - h(t, c_2)| \le K|c_1 - c_2| \text{ in } [0, T].$$

Then either

$$c_1(t) < c_2(t) \text{ on } [0, T],$$

or there is a constant T_0 in $(0, T]$ such that

$$c_1(t) < c_2(t) \text{ in } (T_0, T] \text{ and } c_1(t) \equiv c_2(t) \text{ for all } t \text{ in } [0, T_0].$$

Proof

Either $c_1 < c_2$ in $[0, T]$ or there is some T_0 in $[0, T]$ such that $c_1 = c_2$. Let T_0 be the greatest such time. Suppose that $c_1 < c_2$ at $T_0^* < T_0$. Then Theorem 3.2.2 (Strong Comparison Theorem) implies that $c_1 < c_2$ in $(T_0^*, T]$ which is a contradiction and hence the theorem must follow.❑

Weak and Strong Comparison Theorems for First Order Partial Differential Equations

We now look at weak and strong comparison theorems for first order partial differential equations. The proofs of these theorems are extensions of comparison theorems for ordinary differential equations that we have examined. We shall give such a weak and strong comparison theorem for first order partial differential equations of the form

$$\ell c \equiv \frac{\partial c}{\partial t} - \sum_{i=1}^{m} a_i(t, x)\frac{\partial c}{\partial x_i} = h(t, x, c) \text{ in } (0, T] \times D, \tag{3.2.1}$$

where D is a finite domain in R^m, $T < \infty$ and ℓ has bounded coefficients $a_i(t, x)$

Theorem 3.2.5 (Weak Comparison Theorem) *Suppose that*

(i) *The functions* c_1 *and* c_2 *are defined and are continuous in* $[0, T] \times \overline{D}$, *their first order* x_i *derivatives exist and are continuous in* $(0, T] \times D$ *and their* t *derivatives exist and are uniformly bounded and continuous in the region* $(0, T] \times D$;

(ii) $c_1(0, x) < c_2(0, x)$;

(iii) $c_1 < c_2$ *on* $(0, T] \times \partial D$;

(iv) $\ell c_1 - h(t, x, c_1) < \ell c_2 - h(t, x, c_2)$ *in* $(0, T] \times D$.

Then

$c_1 < c_2$ *in* $[0, T] \times \overline{D}$.

Proof

Let us suppose that $c_1 \geq c_2$ somewhere in $[0, T] \times \overline{D}$. Then, since $c_1 - c_2$ is continuous in $[0, T] \times \overline{D}$, and (ii) and (iii) hold at $t = 0$ and $(0, T] \times \partial D$, respectively, there is a point (t^*, x^*) in $(0, T] \times D$ such that $c_1(t^*, x^*) = c_2(t^*, x^*)$ and $c_1 < c_2$ on $[0, t^*) \times \overline{D}$. But then $\frac{\partial c_1}{\partial t}(t^*, x^*) \geq \frac{\partial c_2}{\partial t}(t^*, x^*)$, $\frac{\partial c_1}{\partial x_i} = \frac{\partial c_2}{\partial x_i}$ and $h(t^*, x^*, c_1) = h(t^*, x^*, c_2)$. Since this violates (iv), at (t^*, x^*), no such (t^*, x^*) exists in $[0, T] \times \overline{D}$.□

If h satisfies a Lipschitz condition then a stronger result can be stated.

Theorem 3.2.6 (Strong Comparison Theorem) *Suppose that*

(i) *The functions* c_1 *and* c_2 *are defined and are continuous in* $[0, T] \times \overline{D}$, *their first order* x_i *derivatives exist and are continuous in* $(0, T] \times D$, *and their* t *derivatives exist and are uniformly bounded and continuous in the region* $(0, T] \times D$;

(ii) $c_1(0, x) < c_2(0, x)$;

(iii) $c_1 \leq c_2$ *on* $(0, T] \times \partial D$;

(iv) $\ell c_1 - h(t, x, c_1) \leq \ell c_2 - h(t, x, c_2)$ *in* $(0, T] \times D$.

Then

$c_1 \leq c_2$ *in* $[0, T] \times \overline{D}$.

Proof

Let

$$w = c_2 + \lambda e^{2Kt}.$$

Then

$$\begin{aligned} \ell c_1 - h(t, x, w) &= \ell c_1 - h(t, x, w) + 2K\lambda e^{2Kt} + h(t, x, c_2) - h(t, x, c_2) \\ &\leq \ell c_1 - h(t, x, c_1) + 2K\lambda e^{2Kt} - [h(t, x, w) - h(t, x, c_2)] \\ &\leq \ell c_1 - h(t, x, c_1) + 2K\lambda e^{2Kt} - K|w - c_2| \\ &\leq \ell c_1 - h(t, x, c_1) + 2K\lambda e^{2Kt} - K\lambda e^{2Kt} \\ &\leq \ell c_1 - h(t, x, c_1) + K\lambda e^{2Kt} \\ &< \ell c_1 - h(t, x, c_1). \end{aligned}$$

Now $w(0, x) < c_1(0, x)$ and $w < c_1$ on $(0, T] \times \partial D$, so by Theorem 3.2.5 (Weak Comparison Theorem), for ordinary differential equations, $w < c_1$ on $[0, T] \times \overline{D}$ for all λ which implies that $c_1 \leq c_2$ on $[0, T] \times \overline{D}$.❑

The following theorem provides a stronger result and spells out the consequences of the existence of contact points of these comparison functions.

Theorem 3.2.7 (Strong Comparison (Contact) Theorem) *Suppose that*

(i) *The functions c_1 and c_2 are defined and are continuous in $[0, T] \times \overline{D}$, their first order x_i derivatives exist and are continuous in $(0, T] \times D$ and their t derivatives exist and are uniformly bounded and continuous in the region $(0, T] \times D$;*

(ii) $c_1(t, x) \leq c_2(t, x)$ *in* $[0, T] \times \overline{D}$;

(iii) $\ell c_1 - h(t, x, c_1) \leq \ell c_2 - h(t, x, c_2)$ *in* $(0, T] \times D$;

(iv) *The function h is Lipschitz continuous in c so that there is a finite constant $K > 0$ for which*

$$|h(t, x, c_1) - h(t, x, c_2)| \leq K|c_1 - c_2| \text{ in } [0,T] \times \overline{D} \times R.$$

Then either

$$c_1(t, x) < c_2(t, x) \text{ in } [0, T] \times \overline{D}$$

or there is a constant T_0 in $(0, T]$ and a point x^* in $\overline{D}$ such that

$c_1(t, x) < c_2(t, x)$ in $(T_0, T] \times \overline{D}$ and $c_1 \equiv c_2$ at those points which lie in $[0, T_0] \times \overline{D}$ and also lie along the characteristic curve given by $\dfrac{dx}{dt} = a(t,x)$, $x = x^*$ at T_0 for t in $[0, T_0]$.

Proof

Either $c_1 < c_2$ in $[0, T] \times \overline{D}$ or there is a constant T_0 in $(0, T]$ and a point x^* in $\overline{D}$ such that $c_1 = c_2$ at (T_0, x^*) in $(0, T] \times \overline{D}$. Let $\ell c_1 = h(t, x, c_1) + A_1(t, x, c_1)$ and $\ell c_2 = h(t, x, c_2) + A_2(t, x, c_2)$ where $A_1 \leq A_2$

in $(0, T]\times\overline{D}$. Then along the characteristic curve $\frac{dx}{dt}=a(t, x)$, $x=x^*$ at T_0, we have $\frac{dc_1}{dt}=h(t, x, c_1)+A_1(t, x, c_1)$ and $\frac{dc_2}{dt}=h(t, x, c_2)+A_1(t, x, c_2)$ holding, so that $\frac{dc_1}{dt}-h(t, x, c_1)\le\frac{dc_2}{dt}-h(t, x, c_2)$ in $(0, T]\times\overline{D}$, and hence from (ii) and (iv) and Theorem 3.2.4, if $c_1(T_0, x^*)=c_2(T_0, x^*)$ then $c_1(t, x)\equiv c_2(t, x)$ for t in $[0, T_0]$, x on the characteristic curve and $(t, x)\in[0, T]\times\overline{D}$.❑

Weak and Strong Comparison Theorems for Parabolic Differential Equations

We now give weak and strong comparison theorems for quasilinear parabolic equations in one dependent variable of the form

$$\mathscr{L}c\equiv\frac{\partial c}{\partial t}-\sum_{i,j=1}^{m}a_{ij}(t, x)\frac{\partial^2 c}{\partial x_i\partial x_j}-\sum_{i=1}^{m}b_i(t, x)\frac{\partial c}{\partial x_i}=h(t, x, c)\ \text{in}\ (0, T]\times D, \tag{3.2.2}$$

where D is a finite domain in R^m, $T<\infty$ and $\mathscr{L}$ is a uniformly parabolic operator with bounded coefficients $a_{ij}(t, x)$ and $b_i(t, x)$. The boundary ∂D of D must satisfy the inner sphere property which requires every point on ∂D to lie on the surface of an open sphere contained in D.

The following two theorems are standard. The proofs follow along the lines for comparison theorems already discussed (see FRIEDMAN [93, 94]).

Theorem 3.2.8 (Weak Comparison Theorem) *Suppose that*

(i) *The functions c_1 and c_2 are defined and are continuous in $[0, T]\times\overline{D}$, their first order x_i derivatives exist and are continuous in $(0, T]\times\overline{D}$, their second order x_{ij} derivatives exist and are uniformly bounded and continuous in the region $(0, T]\times D$ and their t derivatives exist and are uniformly bounded and continuous in the region $(0, T]\times D$;*

(ii) $c_1(0, x)<c_2(0, x)$;

(iii) $\mathscr{L}c_1-h(t, x, c_1)<\mathscr{L}c_2-h(t, x, c_2)$ *in* $(0, T]\times D$;

(iv) $\alpha(t, x)c_1+\beta(t, x)\frac{\partial c_1}{\partial n}<\alpha(t, x)c_2+\beta(t, x)\frac{\partial c_2}{\partial n}$ *on* $(0, T]\times\partial D$,

where $\alpha(t, x)\ge 0$, $\beta(t, x)\ge 0$ on $(0, T]\times\partial D$ and $\alpha+\beta>0$ at each point.

Then

$c_1<c_2$ *in* $[0, T]\times\overline{D}$.

If, $h(t, x, c)$ satisfies a Lipschitz condition, then a stronger result can be stated.

Theorem 3.2.9 (Strong Comparison Theorem) *Suppose that*

(i) *The functions c_1 and c_2 are defined and are continuous in $[0, T]\times\overline{D}$, their first order x_i derivatives exist and are continuous in $(0, T]\times\overline{D}$, their second order x_{ij} derivatives exist and are uniformly bounded and continuous in the region $(0, T]\times D$ and their t derivatives exist and are uniformly bounded and continuous in the region $(0, T]\times D$;*

(ii) $c_1(0, x)\le c_2(0, x)$;

(iii) $\mathscr{L}c_1 - h(t, x, c_1) \le \mathscr{L}c_2 - h(t, x, c_2)$ *in* $(0, T] \times D$;

(iv) $\alpha(t, x)c_1 + \beta(t, x)\dfrac{\partial c_1}{\partial n} \le \alpha(t, x)c_2 + \beta(t, x)\dfrac{\partial c_2}{\partial n}$ *on* $(0, T] \times \partial D$,

where $\alpha(t, x) \ge 0$, $\beta(t, x) \ge 0$ *on* $(0, T] \times \partial D$ *and* $\alpha + \beta > 0$ *at each point*;

(v) *The function h is Lipschitz continuous in c so that there is a finite constant* $K > 0$ *for which*

$|h(t, x, c_1) - h(t, x, c_2)| \le K|c_1 - c_2|$ *in* $[0, T] \times \overline{D} \times R$.

Then

$$c_1 \le c_2 \text{ in } [0, T] \times \overline{D}.$$

The following theorem provides a stronger result and spells out the consequences of the existence of contact points of these comparison functions.

Theorem 3.2.10 (Strong Comparison (Contact) Theorem) *Suppose that*

(i) *The functions* c_1 *and* c_2 *are defined and are continuous in* $[0, T] \times \overline{D}$, *their first order* x_i *derivatives exist and are continuous in* $(0, T] \times \overline{D}$, *their second order* x_{ij} *derivatives exist and are uniformly bounded and continuous in the region* $(0, T] \times D$ *and their t derivatives exist and are uniformly bounded and continuous in the region* $(0, T] \times D$;

(ii) $c_1 \le c_2$ *in* $[0, T] \times \overline{D}$;

(iii) $\mathscr{L}c_1 - h(t, x, c_1) \le \mathscr{L}c_2 - h(t, x, c_2)$ *in* $(0, T] \times D$;

(iv) $\alpha(t, x)c_1 + \beta(t, x)\dfrac{\partial c_1}{\partial n} \le \alpha(t, x)c_2 + \beta(t, x)\dfrac{\partial c_2}{\partial n}$ *on* $(0, T] \times \partial D$,

where $\alpha(t, x) \ge 0$, $\beta(t, x) \ge 0$ *on* $(0, T] \times \partial D$ *and* $\alpha + \beta > 0$ *at each point*;

(v) *The function h is Lipschitz continuous in c so that there is a finite constant* $K > 0$ *for which*

$|h(t, x, c_1) - h(t, x, c_2)| \le K|c_1 - c_2|$ *in* $[0, T] \times \overline{D} \times R$.

Then either

$$c_1 < c_2 \text{ in } [0, T] \times \overline{D}, \tag{3.2.3}$$

or there is a constant T_0 in $(0, T]$ *such that*

$$c_1 < c_2 \text{ in } (T_0, T] \times D \text{ and } c_1 \equiv c_2 \text{ in } [0, T_0] \times \overline{D}. \tag{3.2.4}$$

If $\beta > 0$ *on* $(0, T] \times \partial D$, (3.2.4) *can be replaced by the stronger result*

$$c_1 < c_2 \text{ in } (T_0, T] \times \overline{D} \text{ and } c_1 \equiv c_2 \text{ in } [0, T_0] \times \overline{D}. \tag{3.2.5}$$

Proof

Define functions v_1 and v_2 by

$$c_1 = e^{-Kt}v_1, \; c_2 = e^{-Kt}v_2, \tag{3.2.6}$$

where K is the Lipschitz constant for h, so that

$$v_1 \le v_2 \text{ in } [0, T] \times \overline{D}, \tag{3.2.7}$$

and

$$\mathcal{L}v_1 \le \mathcal{L}v_2 \text{ in } (0, T] \times D. \tag{3.2.8}$$

Either $v_1 < v_2$ and hence $c_1 < c_2$ in $(0, T] \times \overline{D}$ or there is a T_0 in $(0, T]$ such that $v_1 < v_2$ in $(T_0, T] \times \overline{D}$ and $v_1 = v_2$ at a point P in $\overline{D}$ at time T_0. But if P is in D, this implies that $v_1 \equiv v_2$ and hence $c_1 \equiv c_2$ in $[0, T_0] \times \overline{D}$ by the strong comparison theorem of Nirenberg for parabolic equations (NIRENBERG [204]). On the other hand, if $v_1 = v_2$ at P on ∂D at time T_0, and $\beta > 0$ on $(0, T] \times \partial D$, then from (v), $\frac{\partial v_1}{\partial n} \le \frac{\partial v_2}{\partial n}$ at P while at the same time, from condition (iii), $\frac{\partial v_1}{\partial n} \ge \frac{\partial v_2}{\partial n}$ there, so that $\frac{\partial v_1}{\partial n} = \frac{\partial v_2}{\partial n}$ at P. In this case the strong comparison theorem of Friedman implies $v_1 \equiv v_2$ in $[0, T_0] \times \overline{D}$ (FRIEDMAN [93]), so that our conclusions (3.2.3) and (3.2.5) are established. If β can vanish on $(0, T] \times \partial D$, there is a T_0 such that $v_1 < v_2$ in $(T_0, T] \times D$ and $v_1 = v_2$ at a point P in D at time T_0. The Nirenberg theorem then establishes (3.2.4).❑

3.2.2 Generalised Weak and Strong Comparison Theorems

We have developed a number of comparison theorems for scalar equations. Extensions of these results to systems of equations where c_1, c_2 and h are taken as n-vectors in previous theorems will not do. A simple counterexample for ordinary differential equations is given by MCNABB [186] and a counterexample for multicomponent diffusion systems is given by WAKE [302]. However, an extension can be obtained by the concurrent use of upper and lower bounds in the formulation of the comparison theorems by redefining h. We therefore look for comparison theorems for the system S_n, B_n by defining the following functions

$$\underline{f}_i(t, x, \underline{c}_k, \overline{c}_l) = \inf f_i(t, x, \theta_j), \tag{3.2.9}$$

$$\overline{f}_i(t, x, \underline{c}_k, \overline{c}_l) = \sup f_i(t, x, \theta_j), \tag{3.2.10}$$

$$\underline{F}_i(t, z, \underline{C}_k, \overline{C}_l) = \inf F_i(t, z, \Theta_j), \tag{3.2.11}$$

$$\overline{F}_i(t, z, \underline{C}_k, \overline{C}_l) = \sup F_i(t, z, \Theta_j), \tag{3.2.12}$$

for

$$\theta_i = \underline{c}_i \text{ in } \underline{f}_i,\ \theta_i = \overline{c}_i \text{ in } \overline{f}_i, \tag{3.2.13}$$

$$\Theta_i = \underline{C}_i \text{ in } \underline{F}_i,\ \Theta_i = \overline{C}_i \text{ in } \overline{F}_i, \tag{3.2.14}$$

where,

$$\theta_{\substack{j\\ j\neq i}} \in [\underline{c}_j \wedge \overline{c}_j,\ \underline{c}_j \vee \overline{c}_j], \tag{3.2.15}$$

$$\Theta_{\substack{j\\ j\neq i}} \in [\underline{C}_j \wedge \overline{C}_j,\ \underline{C}_j \vee \overline{C}_j], \tag{3.2.16}$$

i.e., θ_j lies in the closed interval bounded by $\underline{c}_j$ and $\overline{c}_j$ for all $j \neq i$ and Θ_j lies in the closed interval bounded by $\underline{C}_j$ and $\overline{C}_j$ for all $j \neq i$.

Theorem 3.2.11 (Generalised Weak Comparison Theorem)
Suppose (c_i, C_i) is a solution of the system S_n, B_n and the functions $\underline{c}_i$, $\overline{c}_i$, $\underline{C}_i$ and $\overline{C}_i$ are defined and satisfy the following continuity properties and inequalities:

(i) *For components $i \in I$, where $D_i > 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $[0, T] \times \overline{\Omega} \times \Lambda$, their first-order x_j-derivatives exist in $(0, T] \times \overline{\Omega} \times \Lambda$, their second order $x_j x_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(ii) *For components $i \in I$, where $D_i = H_i = 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $[0, T] \times \overline{\Omega} \times \Lambda$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(iii) *For components $i \in J$, where $\mathcal{D}_i > 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T] \times \overline{\Lambda}$, their first order z derivatives exist in $(0, T] \times \overline{\Lambda}$, their second order $z_j z_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(iv) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T] \times \overline{\Lambda}$, their first order z_j derivatives exist in $(0, T] \times \Lambda$ and their first order t-derivatives are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(v) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T] \times \overline{\Lambda}$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(vi) $\underline{c}_i < c_i < \overline{c}_i$ *in* $\overline{\Omega} \times \Lambda$ *and* $\underline{C}_i < C_i < \overline{C}_i$ *in* $\overline{\Lambda}$ *at* $t = 0$; **(3.2.17)**

(vii)
$$\begin{aligned} &\frac{\partial \underline{c}_i}{\partial t} - D_i \nabla_x^2 \underline{c}_i - \underline{f}_i(t, x, \underline{c}_k, \overline{c}_l) \\ &< \frac{\partial c_i}{\partial t} - D_i \nabla_x^2 c_i - f_i(t, x, c_j) \\ &< \frac{\partial \overline{c}_i}{\partial t} - D_i \nabla_x^2 \overline{c}_i - \overline{f}_i(t, x, \underline{c}_k, \overline{c}_l) \text{ in } (0, T]\times\Omega\times\Lambda; \end{aligned} \tag{3.2.18}$$

(viii)
$$\frac{\partial \underline{c}_i}{\partial n} < \frac{\partial c_i}{\partial n} < \frac{\partial \overline{c}_i}{\partial n} \text{ on } (0, T]\times\partial\Omega_1\times\Lambda; \tag{3.2.19}$$

(ix)
$$D_i \frac{\partial \underline{c}_i}{\partial n} - H_i(\underline{C}_i - \underline{c}_i) < D_i \frac{\partial c_i}{\partial n} - H_i(C_i - c_i) < D_i \frac{\partial \overline{c}_i}{\partial n} - H_i(\overline{C}_i - \overline{c}_i) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda; \tag{3.2.20}$$

(x)
$$\begin{aligned} &\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \underline{C}_i + u \cdot \nabla \underline{C}_i + H_i \int_{\partial\Omega_2} (\underline{C}_i - \underline{c}_i) - \underline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \\ &< \frac{\partial C_i}{\partial t} - \mathcal{D}_i \nabla^2 C_i + u \cdot \nabla C_i + H_i \int_{\partial\Omega_2} (C_i - c_i) - F_i(t, z, C_j) \\ &< \frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \overline{C}_i + u \cdot \nabla \overline{C}_i + H_i \int_{\partial\Omega_2} (\overline{C}_i - \overline{c}_i) - \overline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \text{ in } (0, T]\times\Lambda; \end{aligned} \tag{3.2.21}$$

(xi) $\underline{C}_{i,1} < C_{i,1} < \overline{C}_{i,1}$, **(3.2.22)**

$v_1 = -u \cdot n_1$ is uniformly bounded and continuous in $(0, T]\times\partial\Lambda$,

$$\upsilon_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} = \upsilon_1 \underline{C}_{i,1}, \quad \upsilon_1 C_i + \mathcal{D}_i \frac{\partial C_i}{\partial n_1} = \upsilon_1 C_{i,1}, \quad \upsilon_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} = \upsilon_1 \overline{C}_{i,1} \text{ on } (0, T]\times\partial\Lambda_1, \tag{3.2.23}$$

so that

$$\upsilon_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} < \upsilon_1 C_i + \mathcal{D}_i \frac{\partial C_i}{\partial n_1} < \upsilon_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} \text{ on} (0, T]\times \partial\Lambda_1; \tag{3.2.24}$$

(xii) $$\frac{\partial \underline{C}_i}{\partial n_\alpha} < \frac{\partial C_i}{\partial n_\alpha} < \frac{\partial \overline{C}_i}{\partial n_\alpha} \text{ on} (0, T]\times \partial\Lambda_\alpha, \ \alpha = 2, 3. \tag{3.2.25}$$

Then $\underline{c}_i < c_i < \overline{c}_i$ *in* $[0, T]\times\overline{\Omega}\times\Lambda$ *and* $\underline{C}_i < C_i < \overline{C}_i$ *in* $[0, T]\times\overline{\Lambda}$.

Proof

We will only look at the case when D_i, $\mathcal{D}_i > 0$ for all i. The proofs for the other cases follow along similar lines of Theorem 3.2.1 (Weak Comparison Theorem) for ordinary differential equations and Theorem 3.2.5 (Weak Comparison Theorem) for first order partial differential equations.

We let $u_i = c_i - \underline{c}_i$ and $v_i = c_i - \overline{c}_i$ in $[0, T]\times\overline{\Omega}\times\Lambda$ and $U_i = C_i - \underline{C}_i$ and $V_i = C_i - \overline{C}_i$ in $[0, T]\times\overline{\Lambda}$. Then if the conclusion is not true then either there exists a point (t^*, x^*, z^*) in $[0, T]\times\overline{\Omega}\times\Lambda$ and an index $i\in I$ such that $u_j(t, x, z)\le 0\le v_j(t, x, z)$ on $[0, t^*]\times\overline{\Omega}\times\Lambda$, $j \neq i$ and $u_i(t, x, z) < 0 < v_i(t, x, z)$ on $[0, t^*]\times\overline{\Omega}\times\Lambda$, or there exists a point (t^*, x^*) in $[0, T]\times\overline{\Lambda}$ and an index $i\in J$ such that $U_j(t, z)\le 0\le V_j(t, z)$ on $[0, t^*]\times\overline{\Lambda}$, $j\neq i$ and $U_i(t, z) < 0 < V_i(t, z)$ on $[0, t^*)\times\overline{\Lambda}$.

Suppose firstly that there exists such a point (t^*, x^*, z^*) in $[0, T]\times\overline{\Omega}\times\Lambda$. By continuity, we have either $u_i(t^*, x^*, z^*) = 0$ or $v_i(t^*, x^*, z^*) = 0$.

If $(t^*, x^*, z^*)\in(0, T]\times\partial\Omega_1\times\Lambda$, then either $\frac{\partial u_i}{\partial n}\le 0$ or $\frac{\partial v_i}{\partial n}\ge 0$, which is impossible by (viii)

If $(t^*, x^*, z^*)\in(0, T]\times\Omega\times\Lambda$, then (t^*, x^*, z^*) is either a point of minimum of u_i or a point of maximum of v_i and these minimum and maximum values at these points are equal to zero. Hence if $(t^*, x^*, z^*)\in (0, T]\times\Omega\times\Lambda$, we have either

$$u_i(t^*, x^*, z^*) = 0, \ \frac{\partial u_i}{\partial x_j}(t^*, x^*, z^*) = 0, \ \sum_{j=1}^{n}\lambda_i^2\frac{\partial^2 u_i}{\partial x_j^2}(t^*, x^*, z^*)\ge 0,$$

or

$$v_i(t^*, x^*, z^*) = 0, \ \frac{\partial v_i}{\partial x_j}(t^*, x^*, z^*) = 0, \ \sum_{j=1}^{n}\lambda_i^2\frac{\partial^2 v_i}{\partial x_j^2}(t^*, x^*, z^*)\le 0.$$

Suppose that the first alternative holds, then it implies that at (t^*, x^*, z^*),

$$\underline{c}_i(t^*, x^*, z^*) = c_i(t^*, x^*, z^*),$$

$$\frac{\partial \underline{c}_i}{\partial x_j}(t^*, x^*, z^*) = \frac{\partial c_i}{\partial x_j}(t^*, x^*, z^*),$$

$$\sum_{j=1}^{n}\lambda_i^2\left(\frac{\partial^2 c_i}{\partial x_j^2}(t^*, x^*, z^*) - \frac{\partial^2 \underline{c}_i}{\partial x_j^2}(t^*, x^*, z^*)\right)\ge 0.$$

Thus $\nabla_x^2 u_i = \nabla_x^2(c_i - \underline{c}_i)\ge 0$ at the point (t^*, x^*, z^*). Since $\frac{\partial u_i}{\partial t} = \frac{\partial}{\partial t}(c_i - \underline{c}_i)\le 0$ also, it follows that

$$\frac{\partial c_i}{\partial t} - \frac{\partial \underline{c}_i}{\partial t} - D_i\nabla_x^2 c_i + D_i\nabla_x^2 \underline{c}_i \le 0.$$

Hence, we have

$$\frac{\partial \underline{c}_i}{\partial t} - D_i\nabla_x^2 \underline{c}_i - \underline{f}_i(t, x, \underline{c}_k, \overline{c}_l) \ge \frac{\partial c_i}{\partial t} - D_i\nabla_x^2 c_i - f_i(t, x, c_j),$$

at the point (t^*, x^*, z^*) which is a contradiction.

If $(t^*, x^*, z^*) \in (0, T] \times \partial\Omega_2 \times \Lambda$, then either $D_i\frac{\partial u_i}{\partial n} + H_i u_i \le 0$ or $D_i\frac{\partial v_i}{\partial n} + H_i v_i \ge 0$ and so there must exist a point (t^*, z^*) in $[0, T] \times \overline{\Lambda}$ and an index $i \in J$ such that $U_j(t, z) \le 0 \le V_j(t, z)$ on $[0, t^*] \times \overline{\Lambda}$, $j \ne i$ and $U_i(t, z) < 0 < V_i(t, z)$ on $[0, t^*) \times \overline{\Lambda}$.

Suppose there exists such a point in $[0, T] \times \overline{\Lambda}$. By continuity, we have either $U_i(t^*, z^*) = 0$ or $V_i(t^*, z^*) = 0$.

If $(t^*, z^*) \in (0, T] \times \Lambda$, then (t^*, z^*) is either a point of minimum of U_i or a point of maximum of V_i and these minimum and maximum values at these points are equal to zero. Hence if $(t^*, z^*) \in (0, T] \times \Lambda$, we have either

$$U_i(t^*, z^*) = 0, \ \frac{\partial U_i}{\partial z_j}(t^*, z^*) = 0, \ \sum_{j=1}^{n} \lambda_i^2 \frac{\partial^2 U_i}{\partial z_j^2}(t^*, z^*) \ge 0,$$

or

$$V_i(t^*, z^*) = 0, \ \frac{\partial V_i}{\partial z_j}(t^*, z^*) = 0, \ \sum_{j=1}^{n} \lambda_i^2 \frac{\partial^2 V_i}{\partial z_j^2}(t^*, z^*) \le 0.$$

Suppose that the first alternative holds, then it implies that at (t^*, z^*),

$$\underline{C}_i(t^*, z^*) = C_i(t^*, z^*),$$

$$\frac{\partial \underline{C}_i}{\partial z_j}(t^*, z^*) = \frac{\partial C_i}{\partial z_j}(t^*, z^*),$$

$$\sum_{j=1}^{n} \lambda_i^2 \left(\frac{\partial^2 C_i}{\partial z_j^2}(t^*, z^*) - \frac{\partial^2 \underline{C}_i}{\partial z_j^2}(t^*, z^*)\right) \ge 0.$$

Thus $\nabla^2 U_i = \nabla^2(C_i - \underline{C}_i) \ge 0$ at the point (t^*, z^*). Since $\frac{\partial U_i}{\partial t} = \frac{\partial}{\partial t}(C_i - \underline{C}_i) \le 0$ also, it follows that

$$\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2 \underline{C}_i + u\cdot\nabla \underline{C}_i + H_i\int_{\partial\Omega_2}(\underline{C}_i - \underline{c}_i) \ge \frac{\partial C_i}{\partial t} - \mathcal{D}_i\nabla^2 C_i + u\cdot\nabla C_i + H_i\int_{\partial\Omega_2}(C_i - c_i).$$

Hence, we have

$$\begin{aligned} &\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2 \underline{C}_i + u\cdot\nabla \underline{C}_i + H_i\int_{\partial\Omega_2}(\underline{C}_i - \underline{c}_i) - \underline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \\ &\ge \frac{\partial C_i}{\partial t} - \mathcal{D}_i\nabla^2 C_i + u\cdot\nabla C_i + H_i\int_{\partial\Omega_2}(C_i - c_i) - F_i(t, z, C_j), \end{aligned}$$

at the point (t^*, z^*) which is a contradiction. The second alternative is treated similarly.

If $(t^*, z^*) \in (0, T] \times \partial\Lambda_1$, then $\upsilon_1 U_i + \mathcal{D}_i \dfrac{\partial U_i}{\partial n_1} \leq 0$ or $\upsilon_1 V_i + \mathcal{D}_i \dfrac{\partial V_i}{\partial n_1} \geq 0$, which is impossible by (ix).

If $(t^*, z^*) \in (0, T] \times \partial\Lambda_\alpha$, $\alpha = 2, 3$, then either $\dfrac{\partial U_i}{\partial n_\alpha} \leq 0$ or $\dfrac{\partial V_i}{\partial n_\alpha} \geq 0$, which is impossible by (xii).

Thus, we get $u_i(t, x, z) < 0 < v_i(t, x, z)$ on $[0, T) \times \overline{\Omega} \times \Lambda$ and $U_i(t, z) < 0 < V_i(t, z)$ on $[0, T) \times \overline{\Lambda}$ for all i. We would arrive at the same conclusions if we suppose firstly that there exists such a point (t^*, z^*) in $[0, T) \times \overline{\Lambda}$ and this proves the claim of the theorem.❑

If f_i and F_i satisfy a Lipschitz condition of the following form, a stronger result can be stated which allow general inequalities in (3.2.17)–(3.2.25). We shall need the following assumption on f_i and F_i.

(H_1) f_i and F_i satisfy a uniform Lipschitz condition in c_j and C_j respectively on any finite interval, so that there are positive constants k_i and K_i such that

$$\left.\begin{aligned} |f_i(t, x, c_j) - f_i(t, x, c_j^*)| &\leq k_i \sup_j (|c_j - c_j^*|), \\ |F_i(t, z, C_j) - F_i(t, z, C_j^*)| &\leq K_i \sup_j (|C_j - C_j^*|). \end{aligned}\right\} \qquad (3.2.26)$$

It can be shown that our assumptions (H_1) of Lipschitz continuity properties for the functions f_i, F_i with respect to the variables c_j and C_j imply similar properties for $\underline{f}_i$, $\bar{f}_i$, $\underline{F}_i$ and $\overline{F}_i$ in the variables $\underline{c}_k$, $\bar{c}_l$, $\underline{C}_k$ and $\overline{C}_l$. We will first require the following lemma:

Lemma 3.2.1

Suppose that we choose the points x_1, x_2, y_1 and y_2 where $x_1 < y_1$ and $x_2 < y_2$ and suppose that there exists $\theta \in [x_1, y_1]$. Then we can always find $\phi \in [x_2, y_2]$ such that

$$\min_\phi |\theta - \phi| \leq \max\{|x_1 - x_2|, |y_1 - y_2|\}.$$

Proof

Either $\theta \in [x_2, y_2]$ or $\theta \notin [x_2, y_2]$. If $\theta \in [x_2, y_2]$, we may take $\phi = \theta$ so that $\min_\phi |\theta - \phi| = 0$. If $\theta \notin [x_2, y_2]$, then either $\theta < x_2$ or $\theta > y_2$. If $\theta < x_2$, then $x_1 < \theta < x_2$ and we may take $\phi = x_2$ so that $\min_\phi |\theta - \phi| = \theta - x_2 < |x_1 - x_2|$ or if $\theta > y_2$, then $y_1 > y_2$ and we may take $\phi = y_1$ so that $\min_\phi |\theta - \phi| = \theta - y_2 < |y_1 - y_2|$. Hence, we can always find $\phi \in [x_2, y_2]$ such that $\min_\phi |\theta - \phi| \leq \max\{|x_1 - x_2|, |y_1 - y_2|\}$.❑

We are now able to prove the following

Lemma 3.2.2

Our assumptions (H_1) of Lipschitz continuity properties for the functions f_i, F_i with respect to the variables c_j and C_j imply similar properties for $\underline{f}_i$, $\bar{f}_i$, $\underline{F}_i$ and $\overline{F}_i$ in the variables $\underline{c}_k$, $\bar{c}_l$, $\underline{C}_k$ and $\overline{C}_l$ and so there are positive constants k_i and K_i given by (H_1) such that

$$\left.\begin{aligned} |\underline{f}_i(t, x, \underline{c}_k, \bar{c}_l) - \underline{f}_i(t, x, \underline{c}_k^*, \bar{c}_l^*)| &\leq k_i \sup_{k,l}(|\underline{c}_k - \underline{c}_k^*|, |\bar{c}_l - \bar{c}_l^*|), \\ |\bar{f}_i(t, x, \underline{c}_k, \bar{c}_l) - \bar{f}_i(t, x, \underline{c}_k^*, \bar{c}_l^*)| &\leq k_i \sup_{k,l}(|\underline{c}_k - \underline{c}_k^*|, |\bar{c}_l - \bar{c}_l^*|), \end{aligned}\right\} \qquad (3.2.27)$$

and

$$\left.\begin{aligned} |\underline{F}_i(t, z, \underline{C}_k, \overline{C}_l) - \underline{F}_i(t, z, \underline{C}_k^*, \overline{C}_l^*)| &\le K_i \sup_{k,l}(|\underline{C}_k - \underline{C}_k^*|, |\overline{C}_l - \overline{C}_l^*|), \\ |\overline{F}_i(t, z, \underline{C}_k, \overline{C}_l) - \overline{F}_i(t, z, \underline{C}_k^*, \overline{C}_l^*)| &\le K_i \sup_{k,l}(|\underline{C}_k - \underline{C}_k^*|, |\overline{C}_l - \overline{C}_l^*|). \end{aligned}\right\} \quad \textbf{(3.2.28)}$$

Proof

We will only prove the first inequality. The other inequalities follow similarly.

Assume without loss of generality that $\underline{c}_j < \overline{c}_j$ and $\underline{c}_j^* < \overline{c}_j^*$ so that $|\underline{f}_i(t, x, \underline{c}_k, \overline{c}_l) - \underline{f}_i(t, x, \underline{c}_k^*, \overline{c}_l^*)| = |f_i(t, x, \theta_j) - f_i(t, x, \theta_j^*)|$, where by definition, $\theta_j \in [\underline{c}_j, \overline{c}_j]$ and $\theta_j^* \in [\underline{c}_j^*, \overline{c}_j^*]$ for all j. Suppose that $|f_i(t, x, \theta_j) \ge f_i(t, x, \theta_j^*)|$. Then $|f_i(t, x, \theta_j) - f_i(t, x, \theta_j^*)| \le f_i(t, x, \theta_j) - f_i(t, x, \phi_j)$, where ϕ_j is any point in $[\underline{c}_j^*, \overline{c}_j^*]$. By Lemma 3.2.1, we can choose ϕ_j so that $\min_{\phi_j} |\theta_j - \phi_j| \le \max\{|\underline{c}_j - \underline{c}_j^*|, |\overline{c}_j - \overline{c}_j^*|\}$ for all j. Then for this choice of ϕ_j,

$$\begin{aligned} |f_i(t, x, \theta_j) - f_i(t, x, \theta_j^*)| &\le k_i\, |\theta_j - \phi_j| \\ &= k_i \sup_j |\theta_j - \phi_j| \\ &\le k_i \sup_j(|\underline{c}_j - \underline{c}_j^*|, |\overline{c}_j - \overline{c}_j^*|), \end{aligned}$$

for all j and the theorem follows .❑

This theorem is the basis for the following comparison theorems for solutions of the system S_n, B_n.

Theorem 3.2.12 (Generalised Strong Comparison Theorem)

Suppose (c_i, C_i) is a solution of the system S_n, B_n and the functions $\underline{c}_i$, $\overline{c}_i$, $\underline{C}_i$ and $\overline{C}_i$ are defined and satisfy the following continuity properties and inequalities

(i) *For components $i \in I$, where $D_i > 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $[0, T] \times \overline{\Omega} \times \Lambda$, their first-order x_j-derivatives exist in $(0, T] \times \overline{\Omega} \times \Lambda$, their second order $x_j x_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(ii) *For components $i \in I$, where $D_i = H_i = 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $[0, T] \times \overline{\Omega} \times \Lambda$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(iii) *For components $i \in J$, where $\mathcal{D}_i > 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T] \times \overline{\Lambda}$, their first order z derivatives exist in $(0, T] \times \overline{\Lambda}$, their second order $z_j z_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(iv) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T] \times \overline{\Lambda}$, their first order z_j derivatives exist in $(0, T] \times \Lambda$ and their first order t-derivatives are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(v) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T] \times \overline{\Lambda}$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(vi) $\underline{c}_i \le c_i \le \overline{c}_i$ *in* $\overline{\Omega} \times \Lambda$ *and* $\underline{C}_i \le C_i \le \overline{C}_i$ *in* $\overline{\Lambda}$ *at* $t = 0$; **(3.2.29)**

(vii) $$\frac{\partial \underline{c}_i}{\partial t} - D_i \nabla_x^2 \underline{c}_i - \underline{f}_i(t, x, \underline{c}_k, \overline{c}_l)$$
$$\le \frac{\partial c_i}{\partial t} - D_i \nabla_x^2 c_i - f_i(t, x, c_j) \tag{3.2.30}$$
$$\le \frac{\partial \overline{c}_i}{\partial t} - D_i \nabla_x^2 \overline{c}_i - \overline{f}_i(t, x, \underline{c}_k, \overline{c}_l) \text{ in } (0, T]\times\Omega\times\Lambda;$$

(viii) $$\frac{\partial \underline{c}_i}{\partial n} \le \frac{\partial c_i}{\partial n} \le \frac{\partial \overline{c}_i}{\partial n} \text{ on } (0, T]\times\partial\Omega_1\times\Lambda; \tag{3.2.31}$$

(ix) $$D_i \frac{\partial \underline{c}_i}{\partial n} - H_i(\underline{C}_i - \underline{c}_i) \le D_i \frac{\partial c_i}{\partial n} - H_i(C_i - c_i) \le D_i \frac{\partial \overline{c}_i}{\partial n} - H_i(\overline{C}_i - \overline{c}_i) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda; \tag{3.2.32}$$

(x) $$\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \underline{C}_i + u\cdot\nabla \underline{C}_i + H_i \int_{\partial\Omega_2} (\underline{C}_i - \underline{c}_i) - \underline{F}_i(t, z, \underline{C}_k, \overline{C}_l)$$
$$\le \frac{\partial C_i}{\partial t} - \mathcal{D}_i \nabla^2 C_i + u\cdot\nabla C_i + H_i \int_{\partial\Omega_2} (C_i - c_i) - F_i(t, z, C_j) \tag{3.2.33}$$
$$\le \frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \overline{C}_i + u\cdot\nabla \overline{C}_i + H_i \int_{\partial\Omega_2} (\overline{C}_i - \overline{c}_i) - \overline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \text{ in } (0, T]\times\Lambda;$$

(xi) $$\underline{C}_{i,1} \le C_{i,1} \le \overline{C}_{i,1}, \tag{3.2.34}$$

$v_1 = -u\cdot n_1$ is uniformly bounded and continuous in $(0, T]\times\partial\Lambda_1$,

$$v_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} = v_1 \underline{C}_{i,1}, \quad v_1 C_i + \mathcal{D}_i \frac{\partial C_i}{\partial n_1} = v_1 C_{i,1}, \quad v_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} = v_1 \overline{C}_{i,1} \text{ on } (0, T]\times\partial\Lambda_1, \tag{3.2.35}$$

so that

$$v_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} \le v_1 C_i + \mathcal{D}_i \frac{\partial C_i}{\partial n_1} \le v_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} \text{ on } (0, T]\times\partial\Lambda_1; \tag{3.2.36}$$

(xii) $$\frac{\partial \underline{C}_i}{\partial n_\alpha} \le \frac{\partial C_i}{\partial n_\alpha} \le \frac{\partial \overline{C}_i}{\partial n_\alpha} \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha = 2, 3; \tag{3.2.37}$$

(xiii) *f_i and F_i satisfy the uniform Lipschitz condition (H_1).*

Then $\underline{c}_i \le c_i \le \overline{c}_i$ *in* $[0, T]\times\overline{\Omega}\times\Lambda$ *and* $\underline{C}_i \le C_i \le \overline{C}_i$ *in* $[0, T]\times\overline{\Lambda}$.

Proof

Construct the functions :

$$\underline{c}_i^\lambda = \underline{c}_i - \lambda e^{\kappa t},\ \overline{c}_i^\lambda = \overline{c}_i + \lambda e^{\kappa t},\ \underline{C}_i^\lambda = \underline{C}_i - \lambda e^{\kappa t},\ \overline{C}_i^\lambda = \overline{C}_i + \lambda e^{\kappa t},\ \lambda > 0,\ \kappa > 0. \tag{3.2.38}$$

The conditions of Theorem 3.2.11 (Generalised Weak Comparison Theorem) can be shown to be satisfied by these functions. We give the details for the only difficult aspect; to show that assumptions (vii) and (x) can hold for all $\lambda > 0$ if κ is large enough. Our assumptions of Lipschitz continuity properties for the functions f_i and F_i with respect to the variables c_j and C_j imply similar properties for $\underline{f}_i$, $\overline{f}_i$, $\underline{F}_i$ and $\overline{F}_i$ in the variables $\underline{c}_k$, $\overline{c}_l$, $\underline{C}_k$ and $\overline{C}_l$ by Lemma 3.2.2. The inequalities (3.2.30) and (3.2.33) in assumptions (vii) and (x) follow for our functions $\underline{c}_i^\lambda$, $\overline{c}_i^\lambda$, $\underline{C}_i^\lambda$ and $\overline{C}_i^\lambda$ if κ is chosen bigger than $\underline{k}_i$, $\overline{k}_i$, $\underline{K}_i$ and $\overline{K}_i$. We give the argument for the first inequality of (3.2.30):

$$
\begin{aligned}
&[\frac{\partial c_i}{\partial t} - D_i\nabla_x^2 c_i - f_i(t, x, c_j)] - [\frac{\partial \underline{c}_i^\lambda}{\partial t} - D_i\nabla_x^2 \underline{c}_i^\lambda - \underline{f}_i(t, x, \underline{c}_k^\lambda, \overline{c}_l^\lambda)] \\
&= \varepsilon + \lambda\kappa e^{\kappa t} + \underline{f}_i(t, x, \underline{c}_k - \lambda e^{\kappa t}, \overline{c}_l + \lambda e^{\kappa t}) - \underline{f}_i(t, x, \underline{c}_k^\lambda, \overline{c}_l^\lambda) \\
&\geq \varepsilon + \lambda(\kappa - \underline{k}_i)e^{\kappa t} \qquad \mathbf{(3.2.39)} \\
&> 0,
\end{aligned}
$$

where $\varepsilon = [\frac{\partial c_i}{\partial t} - D_i\nabla_x^2 c_i - f_i(t, x, c_j)] - [\frac{\partial \underline{c}_i}{\partial t} - D_i\nabla_x^2 \underline{c}_i - \underline{f}_i(t, x, \underline{c}_k, \overline{c}_l)] > 0$ from (3.2.30).

The other inequalities follow in a similar fashion. Hence for all $\lambda > 0$, we have from Theorem 3.2.11,

$$\underline{c}_i^\lambda < c_i^\lambda < \overline{c}_i^\lambda \text{ in } [0, T]\times\overline{\Omega}\times\Lambda \text{ and } \underline{C}_i^\lambda < C_i^\lambda < \overline{C}_i^\lambda \text{ in } [0, T]\times\overline{\Lambda}, \qquad \mathbf{(3.2.40)}$$

and therefore in the limit as λ tends to zero,

$$\underline{c}_i \leq c_i \leq \overline{c}_i \text{ in } [0, T]\times\overline{\Omega}\times\Lambda \text{ and } \underline{C}_i \leq C_i \leq \overline{C}_i \text{ in } [0, T]\times\overline{\Lambda}, \qquad \mathbf{(3.2.41)}$$

and the result follows. ❑

We have seen some generalised weak and strong comparison theorems. While these theorems are useful for solutions of S_n, B_n where initial values at $t = 0$ are given, they provide no information about the steady state solutions for which only boundary value data is given. The following theorem provides a stronger result and spells out the consequences of the existence of contact points of these comparison functions. Its corollary provides useful information about the steady state solutions.

Theorem 3.2.13 (Generalised Strong Comparison (Contact) Theorem)
Suppose (c_i, C_i) is a solution of the system S_n, B_n and the functions $\underline{c}_i$, $\overline{c}_i$, $\underline{C}_i$ and $\overline{C}_i$ are defined and satisfy the following continuity properties and inequalities:

(i) *For components $i \in I$, where $D_i > 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $[0, T]\times\overline{\Omega}\times\Lambda$, their first-order x_j-derivatives exist in $(0, T]\times\overline{\Omega}\times\Lambda$, their second order x_jx_k-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T]\times\Omega\times\Lambda$;*

(ii) *For components $i \in I$, where $D_i = H_i = 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $[0, T]\times\overline{\Omega}\times\Lambda$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T]\times\Omega\times\Lambda$;*

(iii) *For components $i \in J$, where $\mathcal{D}_i > 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T]\times\overline{\Lambda}$, their first order z derivatives exist in $(0, T]\times\overline{\Lambda}$, their second order z_jz_k-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T]\times\Lambda$;*

(iv) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \not\equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $[0, T]\times\overline{\Lambda}$, their first order z_j derivatives exist in $(0, T]\times\Lambda$ and their first order t-derivatives are continuous and uniformly bounded in $(0, T]\times\Lambda$;*

(v) *For components* $i \in J$, *where* $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, $\underline{C}_i$, C_i *and* $\overline{C}_i$ *are continuous in* $[0, T] \times \overline{\Lambda}$ *and their first order t-derivatives exist and are continuous and uniformly bounded in* $(0, T] \times \Lambda$;

(vi) $\underline{c}_i \le c_i \le \overline{c}_i$ *in* $[0, T] \times \overline{\Omega} \times \Lambda$ *and* $\underline{C}_i \le C_i \le \overline{C}_i$ *in* $[0, T] \times \overline{\Lambda}$; **(3.2.42)**

(vii)
$$\begin{aligned}&\frac{\partial \underline{c}_i}{\partial t} - D_i \nabla_x^2 \underline{c}_i - \underline{f}_i(t, x, \underline{c}_k, \overline{c}_l)\\ &\le \frac{\partial c_i}{\partial t} - D_i \nabla_x^2 c_i - f_i(t, x, c_j)\\ &\le \frac{\partial \overline{c}_i}{\partial t} - D_i \nabla_x^2 \overline{c}_i - \overline{f}_i(t, x, \underline{c}_k, \overline{c}_l) \text{ in } (0, T] \times \Omega \times \Lambda;\end{aligned} \tag{3.2.43}$$

(viii)
$$\frac{\partial \underline{c}_i}{\partial n} \le \frac{\partial c_i}{\partial n} \le \frac{\partial \overline{c}_i}{\partial n} \text{ on } (0, T] \times \partial\Omega_1 \times \Lambda; \tag{3.2.44}$$

(ix)
$$D_i \frac{\partial \underline{c}_i}{\partial n} - H_i(\underline{C}_i - \underline{c}_i) \le D_i \frac{\partial c_i}{\partial n} - H_i(C_i - c_i) \le D_i \frac{\partial \overline{c}_i}{\partial n} - H_i(\overline{C}_i - \overline{c}_i) \text{ on } (0, T] \times \partial\Omega_2 \times \Lambda; \tag{3.2.45}$$

(x)
$$\begin{aligned}&\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \underline{C}_i + u \cdot \nabla \underline{C}_i + H_i \int_{\partial\Omega_2} (\underline{C}_i - \underline{c}_i) - \underline{F}_i(t, z, \underline{C}_k, \overline{C}_l)\\ &\le \frac{\partial C_i}{\partial t} - \mathcal{D}_i \nabla^2 C_i + u \cdot \nabla C_i + H_i \int_{\partial\Omega_2} (C_i - c_i) - F_i(t, z, C_j)\\ &\le \frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \overline{C}_i + u \cdot \nabla \overline{C}_i + H_i \int_{\partial\Omega_2} (\overline{C}_i - \overline{c}_i) - \overline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \text{ in } (0, T] \times \Lambda;\end{aligned} \tag{3.2.46}$$

(xi)
$$\underline{C}_{i,1} \le C_{i,1} \le \overline{C}_{i,1}, \tag{3.2.47}$$

$v_1 = -u \cdot n_1$ *is uniformly bounded and continuous in* $(0, T] \times \partial\Lambda_1$,

$$v_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} = v_1 \underline{C}_{i,1}, \quad v_1 C_i + \mathcal{D}_i \frac{\partial C_i}{\partial n_1} = v_1 C_{i,1}, \quad v_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} = v_1 \overline{C}_{i,1} \text{ on } (0, T] \times \partial\Lambda_1, \tag{3.2.48}$$

so that

$$v_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} \le v_1 C_i + \mathcal{D}_i \frac{\partial C_i}{\partial n_1} \le v_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} \text{ on } (0, T] \times \partial\Lambda_1; \tag{3.2.49}$$

(xii)
$$\frac{\partial \underline{C}_i}{\partial n_\alpha} \le \frac{\partial C_i}{\partial n_\alpha} \le \frac{\partial \overline{C}_i}{\partial n_\alpha} \text{ on } (0, T] \times \partial\Lambda_\alpha, \ \alpha = 2, 3; \tag{3.2.50}$$

(xiii) f_i *and* F_i *satisfy the uniform Lipschitz condition* (H_1).

Then

(I) *For components* $i \in I$, *where* $D_i, H_i > 0$, $\mathcal{D}_i > 0$, *either* $\underline{c}_i < c_i < \overline{c}_i$ *in* $(0, T] \times \overline{\Omega} \times \Lambda$ *and* $\underline{C}_i < C_i < \overline{C}_i$ *in* $(0, T] \times \overline{\Lambda}$ *or there are constants* T_i *in* $(0, T]$ *such that* $\underline{c}_i < c_i < \overline{c}_i$ *in* $(T_i, T] \times \overline{\Omega} \times \Lambda$, $c_i \equiv \overline{c}_i$ *(or* $c_i \equiv \underline{c}_i$*) in* $[0, T_i] \times \overline{\Omega} \times \Lambda$, $\underline{C}_i < C_i < \overline{C}_i$ *in* $(T_i, T] \times \overline{\Lambda}$ *and* $C_i \equiv \overline{C}_i$ *(or* $C_i \equiv \underline{C}_i$*) in* $[0, T_i] \times \overline{\Lambda}$.

(II) *For components* $i \in I$, *where* $D_i, H_i > 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, *either* $\underline{c}_i < c_i < \overline{c}_i$ *in* $(0, T] \times \overline{\Omega} \times \Lambda$ *and* $\underline{C}_i < C_i < \overline{C}_i$ *in* $(0, T] \times \overline{\Lambda}$ *or there are constants* T_i *in* $(0, T]$ *such that* $\underline{c}_i < c_i < \overline{c}_i$ *in* $(T_i, T] \times \overline{\Omega} \times \Lambda$, $\underline{C}_i < C_i < \overline{C}_i$ *in* $(T_i, T] \times \overline{\Lambda}$ *and there is at least one point* z^* *in* $\overline{\Lambda}$ *such that*

$c_i \equiv \bar{c}_i$ (or $c_i \equiv \underline{c}_i$) in $[0, T_i]\times\bar{\Omega}\times\Lambda$ and $C_i \equiv \bar{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i]\times\bar{\Lambda}$ along the characteristic curve given by $\frac{dz}{dt} = u(t, z)$, $z = z^*$ at T_i for t in $[0, T_i]$ or until z reaches the boundary $\partial\Lambda_1$.

(III) *For components $i \in I$, where D_i, $H_i > 0$, $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \equiv 0$, either $\underline{c}_i < c_i < \bar{c}_i$ in $(0, T]\times\bar{\Omega}\times\Lambda$ and $\underline{C}_i < C_i < \bar{C}_i$ in $(0, T]\times\bar{\Lambda}$ or there are constants T_i in $(0, T]$ such that $\underline{c}_i < c_i < \bar{c}_i$ in $(T_i, T]\times\bar{\Omega}\times\Lambda$ and $\underline{C}_i < C_i < \bar{C}_i$ in $(T_i, T]\times\bar{\Lambda}$ and there is at least one point z^* in $\bar{\Lambda}$ such that $c_i \equiv \bar{c}_i$ (or $c_i \equiv \underline{c}_i$) in $[0, T_i]\times\bar{\Omega}\times\Lambda$ and $C_i \equiv \bar{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i]\times\bar{\Lambda}$ for t in $[0, T_i]$ at z^*.*

(IV) *For components $i \in I$, where $D_i = H_i = 0$, either $\underline{c}_i < c_i < \bar{c}_i$ in $(0, T]\times\bar{\Omega}\times\Lambda$ or there are constants T_i in $(0, T]$ such that $\underline{c}_i < c_i < \bar{c}_i$ in $(T_i, T]\times\bar{\Omega}\times\Lambda$ and there is at least one point $(x^*_i\ z^*)$ in $\bar{\Omega}^*\times\Lambda$ such that $c_i \equiv \bar{c}_i$ (or $c_i \equiv \underline{c}_i$) in $[0, T_i]\times\bar{\Omega}^*\times\Lambda$ for t in $[0, T_i]$ at $(x^*_i\ z^*)$, where $\bar{\Omega}^*$ is some simply connected part of Ω containing x^*.*

(V) *For components $i \in J$, where $D_i = H_i = 0$, $\mathcal{D}_i > 0$, either $\underline{C}_i < C_i < \bar{C}_i$ in $(0, T]\times\bar{\Lambda}$ or there are constants T_i in $(0, T]$ such that $\underline{C}_i < C_i < \bar{C}_i$ in $(T_i, T]\times\bar{\Lambda}$ and $C_i \equiv \bar{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i]\times\bar{\Lambda}$.*

(VI) *For components $i \in J$, where $D_i = H_i = 0$, $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \not\equiv 0$, either $\underline{C}_i < C_i < \bar{C}_i$ in $(0, T]\times\bar{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{C}_i < C_i < \bar{C}_i$ in $(T_i, T]\times\bar{\Lambda}$ and there is at least one point z^* in $\bar{\Lambda}$ such that $C_i \equiv \bar{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i]\times\bar{\Lambda}$ along the characteristic curve given by $\frac{dz}{dt} = u(t, z)$, $z = z^*$ at T_i for t in $[0, T_i]$ or until z reaches the boundary $\partial\Lambda_1$.*

(VII) *For components $i \in J$, where $D_i = H_i = 0$, $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \equiv 0$, either $\underline{C}_i < C_i < \bar{C}_i$ in $(0, T]\times\bar{\Lambda}$ or there are constants T_i in $(0, T]$ such that $\underline{C}_i < C_i < \bar{C}_i$ in $(T_i, T]\times\bar{\Lambda}$ and at least one point z^* in $\bar{\Lambda}$ such that $C_i \equiv \bar{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i]\times\bar{\Lambda}$ for t in $[0, T_i]$ at z^*.*

Proof

Let us define

$$\phi_i(t, x, u_i) \equiv f_i(t, x, c_i^*) \text{ where } c_i^* = u_i \text{ and } c_j^* = c_j \text{ for } j \neq i, \tag{3.2.51}$$

and

$$\Phi_i(t, z, U_i) \equiv F_i(t, z, C_j^*) \text{ where } C_i^* = U_i \text{ and } C_j^* = C_j \text{ for } j \neq i. \tag{3.2.52}$$

Then from (vi) and (ix), we have,

$$D_i\frac{\partial \underline{c}_i}{\partial n} + H_i\underline{c}_i \le D_i\frac{\partial c_i}{\partial n} + H_i c_i \le D_i\frac{\partial \bar{c}_i}{\partial n} + H_i\bar{c}_i, \tag{3.2.53}$$

from (vi), (vii) and the definition of $\underline{f}_i$, $\bar{f}_i$ and ϕ_i, we have

$$\frac{\partial \underline{c}_i}{\partial t} - D_i\nabla_x^2\underline{c}_i - \phi_i(t, x, \underline{c}_i) \le \frac{\partial c_i}{\partial t} - D_i\nabla_x^2 c_i - \phi_i(t, x, c_i) \le \frac{\partial \bar{c}_i}{\partial t} - D_i\nabla_x^2\bar{c}_i - \phi_i(t, x, \bar{c}_i), \tag{3.2.54}$$

and from (vii), (x) and the definition of $\underline{F}_i$, $\bar{F}_i$ and Φ_i, we have,

$$\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2\underline{C}_i + u\cdot\nabla\underline{C}_i + H_i\mathcal{A}\underline{C}_i - \Phi_i(t, z, \underline{C}_i)$$

$$\le \frac{\partial C_i}{\partial t} - \mathcal{D}_i\nabla^2 C_i + u\cdot\nabla C_i + H_i\mathcal{A}C_i - \Phi_i(t, z, C_i) \tag{3.2.55}$$

$$\leq \frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \overline{C}_i + u \cdot \nabla \overline{C}_i + H_i \mathcal{A} \overline{C}_i - \Phi_i(t, z, \overline{C}_i).$$

The inequalities governing the functions $\underline{c}_i$, c_i, $\overline{c}_i$, $\underline{C}_i$, C_i and $\overline{C}_i$ are now all uncoupled and our conclusion is a consequence of Theorem 3.2.4 (Strong Comparison (Contact) Theorem) for ordinary differential equations, Theorem 3.2.7 (Strong Comparison (Contact) Theorem) for first order partial differential equations and Theorem 3.2.10 (Strong Comparison (Contact) Theorem) for parabolic equations.

(I) For components $i \in I$, where D_i, $H_i > 0$, $\mathcal{D}_i > 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $(0, T] \times \overline{\Omega} \times \Lambda$ and $\underline{C}_i < C_i < \overline{C}_i$ in $(0, T] \times \overline{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{c}_i < c_i < \overline{c}_i$ in $(T_i, T] \times \overline{\Omega} \times \Lambda$, $\underline{C}_i < C_i < \overline{C}_i$ in $(T_i, T] \times \overline{\Lambda}$, $c_i = \overline{c}_i$ $(= \underline{c}_i)$ at a point (T_i, x^*, z^*), where $(x^*, z^*) \in \overline{\Omega} \times \Lambda$ and $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*) where $z^* \in \overline{\Lambda}$.

Suppose that $c_i = \overline{c}_i$ at a point (T_i, x^*, z^*). Theorem 3.2.10 then implies $c_i \equiv \overline{c}_i$ in $(0, T_i] \times \overline{\Omega}^* \times \Lambda$, where $\overline{\Omega}^*$ is some simply connected part of Ω at (T_i, z^*) containing x^*. Condition (ix) shows $C_i = \overline{C}_i$ at (T_i, z^*) and hence $C_i \equiv \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$. This same result is obtained from the alternative assumption that $C_i = \overline{C}_i$ at a point (T_i, z^*). Condition (x) now implies $c_i = \overline{c}_i$ on $\partial\Omega \times \overline{\Lambda}$ at $t = T_i$ and hence $c_i \equiv \overline{c}_i$ in $[0, T_i] \times \overline{\Omega} \times \Lambda$ and $C_i \equiv \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$.

(II) For components $i \in I$, where D_i, $H_i > 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $(0, T] \times \overline{\Omega} \times \Lambda$ and $\underline{C}_i < C_i < \overline{C}_i$ in $(0, T] \times \overline{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{c}_i < c_i < \overline{c}_i$ in $(T_i, T] \times \overline{\Omega} \times \Lambda$, $\underline{C}_i < C_i < \overline{C}_i$ in $(T_i, T] \times \overline{\Lambda}$, $c_i = \overline{c}_i$ $(= \underline{c}_i)$ at a point (T_i, x^*, z^*), where $(x^*, z^*) \in \overline{\Omega} \times \Lambda$ and $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*) where $z^* \in \overline{\Lambda}$.

Suppose that $c_i = \overline{c}_i$ at a point (T_i, x^*, z^*). Theorem 3.2.10 then implies $c_i \equiv \overline{c}_i$ in $(0, T_i] \times \overline{\Omega}^* \times \Lambda$, where $\overline{\Omega}^*$ is some simply connected part of Ω at (T_i, z^*) containing x^*. Condition (ix) shows $C_i = \overline{C}_i$ at (T_i, z^*) and hence $C_i \equiv \overline{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i] \times \overline{\Lambda}$ along the characteristic curve given by $\frac{dz}{dt} = u(t, z)$, $z = z^*$ at T_i for t in $[0, T_i]$ or until z reaches the boundary $\partial\Lambda_1$. This same result is obtained from the alternative assumption that $C_i = \overline{C}_i$ at a point (T_i, z^*). Condition (x) now implies $c_i = \overline{c}_i$ on $\partial\Omega \times \Lambda$ at $t = T_i$ and hence $c_i \equiv \overline{c}_i$ in $[0, T_i] \times \overline{\Omega} \times \Lambda$ and $C_i \equiv \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$ along the characteristic curve given by $\frac{dz}{dt} = u(t, z)$, $z = z^*$ at T_i for t in $[0, T_i]$ or until z reaches the boundary $\partial\Lambda_1$.

(III) For components $i \in I$, where D_i, $H_i > 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $(0, T] \times \overline{\Omega} \times \Lambda$ and $\underline{C}_i < C_i < \overline{C}_i$ in $(0, T] \times \overline{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{c}_i < c_i < \overline{c}_i$ in $(T_i, T] \times \overline{\Omega} \times \Lambda$, $\underline{C}_i < C_i < \overline{C}_i$ in $(T_i, T] \times \overline{\Lambda}$, $c_i = \overline{c}_i$ $(= \underline{c}_i)$ at a point (T_i, x^*, z^*), where $(x^*, z^*) \in \overline{\Omega} \times \Lambda$ and $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*) where $z^* \in \overline{\Lambda}$.

Suppose that $c_i = \overline{c}_i$ at a point (T_i, x^*, z^*). Theorem 3.2.10 then implies $c_i \equiv \overline{c}_i$ in $(0, T_i] \times \overline{\Omega}^* \times \Lambda$, where $\overline{\Omega}^*$ is some simply connected part of Ω at (T_i, z^*) containing x^*. Condition (ix) shows $C_i = \overline{C}_i$ at (T_i, z^*) and hence $C_i \equiv \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$ at z^*. This same result is obtained from the alternative assumption that $C_i = \overline{C}_i$ at a point (T_i, z^*). Condition (x) now implies $c_i = \overline{c}_i$ on $\partial\Omega \times \overline{\Lambda}$ at $t = T_i$ and hence $c_i \equiv \overline{c}_i$ in $[0, T_i] \times \overline{\Omega} \times \Lambda$ and $C_i \equiv \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$ for t in $[0, T_i]$ at z^* in $\overline{\Lambda}$.

(IV) For components $i \in I$, where $D_i = H_i = 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $(0, T] \times \overline{\Omega} \times \Lambda$, or there are constants T_i in $(0, T]$ such that $\underline{c}_i < c_i < \overline{c}_i$ in $(T_i, T] \times \overline{\Omega} \times \Lambda$ and $c_i = \overline{c}_i$ $(= \underline{c}_i)$ at a point (T_i, x^*, z^*), where $(x^*, z^*) \in \overline{\Omega} \times \Lambda$.

Suppose that $c_i = \overline{c}_i$ at a point (T_i, x^*, z^*). Theorem 3.2.4 then implies $c_i \equiv \overline{c}_i$ in $(0, T_i] \times \overline{\Omega}^* \times \Lambda$, at (x^*, z^*), where $\overline{\Omega}^*$ is some simply connected part of Ω at (T_i, z^*) containing x^*.

(V) For components $i \in J$, where $D_i = H_i = 0$, $\mathcal{D}_i > 0$, either $\underline{C}_i < C_i < \overline{C}_i$ in $(0, T] \times \overline{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{C}_i < C_i < \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$ and $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*) where $z^* \in \overline{\Lambda}$.

Suppose that $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*). Theorem 3.2.10 then implies $C_i \equiv \overline{C}_i$ in $[0, T_i] \times \overline{\Lambda}$.

(VI) For components $i \in J$, where $D_i = H_i = 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, either $\underline{C}_i < C_i < \overline{C}_i$ in $(0, T] \times \overline{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{C}_i < C_i < \overline{C}_i$ in $(T_i, T] \times \overline{\Lambda}$ and $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*) where $z^* \in \overline{\Lambda}$.

Suppose that $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*). Theorem 3.2.7 then implies $C_i \equiv \overline{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i] \times \overline{\Lambda}$ along the characteristic curve given by $\dfrac{dz}{dt} = u(t, z)$, $z = z^*$ at T_i for t in $[0, T_i]$ or until z reaches the boundary $\partial\Lambda_1$.

(VII) For components $i \in J$, where $D_i = H_i = 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, either $\underline{C}_i < C_i < \overline{C}_i$ in $(0, T] \times \overline{\Lambda}$, or there are constants T_i in $(0, T]$ such that $\underline{C}_i < C_i < \overline{C}_i$ in $(T_i, T] \times \overline{\Lambda}$ and $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*) where $z^* \in \overline{\Lambda}$.

Suppose that $C_i = \overline{C}_i$ $(= \underline{C}_i)$ at a point (T_i, z^*). Theorem 3.2.4 then implies $C_i \equiv \overline{C}_i$ (or $C_i \equiv \underline{C}_i$) in $[0, T_i] \times \overline{\Lambda}$ for t in $[0, T_i]$ at z^*.❑

An immediate corallary that is independent of time t is the following where we assume that the functions f_i and F_i are independent of t, so that $\underline{f}_i$, $\overline{f}_i$ $\underline{F}_i$ and $\overline{F}_i$ are independent of t.

Corollary 3.2.1
Suppose (c_i, C_i) is a steady state solution of the system S_n, B_n and the functions $\underline{c}_i$, $\overline{c}_i$, $\underline{C}_i$ and $\overline{C}_i$ are defined and satisfy the following continuity properties and inequalities:

(i) *For components $i \in I$, where $D_i > 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $\overline{\Omega} \times \Lambda$, their first-order x_j-derivatives exist in $\overline{\Omega} \times \Lambda$ and their second order x_jx_k-derivatives exist and are continuous and uniformly bounded in $\Omega \times \Lambda$;*

(ii) *For components $i \in I$, where $D_i = H_i = 0$, $\underline{c}_i$, c_i and $\overline{c}_i$ are continuous in $\overline{\Omega} \times \Lambda$;*

(iii) *For components $i \in J$, where $\mathcal{D}_i > 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $\overline{\Lambda}$, their first order z derivatives exist in $\overline{\Lambda}$ and their second order z_jz_k-derivatives are continuous and are uniformly bounded in Λ;*

(iv) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $\overline{\Lambda}$ and their first order z_j derivatives exist in Λ and are uniformly bounded in Λ;*

(v) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, $\underline{C}_i$, C_i and $\overline{C}_i$ are continuous in $\overline{\Lambda}$;*

(vi) $\underline{c}_i \le c_i \le \overline{c}_i$ *in* $\overline{\Omega} \times \Lambda$ *and* $\underline{C}_i \le C_i \le \overline{C}_i$ *in* $\overline{\Lambda}$; **(3.2.56)**

(vii) $-D_i\nabla_x^2\underline{c}_i - \underline{f}_i(x, \underline{c}_k, \overline{c}_l) \le -D_i\nabla_x^2 c_i - f_i(x, c_j) \le -D_i\nabla_x^2\overline{c}_i - \overline{f}_i(x, \underline{c}_k, \overline{c}_l)$ *in* $\Omega \times \Lambda$; **(3.2.57)**

(viii) $\dfrac{\partial \underline{c}_i}{\partial n} \le \dfrac{\partial c_i}{\partial n} \le \dfrac{\partial \overline{c}_i}{\partial n}$ *on* $\partial\Omega_1 \times \Lambda$; **(3.2.58)**

(ix) $$D_i\frac{\partial \underline{c}_i}{\partial n} - H_i(\underline{C}_i - \underline{c}_i) \le D_i\frac{\partial c_i}{\partial n} - H_i(C_i - c_i) \le D_i\frac{\partial \overline{c}_i}{\partial n} - H_i(\overline{C}_i - \overline{c}_i) \text{ on } \partial\Omega_2\times\Lambda; \tag{3.2.59}$$

(x) $$\begin{aligned}&-\mathcal{D}_i\nabla^2\underline{C}_i + u\cdot\nabla\underline{C}_i + H_i\int_{\partial\Omega_2}(\underline{C}_i - \underline{c}_i) - \underline{F}_i(z, \underline{C}_k, \overline{C}_l)\\ &\le -\mathcal{D}_i\nabla^2 C_i + u\cdot\nabla C_i + H_i\int_{\partial\Omega_2}(C_i - c_i) - F_i(z, C_j)\\ &\le -\mathcal{D}_i\nabla^2\overline{C}_i + u\cdot\nabla\overline{C}_i + H_i\int_{\partial\Omega_2}(\overline{C}_i - \overline{c}_i) - \overline{F}_i(z, \underline{C}_k, \overline{C}_l) \text{ in } \Lambda;\end{aligned} \tag{3.2.60}$$

(xi) $$\underline{C}_{i,1} \le C_{i,1} \le \overline{C}_{i,1}, \tag{3.2.61}$$

$v_1 = -u\cdot n_1$ is uniformly bounded and continuous in $\partial\Lambda_1$,

$$v_1\underline{C}_i + \mathcal{D}_i\frac{\partial\underline{C}_i}{\partial n_1} = v_1\underline{C}_{i,1},\quad v_1 C_i + \mathcal{D}_i\frac{\partial C_i}{\partial n_1} = v_1 C_{i,1},\quad v_1\overline{C}_i + \mathcal{D}_i\frac{\partial\overline{C}_i}{\partial n_1} = v_1\overline{C}_{i,1} \text{ on } \partial\Lambda_1, \tag{3.2.62}$$

so that

$$v_1\underline{C}_i + \mathcal{D}_i\frac{\partial\underline{C}_i}{\partial n_1} \le v_1 C_i + \mathcal{D}_i\frac{\partial C_i}{\partial n_1} \le v_1\overline{C}_i + \mathcal{D}_i\frac{\partial\overline{C}_i}{\partial n_1} \text{ on } \partial\Lambda_1; \tag{3.2.63}$$

(xii) $$\frac{\partial\underline{C}_i}{\partial n_\alpha} \le \frac{\partial C_i}{\partial n_\alpha} \le \frac{\partial\overline{C}_i}{\partial n_\alpha} \text{ on } \partial\Lambda_\alpha,\ \alpha = 2, 3; \tag{3.2.64}$$

(xiii) *f_i and F_i satisfy the uniform Lipschitz condition (H_1).*

Then

(I) *For components $i \in I$, where $D_i, H_i > 0$, $\mathcal{D}_i > 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $\overline{\Omega}\times\Lambda$ and $\underline{C}_i < C_i < \overline{C}_i$ in $\overline{\Lambda}$ or $c_i \equiv \overline{c}_i$ (or $c_i \equiv \underline{c}_i$) in $\overline{\Omega}\times\Lambda$ and $C_i \equiv \overline{C}_i$ (or $C_i \equiv \underline{C}_i$) in $\overline{\Lambda}$.*

(II) *For components $i \in I$, where $D_i, H_i > 0$, $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \not\equiv 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $\overline{\Omega}\times\Lambda$ and $\underline{C}_i < C_i < \overline{C}_i$ in $\overline{\Lambda}$, or $c_i \equiv \overline{c}_i$ (or $c_i \equiv \underline{c}_i$) in $\overline{\Omega}\times\Lambda$ and there is at least one point z^* in $\overline{\Lambda}$ such that $C_i \equiv \overline{C}_i$ (or $C_i \equiv \underline{C}_i$) in $\overline{\Lambda}$ along the characteristic curve given by $\dfrac{dz}{dz_1} = \dfrac{u(z)}{u_1(z)}$, $z = z^*$ at z_1 for z_1 in $\overline{\Lambda}_1$ until z reaches the boundary $\partial\Lambda_1$ (Here u_1 is chosen without loss of generality to be the first component of $u(z)$ that is nonzero, z_1 corresponds to this component and $\overline{\Lambda} \equiv \overline{\Lambda}_1 \cup \overline{\Lambda}_{n-1}$ where $\overline{\Lambda}_1$ is the interval $[a, b]$ with $a, b \in R$).*

(III) *For components $i \in I$, where $D_i, H_i > 0$, $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \equiv 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $\overline{\Omega}\times\Lambda$ and $\underline{C}_i < C_i < \overline{C}_i$ in $\overline{\Lambda}$ or there is at least one point z^* in $\overline{\Lambda}$ such that $c_i \equiv \overline{c}_i$ (or $c_i \equiv \underline{c}_i$) in $\overline{\Omega}\times\Lambda$ and $C_i \equiv \overline{C}_i$ (or $C_i \equiv \underline{C}_i$) in $\overline{\Lambda}$ at z^*.*

(IV) *For components $i \in I$, where $D_i = H_i = 0$, either $\underline{c}_i < c_i < \overline{c}_i$ in $\overline{\Omega}\times\Lambda$ or there is at least one point z^* in $\overline{\Lambda}$ such that $c_i \equiv \overline{c}_i$ (or $c_i \equiv \underline{c}_i$) in $\overline{\Omega}^*\times\Lambda$ at the point (x^*, z^*), where $\overline{\Omega}^*$ is some simply connected part of Ω at z^* containing x^*.*

(V) *For components* $i \in J$, *where* $D_i = H_i = 0$, $\mathcal{D}_i > 0$, *either* $\underline{C}_i < C_i < \overline{C}_i$ *in* $\overline{\Lambda}$ *or* $C_i \equiv \overline{C}_i$ (*or* $C_i \equiv \underline{C}_i$) *in* $\overline{\Lambda}$.

(VI) *For components* $i \in J$, *where* $D_i = H_i = 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, *either* $\underline{C}_i < C_i < \overline{C}_i$ *in* $\overline{\Lambda}$ *or there is at least one point* z^* *in* $\overline{\Lambda}$ *such that* $C_i \equiv \overline{C}_i$ (*or* $C_i \equiv \underline{C}_i$) *along the characteristic curve given by* $\dfrac{dz}{dz_1} = \dfrac{u(z)}{u_1(z)}$, $z = z^*$ *at* z_1 *for* z_1 *in* $\overline{\Lambda}_1$ *until* z *reaches the boundary* $\partial\Lambda_1$.

(VII) *For components* $i \in J$, *where* $D_i = H_i = 0$, $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, *either* $\underline{C}_i < C_i < \overline{C}_i$ *in* $\overline{\Lambda}$ *or there is at least one point* z^* *in* $\overline{\Lambda}$ *such that* $C_i \equiv \overline{C}_i$ (*or* $C_i \equiv \underline{C}_i$) *in* $\overline{\Lambda}$ *at* z^*.

Remark 3.2.1

Consider the system where D_i, $\mathcal{D}_i > 0$ for all i. From conditions (vii) and (x) of Theorem 3.2.13 (Generalised Strong Comparison (Contact) Theorem), we must also have $f_i(t, x, c_j) = \bar{f}_i(t, x, \underline{c}_k, \bar{c}_l)$ $(= \underline{f}_i(t, x, \underline{c}_k, \bar{c}_l))$ in $[0, T_i] \times \overline{\Omega} \times \Lambda$ and $F_i(t, z, C_j) = \overline{F}_i(t, z, \underline{C}_k, \overline{C}_l)$ $(= \underline{F}_i(t, z, \underline{C}_k, \overline{C}_l))$ in $[0, T_i] \times \overline{\Lambda}$ if f_i and F_i are strictly monotone increasing in c_j and C_j, respectively. These imply c_j coincides with one of the bounds $\bar{c}_j$ or $\underline{c}_j$ and hence $T_i = T_j$ or else $\bar{f}_i$ is independent of $\bar{c}_j$ or $\underline{c}_j$ and in this range the inequalities for $\bar{c}_j$ ($\underline{c}_j$) become uncoupled from the $\bar{c}_i$, $\underline{c}_i$ system and T_i and T_j may be unrelated. There are similar consequences for $\overline{F}_i$ and the $\overline{C}_i$, $\underline{C}_i$ system. From conditions (vii) and (x) of Corollary 3.2.1, we see that similar consequences also hold for the time independent case.

Our next comparison theorem for solutions of S_n, B_n shows the consequences of Theorem 3.2.13 if some of the inequalities are strict. Let us consider the case where strict inequalities are required of the initial conditions and the boundary condition at $\partial\Lambda_1$ and therefore, the severe constraints that (vi) in Theorem 3.2.13 hold at the outset and (xi) hold at the boundary $\partial\Lambda_1$ are relinquished. Similar theorems hold if strict inequalities are required of the differential inequalities.

Theorem 3.2.14

Assume that our assumptions in Theorem 3.2.13 *all hold with the exception of* (vi) *which is replaced by the following*

(vi') $\underline{c}_i < c_i < \bar{c}_i$ *in* $\overline{\Omega} \times \Lambda$ *and* $\underline{C}_i < C_i < \overline{C}_i$ *in* $\overline{\Lambda}$ *at* $t = 0$, **(3.2.65)**

and for components $i \in J$, *where* $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, (xi) *is replaced by the following*

(xi') $\underline{C}_{i,1} < C_{i,1} < \overline{C}_{i,1}$ on $(0, T] \times \partial\Lambda_1$. **(3.2.66)**

Then the inequalities in (3.2.65) *hold for all* t *in* $[0, T]$.

Proof

If the inequalities (3.2.65) are violated in $[0, T]$, then there is a first time t^* when the strict inequality is violated. At such a t^* there are points in $\overline{\Lambda}$ where, at a point in $\overline{\Omega} \times \Lambda$, one, some or all of the following happen:

$$c_i = \underline{c}_i,\ c_i = \bar{c}_i,\ C_i = \underline{C}_i,\ C_i = \overline{C}_i, \tag{3.2.67}$$

for some value or values of i.

Suppose this happens at $(t^*_, x^*_, z^*)$. Then from Theorem 3.2.13 this implies that $\underline{c}_i$ or $\overline{c}_i \equiv c_i$ in $[0, t^*]\times\overline{\Omega}\times\Lambda$ at $(x^*_, z^*)$ and hence this same equality is satisfied at $(0, x^*_, z^*)$. If we suppose that this happens at $(t^*_, z^*)$ then Theorem 3.2.13 implies that $\underline{C}_i$ or $\overline{C}_i \equiv C_i$ in $[0, t^*]\times\overline{\Lambda}$ at z^* and hence this same equality is satisfied at $(0, z^*)$ or in the case of components $i\in J$, where $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \not\equiv 0$, this equality may be satisfied at $\partial\Lambda_1$. This is contrary to assumptions, hence the strict inequality (3.2.65) must hold for all t in $[0, T]$.□

It is interesting to note that theorems analagous to theorems 3.2.11 (Generalised Weak Comparison Theorem) and 3.2.12 (Generalised Strong Comparison Theorem) do not hold in general in the case of the corresponding steady state or time independent problem $\hat{S}_n$, $\hat{B}_n$. For example, consider the problem

$$-\frac{\partial^2 c}{\partial x^2} = 8c+1 \text{ for } 0 < x < 1, 0 < z < 1,$$
$$\frac{\partial c}{\partial x} = 0 \text{ at } x = 0, 0 < z < 1,$$
$$\frac{\partial c}{\partial x} + c = C \text{ at } x = 1, 0 < z < 1,$$
$$-\frac{d^2C}{dz^2}+\frac{dC}{dz}+\left.\frac{\partial c}{\partial x}\right|_{x=1} = 0 \text{ in } 0 < z < 1,$$
$$C+\frac{\partial C}{\partial z} = 1 \text{ at } z = 1,$$
$$\frac{\partial C}{\partial z} = 0 \text{ at } z = 0.$$

The functions $\underline{c} = (4x^4+3)z$, $\overline{c} = 8x^2z$, $\underline{C} = z^2$ and $\overline{C} = z^2+z$ satisfy the following inequalities:

$$\begin{aligned}[-\frac{\partial^2\overline{c}}{\partial x^2}-(8\overline{c}+1)]-[-\frac{\partial^2\underline{c}}{\partial x^2}-(8\underline{c}+1)] &= [-16z-(8\cdot 8x^2z+1)]-[-48x^2z-(8(4x^4+3)z+1)]\\ &= [-16z-64x^2z-1]-[-48x^2z-32x^4z-24z-1)]\\ &= (32x^4-16x^2+8)z\\ &= [2(4x^2-1)^2+6]z\\ &> 0 \text{ in } 0 < x < 1, 0 < z < 1,\end{aligned}$$

$$\frac{\partial\overline{c}}{\partial x} = \frac{\partial\underline{c}}{\partial x} = 0 \geq 0 \text{ at } x = 0, 0 < z < 1,$$

$$[\frac{\partial\overline{c}}{\partial x}-(\overline{C}-\overline{c})]-[\frac{\partial\underline{c}}{\partial x}-(\underline{C}-\underline{c})] = [16z-(\overline{C}-8z)]-[16z-(\underline{C}-7z)] = \underline{C}-\overline{C}+z = 0 \geq 0 \text{ at } x = 1, 0 < z < 1,$$

$$\begin{aligned}[-\frac{d^2\overline{C}}{dz^2}+\frac{d\overline{C}}{dz}+\left.\frac{\partial\overline{c}}{\partial x}\right|_{x=1}]-[-\frac{d^2\underline{C}}{dz^2}+\frac{d\underline{C}}{dz}+\left.\frac{\partial\underline{c}}{\partial x}\right|_{x=1}] &= [-2+(2z+1)+16z]-[-2+2z+16z]\\ &= 1 \geq 0 \text{ in } 0 < z < 1,\end{aligned}$$

$$[\overline{C}+\frac{\partial\overline{C}}{\partial z}] - [\underline{C}+\frac{\partial\underline{C}}{\partial z}] = [(z^2+z)+(2z+1)]-[z^2+2z] = z+1 \geq 0 \text{ at } z = 1,$$

$$\frac{\partial\overline{C}}{\partial z} = 1, \frac{\partial\underline{C}}{\partial z} = 0 \text{ at } z = 0.$$

Thus,

$$[-\frac{\partial^2 \overline{c}}{\partial x^2} - (8\overline{c}+1)] > [-\frac{\partial^2 \underline{c}}{\partial x^2} - (8\underline{c}+1)] \text{ for } 0 < x < 1, 0 < z < 1,$$

$$\frac{\partial \overline{c}}{\partial x} \geq \frac{\partial \underline{c}}{\partial x} \text{ at } x = 0, 0 < z < 1,$$

$$[\frac{\partial \overline{c}}{\partial x} - (\overline{C} - \overline{c})] \geq [\frac{\partial \underline{c}}{\partial x} - (\underline{C} - \underline{c})] \text{ at } x = 1, 0 < z < 1,$$

$$[-\frac{d^2\overline{C}}{dz^2} + \frac{dC}{dz} + \left.\frac{\partial \overline{c}}{\partial x}\right|_{x=1}] \geq [-\frac{d^2\underline{C}}{dz^2} + \frac{d\underline{C}}{dz} + \left.\frac{\partial \underline{c}}{\partial x}\right|_{x=1}] \text{ for } 0 < z < 1,$$

$$\frac{\partial \overline{C}}{\partial z} \geq \frac{\partial \underline{C}}{\partial z} \text{ at } z = 0,$$

$$[\overline{C} + \frac{\partial \overline{C}}{\partial z}] \geq [\underline{C} + \frac{\partial \underline{C}}{\partial z}] \text{ at } z = 1.$$

If theorems analogous to Theorems 3.2.12 (Generalised Strong Comparison Theorem) held, we would also expect that at least that $\underline{c} \leq \overline{c}$ for all $0 \leq x \leq 1$, $0 < z < 1$ and $\underline{C} \leq \overline{C}$ for $0 < z < 1$. Clearly, from the definition of $\underline{C}$ and $\overline{C}$, we have $\underline{C} \leq \overline{C}$ for all z. However, when $x = \frac{1}{2}$, $\underline{c}(\frac{1}{2}) = (4(\frac{1}{2})^4 + 3)z = 3\frac{1}{4}z$, $\overline{c}(\frac{1}{2}) = 8(\frac{1}{2})^2 z = 2z$ and $3\frac{1}{4}z \nless 2z$, so theorems analogous to Theorems 3.2.12 do not hold in this case.

Remark 3.2.2

Equations S_n, B_n have been chosen with bioreactor applications in mind, but the theory can be readily generalised in a number of ways. Our proofs are still valid for $D_i\nabla_x^2 c_i$ replaced by $\nabla_x \cdot (D_i(x, c_i)\nabla_x c_i)$ and $\mathcal{D}_i\nabla^2 C_i$ replaced by $\nabla \cdot (\mathcal{D}_i(z, C_i)\nabla C_i)$, provided that we have uniform ellipticity conditions for these more general equations. Furthermore, the mass transfer coefficients H_i could be functions of x and t, provided that these functions are still positive and satisfy appropriate continuity properties, and a wider class of coupling functions is permissible, since f_i and F_i may be permitted to depend on ∇c_i and ∇C_i, respectively.

In section 3.3 we discuss the uniqueness of solutions of the system S_n, B_n.

3.3 Uniqueness of Solutions to the Unsteady State Problem

The numerical analyst needs a knowledge of classical theory in order to decide whether a problem has a solution and whether it is a unique solution or not. The experimentalists who try to validate mathematical models also need to know which solution they are comparing their experimental data against if there is more than one solution.

We use Theorem 3.2.12 (Generalised Strong Comparison Theorem) to show that solutions of system S_n, B_n are uniquely specified by the functions $c_{i,0}$, $C_{i,0}$ and $C_{i,1}$.

Theorem 3.3.1 (Generalised Uniqueness Theorem)

Suppose (c_i, C_i) is a solution of the system S_n, B_n which satisfies the following continuity properties

(i) *For components $i \in I$, where $D_i, H_i > 0$, c_i are continuous in $[0, T] \times \overline{\Omega} \times \Lambda$, their first-order x_j-derivatives exist in $(0, T] \times \overline{\Omega} \times \Lambda$, their second order $x_j x_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(ii) *For components $i \in I$, where $D_i = H_i = 0$, c_i are continuous in $[0, T] \times \overline{\Omega} \times \Lambda$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(iii) *For components $i \in J$, where $\mathcal{D}_i > 0$, C_i are continuous in $[0, T] \times \overline{\Lambda}$, their first order z derivatives exist in $(0, T] \times \overline{\Lambda}$, their second order $z_j z_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(iv) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, C_i are continuous in $[0, T] \times \overline{\Lambda}$, their first order z_j derivatives exist in $(0, T] \times \Lambda$ and their first order t-derivatives are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(v) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, C_i are continuous in $[0, T] \times \overline{\Lambda}$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(vi) *f_i and F_i satisfy the uniform Lipschitz condition (H_1).*

Then there can be at most one solution to the system S_n, B_n.

Proof

Theorem 3.2.12 (Generalised Strong Comparison Theorem) implies uniqueness of the initial value problem S_n, B_n, since if (c_{i1}, C_{i1}) and (c_{i2}, C_{i2}) are two solutions coinciding at $t = 0$, and at $\partial\Lambda_1$, then

$$c_{i1} \le c_{i2} \le c_{i1} \text{ and } C_{i1} \le C_{i2} \le C_{i1}, \tag{3.3.1}$$

and therefore c_{i1} coincides with c_{i2} and C_{i1} with C_{i2} for $t > 0$. ❑

Remark 3.3.1

It should be pointed out that although the uniqueness conclusion for the system S_n, B_n for given initial conditions holds for all finite T, it has little relevance to questions concerning the uniqueness of the steady-state problem $\hat{S}_n$, $\hat{B}_n$. There may be many steady state solutions of the system S_n, B_n satisfying all but the initial conditions of section 3.2 but we see from Theorem 3.2.12, that each must arise from different initial conditions.

In section 3.4 we shall present some imbedding results for the system S_n, B_n.

3.4 Imbedding Results

In this section, we see that for the purposes of uniqueness, stability and existence theorems, we may assume at the outset that the system S_n, B_n is a quasimonotone system, i.e. f_i and F_i are monotone nondecreasing in c_j and C_j respectively for $j \neq i$. This is not a restriction on these theorems of this chapter since if this monotone property is not satisfied, then the system S_n, B_n with general functions f_i and F_i can be imbedded in a system S_{2n}, B_{2n} of the same form where $f_i(t, x, c_j)$ is replaced by $\bar{f}_i(t, x, \underline{c}_k, \overline{c}_l)$ for the first $n(I)$ dependent variables $\overline{c}_i$ and by $\underline{f}_i(t, x, \underline{c}_k, \overline{c}_l)$ for the next $n(I)$ dependent variables $\underline{c}_i$. Also, $F_i(t, z, C_j)$ is replaced by $\overline{F}_i(t, z, \underline{C}_k, \overline{C}_l)$ for the first $n(J)$ dependent variables $\overline{C}_i$ and by $\underline{F}_i(t, z, \underline{C}_k, \overline{C}_l)$ for the next $n(J)$ dependent variables $\underline{C}_i$. It can be shown that solutions of this new system generate solutions of the original system and therefore uniqueness, stability and existence can be implied in the original system.

We consider the new system S_{2n}, B_{2n} of up to twice the order satisfied by $\underline{c}_i$, $\overline{c}_i$, $\underline{C}_i$ and $\overline{C}_i$ in the following equations:

$$\frac{\partial \underline{c}_i}{\partial t} - D_i \nabla_x^2 \underline{c}_i = \underline{f}_i(t, x, \underline{c}_k, \overline{c}_l), \quad \frac{\partial \overline{c}_i}{\partial t} - D_i \nabla_x^2 \overline{c}_i = \overline{f}_i(t, x, \underline{c}_k, \overline{c}_l) \text{ in } (0, T]\times\Omega\times\Lambda,$$

$$\frac{\partial \underline{c}_i}{\partial n} = 0, \quad \frac{\partial \overline{c}_i}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda,$$

$$D_i \frac{\partial \underline{c}_i}{\partial n} = H_i(\underline{C}_i - \underline{c}_i), \quad D_i \frac{\partial \overline{c}_i}{\partial n} = H_i(\overline{C}_i - \overline{c}_i) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \underline{C}_i + u\cdot\nabla \underline{C}_i + H_i \int_{\partial\Omega_2} (\underline{C}_i - \underline{c}_i) = \underline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \text{ in } (0, T]\times\Lambda,$$

$$\frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i \nabla^2 \overline{C}_i + u\cdot\nabla \overline{C}_i + H_i \int_{\partial\Omega_2} (\overline{C}_i - \overline{c}_i) = \overline{F}_i(t, z, \underline{C}_k, \overline{C}_l) \text{ in } (0, T]\times\Lambda,$$

$$\upsilon_1 \underline{C}_i + \mathcal{D}_i \frac{\partial \underline{C}_i}{\partial n_1} = \upsilon_1 \underline{C}_{i,1}, \quad \upsilon_1 \overline{C}_i + \mathcal{D}_i \frac{\partial \overline{C}_i}{\partial n_1} = \upsilon_1 \overline{C}_{i,1} \text{ on } (0, T]\times\partial\Lambda_1,$$

$$\frac{\partial \underline{C}_i}{\partial n_\alpha} = 0, \quad \frac{\partial \overline{C}_i}{\partial n_\alpha} = 0 \text{ on } (0, T]\times\partial\Lambda_\alpha, \ \alpha = 2, 3,$$

$$\underline{c}_i(0, x, z) = c_{i,0}, \quad \overline{c}_i(0, x, z) = c_{i,0} \text{ in } \Omega\times\Lambda,$$

$$\underline{C}_i(0, z) = C_{i,0}, \quad \overline{C}_i(0, z) = C_{i,0} \text{ in } \Lambda,$$

where $\underline{f}_i$, $\overline{f}_i$ $\underline{F}_i$ and $\overline{F}_i$ are defined in (3.2.7)-(3.2.14).

Note that the functions $\{\overline{f}_i, -\underline{f}_i\}$ and $\{\overline{F}_i, -\underline{F}_i\}$ obey a mixed quasimonotone property (mqmp) in the sense of LADDE *et al.*[153, p.161], i.e, the functions $\overline{f}_i$ and $-\underline{f}_i$ are monotone nondecreasing in $\overline{c}_l$ and monotone nonincreasing in $\underline{c}_k$ for all $i \neq k, l$ and the functions $\overline{F}_i$ and $-\underline{F}_i$ are monotone nondecreasing in $\overline{C}_l$ and monotone nonincreasing in $\underline{C}_k$ for all $i \neq k, l$.

If we therefore slightly modify the system S_{2n}, B_{2n} as suggested by MCNABB [186], by introducing new variables $v_i = \overline{c}_i$, $v_{n(I)+i} = -\underline{c}_i$ for $i=1,..,n(I)$ and $V_i = \overline{C}_i$, $V_{n(J)+i} = -\underline{C}_i$ for $i=1,..,n(J)$ and if we set $f_i^* = \overline{f}_i$, $f_{n(I)+i}^* = -\underline{f}_i$ for $i=1,..,n(I)$ and $F_i^* = \overline{F}_i$, $F_{n(J)+i}^* = -\underline{F}_i$ for $i=1,..,n(J)$ then we obtain a new system S_{2n}^*, B_{2n}^* for which f_i^* and F_i^* are nondecreasing functions of v_j and V_j, respectively, for all $j \neq i$. It can be shown by Lemma 3.2.2, that these new functions have the Lipschitz properties that were imposed on the original functions f_i and F_i.

Every solution (c_i, C_i) of S_n, B_n generates a solution $v_i = c_i$, $v_{n(I)+i} = -c_i$ and $V_i = C_i$, $V_{n(J)+i} = -C_i$ of the new system S_{2n}^*, B_{2n}^* with the special property that for $i \leq n(I)$, $v_i + v_{n(I)+i} \equiv 0$ in $[0, T]\times\overline{\Omega}\times\Lambda$ and for $i \leq n(J)$, $V_i + V_{n(J)+i} \equiv 0$ in $[0, T]\times\overline{\Lambda}$. Conversely, any solution (v_i, V_i) of the new system S_{2n}^*, B_{2n}^* with the special property that for $i \leq n(I)$, $v_i + v_{n(I)+i} \equiv 0$ in $[0, T]\times\overline{\Omega}\times\Lambda$ at $t = 0$ and for $i \leq n(J)$, $V_i + V_{n(J)+i} \equiv 0$ in $\overline{\Lambda}$ at $t = 0$ and $V_{i,1} + V_{n(J)+i,1} \equiv 0$ on $(0, T]\times\partial\Lambda_1$, is shown in the following theorem to give rise to a solution of the system S_n, B_n.

Theorem 3.4.1.

The general system S_n, B_n for which f_i and F_i are Lipschitz continuous in c_j and C_j respectively, may be imbedded in a system S_{2n}^*, B_{2n}^* of twice the order which is coupled by monotone functions f_i^* and F_i^* of *the new dependent variables v_i and V_i. Moreover, all the solutions (c_i, C_i) of the system S_n, B_n are solutions of the new system, where*

$$v_i = c_i,\ v_{n(I)+i} = -c_i \text{ for } i=1,..,n(I) \tag{3.4.1}$$

and

$$V_i = C_i,\ V_{n(J)+i} = -C_i \text{ for } i=1,..,n(J) \tag{3.4.2}$$

and all the solutions (v_i, V_i) of S_{2n}^*, B_{2n}^* for which

$$w_i = v_i + v_{n(I)+i} = 0 \text{ in } \Omega\times\Lambda \text{ at } t = 0, \tag{3.4.3}$$

$$W_i = V_i + V_{n(J)+i} = 0 \text{ in } \Lambda \text{ at } t = 0, \tag{3.4.4}$$

$$\frac{\partial w_i}{\partial t} - D_i\nabla_x^2 w_i = f_i^*(t, x, v_j) + f_{n(I)+i}^*(t, x, v_k) \text{ in } (0, T]\times\Omega\times\Lambda, \tag{3.4.5}$$

$$\frac{\partial w_i}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda, \tag{3.4.6}$$

$$D_i\frac{\partial w_i}{\partial n} - H_i(W_i - w_i) = 0 \text{ on } (0, T]\times\partial\Omega_2\times\Lambda, \tag{3.4.7}$$

$$\frac{\partial W_i}{\partial t} - \mathcal{D}_i\nabla_x^2 W_i + u\cdot\nabla W_i = F_i^*(t, z, V_j) + F_{n(J)+i}^*(t, z, V_k) - H_i\int_{\partial\Omega_2}(W_i - w_i) \text{ in } (0, T]\times\Lambda, \tag{3.4.8}$$

$$\upsilon_1 W_i + \mathcal{D}_i\frac{\partial W_i}{\partial n_1} = W_{i,1} = V_{i,1} + V_{n(J)+i,1} = 0 \text{ on } (0, T]\times\partial\Lambda_1, \tag{3.4.9}$$

$$\frac{\partial W_i}{\partial n_\alpha} = 0 \text{ on } (0, T]\times\partial\Lambda_\alpha, \alpha = 2, 3, \tag{3.4.10}$$

with $w_i = v_i + v_{n(I)+i}$ for all $i = 1,..,n(I)$ and $W_i = V_i + V_{n(J)+i}$, for all $i = 1,..,n(J)$ generate solutions (c_i, C_i) of the system S_n, B_n.

Proof

We first note that if we set $\underline{c}_i \equiv \bar{c}_i \equiv c_i$ and $\underline{C}_i \equiv \overline{C}_i \equiv C_i$ for all t, where (c_i, C_i) is a solution of S_n, B_n, then we have a solution of the new system S_{2n}, B_{2n}, so that the solution set of this new system contains all of the solutions of the original system S_n, B_n. In this system, we make the variable change

$$v_i = \bar{c}_i,\ v_{n(I)+i} = -\underline{c}_i, \text{ for } i=1,..,n(I), \tag{3.4.11}$$

$$V_i = \overline{C}_i,\ V_{n(J)+i} = -\underline{C}_i, \text{ for } i=1,..,n(J), \tag{3.4.12}$$

so that the coupling functions f_i^* and F_i^* are nondecreasing functions of all the new dependent variables v_j and V_j, respectively, for all $j \neq i$. Denote this system by S_{2n}^*, B_{2n}^*.

The solutions of S_n, B_n generate solutions in S_{2n}^*, B_{2n}^* for which $w_i = v_i + v_{n(I)+i} = 0$ for $i=1,..,n(I)$ in $[0, T]\times\overline{\Omega}\times\Lambda$ and $W_i = V_i + V_{n(J)+i} = 0$ for $i=1,..,n(J)$ in $[0, T]\times\overline{\Lambda}$.

Suppose we have a solution (v_i, V_i) of S_{2n}^*, B_{2n}^* for which (w_i, W_i) defined above satisfy $w_i = W_i = 0$ everywhere at $t = 0$ and conditions (3.4.5)-(3.4.10) are satisfied. We then obtain the following system of equations, S_n^* for (w_i, W_i):

$$\begin{aligned}\frac{\partial w_i}{\partial t}-D_i\nabla_x^2 w_i &= f_i^*(t,x,v_j)+f_{n(I)+i}^*(t,x,v_k)\\ &=\bar{f}_i(t,x,\underline{c}_j,\bar{c}_k)-\underline{f}_i(t,x,\underline{c}_j,\bar{c}_k)\\ &=\bar{f}_i(t,x,\bar{c}_j-w_j,\bar{c}_k)-\underline{f}_i(t,x,\bar{c}_j-w_j,\bar{c}_k)\ \text{in}\ (0,T]\times\Omega\times\Lambda,\end{aligned} \tag{3.4.13}$$

$$\begin{aligned}\frac{\partial W_i}{\partial t}-\mathcal{D}_i\nabla_x^2 W_i+u\cdot\nabla W_i &= F_i^*(t,z,V_j)+F_{n(J)+i}^*(t,z,V_k)-H_i\int_{\partial\Omega_2}(W_i-w_i)\\ &=\bar{F}_i(t,z,\underline{C}_j,\bar{C}_k)-\underline{F}_i(t,z,\underline{C}_j,\bar{C}_k)-H_i\int_{\partial\Omega_2}(W_i-w_i)\\ &=\bar{F}_i(t,z,\bar{C}_j-W_j,\bar{C}_k)-\underline{F}_i(t,z,\bar{C}_j-W_j,\bar{C}_k)-H_i\int_{\partial\Omega_2}(W_i-w_i)\ \text{in}\ (0,T]\times\Lambda,\end{aligned} \tag{3.4.14}$$

$$D_i\frac{\partial w_i}{\partial n}=H_i(W_i-w_i)\ \text{on}\ (0,T]\times\partial\Omega_2\times\Lambda. \tag{3.4.15}$$

In addition, (w_i, W_i) satisfies the boundary conditions B_n^* given by B_n with zero initial conditions and $W_{i,1}=V_{i,1}+V_{n(J)+i,1}=0$.

But $\bar{f}_i(t,x,\bar{c}_j-w_j,\bar{c}_k)-\underline{f}_i(t,x,\bar{c}_j-w_j,\bar{c}_k)$ and $\bar{F}_i(t,z,\bar{C}_j-W_j,\bar{C}_k)-\underline{F}_i(t,z,\bar{C}_j-W_j,\bar{C}_k)$ $-H_i\int_{\partial\Omega_2}(W_i-w_i)$ vanish when $W_j\equiv w_j\equiv 0$ for all j, and since $(w_i, W_i)\equiv 0$ is a solution of this initial value problem and by Theorem 3.3.1 (Generalised Uniqueness theorem), is the only solution, we conclude that $w_i\equiv 0$ in $[0,T]\times\bar{\Omega}\times\Lambda$ and $W_i\equiv 0$ in $[0,T]\times\bar{\Lambda}$. The conclusion of our theorem must follow.❑

An immediate consequence of these imbedding results is that existence, uniqueness and stability results for the system S_{2n}^*, B_{2n}^* implies existence, uniqueness and stability for the corresponding solution of S_n, B_n. Of course, solutions of S_n, B_n may be stable in S_n, B_n, but unstable in the larger setting S_{2n}^*, B_{2n}^*. A direct implication of these results is that nonexistence results of the system S_{2n}^*, B_{2n}^* implies nonexistence for the system S_n, B_n. There are other implications of these imbedding results that are discussed in section 3.7.

Remark 3.4.1
Note that the functions

$$\bar{f}_i(t,x,\bar{c}_j-w_j,\bar{c}_k)-\underline{f}_i(t,x,\bar{c}_j-w_j,\bar{c}_k)$$

and

$$\bar{F}_i(t,z,\bar{C}_j-W_j,\bar{C}_k)-\underline{F}_i(t,z,\bar{C}_j-W_j,\bar{C}_k)-H_i\int_{\partial\Omega_2}(W_i-w_i),$$

in the right hand sides of (3.4.14) and (3.4.15) are monotone nondecreasing in w_j and W_j, respectively.

In section 3.5 we shall study the stability of solutions of the system S_n, B_n and uniqueness of soutions to the steady state system $\hat{S}_n$, $\hat{B}_n$.

3.5 Stability of Solutions and Uniqueness of Solutions to the Steady State Problem

In this section, we establish some useful sufficient conditions for the global stability of all solutions of the general system S_n, B_n. By global stability of a solution (c_i, C_i) of S_n, B_n, we mean that arbitrary changes in $c_{i,0}$ and $C_{i,0}$ decay to zero with increasing t. Such stability implies the uniqueness of the solutions to the steady state problem, since if (c_{i1}, C_{i1}) and (c_{i2}, C_{i2}) are two steady state solutions of S_n, B_n satisfying the same boundary conditions, the disturbances $(c_{i2} - c_{i1}, C_{i2} - C_{i1})$ in the initial conditions of (c_{i1}, C_{i1}) must decay to zero, implying that only one of these could be a time independent solution.

We assume at the outset that the system S_n, B_n is a quasimonotone system, i.e. f_i and F_i are monotone nondecreasing in c_j and C_j respectively for $j \neq i$. This is not a restriction on the theorems of this section since if this monotone property is not satisfied, then the system S_n, B_n with general functions f_i and F_i can be imbedded in a system S_{2n}, B_{2n} of the same form where $f_i(t, x, c_j)$ is replaced by $\bar{f}_i(t, x, \underline{c}_k, \bar{c}_l)$ for the first $n(I)$ dependent variables $\bar{c}_i$ and by $\underline{f}_i(t, x, \underline{c}_k, \bar{c}_l)$ for the next $n(I)$ dependent variables $\underline{c}_i$. Also, $F_i(t, z, C_j)$ is replaced by $\bar{F}_i(t, z, \underline{C}_k, \bar{C}_l)$ for the first $n(J)$ dependent variables $\bar{C}_i$ and by $\underline{F}_i(t, z, \underline{C}_k, \bar{C}_l)$ for the next $n(J)$ dependent variables $\underline{C}_i$. The stability and uniqueness results obtained for this new system then apply to the original system by the imbedding results of section 3.4.

Suppose (c_i, C_i) is a solution of a quasimonotone system S_n, B_n for which the velocity distribution u is independent of time. We set out to find positive functions (u_i, U_i) and conditions on f_i and F_i so that $(c_i + \lambda u_i, C_i + \lambda U_i)$ are upper functions and $(c_i - \lambda u_i, C_i - \lambda U_i)$ are lower functions for all $\lambda > 0$. When such functions (u_i, U_i) exist, they give us a family of comparison functions associated with (c_i, C_i) for all $\lambda > 0$ which have a bearing on the stability of the solutions of the system S_n, B_n, including the steady state ones and provide a means of establishing conditions under which these are unique. We first note that the functions (u_i, U_i) need to satisfy the following conditions if they are to generate upper and lower functions for all $\lambda > 0$:

(i) *For components $i \in I$, where $D_i, H_i > 0$, u_i are continuous in $[0, T] \times \bar{\Omega} \times \Lambda$, their first-order x_j-derivatives exist in $(0, T] \times \bar{\Omega} \times \Lambda$, their second order $x_j x_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(ii) *For components $i \in I$, where $D_i = H_i = 0$, u_i are continuous in $[0, T] \times \bar{\Omega} \times \Lambda$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Omega \times \Lambda$;*

(iii) *For components $i \in J$, where $\mathcal{D}_i > 0$, U_i are continuous in $[0, T] \times \bar{\Lambda}$, their first order z derivatives exist in $(0, T] \times \bar{\Lambda}$, their second order $z_j z_k$-derivatives and first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(iv) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla U_i \not\equiv 0$, U_i are continuous in $[0, T] \times \bar{\Lambda}$, their first order z_j derivatives exist in $(0, T] \times \Lambda$ and their first order t-derivatives are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(v) *For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla U_i \equiv 0$, U_i are continuous in $[0, T] \times \bar{\Lambda}$ and their first order t-derivatives exist and are continuous and uniformly bounded in $(0, T] \times \Lambda$;*

(vi) $u_i > 0$ *in* $\bar{\Omega} \times \Lambda$ *and* $U_i > 0$ *in* $\bar{\Lambda}$ *at* $t = 0$; **(3.5.1)**

(vii) $\dfrac{\partial u_i}{\partial n} \geq 0$ *on* $(0, T] \times \partial\Omega_1 \times \Lambda$; **(3.5.2)**

(viii) $D_i \dfrac{\partial u_i}{\partial n} - H_i(U_i - u_i) \geq 0 \; on \; (0,\, T] \times \partial\Omega_2 \times \Lambda;$ **(3.5.3)**

(ix) $\upsilon_1 U_i + \mathscr{D}_i \dfrac{\partial U_i}{\partial n_1} = \upsilon_1 U_{i,1} \geq 0 \; on \; (0,\, T] \times \partial\Lambda_1;$ **(3.5.4)**

(x) $\dfrac{\partial U_i}{\partial n_\alpha} \geq 0 \; on \; (0,\, T] \times \partial\Lambda_\alpha, \alpha = 2,\, 3;$ **(3.5.5)**

(xi) $\dfrac{\partial u_i}{\partial t} - D_i \nabla_x^2 u_i \geq \dfrac{1}{\lambda}[f_i(t,\, x,\, c_j + \lambda u_j) - f_i(t,\, x,\, c_j)] \; in \; (0,\, T] \times \Omega \times \Lambda;$ **(3.5.6)**

(xii) $\dfrac{\partial U_i}{\partial t} - \mathscr{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \int_{\partial\Omega_2} (U_i - u_i) \geq \dfrac{1}{\lambda}[F_i(t,\, z,\, C_j + \lambda U_j) - F_i(t,\, z,\, C_j)] \; in \; (0,\, T] \times \Lambda.$ **(3.5.7)**

If f_i and F_i are assumed to be differentiable, then it follows from the mean value theorem that the right hand sides of (3.5.6) and (3.5.7) are equal to $\sum_{j=1}^{n} \dfrac{\partial f_i}{\partial c_j}(t,\, x,\, c_j + \lambda_i^* u_j) u_j$ and $\sum_{j=1}^{n} \dfrac{\partial F_i}{\partial C_j}(t,\, z,\, C_j + \lambda_i^{**} U_j) U_j$ respectively, for some $\lambda_i^*, \lambda_i^{**}$ in $(0,\, \lambda)$.

The following conditions on the derivatives of f_i, F_i and on the solutions $(u_i,\, U_i)$ of a linear system of equations $P(\varepsilon)$ derived from S_n, B_n are sufficient to provide a family of upper and lower functions of the type we seek.

Assume there exists constants a_{ij} such that $\dfrac{\partial f_i}{\partial c_j}(t,\, x,\, \theta_k) \leq a_{ij}$ for all $(t,\, x,\, z)$ in $[0,\, T] \times \overline{\Omega} \times \Lambda$ and for all θ_k and assume also that there exists constants A_{ij} such that $\dfrac{\partial F_i}{\partial C_j}(t,\, z,\, \Theta_k) \leq A_{ij}$ for all $(t,\, z)$ in $[0,\, T] \times \overline{\Lambda}$ and for all Θ_k. Note that $a_{ij} \geq 0$ and $A_{ij} \geq 0$ for $i \neq j$ since we have already assumed that f_i and F_i were quasimonotone nondecreasing. We look for positive functions, $(u_i,\, U_i)$ of separated variables form

$$u_i = e^{-\varepsilon t} w_i, \tag{3.5.8}$$

and

$$U_i = e^{-\varepsilon t} W_i, \tag{3.5.9}$$

for some $\varepsilon > 0$, satisfying the linear inequalities (3.5.1)-(3.5.5), together with the following linearised versions of (3.5.6)-(3.5.7):

$$\frac{\partial u_i}{\partial t} - D_i \nabla_x^2 u_i - \sum_j a_{ij} u_j \geq 0 \text{ in } (0,\, T] \times \Omega \times \Lambda, \tag{3.5.10}$$

and

$$\frac{\partial U_i}{\partial t} - \mathscr{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \mathscr{A} U_i - \sum_j A_{ij} U_j \geq H_i \int_{\partial\Omega_2} u_i \text{ in } (0,\, T] \times \Lambda. \tag{3.5.11}$$

Such functions exist and generate upper and lower functions for any solution of S_n, B_n and any $\lambda > 0$, if we can find w_i and W_i positive in $\overline{\Omega} \times \Lambda$ and $\overline{\Lambda}$ respectively, satisfying the inequalities (3.5.12)-(3.5.17) below. The functions u_i and U_i defined by (3.5.8)-(3.5.9) then satisfy the inequalities (3.5.1)-(3.5.5) and (3.5.10)-(3.5.11). Matrix notation is convenient for the linearised system which follow.

Let w denote the $n(I)$-vector with components w_i and let $D, H, I_{n(I)}$ denote the diagonal $n(I)$th order matrices with diagonal elements D_i, H_i and 1 where $I_{n(I)}$ is the $n(I) \times n(I)$ unit matrix. Let W, W_1 denote the $n(J)$-vector with components W_i, $W_{i,1}$ and let $\mathscr{D}, I_{n(J)}$ denote diagonal $n(J)$th order matrices with diagonal elements $\mathscr{D}_i$ and 1 where $I_{n(J)}$ is the $n(J) \times n(J)$ unit matrix. Also, let a and A be the matrices with elements a_{ij} and A_{ij} respectively. The vectors $(w,\, W)$ are required to be positive solutions of the matrix system $P(\varepsilon)$:

$$D\nabla_x^2 w + (\varepsilon I + a)w \le 0 \text{ in } \Omega\times\Lambda, \tag{3.5.12}$$

$$\frac{\partial w}{\partial n} \ge 0 \text{ on } \partial\Omega_1\times\Lambda, \tag{3.5.13}$$

$$D\frac{\partial w}{\partial n} \ge H(W-w) \text{ on } \partial\Omega_2\times\Lambda, \tag{3.5.14}$$

$$\mathscr{D}\nabla^2 W - u\cdot\nabla W + (\varepsilon I - \mathscr{A}H + A)W + H\int_{\partial\Omega_2} w \le 0 \text{ in } \Lambda, \tag{3.5.15}$$

$$\upsilon_1 W + \mathscr{D}\frac{\partial W}{\partial n_1} \ge \upsilon_1 W_1 (>0) \text{ on } \partial\Lambda_1, \tag{3.5.16}$$

$$\frac{\partial W}{\partial n_\alpha} \ge 0 \text{ on } \partial\Lambda_\alpha, \alpha = 2, 3. \tag{3.5.17}$$

Theorem 3.5.2

If (w, W) have positive components in $\overline{\Omega}\times\Lambda$ and $\overline{\Lambda}$ which are solutions of $P(\varepsilon)$ for some $\varepsilon > 0$, then all solutions of S_n, B_n (including the steady state ones) are globally stable.

Proof

Let (c_{i1}, C_{i1}) be a solution of problem S_n, B_n satisfying the continuity requirement of the Theorems 3.2.12 (Generalised Strong Comparison theorem). Consider the functions

$$\overline{c}_{i1} = c_{i1} + \lambda e^{-\varepsilon t} w_i,\ \underline{c}_{i1} = c_{i1} - \lambda e^{-\varepsilon t} w_i,\ \overline{C}_{i1} = C_{i1} + \lambda e^{-\varepsilon t} W_i,\ \underline{C}_{i1} = C_{i1} - \lambda e^{-\varepsilon t} W_i, \tag{3.5.18}$$

where w_i and W_i are positive solutions of problem $P(\varepsilon)$ for some $\varepsilon > 0$.

It is a tedious but trivial exercise to show that when $\lambda > 0$ and $f_i(t, x, c_{j1})$ and $F_i(t, z, C_{j1})$ are monotone nondecreasing in c_{j1} and C_{j1} for $j \ne i$, then $(\underline{c}_{i1}, \underline{C}_{i1})$ and $(\overline{c}_{i1}, \overline{C}_{i1})$ defined by equations (3.5.18) satisfy all the requirements of Theorem 3.2.14. If (c_{i2}, C_{i2}) is any other solution of problem S_n, B_n satisfying the same boundary conditions (2.1.7) (except when $\mathscr{D}_i = 0$, $u\cdot\nabla U_i \not\equiv 0$), but different initial conditions, we may take λ large enough so that (c_{i2}, C_{i2}) is bounded by $(\underline{c}_{i1}, \underline{C}_{i1})$ and $(\overline{c}_{i1}, \overline{C}_{i1})$ at $t = 0$. Theorem 3.2.14 then implies these bounds are sustained for all finite time, and since these bounds decay exponentially (with exponent $-\varepsilon t$) to (c_{i1}, C_{i1}), we see that all solutions are exponentially stable. Moreover, if the steady state problem has a solution, then it is unique and exponentially stable.❑

If $n = n(I) = n(J)$, and all w are coupled to W by (3.5.14), then the system $P(\varepsilon)$ can be uncoupled in the x and z variable by means of the matrix transformation

$$w(x,z) = \theta(x) S W(z), \tag{3.5.19}$$

where $\theta(x)$ satisfies the boundary value problem:

$$D\nabla_x^2\theta + (\varepsilon I + a)\theta = 0 \text{ in } \Omega, \tag{3.5.20}$$

$$\frac{\partial\theta}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{3.5.21}$$

$$D\frac{\partial\theta}{\partial n} = H(S^{-1} - \theta) \text{ on } \partial\Omega_2, \tag{3.5.22}$$

and vector $W(z)$ satisfies the differential inequalities:

$$\mathcal{D}\nabla^2 W - u\cdot\nabla W + (\varepsilon I - \mathcal{A}H + A)W + (H\int_{\partial\Omega_2}\theta)SW \le 0 \text{ in } \Lambda, \tag{3.5.23}$$

$$\upsilon_1 W + \mathcal{D}\frac{\partial W}{\partial n_1} \ge \upsilon_1 W_1(>0) \text{ on } \partial\Lambda_1, \tag{3.5.24}$$

$$\frac{\partial W}{\partial n_\alpha} \ge 0 \text{ on } \partial\Lambda_\alpha, \alpha = 2, 3. \tag{3.5.25}$$

Suppose we impose further conditions on S_n, B_n, by assuming the matrix a is the product of a positive diagonal matrix d and a symmetric matrix b (i.e., $a = db$), a not uncommon feature of kinetic equations, while D and H are proportional so that $H = \gamma D$ for a positive number γ. In these circumstances, the equations for θ may, by a suitable choice of S (in fact $S = T^{-1}$) be expressed in the form $\theta(x)=T\varphi(x)$ whence, by a choice of T shown below, $\varphi(x)$ can be made diagonal. The matrix φ satisfies the equation

$$d(T')^{-1}[T'd^{-1}DT\nabla^2\varphi + T'(\varepsilon d^{-1}+b)T\varphi] = 0 \text{ in } \Omega, \tag{3.5.26}$$

where T' denotes the transpose of T. The matrix T can be chosen so that $T'(\varepsilon d^{-1}+b)T = \mu$, a diagonal matrix and $T'd^{-1}DT = J$, where J is diagonal with the ith diagonal element equal to one if $D_i > 0$ and equal to zero if D_i is zero. We may choose ε so that μ is nonsingular. If $S^{-1} = T$, then in Ω we have

$$J\nabla^2\varphi + \mu\varphi = 0, \tag{3.5.27}$$

and on the boundaries of $\partial\Omega$,

$$J\frac{\partial\varphi}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{3.5.28}$$

$$J\frac{\partial\varphi}{\partial n} = \gamma J(I - \varphi) \text{ on } \partial\Omega_2. \tag{3.5.29}$$

We see that all the components of φ are uncoupled, and $w = T\varphi T^{-1}W$.

Problem $P^*(\varepsilon)$, where the inequalities are replaced by equalities may have non zero solutions when $W_1 = 0$ for certain values of ε (eigenvalues). If ε_1 is the smallest eigenvalue of ε and ε_1 is positive, then in general, we can find a positive $\varepsilon_* < \varepsilon_1$ for which $P(\varepsilon_*)$ has positive solutions (w, W). The argument functions of ε on any closed interval not containing an eigenvalue. When ε is very large and negative, $w = W = K$, a positive (in every component) constant vector is an upper solution of $P^*(\varepsilon)$, while $w = W = 0$ is a lower solution, and so a positive solution exists. As ε is increased, the solution (w, W) must remain positive since it depends continuously on ε and Theorem 3.2.13 (Generalised Strong Comparison (Contact) Theorem) does not allow for the existence of an ε for which $w \ge 0$ in $\overline{\Omega} \times \Lambda$ and $W \ge 0$ in $\overline{\Lambda}$ while one of these vanish at a point in $\overline{\Omega} \times \Lambda$ or $\overline{\Lambda}$. This situation prevails for increasing ε unless w or W have components which tend to infinity as ε increases towards a finite ε_1. If M is the greatest value of all the components of (w, W), then $w^* = \frac{w}{M}$, $W^* = \frac{W}{M}$ is the solution of $P^*(\varepsilon)$ for $W_1^* = \frac{W_1}{M}$ and as ε tends to ε_1 and M tends to infinity, (w^*, W^*) tends to a non zero solution of $P^*(\varepsilon_1)$ with $W_1 = 0$, and so ε_1 is an eigenvalue.

In section 3.6 we shall study the existence of solutions to the system S_n, B_n.

3.6 Existence of Solutions to the Unsteady State Problem

There are many methods of proving existence of solutions. Often a fixed-point algorithm in an abstract function space is used. A number of existence-comparison theorems are available for weakly coupled parabolic systems. These can be established by various methods. Some examples are the work by KUIPER [149] using a functional analytic approach and by AMANN [10] and BEBERNES *et al.* [35-37] in connection with invariant sets. The technique we concentrate on in this section that is intimately connected with the maximum principles is the so called method of sub- and supersolutions or the method of upper and lower solutions.

The theory of monotone operators together with the method of upper and lower solutions can be used to construct convergent monotone sequences and thereby establishes an existence-comparison theorem, provided that a suitable initial iteration can be chosen. It turns out that this initial iteration can be taken as either an upper solution or a lower solution satisfying certain inequalities associated with the original system. It is shown that the existence of a lower solution $\underline{\underline{u}}_i$ and an upper solution $\tilde{u}_i$ (these are also known as subsolutions and supersolutions or under and oversolutions, respectively) with $\underline{\underline{u}}_i \leq \tilde{u}_i$ guarantees the existence of at least one solution u_i in the interval $[\underline{\underline{u}}_i, \tilde{u}_i]$. More precisely, there exists a minimal solution $\underline{u}_i$ and a maximal solution $\overline{u}_i$ in the interval $[\underline{\underline{u}}_i, \tilde{u}_i]$ such that the solution u_i satisfies $\underline{u}_i \leq u_i \leq \overline{u}_i$. The minimal and maximal solutions will, respectively, be obtained as the supremum of all possible lower solutions and the infimum of all possible upper solutions.

The theory of monotone operators together with the method of upper and lower solutions in proving existence theorems for scalar parabolic equations is usually attributed to SATTINGER [257]. Similar results are also available for scalar elliptic equations (HUDJAEV [133], KELLER [141], AMANN [5]). In these cases, the nonlinear term is assumed to be quasimonotone nondecreasing in the sense that the nonlinear term could be made monotone nondecreasing by the addition of a suitably large enough linear term. This method of proving existence theorems can also be extended to systems of equations and had been used earlier for multicomponent parabolic systems where some diffusion coefficients were allowed to vanish (MCNABB [182]). It has also been used for infinite systems of ordinary differential equations (CHANDRA, *et al.* [66]). All these techniques employ the maximum principle or an appropriate comparison theorem and in particular for systems, all these results require the nonlinearities $f_i(t, x, c_j)$ to be quasimonotone nondecreasing (nonincreasing) in the sense that f_i is monotone nondecreasing (nonincreasing) in c_j for all $j \neq i$ and there exists a constant M_i (the Lipschitz constant if f_i is Lipschitz continuous in c_j) so that $f_i + Mc_i$ is monotone nondecreasing (nonincreasing). The method of upper and lower solutions can also be applied to systems where the restriction that f_i is quasimonotone nondecreasing (nonincreasing) is not satisfied but instead the nonlinearities may satisfy other monotone properties. NORMAN [205] and CHANDRA, *et al.* [65] gave an example of a system which obeyed a mixed quasimonotone property (mqmp) in the sense that for all i, the nonlinearities $f_i(t, x, c_j)$ are quasimonotone nondecreasing in c_i, monotone nondecreasing in the variables $c_j, j \neq i$ and monotone nonincreasing in the the variables $c_k, k \neq i, j$. PAO [216] categorised systems of parabolic equations into three basic types according to their relative quasimonotone property (a) type I where the nonlinearities $f_i(t, x, c_j)$ were quasimonotone nondecreasing in the variables c_j, (b) type II where the nonlinearities were quasimonotone nonincreasing in the variables c_j, and (c) type III where for some i, the nonlinearities were quasimonotone nondecreasing in c_j, and for all remaining i, the nonlinearities were quasimonotone nonincreasing in c_j. For mixed quasimonotone systems, type I, type II and type III systems, an existence-comparison theorem in terms of upper and lower solutions could still be established along the monotone and regularity arguments of SATTINGER [257] for scalar equations. These techniques could also be applied to other systems of differential equations provided that the nonlinearities obey some sort of a monotone property. LADDE, *et al.* [153] defined monotone iterative techniques for systems of first order differential equations, second order differential equations, elliptic equations, parabolic equations and first order partial differential equations where the nonlinearity possesses a mixed quasimonotone property (mqmp). These solutions are defined in terms of coupled quasisolutions. Coupled upper and lower quasisolutions are defined by using the mixed quasimonotone property (mqmp) and quasisolutions may be constructed by monotone iteration. It is then required to show that these quasisolutions are actual solutions. The stability for solutions of reaction diffusion systems may also be examined by the method of quasisolutions (LAKSHMIKANTHAM and VATSALA [158]) as well as other qualitative properties of such solutions.

It is not always necessary that in order to establish such an existence-comparison theorem in terms of upper and lower solutions that the nonlinearities must obey a monotone property . A monotone iteration technique was developed by KHAVANIN and LAKSHMIKANTHAM [145] for weakly coupled first and second order boundary value problems. This technique, known as the method of mixed monotony made it possible to construct monotone sequences even when the nonlinearities did not possess any monotone properties. CARL [46], also proposed a monotone scheme for the solutions of weakly coupled systems of reaction-diffusion equations without any monotonicity property required of the nonlinear reaction terms. The considerations including the definitions of upper and lower solutions are all taken within the framework of weak solutions. CARL and GROSSMAN [47] proposed a method of imbedding a system of n equations into a system of $2n$ equations and obtaining existence and enclosing theorems for elliptic and parabolic systems with nonmonotone nonlinearities in terms of upper and lower solutions. These theorems implied existence of solutions of the original system and the method was allowed to work under very low regularity conditions. Their definition of coupled upper and lower solutions coincides with the notion of coupled upper and lower quasisolutions defined by LADDE *et al.* [153]. This method of imbedding a system of n reaction diffusion equations where reaction functions had no monotonicity requirement into a system of order $2n$ with reaction functions redefined had also been proposed by MCNABB [186] for systems of ordinary differential equations and parabolic systems. However, it was furthermore shown that this system of twice the order may be modified to give a quasimonotone nondecreasing system of the type given earlier by MCNABB [182]. All the earlier notions of monotone iteration were then applicable and coupled upper and lower solutions could be uncoupled into upper and lower solutions. These results also show that stability, uniqueness and existence results of this new system implies stability, uniqueness and existence results of the original system.

Most of the discussions in the current literature are devoted to systems which are coupled through the reaction functions in the diffusion equations. However, in many situations, the nonlinearities may occur in the boundary conditions as well as in the equations. KELLER [141] and AMANN [5, 6, 8] considered a class of mildly nonlinear scalar elliptic boundary value problems that are suggested by several steady state diffusion processes of interest where the nonlinearities are in the boundary conditions and ARONSON and PELETIER [23] considered an interesting problem of an initial boundary value problem that is in the presence of several distinct steady states that is coupled in the boundary conditions. PAO [211] studied a scalar parabolic equation with nonlinear boundary conditions in an unbounded or bounded domain. The nonlinearities in the reaction functions as well as in the boundary conditions are assumed to be quasimonotone. The question of stability of such a parabolic equation in bounded domains was also examined by PAO [212] by using this monotone property in the boundary conditions. PAO [215] considers a system of two reaction diffusion equations which are coupled through the boundary conditions and not in the reaction functions. The nonlinearities in the boundary conditions are defined as earlier for reaction functions in terms of type I, type II and type III functions depending on their relative quasimonotone property and a montone iteration scheme is proposed for each type. It is this monotone property together with suitable maximum principles which guarantee the use of monotone iterations in proving existence theorems. There has been no literature on systems of coupled reaction diffusion equations which are also coupled through the boundary conditions where there are no monotone properties in both the reaction functions and the boundary conditons.

Our generalised particle reactor equations S_n, B_n form a system of up to $2n$ weakly coupled, degenerate equations which may be a combination of ordinary differential equations, first order partial differential equations and parabolic equations. The degeneracy is is not only concerned with the possibility of D_i or $\mathcal{D}_j$ being zero for some i, j but is also associated with the fact that in the case that D_i is nonzero, the Laplacian for the c_i equations involves only the x dependent variables whereas for the C_i equations it involves only the z dependent variables. The weak coupling is also non standard in that through equation (2.1.6) the C_i equations have a functional connection to the c_i variables via $\int_{\partial\Omega_2} D_i \frac{\partial c_i}{\partial n}$. Our reaction diffusion system within a particle is therefore not only coupled through the boundary conditions but the nonlinearity in the boundary conditions are more general than the examples discussed by PAO [215] and are given as coupled functionals (see PARSHOTAM *et al.* [224] and WAKE [304] for examples of functional boundary value problems), i.e. in the sense that the boundary data is given by solutions to coupled reaction convection equations. These reaction convection equations may also have reaction functions which have no monotonicity requirement.

Despite all these features we are able to show in this section that this system is governed by generalised existence theorems similar in type to those for weakly coupled parabolic systems in MCNABB [182]. However, additional smoothness properties such as Hölder continuity conditions on f_i and F_i are required for our generalised existence theorem.

In general, the methods of proving existence of nonlinear differential equations consists of three steps:

(i) Construction of a sequence of approximate solutions;
(ii) Showing that the constructed sequence of approximate solutions converges to a limit function;
(iii) Proving that this limit function is actually a solution of the given problem.

Steps (i) and (iii) are standard and straighforward. It is, however step (ii) that needs attention. In this section, we shall construct a sequence of approximate solutions by setting up an iteration scheme of linear equations. The additional continuity properties are required for the existence of these linear equations. We show that this constructed sequence of approximate solutions converges monotonically and uniformly (in appropriate spaces) to a limit function which is actually a solution of the system S_n, B_n.

We demonstrate in this section that solutions of problem S_n, B_n specified by $c_{i,0}$, $C_{i,0}$ and $C_{i,1}$ exist. By a solution, we shall understand a *classical* solution (c_i, C_i) of S_n, B_n where

(i) For components $i \in I$ where $D_i, H_i > 0$, c_i are continuous in $[0, T]\times\overline{\Omega}\times\Lambda$, have continuous first order x_j derivatives in $(0, T]\times\overline{\Omega}\times\Lambda$, continuous second order x_j derivatives in $(0, T]\times\Omega\times\Lambda$ and continuous first order t derivatives in $(0, T]\times\Omega\times\Lambda$. In this case, we shall look for *classical solutions* of the form $c_i(t, x, z) \in C^{1,2,0}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$.

(ii) For components $i \in I$ where $D_i = H_i = 0$, c_i are continuous in $[0, T]\times\overline{\Omega}\times\Lambda$ and have continuous first order t derivatives in $(0, T]\times\Omega\times\Lambda$. In this case, we shall look for *classical solutions* of the form $c_i(t, x, z) \in C^{1,0,0}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$.

(iii) For components $i \in J$ where $\mathcal{D}_i > 0$, C_i are continuous in $[0, T] \times \overline{\Lambda}$, have continuous first order z_j derivatives in $(0, T] \times \overline{\Lambda}$, continuous second order z_j derivatives in $(0, T] \times \Lambda$ and continuous first order t derivatives in $(0, T] \times \Lambda$. In this case we shall look for *classical solutions* of the form $C_i(t, z) \in C^{1,2}[(0, T] \times \overline{\Lambda}, R^{n(J)}]$.

(iv) For components $i \in J$ where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, C_i are continuous in $[0, T] \times \overline{\Lambda}$, have continuous first order z_j derivatives in $(0, T] \times \Lambda$ and continuous first order t derivatives in $(0, T] \times \Lambda$. In this case we shall look for *classical solutions* of the form $C_i(t, z) \in C^{1,1}[(0, T] \times \overline{\Lambda}, R^{n(J)}]$.

(v) For components $i \in J$ where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, C_i are continuous in $[0, T] \times \overline{\Lambda}$ and have continuous first order t derivatives in $(0, T] \times \Lambda$. In this case we shall look for *classical solutions* of the form $C_i(t, z) \in C^{1,0}[(0, T] \times \overline{\Lambda}, R^{n(J)}]$.

Comparison theorems are used in this section in conjunction with theorems on *a priori* estimates and existence of linear parabolic equations to derive estimates of the system S_n, B_n and to prove the existence of solutions to this system. There may be some cases where D_i or $\mathcal{D}_i$ may be zero and these cases are treated by using standard results.

We shall need some additional continuity properties to establish existence of the corresponding linear system and make the following assumptions on $f_i(t, x, c_j)$ and $F_i(t, z, C_j)$.

(H_2) (i) $f_i(t, x, c_j) \in C^{\alpha/2, \alpha}[[0, T] \times \overline{\Omega} \times R^{n(I)}, R^{n(I)}]$, i.e., $f_i(t, x, c_j)$ is Hölder continuous in t and x with exponent $\alpha/2$ and α, respectively, for each fixed value of c_j.

(ii) $F_i(t, z, C_j) \in C^{\alpha/2, \alpha}[[0, T] \times \overline{\Lambda} \times R^{n(J)}, R^{n(J)}]$, i.e., $F_i(t, z, C_j)$ is Hölder continuous in t and z with exponent $\alpha/2$ and α respectively, for each fixed value of C_j.

From Lemma 3.1.3, we see that exponents α in both cases may be assumed to be identical.

3.6.1 The Monotone System S_n, B_n

We may assume at the outset that the system S_n, B_n is a monotone system in the sense that $f_i(t, x, c_j)$ is monotone nondecreasing in c_i and $F_i(t, z, C_j)$ is monotone nondecreasing in C_i. This is not a restriction on the theorems of this section since if this monotone property is not satisfied we may make the following substitution to obtain a system of the same type but with new functions that are monotone nondecreasing in c_i and C_i. We first observe that if (c_i, C_i) is a solution of S_n, B_n, then the functions (w_i, W_i) defined by

$$c_i = e^{-Kt} w_i \tag{3.6.1}$$

and

$$C_i = e^{-Kt} W_i, \tag{3.6.2}$$

satisfies the following system of equations:

$$\frac{\partial w_i}{\partial t} - D_i \nabla_x^2 w_i = K w_i + e^{Kt} f_i(t, x, e^{-Kt} w_j) \text{ in } (0, T] \times \Omega \times \Lambda,$$
$$\frac{\partial w_i}{\partial n} = 0 \text{ on } (0, T] \times \partial\Omega_1 \times \Lambda,$$

$$D_i \frac{\partial w_i}{\partial n} = H_i(W_i - w_i) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial W_i}{\partial t} - \mathcal{D}_i\nabla^2 W_i + u\cdot\nabla W_i + H_i\int_{\partial\Omega_2}(W_i - w_i) = KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j) \text{ in } (0, T]\times\Lambda,$$

$$\upsilon_1 W_i + \mathcal{D}_i\frac{\partial W_i}{\partial n_1} = \upsilon_1 e^{Kt}C_{i,1} \text{ on } (0, T]\times\partial\Lambda_1,$$

$$\frac{\partial W_i}{\partial n_\alpha} = 0 \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha=2,3,$$

$$w_i(0, x, z) = c_{i,0} \text{ in } \Omega\times\Lambda,$$

$$W_i(0, z) = C_{i,0} \text{ in } \Lambda.$$

This system is similar to the original system S_n, B_n with the nonlinear coupling function $f_i(t, x, c_j)$ for c_j components replaced by

$$Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j), \tag{3.6.3}$$

and nonlinear coupling function $F_i(t, z, C_j)$ for the C_j components replaced by

$$KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j). \tag{3.6.4}$$

These functions satisfy a monotone property given by the following lemma:

Lemma 3.6.1
Our assumptions (H_1) of Lipschitz continuity properties for the functions f_i and F_i with respect to c_j and C_j, imply that the functions $Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)$ and $KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j)$ with $c_i = e^{-Kt}w_i$ and $C_i = e^{-Kt}W_i$, are monotone nondecreasing in w_i and W_i, respectively.

Proof
Assume that $w_j \le w_j^*$ so that $c_j \le c_j^*$.
From (H_1), we see that

$$K_i(c_j - c_j^*) \le f_i(t, x, c_j) - f_i(t, x, c_j^*) \le -K_i(c_j - c_j^*),$$

and therefore,

$$\begin{aligned}
&[Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)] - [Kw_i^* + e^{Kt}f_i(t, x, e^{-Kt}w_j^*)] \\
&\qquad = Ke^{Kt}(c_i - c_i^*) + e^{Kt}[f_i(t, x, c_j) - f_i(t, x, c_j^*)] \\
&\qquad \le -e^{Kt}[K(c_i^* - c_i) - K_i(c_j^* - c_j)] \\
&\qquad \le 0,
\end{aligned}$$

if K is chosen to be large enough. This shows that

$$Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j) \le Kw_i^* + e^{Kt}f_i(t, x, e^{-Kt}w_j^*),$$

so that this new coupling function $Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)$ is monotone nondecreasing in w_i. A similar argument holds if we have to show that $KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j)$ is monotone nondecreasing in W_i.□

Remark 3.6.1

The substitution $c_i = e^{-Kt}w_i$ and $C_i = e^{-Kt}W_i$ which gives us a similar system with new functions $Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)$ and $KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j)$ from f_i and F_i and which are monotone nondecreasing in c_i and C_i, respectively is discussed by FRIEDMAN [94, p.202] and PAO [208]. Note that if K is chosen large enough our new functions are strictly monotone increasing in c_i and C_i.

Remark 3.6.2

From the Lipschitz continuity properties of the functions f_i and F_i, it can be shown that $f_i + k_i c_i$ and $F_i + K_i C_i$ are monotone nondecreasing in c_i and C_i, respectively, where k_i and K_i are Lipschitz constants of f_i and F_i, respectively (PAO [211]). If furthermore, the functions f_i and F_i are monotone nodecreasing in c_j and C_j, respectively, for $j \neq i$, then f_i and F_i will be quasimonotone nondecreasing.

It can also be shown that these new functions also satisfy the same Lipschitz and Hölder continuity properties as our original functions.

Lemma 3.6.2

Our assumptions (H_1) *of Lipschitz continuity properties for the functions* f_i *and* F_i *with respect to the variables* c_j *and* C_j *imply similar Lipschitz continuity properties for the functions* $Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)$ *and* $KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j)$ *with respect to the variables* w_j *and* W_j, *where* $c_i = e^{-Kt}w_i$ *and* $C_i = e^{-Kt}W_i$.

Proof

We need to only show that

$$
\begin{aligned}
&|[Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)] - [Kw_i^* + e^{Kt}f_i(t, x, e^{-Kt}w_j^*)]| \\
&\qquad \leq K|w_i - w_i^*| + e^{Kt}|f_i(t, x, e^{-Kt}w_j) - f_i(t, x, e^{-Kt}w_j^*)| \\
&\qquad \leq K|w_i - w_i^*| + e^{Kt}k_i|e^{-Kt}(w_j - w_j^*)| \\
&\qquad \leq K|w_i - w_i^*| + k_i|w_j - w_j^*| \\
&\qquad \leq k \sup_j |w_j - w_j^*|,
\end{aligned}
$$

where,

$$k = \max_j (K, k_j).$$

The first part of the proof is complete and the rest of the proof follows similarly.❑

Lemma 3.6.3

Our assumptions (H_1) *of Lipschitz continuity properties for the functions* f_i, *with respect to the variables* c_j *and assumptions* (H_2) *of Hölder continuity properties for the functions* f_i, *with respect to the variables* t *and* x *with* c_j *fixed imply similar Hölder continuity properties for the functions* $Kw_i + e^{Kt}f_i(t, x, e^{-Kt}w_j)$ *with respect to the variables* t *and* x *with* w_j *fixed, where* $c_i = e^{-Kt}w_i$. *Similarly, our assumptions* (H_1) *of Lipschitz continuity properties for the functions* F_i, *with respect to the variables* C_j *and assumptions* (H_2) *of Hölder continuity properties for the functions* F_i, *with respect to the variables* t *and* z *with* C_j *fixed imply similar Hölder continuity properties for the functions* $KW_i + e^{Kt}F_i(t, z, e^{-Kt}W_j)$ *with respect to the variables* t *and* z *with* W_j *fixed, where* $C_i = e^{-Kt}W_i$.

Proof

We shall only show that $f_i(t, x, e^{-Kt}w_j)$ is Hölder continuous in t. The rest of the proof is similar and follows from Lemma 3.1.1 and Lemma 3.1.2.

$$
\begin{aligned}
&|f_i(t, x, e^{-Kt}w_j) - f_i(t^*, x, e^{-Kt^*}w_j)| \\
&\quad = |f_i(t, x, e^{-Kt}w_j) - f_i(t^*, x, e^{-Kt}w_j) + f_i(t^*, x, e^{-Kt}w_j) - f_i(t^*, x, e^{-Kt^*}w_j)| \\
&\quad \le |f_i(t, x, e^{-Kt}w_j) - f_i(t^*, x, e^{-Kt}w_j)| + |f_i(t^*, x, e^{-Kt}w_j) - f_i(t^*, x, e^{-Kt^*}w_j)| \\
&\quad \le k_t(f_i)|t - t^*|^{\alpha/2} + k_i(f_i)|e^{-Kt}w_j - e^{-Kt^*}w_j| \\
&\quad \le k_t(f_i)|t - t^*|^{\alpha/2} + k_i(f_i)|w_j||e^{-Kt} - e^{-Kt^*}| \\
&\quad \le k_t(f_i)|t - t^*|^{\alpha/2} + k_i(f_i)|w_j|KT^{1-\alpha/2}|t - t^*|^{\alpha/2} \\
&\quad \le k|t - t^*|^{\alpha/2},
\end{aligned}
$$

where

$$k = k_t(f_i) + k_i(f_i)|w_j|KT^{1-\alpha/2}. \square$$

Remark 3.6.3

Note also that we may just as well have chosen the substitution $c_i = e^{-Kx_1}w_i$ and $C_i = e^{-Kz_1}W_i$, (where x_1 and z_1 are chosen without loss of generality to be the first components of x and z) instead of (3.6.1)-(3.6.2) and arrived at the same conclusions in Lemma 3.6.1, Lemma 3.6.2 and Lemma 3.6.3.

We may assume that the substitution (3.6.1)-(3.6.2) has been made and that $f_i(t, x, c_j)$ is monotone nondecreasing in c_i and $F_i(t, z, C_j)$ is monotone nondecreasing in C_i. If, on the other hand the monotone property is not satisfied by all the other variables in these two functions, then the system S_n, B_n with general functions f_i and F_i can be imbedded in a system S_{2n}, B_{2n} of the same form where $f_i(t, x, c_j)$ is replaced by $\bar{f}_i(t, x, \underline{c}_k, \bar{c}_l)$ for the first $n(I)$ dependent variables $\bar{c}_i$ and by $\underline{f}_i(t, x, \underline{c}_k, \bar{c}_l)$ for the next $n(I)$ dependent variables $\underline{c}_i$. Also, $F_i(t, z, C_j)$ is replaced by $\overline{F}_i(t, z, \underline{C}_k, \overline{C}_l)$ for the first $n(J)$ dependent variables $\overline{C}_i$ and by $\underline{F}_i(t, z, \underline{C}_k, \overline{C}_l)$ for the next $n(J)$ dependent variables $\underline{C}_i$. The existence results obtained for this new system of twice the order satisfied by $(\underline{c}_i, \underline{C}_i)$ and $(\bar{c}_i, \overline{C}_i)$ then implies a solution of our original system S_n, B_n by the imbedding results of section 3.4.

It has been shown in Lemma 3.2.2 that the functions $\underline{f}_i$, $\bar{f}_i$, $\underline{F}_i$ and $\overline{F}_i$ satisfy the same Lipschitz continuity properties as our original functions f_i and F_i in the system S_n, B_n. It can also be shown in the following lemma that these new functions satisfy the same Hölder continuity properties as our original functions.

Lemma 3.6.4

Our assumptions (H_2) of Hölder continuity properties for the functions f_i, with respect to the variables t and x with c_j fixed, imply similar Hölder continuity properties for $\underline{f}_i$ and $\bar{f}_i$ with respect to the variables t and x with $\underline{c}_k$ and $\bar{c}_l$ fixed and so there are constants k_t and k_x such that

$$
\left.
\begin{aligned}
|\underline{f}_i(t, x, \underline{c}_k, \bar{c}_l) - \underline{f}_i(t^*, x, \underline{c}_k, \bar{c}_l)| &\le k_t(\underline{f}_i)|t - t^*|^{\alpha/2}, \\
|\bar{f}_i(t, x, \underline{c}_k, \bar{c}_l) - \bar{f}_i(t^*, x, \underline{c}_k, \bar{c}_l)| &\le k_t(\bar{f}_i)|t - t^*|^{\alpha/2}, \\
|\underline{f}_i(t, x, \underline{c}_k, \bar{c}_l) - \underline{f}_i(t, x^*, \underline{c}_k, \bar{c}_l)| &\le k_x(\underline{f}_i)\|x - x^*\|^{\alpha}, \\
|\bar{f}_i(t, x, \underline{c}_k, \bar{c}_l) - \bar{f}_i(t, x^*, \underline{c}_k, \bar{c}_l)| &\le k_x(\bar{f}_i)\|x - x^*\|^{\alpha}.
\end{aligned}
\right\}
\qquad \textbf{(3.6.5)}
$$

Similarly, our assumptions (H_2) of Hölder continuity properties for the functions F_i with respect to the variables t and z with C_j fixed, imply similar Hölder continuity properties for $\underline{F}_i$ and $\overline{F}_i$ with respect to the variables t and z with $\underline{C}_k$ and $\overline{C}_l$ fixed and so there are constants K_t and K_z, such that

$$\left.\begin{aligned}
|\underline{F}_i(t, z, \underline{C}_k, \overline{C}_l)-\underline{F}_i(t^*, z, \underline{C}_k, \overline{C}_l)| &\le K_t(\underline{F}_i)|t-t^*|^{\alpha/2},\\
|\overline{F}_i(t, z, \underline{C}_k, \overline{C}_l)-\overline{F}_i(t^*, z, \underline{C}_k, \overline{C}_l)| &\le K_t(\overline{F}_i)|t-t^*|^{\alpha/2},\\
|\underline{F}_i(t, z, \underline{C}_k, \overline{C}_l)-\underline{F}_i(t, z^*, \underline{C}_k, \overline{C}_l)| &\le K_z(\underline{F}_i)\|z-z^*\|^{\alpha},\\
|\overline{F}_i(t, z, \underline{C}_k, \overline{C}_l)-\overline{F}_i(t, z^*, \underline{C}_k, \overline{C}_l)| &\le K_z(\overline{F}_i)\|z-z^*\|^{\alpha}.
\end{aligned}\right\} \tag{3.6.6}$$

Proof

Since $\underline{c}_k$, $\overline{c}_l$, $\underline{C}_k$ and $\overline{C}_l$ are fixed, this lemma follows directly from the definitions of $\underline{f}_i$, $\bar{f}_i$, $\underline{F}_i$ and $\overline{F}_i$ in (3.2.9)-(3.2.12) and assumption (H_2).❑

For the purposes of our existence proof, we may henceforth assume our coupling functions f_i and F_i are monotone nondecreasing in the variables c_j and C_j, respectively, for all j.

Remark 3.6.4

CARL and GROSSMAN [47] have an analogous definition for the functions $\underline{f}_i$ and $\bar{f}_i$. It is shown that if $f_i(t, x, u)$ are *Carathéodory type* functions, that is for almost all $x \in \Omega$, the functions f_i are continuous on R^m, and for all $u \in R^m$, the functions f_i are measurable on Ω, then so are the functions $\underline{f}_i$ and $\bar{f}_i$. This is proved using a measurable selection theorem which is usually known from optimisation theory.

3.6.2 Upper and Lower Solutions and Monotone Iteration

We shall now introduce the concepts of upper and lower solutions relative to the monotone system S_n, B_n.

Definition 3.6.1.

Assume that

(i) For components $i \in I$, where $D_i > 0$, $\underset{\sim}{c}_i$ and $\tilde{c}_i$ are continuous functions in $[0, T]\times\overline{\Omega}\times\Lambda$ with continuous first order x_j derivatives in $(0, T]\times\overline{\Omega}\times\Lambda$, continuous second order x_j derivatives in $(0, T]\times\Omega\times\Lambda$ and continuous first order t derivatives in $(0, T]\times\Omega\times\Lambda$;

(ii) For components $i \in I$, where $D_i = H_i = 0$, $\underset{\sim}{c}_i$ and $\tilde{c}_i$ are continuous functions in $[0, T]\times\overline{\Omega}\times\Lambda$ with continuous first order t derivatives in $(0, T]\times\Omega\times\Lambda$;

(iii) For components $i \in J$, where $\mathcal{D}_i > 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $[0, T]\times\overline{\Lambda}$, with continuous first order z_j derivatives in $(0, T]\times\overline{\Lambda}$, continuous second order z_j derivatives in $(0, T]\times\Lambda$ and continuous first order t derivatives in ;

(iv) For components $i \in J$, where $\mathcal{D}_i = 0$, $u\cdot\nabla\underset{\sim}{C}_i$, $u\cdot\nabla\tilde{C}_i \not\equiv 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $[0, T]\times\overline{\Lambda}$, with continuous first order z_j derivatives in $(0, T]\times\Lambda$ and continuous first order t derivatives in $(0, T]\times\Lambda$;

(v) For components $i \in J$ where $\mathcal{D}_i = 0$, $u\cdot\nabla\underset{\sim}{C}_i$, $u\cdot\nabla\tilde{C}_i \equiv 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $[0, T]\times\overline{\Lambda}$, with continuous first order t derivatives in $(0, T]\times\Lambda$;

The ordered pair of functions $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ with $\underset{\sim}{c}_i \le \tilde{c}_i$ on $[0,\ T]\times\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_i \le \tilde{C}_i$ on $[0,\ T]\times\overline{\Lambda}$ are said to be *lower* and *upper solutions* of S_n, B_n respectively, if they satisfy:

$$\frac{\partial \underset{\sim}{c}_i}{\partial t} - D_i\nabla_x^2 \underset{\sim}{c}_i \le f_i(t,\ x,\ \underset{\sim}{c}_j) \text{ in } (0,\ T]\times\Omega\times\Lambda,$$

$$\frac{\partial \underset{\sim}{c}_i}{\partial n} \le 0 \text{ on } (0,\ T]\times\partial\Omega_1\times\Lambda,$$

$$D_i\frac{\partial \underset{\sim}{c}_i}{\partial n} \le H_i(\underset{\sim}{C}_i - \underset{\sim}{c}_i) \text{ on } (0,\ T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial \underset{\sim}{C}_i}{\partial t} - \mathcal{D}_i\nabla^2 \underset{\sim}{C}_i + u\cdot\nabla \underset{\sim}{C}_i + H_i\int_{\partial\Omega_2}(\underset{\sim}{C}_i - c_i) \le F_i(t,\ z,\ \underset{\sim}{C}_j) \text{ in } (0,\ T]\times\Lambda,$$

$$\upsilon_1 \underset{\sim}{C}_i + \mathcal{D}_i\frac{\partial \underset{\sim}{C}_i}{\partial n_1} \le \upsilon_1 C_{i,1} \text{ on } (0,\ T]\times\partial\Lambda_1,$$

$$\frac{\partial \underset{\sim}{C}_i}{\partial n_\alpha} \le 0 \text{ on } (0,\ T]\times\partial\Lambda_\alpha,\ \alpha = 2,\ 3,$$

$$\underset{\sim}{c}_i(0,\ x,\ z) \le c_{i,0} \text{ in } \Omega\times\Lambda,$$

$$\underset{\sim}{C}_i(0,\ z) \le C_{i,0} \text{ in } \Lambda,$$

and

$$\frac{\partial \tilde{c}_i}{\partial t} - D_i\nabla_x^2 \tilde{c}_i \ge f_i(t,\ x,\ \tilde{c}_j) \text{ in } (0,\ T]\times\Omega\times\Lambda,$$

$$\frac{\partial \tilde{c}_i}{\partial n} \ge 0 \text{ on } (0,\ T]\times\partial\Omega_1\times\Lambda,$$

$$D_i\frac{\partial \tilde{c}_i}{\partial n} \ge H_i(\tilde{C}_i - \tilde{c}_i) \text{ on } (0,\ T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial \tilde{C}_i}{\partial t} - \mathcal{D}_i\nabla^2 \tilde{C}_i + u\cdot\nabla \tilde{C}_i + H_i\int_{\partial\Omega_2}(\tilde{C}_i - \tilde{c}_i) \ge F_i(t,\ z,\ \tilde{C}_j) \text{ in } (0,\ T]\times\Lambda,$$

$$\upsilon_1 \tilde{C}_i + \mathcal{D}_i\frac{\partial \tilde{C}_i}{\partial n_1} \ge \upsilon_1 C_{i,1} \text{ on } (0,\ T]\times\partial\Lambda_1,$$

$$\frac{\partial \tilde{C}_i}{\partial n_\alpha} \ge 0 \text{ on } (0,\ T]\times\partial\Lambda_\alpha,\ \alpha = 2,\ 3,$$

$$\tilde{c}_i(0,\ x,\ z) \ge c_{i,0} \text{ in } \Omega\times\Lambda,$$

$$\tilde{C}_i(0,\ z) \ge C_{i,0} \text{ in } \Lambda,$$

respectively.

The strong comparison theorem shows that if $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ are *lower* and *upper* solutions of S_n, B_n and $(c_i,\ C_i)$ is a solution of S_n, B_n, then $\underset{\sim}{c}_i \le c_i \le \tilde{c}_i$ and $\underset{\sim}{C}_i \le C_i \le \tilde{C}_i$.

The existence of monotone sequences depend therefore on a suitable pair of lower and upper solutions. This is by no means ensured without addition restrictions on the nonlinear reaction functions. PAO [222] gives sufficient conditions for the existence of lower and upper solutions for parabolic equations. These will require that f_i or $\dfrac{\partial f_i}{\partial c_j}$ to be uniformly bounded and F_i or $\dfrac{\partial F_i}{\partial C_j}$ to be uniformly bounded. CARL

[46] gives a method to show how these lower and upper solutions can be constructed. TAM [278-281] used comparison theorems to construct upper and lower solutions for parabolic equations and compared these solutions with the exact numerical solutions. It is important to note that these lower and upper solutions provide lower and upper bounds for solutions and that these bounds can be improved by monotone iterative techniques. We shall for the purposes of an existence theorem, assume that upper and lower solutions exist.

In order to establish an existence theorem for S_n, B_n in terms of upper and lower solutions, we define a transformation $\mathcal{T}$, by

$$(c_i^{(k)}, C_i^{(k)}) = \mathcal{T}(c_j^{(k-1)}, C_j^{(k-1)}), \tag{3.6.7}$$

and consider the sequences $\{(c_i^{(k)}, C_i^{(k)})\}$ where $c_i^{(k)}$ is obtained from the linear system

$$\frac{\partial c_i^{(k)}}{\partial t} - D_i \nabla_x^2 c_i^{(k)} = f_i(t, x, c_j^{(k-1)}) \text{ in } (0, T]\times\Omega\times\Lambda, \tag{3.6.8}$$

$$\frac{\partial c_i^{(k)}}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda, \tag{3.6.9}$$

$$D_i \frac{\partial c_i^{(k)}}{\partial n} + H_i c_i^{(k)} = H_i C_i^{(k-1)} \text{ on } (0, T]\times\partial\Omega_2\times\Lambda, \tag{3.6.10}$$

$$c_i^{(k)}(0, x, z) = c_{i,0} \text{ in } \Omega\times\Lambda, \tag{3.6.11}$$

and $C_i^{(k)}$ is obtained from the linear system

$$\frac{\partial C_i^{(k)}}{\partial t} - \mathcal{D}_i \nabla^2 C_i^{(k)} + u\cdot\nabla C_i^{(k)} + H_i \mathcal{A} C_i^{(k)} = F_i(t, z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)} \text{ in } (0, T]\times\Lambda, \tag{3.6.12}$$

$$\upsilon_1 C_i^{(k)} + \mathcal{D}_i \frac{\partial C_i^{(k)}}{\partial n_1} = \upsilon_1 C_{i,1} \text{ on } (0, T]\times\partial\Lambda_1, \tag{3.6.13}$$

$$\frac{\partial C_i^{(k)}}{\partial n_\alpha} = 0 \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha = 2, 3, \tag{3.6.14}$$

$$C_i^{(k)}(0, z) = C_{i,0} \text{ in } \Lambda, \tag{3.6.15}$$

with $\underset{\sim}{c}_j \le c_j^{(k-1)} \le \tilde{c}_j$ on $[0, T]\times\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_j \le C_j^{(k-1)} \le \tilde{C}_j$ on $[0, T]\times\overline{\Lambda}$ for $k = 1,\ldots$.

For each k, the system (3.6.8) consists of $n(I)$ linear, completely uncoupled initial value problems with boundary and initial conditions given by (3.6.9)-(3.6.11) and this system is uncoupled from the system (3.6.12) which consists of $n(J)$ linear, completely uncoupled initial value problems with initial and boundary conditions given by (3.6.13)-(3.6.15).

Since $c_i^{(k)}(t, x, z)$ is not differentiated with respect to z in (3.6.8), Λ may be considered to be a parameter space in (3.6.8)-(3.6.11). For functions $c_i^{(k)}(t, x, z)$ where $D_i = H_i = 0$, Ω may also be considered to be a parameter space and for functions $C_i^{(k)}(t, z)$, where $\mathcal{D}_i = 0$, $u\cdot\nabla C_i^{(k-1)} \equiv 0$, we may similarly treat Λ as a parameter space. The existence and uniqueness of sequences $\{(c_i^{(k)}, C_i^{(k)})\}$ may therefore follow from solving standard scalar systems of linear parabolic equations (LADYSHENKAYA [155] or FRIEDMAN [94]) which may or may not depend on parameters, systems of ordinary differential equations which depend on parameters (HARTMAN [119, p. 93]) and systems of first order partial differential equations (LAKSHMIKANTHAM *et al.*[160]).

All these theorems will require Hölder continuity properties on the functions $f_i(t, x, c_j^{(k-1)})$ and $F_i(t, z, C_j^{(k-1)})+H_i\int_{\partial\Omega_2} c_i^{(k-1)}$ which are satisfied if either $c_j^{(k-1)} \in C^{(1+\alpha)/2,1+\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$, $c_j^{(k-1)} \in C^{\alpha/2,\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$, $C_j^{(k-1)} \in C^{(1+\alpha)/2,1+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ or $C_j^{(k-1)} \in C^{\alpha/2,\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$.

These theorems will also require Hölder continuity properties in the boundary and initial conditions and so we make the following assumptions on $c_{i,0}$, $C_{i,0}$ and $C_{i,1}$. We will assume that $\partial\Omega$ and $\partial\Lambda$ belong to class $C^{2+\alpha}$.

(H_3)

(i) For components $i \in I$, where $D_i, H_i > 0$,

$$c_{i,0} \in C^{2+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}];$$

(ii) For components $i \in I$, where $D_i = H_i = 0$,

$$c_{i,0} \in C^{\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}];$$

(iii) For components $i \in J$, where $\mathcal{D}_i > 0$,

$$C_{i,0} \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}] \text{ and } C_{i,1} \in C^{(1+\alpha)/2,1+\alpha}[(0, T]\times\partial\Lambda_1, R^{n(J)}];$$

(iv) For components $i \in J$, where $\mathcal{D}_i = 0$ and $u\cdot\nabla C_i \not\equiv 0$,

$$C_{i,0} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}] \text{ and } C_{i,1} \in C^{\alpha/2,\alpha}[(0, T]\times\partial\Lambda_1, R^{n(J)}];$$

(v) For components $i \in J$, where $\mathcal{D}_i = 0$ and $u\cdot\nabla C_i \equiv 0$,

$$C_{i,0} \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}].$$

The velocity distribution vector function $u(t, z)$ is also required to satisfy the following Hölder continuity property:

(H_4) $u(t, z) \in C^{\alpha/2,\alpha}[(0, T]\times\overline{\Lambda}, R^n]$.

For components $i \in J$, where $\mathcal{D}_i = 0$, $u\cdot\nabla C_i \not\equiv 0$, we shall also need the following additional assumptions

(H_5)

(i) For each $(t_0, z_0) \in [0,T]\times\overline{\Lambda}$, there exists a unique solution $z(t, t_0, z_0)$ of

$$\frac{dz}{dt} = u(t, z),\ z(t_0) = z_0, \text{ on } [0, T]; \tag{3.6.16}$$

(ii) $z(t, t_0, z_0)$ is continuously differentiable with respect to (t_0, z_0);

(iii) The relationship

$$\frac{\partial z}{\partial t_0}(t, t_0, z_0)+\frac{\partial z}{\partial z_0}(t, t_0, z_0)u(t_0, z_0)\neq 0, \tag{3.6.17}$$

holds.

(H_6)

(i) For each $z_0 \in \overline{\Lambda}$ and $Y_{i0} \in R^{n(J)}$, there exists a unique solution $Y_i(t, 0, Y_{i0}; z_0)$ of

$$\frac{\partial Y_i}{\partial t} = F_i(t,\, z(t,\, t_0,\, z_0),\, C_j^{(k-1)}) - H_i \mathscr{A} Y_i + H_i \int_{\partial\Omega_2} c_i^{(k-1)}(t,\, x,\, z(t,\, t_0,\, z_0)),\; Y_i(0) = Y_{i0}, \quad \textbf{(3.6.18)}$$

on $[0, T]$, where $z(t, t_0, z_0)$ is the unique solution of (3.6.16);

(ii) $Y_i(t, 0, Y_{i0}; z_0)$ is continuously differentiable with respect to (Y_{i0}, z_0).

Note that assumptions (H_3)-(H_5) will hold in either our original system S_n, B_n or the monotone system S_{2n}, B_{2n} and (H_6) can be shown to hold in the monotone system S_{2n}, B_{2n} if it holds in our original system S_n, B_n.

Lemma 3.6.5

Consider the IBVP (3.6.8)–(3.6.15) and suppose that the assumptions (H_1)–(H_4) hold. Let there exist $(\underset{\sim}{c}_i,\, \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\, \tilde{C}_i)$ which are lower and upper solutions of S_n, B_n with $\underset{\sim}{c}_j \le c_j^{(k-1)} \le \tilde{c}_j$ on $[0, T]\times\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_j \le C_j^{(k-1)} \le \tilde{C}_j$ on $[0, T]\times\overline{\Lambda}$.

Assume that

(i) *For components $j \in I$, where $D_j, H_j > 0$, $c_j^{(k-1)} \in C^{(1+\alpha)/2, 1+\alpha, \alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$;*

(ii) *For components $j \in I$, where $D_j = H_j = 0$, $c_j^{(k-1)} \in C^{\alpha/2, \alpha, \alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$;*

(iii) *For components $j \in J$, where $\mathscr{D}_j > 0$, $C_j^{(k-1)} \in C^{(1+\alpha)/2, 1+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$;*

(iv) *For components $j \in J$, where $\mathscr{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \not\equiv 0$, $C_j^{(k-1)} \in C^{(1+\alpha)/2, \alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$, and assumptions ($H_5$)-($H_6$) hold;*

(v) *For components $j \in J$, where $\mathscr{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \equiv 0$, $C_j^{(k-1)} \in C^{(1+\alpha)/2, \alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$.*

Then the IBVP (3.6.8)-(3.6.15) possesses a unique solution $(c_i^{(k)}, C_i^{(k)})$, where

(I) *For components $i \in I$, where $D_i, H_i > 0$, $c_i^{(k)} \in C^{1+\alpha/2, 2+\alpha, \alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$;*

(II) *For components $i \in I$, where $D_i = H_i = 0$, $c_i^{(k)} \in C^{1+\alpha/2, \alpha, \alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$;*

(III) *For components $i \in J$, where $\mathscr{D}_i > 0$, $C_i^{(k)} \in C^{1+\alpha/2, 2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$;*

(IV) *For components $i \in J$, where $\mathscr{D}_i = 0$, $u\cdot\nabla C_i^{(k)} \not\equiv 0$, $C_i^{(k)} \in C^{1+\alpha/2, 1+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$;*

(V) *For components $i \in J$, where $\mathscr{D}_i = 0$, $u\cdot\nabla C_i^{(k)} \equiv 0$, $C_i^{(k)} \in C^{1+\alpha/2, \alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$.*

Furthermore, in all cases $c_i^{(k)}$ and $C_i^{(k)}$ satisfy the inequalities $\underset{\sim}{c}_i \le c_i^{(k)} \le \tilde{c}_i$ in $[0, T]\times\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_i \le C_i^{(k)} \le \tilde{C}_i$ in $[0, T]\times\overline{\Lambda}$.

Proof

We first consider the case when D_j, $\mathscr{D}_j > 0$ for all j. It is obvious that for equations (3.6.8)-(3.6.11), all conditions of Theorem 3.1.2 except for those listed in assumption (iv) are satisfied. Note that the function $C_j^{(k-1)}$ in the boundary condition of $c_i^{(k)}$ are functions of t and z but are independent of x. The function $C_j^{(k-1)}$ therefore satisfies the Hölder continuity property in t required by assumption (v) of Theorem 3.1.2 and z may be treated as a parameter. It is therefore enough to show that $f_i(t, x, c_j^{(k-1)}) \in C^{\alpha/2, \alpha, \alpha}[[0, T]\times\overline{\Omega}\times\Lambda\times R^{n(I)}, R^{n(I)}]$.

We have

$$|f_i(t, x, c_j^{(k-1)}(t, x, z)) - f_i(t^*, x, c_j^{(k-1)}(t^*, x, z))| \le k_t(f_i)[|t-t^*|^{\alpha/2} + |c_j^{(k-1)}(t, x, z) - c_j^{(k-1)}(t^*, x, z)|]$$
$$\le k_t(f_i)[|t-t^*|^{\alpha/2} + k_t(c_j^{(k-1)})|t-t^*|^{(1+\alpha)/2}]$$
$$\le k_t(f_i(t, x, c_j^{(k-1)}))|t-t^*|^{\alpha/2},$$

where,

$$k_t(f_i(t, x, c_j^{(k-1)})) = k_t(f_i)(1 + k_t(c_i^{(k-1)})T^{1/2}). \tag{3.6.19}$$

Also,

$$|f_i(t, x, c_j^{(k-1)}(t, x, z)) - f_i(t, x^*, c_j^{(k-1)}(t, x^*, z^*))| \le k_{x,z}(f_i)[\|x-x^*\|^{\alpha} + |c_j^{(k-1)}(t, x, z) - c_j^{(k-1)}(t, x^*, z^*)|]$$
$$\le k_{x,z}(f_i)[\|x-x^*\|^{\alpha} + k_{x,z}(c_j^{(k-1)})(|c_j^{(k-1)}|_{C^1}(d(\overline{\Omega}))^{1-\alpha}\|x-x^*\|^{\alpha} + \|z-z^*\|^{\alpha})]$$
$$\le k_{x,z}(f_i(t, x, c_j^{(k-1)}))(\|x-x^*\|^{\alpha} + \|z-z^*\|^{\alpha}),$$

where,

$$k_{x,z}(f_i(t, x, c_j^{(k-1)})) = k_{x,z}(f_i)(max\{1 + k_{x,z}(c_j^{(k-1)})|c_j^{(k-1)}|_{C^1}(d(\overline{\Omega}))^{1-\alpha}, k_{x,z}(c_j^{(k-1)})\}). \tag{3.6.20}$$

These two equations together show that

$$f_i(t, x, c_j^{(k-1)}) \in C^{\alpha/2,\alpha,\alpha}[[0, T]\times\overline{\Omega}\times\Lambda\times R^{n(l)}, R^{n(l)}], \tag{3.6.21}$$

i.e., $f_i(t, x, c_j^{(k-1)})$ is Hölder continuous in t and (x, z) with exponent $\alpha/2$ and α, respectively.

For a given z in Λ, it follows from Theorem 3.1.2 that (3.6.8)-(3.6.11) has a unique solution $c_i^{(k)}$, where $c_i^{(k)}(t, x; z) \in C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Omega}, R^{n(l)}]$.

To show that $c_i^{(k)}$ is Hölder continuous in z with exponent α, we consider equations (3.6.8)-(3.6.11) with z and z^* and look at the difference of these equations. Note that from the assumptions,

$$|f_i(t, x, c_j^{(k-1)}(t, x, z)) - f_i(t, x, c_j^{(k-1)}(t, x, z^*))| \le k_z(f_i(t, x, c_j^{(k-1)}))\|z-z^*\|^{\alpha},$$

$$|C_j^{(k-1)}(t, z) - C_j^{(k-1)}(t, z^*)| \le K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z-z^*\|^{\alpha},$$

$$|c_{i,0}(x, z) - c_{i,0}(x, z^*)| \le k_z(c_{i,0})\|z-z^*\|^{\alpha},$$

so that

$$-k_z(f_i(t, x, c_j^{(k-1)}))\|z-z^*\|^{\alpha} \le f_i(t, x, c_j^{(k-1)}(t, x, z)) - f_i(t, x, c_j^{(k-1)}(t, x, z^*))$$
$$\le k_z(f_i(t, x, c_j^{(k-1)}))\|z-z^*\|^{\alpha},$$

$$-K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z-z^*\|^{\alpha} \le C_j^{(k-1)}(t, z) - C_j^{(k-1)}(t, z^*)$$
$$\le K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z-z^*\|^{\alpha},$$

$$-k_z(c_{i,0})\|z-z^*\|^\alpha \leq c_{i,0}(x,z)-c_{i,0}(x,z^*) \leq k_z(c_{i,0})\|z-z^*\|^\alpha.$$

It then follows that

$$-k_z(f_i(t,x,c_j^{(k-1)}))\|z-z^*\|^\alpha \leq \frac{\partial}{\partial t}(c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*))-D_i\nabla_x^2(c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*))$$
$$\leq k_z(f_i(t,x,c_j^{(k-1)}))\|z-z^*\|^\alpha, \tag{3.6.22}$$

$$-K_z(C_j^{(k-1)})H_i|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z-z^*\|^\alpha$$
$$\leq D_i\frac{\partial}{\partial n}(c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*))+H_i(c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*))$$
$$\leq K_z(C_j^{(k-1)})H_i|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z-z^*\|^\alpha, \tag{3.6.23}$$

$$-k_z(c_{i,0})\|z-z^*\|^\alpha \leq c_{i,0}(x,z)-c_{i,0}(x,z^*)\leq k_z(c_{i,0})\|z-z^*\|^\alpha. \tag{3.6.24}$$

Letting

$$w_{i1} = \frac{c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*)+k_z(f_i(t,x,c_j^{(k-1)}))\|z-z^*\|^\alpha t}{K\|z-z^*\|^\alpha}, \tag{3.6.25}$$

and

$$w_{i2} = \frac{c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*)-k_z(f_i(t,x,c_j^{(k-1)}))\|z-z^*\|^\alpha t}{K\|z-z^*\|^\alpha}, \tag{3.6.26}$$

where

$$K = max\{k_z(c_{i,0}),\ K_z(C_j^{(k-1)})H_i|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\}, \tag{3.6.27}$$

we obtain the problems

$$\frac{\partial w_{i1}}{\partial t}-D_i\nabla_x^2 w_{i1}\geq 0,\ \frac{D_i}{H_i}\frac{\partial w_{i1}}{\partial n}+w_{i1}\geq -1,\ w_{i1,0}\geq -1, \tag{3.6.28}$$

and

$$\frac{\partial w_{i2}}{\partial t}-D_i\nabla_x^2 w_{i2}\leq 0,\ \frac{D_i}{H_i}\frac{\partial w_{i2}}{\partial n}+w_{i2}\leq 1,\ w_{i2,0}\leq 1. \tag{3.6.29}$$

The problems (3.6.28) and (3.6.29) are equivalent and it follows by Theorem 3.2.9 (Strong Comparison Theorem) for parabolic equations that

$$w_{i1}\geq -1, \tag{3.6.30}$$

and

$$w_{i2}\leq 1. \tag{3.6.31}$$

Therefore

$$-(K+k_z(f_i(t,x,c_j^{(k-1)}))T)\|z-z^*\|^\alpha \le (c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*))$$
$$\le (K+k_z(f_i(t,x,c_j^{(k-1)}))T)\|z-z^*\|^\alpha, \tag{3.6.32}$$

so that

$$|(c_i^{(k)}(t,x,z)-c_i^{(k)}(t,x,z^*))| \le (K+k_z(f_i(t,x,c_j^{(k-1)}))T)\|z-z^*\|^\alpha, \tag{3.6.33}$$

i.e., $c_i^{(k)}$ is Hölder continuous in z.

We see that (3.6.8)-(3.6.11) has a unique solution $c_i^{(k)}$, where

$$c_i^{(k)}(t,x,z)\in C^{1+\alpha/2,2+\alpha,\alpha}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]. \tag{3.6.34}$$

Note that the equation (3.6.32) could also have been obtained by integrating (3.6.22) with boundary and initial conditions (3.6.23)-(3.6.24) and noting that the corresponding Green's function is integrable.

It is obvious that for equations (3.6.12)-(3.6.15), $v_1\in C^{\alpha/2,\alpha}[(0,T]\times\overline{\Lambda}, R^n]$ and all conditions of Theorem 3.1.2 except for those listed in assumption (iv) are satisfied. Therefore, it is enough to show that $F_i(t,z,C_j^{(k-1)})+H_i\int_{\partial\Omega_2}c_i^{(k-1)}\in C^{\alpha/2,\alpha}[[0,T]\times\overline{\Lambda}\times R^{n(J)}, R^{n(J)}]$.

We have

$$\begin{aligned}
&|[F_i(t,z,C_j^{(k-1)}(t,z))+H_i\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z)]-[F_i(t^*,z,C_j^{(k-1)}(t^*,z))+H_i\int_{\partial\Omega_2}c_i^{(k-1)}(t^*,x,z)]|\\
&\quad\le |F_i(t,z,C_j^{(k-1)}(t,z))-F_i(t^*,z,C_j^{(k-1)}(t^*,z))| + H_i\left|\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z)-c_i^{(k-1)}(t^*,x,z)\right|\\
&\quad\le K_t(F_i)[|t-t^*|^{\alpha/2}+|C_j^{(k-1)}(t,z)-C_j^{(k-1)}(t^*,z)|] + H_i\int_{\partial\Omega_2}|c_i^{(k-1)}(t,x,z)-c_i^{(k-1)}(t^*,x,z)|\\
&\quad\le K_t(F_i)[|t-t^*|^{\alpha/2}+K_t(C_j^{(k-1)})|t-t^*|^{(1+\alpha)/2}] + H_ik_t(c_i^{(k-1)})\int_{\partial\Omega_2}|t-t^*|^{(1+\alpha)/2}\\
&\quad\le K_t(F_i)[|t-t^*|^{\alpha/2}+K_t(C_j^{(k-1)})|t-t^*|^{(1+\alpha)/2}]+H_ik_t(c_i^{(k-1)})\mathcal{A}|t-t^*|^{(1+\alpha)/2}\\
&\quad\le K_t(F_i(t,z,C_j^{(k-1)})+H_i\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z))|t-t^*|^{\alpha/2},
\end{aligned}$$

where

$$K_t(F_i(t,z,C_j^{(k-1)})+H_i\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z)) = [1+T^{1/2}[K_t(C_j^{(k-1)})+H_ik_t(c_i^{(k-1)})\mathcal{A}]]. \tag{3.6.35}$$

Also,

$$\begin{aligned}
&|[F_i(t,z,C_j^{(k-1)}(t,z))+H_i\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z)]-[F_i(t,z^*,C_j^{(k-1)}(t,z^*))+H_i\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z^*)]|\\
&\quad\le |F_i(t,z,C_j^{(k-1)}(t,z^*))-F_i(t,z^*,C_j^{(k-1)}(t,z^*))| + H_i\left|\int_{\partial\Omega_2}c_i^{(k-1)}(t,x,z)-c_i^{(k-1)}(t,x,z^*)\right|\\
&\quad\le |F_i(t,z,C_j^{(k-1)}(t,z^*))-F_i(t,z^*,C_j^{(k-1)}(t,z^*))| + H_i\int_{\partial\Omega_2}|c_i^{(k-1)}(t,x,z)-c_i^{(k-1)}(t,x,z^*)|\\
&\quad\le K_z(F_i)[\|z-z^*\|^\alpha+|C_j^{(k-1)}(t,z)-C_j^{(k-1)}(t,z^*)|] + H_ik_z(c_i^{(k-1)})\int_{\partial\Omega_2}\|z-z^*\|^\alpha
\end{aligned}$$

$$\leq K_z(F_i)[\|z-z^*\|^\alpha + K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\Lambda))^{1-\alpha}\|z-z^*\|^\alpha] + H_i k_z(c_i^{(k-1)})\mathscr{A}\|z-z^*\|^\alpha$$
$$\leq K_z(F_i(t, z, C_j^{(k-1)}) + H_i\int_{\partial\Omega_2} c_i^{(k-1)})\|z-z^*\|^\alpha,$$

where

$$K_z(F_i(t, z, C_j^{(k-1)}) + H_i\int_{\partial\Omega_2} c_i^{(k-1)}) = K_z(F_i)[1 + K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}] + H_i k_z(c_i^{(k-1)})\mathscr{A}. \quad \textbf{(3.6.36)}$$

These equations together show that

$$F_i(t, z, C_j^{(k-1)}) + H_i\int_{\partial\Omega_2} c_i^{(k-1)} \in C^{\alpha/2,\alpha}[[0, T]\times\overline{\Lambda}\times R^{n(J)}, R^{n(J)}], \quad \textbf{(3.6.37)}$$

i.e., $F_i(t, z, C_j^{(k-1)}) + H_i\int_{\partial\Omega_2} c_i^{(k-1)}$ is Hölder continuous in t and z with exponent $\alpha/2$ and α respectively.

It follows from Theorem 3.1.2 that (3.6.12)-(3.6.15) has a unique solution $C_i^{(k)}$, where $C_i^{(k)} \in C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$.

To prove (I) and (II) in the general case, we need only observe that $f_i(t, x, c_j^{(k-1)}) \in C^{\alpha/2,\alpha,\alpha}[[0, T]\times\overline{\Omega}\times\Lambda\times R^{n(I)}, R^{n(I)}]$ from (i) and (ii). The proof is similar to that shown earlier.

In the case of (I), we note that for components i, where $D_i, H_i > 0$,

$$c_i^{(k)} \in C^{1+\alpha/2,2+\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}], \quad \textbf{(3.6.38)}$$

by the same argument as above using Theorem 3.1.2.

In the case of (II), we note that for components i, where $D_i = H_i = 0$,

$$c_i^{(k)}(t, x, z) = c_{i,0} + \int_0^t f_i(t', x, c_j^{(k-1)}(t', x, z))dt', \quad \textbf{(3.6.39)}$$

exists and is unique by the Hölder continuity property of $f_i(t, x, c_j^{(k-1)})$ in t, x and z. Also, if $f_i(t, x, c_j^{(k-1)})$ is Hölder continuous in t with exponent $\alpha/2$, then $\frac{\partial c_i^{(k)}}{\partial t}$ is Hölder continuous in t with exponent $\alpha/2$. Furthermore,

$$-k_{x,z}(f_i(t, x, c_j^{(k-1)}))(\|x-x^*\|^\alpha + \|z-z^*\|^\alpha) \leq \frac{\partial}{\partial t}(c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x^*, z^*))$$
$$\leq k_{x,z}(f_i(t, x, c_j^{(k-1)}))(\|x-x^*\|^\alpha + \|z-z^*\|^\alpha), \quad \textbf{(3.6.40)}$$

$$-k_{x,z}(c_{i,0})(\|x-x^*\|^\alpha + \|z-z^*\|^\alpha) \leq c_{i,0}(x, z) - c_{i,0}(x^*, z^*) \leq k_{x,z}(c_{i,0})(\|x-x^*\|^\alpha + \|z-z^*\|^\alpha). \quad \textbf{(3.6.41)}$$

Letting

$$w_{i1} = \frac{c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x, z^*) + k_{x,z}(f_i(t, x, c_j^{(k-1)}))(\|x-x^*\|^\alpha + \|z-z^*\|^\alpha)t}{k_{x,z}(c_{i,0})(\|x-x^*\|^\alpha + \|z-z^*\|^\alpha)}, \quad \textbf{(3.6.42)}$$

and

$$w_{i2} = \frac{c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x, z^*) - k_{x,z}(f_i(t, x, c_j^{(k-1)}))(\|x - x^*\|^\alpha + \|z - z^*\|^\alpha)t}{k_{x,z}(c_{i,0})(\|x - x^*\|^\alpha + \|z - z^*\|^\alpha)}, \tag{3.6.43}$$

we obtain the problems

$$\frac{\partial w_{i1}}{\partial t} \geq 0,\ w_{i1,0} \geq -1, \tag{3.6.44}$$

and

$$\frac{\partial w_{i2}}{\partial t} \leq 0,\ w_{i2,0} \leq 1. \tag{3.6.45}$$

The problems (3.6.44) and (3.6.45) are equivalent and it follows by Theorem 3.2.3 (Strong Comparison Theorem) for ordinary differential equations that

$$w_{i1} \geq -1, \tag{3.6.46}$$

and

$$w_{i2} \leq 1. \tag{3.6.47}$$

Therefore

$$-(k_{x,z}(c_{i,0}) + k_z(f_i(t, x, c_j^{(k-1)}))T)(\|x - x^*\|^\alpha + \|z - z^*\|^\alpha) \leq (c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x, z^*))$$

$$\leq (k_{x,z}(c_{i,0}) + k_z(f_i(t, x, c_j^{(k-1)}))T)(\|x - x^*\|^\alpha + \|z - z^*\|^\alpha), \tag{3.6.48}$$

so that

$$|(c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x, z^*))| \leq (k_{x,z}(c_{i,0}) + k_z(f_i(t, x, c_j^{(k-1)}))T)(\|x - x^*\|^\alpha + \|z - z^*\|^\alpha), \tag{3.6.49}$$

i.e., $c_i^{(k)}$ is Hölder continuous in x and z.

This result also follows by integrating (3.6.40) through with respect to t and applying the initial condition (3.6.41). Altogether, these imply that

$$c_i^{(k)} \in C^{1+\alpha/2,\alpha,\alpha}[(0, T] \times \overline{\Omega} \times \Lambda, R^{n(I)}]. \tag{3.6.50}$$

To prove (III)–(V) in the general case, we need only observe that $F_i(t, z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)} \in C^{\alpha/2,\alpha}$ $[[0, T] \times \overline{\Lambda} \times R^{n(J)}, R^{n(J)}]$ from (i)–(v).

In the case of (III), we note that for components i, where $\mathcal{D}_i > 0$,

$$C_i^{(k)} \in C^{1+\alpha/2,2+\alpha}[(0, T] \times \overline{\Lambda}, R^{n(J)}] \tag{3.6.51}$$

by the same arguments as above using Theorem 3.1.2.

In the case of (IV), we note that for components i, where $\mathcal{D}_i = 0$ and $u \cdot \nabla C_i^{(k)} \equiv 0$,

$$C_i^{(k)}(t, z) = C_{i,0} + \int_0^t F_i(t', z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)}(t', x, z) dt', \tag{3.6.52}$$

exists and is unique by the Hölder continuity property of $F_i(t,\ z,\ C_j^{(k-1)}) + H_i\int_{\partial\Omega_2} c_i^{(k-1)}$ in t and z. By the same argument as for the proof of (II), we see that

$$C_i^{(k)} \in C^{1+\alpha/2,\alpha}[(0,\ T]\times\overline{\Lambda},\ R^{n(J)}]. \tag{3.6.53}$$

In the case of (V), we see that by (H_5) and (H_6), $z(t,\ t_0,\ z_0)$ and $Y_i(t,\ 0,\ Y_{i0};\ z_0)$ are unique solutions of (3.6.16) and (3.6.18), respectively, on $[0,\ T]$. Choose $Y_{i0} = C_{i0}(z_0)$ and note that if $z = z(t,\ 0,\ z_0)$, then because of uniqueness, $z_0 = z(0,\ t,\ z)$. Also, the solution $(z(t,\ 0,\ z_0),\ Y_i(t,\ 0,\ Y_{i0};\ z_0))$ of the systems (3.6.16) and (3.6.18) is a characteristic equation of (3.6.12). Hence, for each solution of (3.6.16) and (3.6.18), we have

$$C_i^{(k)}(t,z(t,\ 0,\ z_0)) = Y_i(t,\ 0,\ C_{i,0}(z_0);\ z_0), \tag{3.6.54}$$

and consequently,

$$C_i^{(k)}(t,z) = Y_i(t,\ 0,\ C_{i,0}(z(0,\ t,\ z));\ z(0,\ t,\ z)). \tag{3.6.55}$$

Now by using assumptions (A_5) and (A_6), it is easy to show that $C_i^{(k)}(t,z)$ defined by (3.6.55) satisfies (3.6.12).

To show uniqueness of solutions of (3.6.12), we suppose, that $C_{i1}^{(k)}$ and $C_{i2}^{(k)}$ are two solutions of (3.6.12) on $[0,\ T]\times\overline{\Lambda}$. By Theorem 3.2.9 (Strong Comparison Theorem) for first order partial differential equations, we see that $C_{i1}^{(k)} \le C_{i2}^{(k)} \le C_{i1}^{(k)}$ and therefore $C_{i1}^{(k)}$ coincides with $C_{i2}^{(k)}$.

The Hölder continuity of $C_i^{(k)}(t,z)$ is obtained by examining the characteristic equations (3.6.16) and (3.6.18), so that

$$C_i^{(k)} \in C^{1+\alpha/2,1+\alpha}[(0,\ T]\times\overline{\Lambda},\ R^{n(J)}]. \tag{3.6.56}$$

Finally, we show that $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ are lower and upper solutions of $(c_i^{(k)},\ C_i^{(k)})$. To show that $(\tilde{c}_i,\ \tilde{C}_i)$ is an upper solution of $(c_i^{(k)},\ C_i^{(k)})$, we need only observe that

$$\frac{\partial}{\partial t}(\tilde{c}_i - c_i^{(k)}) - D_i\nabla_x^2(\tilde{c}_i - c_i^{(k)}) \ge f_i(t,\ x,\ \tilde{c}_j) - f_i(t,\ x,\ c_j^{(k-1)}) \ge 0 \text{ in } (0,\ T]\times\Omega\times\Lambda,$$

$$D_i\frac{\partial}{\partial n}(\tilde{c}_i - c_i^{(k)}) + H_i(\tilde{c}_i - c_i^{(k)}) = H_i(\tilde{C}_i - C_i^{(k-1)}) \ge 0 \text{ on } (0,\ T]\times\partial\Omega_2\times\Lambda,$$

$$\begin{aligned}
&\frac{\partial}{\partial t}(\tilde{C}_i - C_i^{(k)}) - \mathcal{D}_i\nabla^2(\tilde{C}_i - C_i^{(k)}) + u\cdot\nabla(\tilde{C}_i - C_i^{(k)}) + H_i\mathcal{A}(\tilde{C}_i - C_i^{(k)}) \\
&\qquad \ge F_i(t,\ z,\ \tilde{C}_j) - F_i(t,\ z,\ C_i^{(k-1)}) + H_i\int_{\partial\Omega_2}(\tilde{c}_i - c_i^{(k-1)}) \\
&\qquad \ge 0 \text{ in } (0,\ T]\times\Lambda,
\end{aligned}$$

since f_i and F_i are monotone nondecreasing in c_j and C_j, respectively.

We may therefore apply the maximum principle for the parabolic operator or Theorem 3.2.3 (Strong Comparison Theorem) for ordinary differential equations or Theorem 3.2.6 (Strong Comparison Theorem) for first order partial differential equations to conclude that $(\tilde{c}_i,\ \tilde{C}_i) \le (c_i^{(k)},\ C_i^{(k)})$. Similarly, $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ may be shown to be a lower solution of $(c_i^{(k)},\ C_i^{(k)})$ and the theorem is complete.❑

To start off the iterative procedure, we need some continuity properties of $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$. The properties of the mapping $\mathscr{T}$, from $(c_j^{(k-1)}, C_j^{(k-1)})$ into $(c_i^{(k)}, C_i^{(k)})$ are then given by the following lemma.

Lemma 3.6.6.

Consider the IBVP (3.6.8)–(3.6.15) and suppose that the assumptions (H_1)–(H_4) hold. Let there exist $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ which are lower and upper solutions respectively of S_n, B_n.

Assume that

(i) *For components $j \in I$, where $D_j, H_j > 0$, $\underset{\sim}{c}_j, \tilde{c}_j \in C^{1+\alpha/2,2+\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$;*

(ii) *For components $j \in I$, where $D_j = H_j = 0$, $\underset{\sim}{c}_j, \tilde{c}_j \in C^{1+\alpha/2,\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$;*

(iii) *For components $j \in J$, where $\mathscr{D}_j > 0$, $\underset{\sim}{C}_j, \tilde{C}_j \in C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$;*

(iv) *For components $j \in J$, where $\mathscr{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \not\equiv 0$, $\underset{\sim}{C}_j, \tilde{C}_j \in C^{1+\alpha/2,1+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$, and assumptions (H_5)-(H_6) hold;*

(v) *For components $j \in J$, where $\mathscr{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \equiv 0$, $\underset{\sim}{C}_j, \tilde{C}_j \in C^{1+\alpha/2,\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$.*

Then the mapping $\mathscr{T}$, from $(c_j^{(k-1)}, C_j^{(k-1)})$ to $(c_i^{(k)}, C_i^{(k)})$ possesses the following properties:

(I) $(\tilde{c}_i, \tilde{C}_i) \geq \mathscr{T}(\tilde{c}_j, \tilde{C}_j)$, $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \leq \mathscr{T}(\underset{\sim}{c}_j, \underset{\sim}{C}_j)$.

(II) *$\mathscr{T}$ is a monotone operator on the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$.*

Proof

We first consider the case when $D_j, \mathscr{D}_j > 0$ for all components j. The natural imbedding of $C^{1+\alpha/2,2+\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ into $C^{1,2,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ into $C^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ implies that $\underset{\sim}{c}_j, \tilde{c}_j \in C^{1,2,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\underset{\sim}{C}_j, \tilde{C}_j \in C^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$.

The boundedness of Ω and Λ, together with the fact that their boundaries belong to $C^{2+\alpha}$, shows that, if $c_j^{(k-1)}(t, x; z) \in C^{1,2}[(0, T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C_j^{(k-1)}(t, z) \in C^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$, then $c_j^{(k-1)}(t, x; z) \in W_q^{1,2}[(0, T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C_j^{(k-1)}(t, z) \in W_q^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ for $q > 1$. From Lemma 3.1.5, we may take q to be identical in both cases.

This, in view of Theorem 3.1.1 (Imbedding Theorem), yields that $c_j^{(k-1)}(t, x; z) \in C^{(1+\alpha)/2,1+\alpha}[(0, T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C_j^{(k-1)}(t, z) \in C^{(1+\alpha)/2,1+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$. From Lemma 3.1.3, α may be chosen to be identical in both cases. From arguments similar to that shown in the proof of Lemma 3.6.5, we see that $c_j^{(k-1)}(t, x, z) \in C^{(1+\alpha)/2,1+\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$.

It is immediate that the proof of (I) follows from the choices $(c_j^{(k-1)}, C_j^{(k-1)}) = (\underset{\sim}{c}_j, \underset{\sim}{C}_j)$ and $(c_j^{(k-1)}, C_j^{(k-1)}) = (\tilde{c}_j, \tilde{C}_j)$ in Lemma 3.6.5.

All the other possible cases are treated similarly.

We have shown that if $(c_j^{(0)}, C_j^{(0)}) = (\tilde{c}_j, \tilde{C}_j)$ then $(c_i^{(0)}, C_i^{(0)}) \geq \mathscr{T}(c_j^{(0)}, C_j^{(0)}) = (c_i^{(1)}, C_i^{(1)})$ and if $(c_j^{(0)}, C_j^{(0)}) = (\underset{\sim}{c}_j, \underset{\sim}{C}_j)$ then $(c_i^{(0)}, C_i^{(0)}) \leq \mathscr{T}(c_j^{(0)}, C_j^{(0)}) = (c_i^{(1)}, C_i^{(1)})$. We have, in fact proved that the mapping $\mathscr{T}$ maps intervals $[\underset{\sim}{c}_j, \tilde{c}_j]$ and $[\underset{\sim}{C}_j, \tilde{C}_j]$ onto themselves.

To prove (II), let c_{j1}, $c_{j2} \in [\underset{\sim}{c}_j, \tilde{c}_j]$ and C_{j1}, $C_{j2} \in [\underset{\sim}{C}_j, \tilde{C}_j]$ where $(c_{j1}, C_{j1}) \geq (c_{j2}, C_{j2})$ for all components j. We want to show that $\mathcal{T}(c_{j1}, C_{j1}) \geq \mathcal{T}(c_{j2}, C_{j2})$.

Let $(u_i, U_i) = \mathcal{T}(c_{j1}, C_{j1}) - \mathcal{T}(c_{j2}, C_{j2})$. Then the monotone nondecreasing property of f_i and F_i implies that

$$\frac{\partial u_i}{\partial t} - D_i \nabla_x^2 u_i = f_i(t, x, c_{j1}) - f_i(t, x, c_{j2}) \geq 0 \text{ in } (0, T] \times \Omega \times \Lambda, \tag{3.6.57}$$

$$D_i \frac{\partial u_i}{\partial n} + H_i u_i = H_i(C_{i1} - C_{i2}) \geq 0 \text{ on } (0, T] \times \partial\Omega_2 \times \Lambda, \tag{3.6.58}$$

$$\frac{\partial U_i}{\partial t} - \mathcal{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \mathcal{A} U_i = F_i(t, z, C_{j1}) - F_i(t, z, C_{j2}) + H_i \int_{\partial\Omega_2} c_{i1} - c_{i2} \geq 0 \text{ in } (0, T] \times \Lambda, \tag{3.6.59}$$

and from the maximum principle for the parabolic operator or comparison theorems for ordinary differential equations or first order partial differential equations, $(u_i, U_i) \geq 0$ or $\mathcal{T}(c_{j1}, C_{j1}) \geq \mathcal{T}(c_{j2}, C_{j2})$. This shows that $\mathcal{T}$ is a monotone operator on the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$.□

The monotone operator $\mathcal{T}$ will play a central role in the iteration scheme.

Remark 3.6.5

If f_i and F_i are strictly monotone increasing in c_j and C_j, respectively, then by Theorem 3.2.13 (Generalised Strong Comparison (Contact) Theorem), $\mathcal{T}(c_{j1}, C_{j1}) > \mathcal{T}(c_{j2}, C_{j2})$, (unless $\mathcal{T}(c_{j1}, C_{j1}) \equiv \mathcal{T}(c_{j2}, C_{j2})$ in which case the right hand sides of (3.6.57) and (3.6.59) are identically zero; but this happens only if $(c_{j1}, C_{j1}) = (c_{j2}, C_{j2})$, from the strict monotone property of f_i and F_i). We say that the monotone operator $\mathcal{T}$ is monotone operator in the sense of COLLATZ [76], i.e., $(c_{j1}, C_{j1}) \geq (c_{j2}, C_{j2})$ implies that $\mathcal{T}(c_{j1}, C_{j1}) > \mathcal{T}(c_{j2}, C_{j2})$.

Remark 3.6.6

If f_i and F_i are monotone nonincreasing in c_j and C_j, respectively, the operator $\mathcal{T}$ is alternating on the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$ in the sense that $(c_{j1}, C_{j2}) \geq (c_{j2}, C_{j1})$ implies that $\mathcal{T}(c_{j1}, C_{j2}) \leq \mathcal{T}(c_{j2}, C_{j1})$. To prove this, let $(u_i, U_i) = \mathcal{T}(c_{j1}, C_{j2}) - \mathcal{T}(c_{j2}, C_{j1})$. Then the monotone nonincreasing property of f_i and F_i implies that

$$\frac{\partial u_i}{\partial t} - D_i \nabla_x^2 u_i = f_i(t, x, c_{j1}) - f_i(t, x, c_{j2}) \leq 0 \text{ in } (0, T] \times \Omega \times \Lambda, \tag{3.6.60}$$

$$D_i \frac{\partial u_i}{\partial n} + H_i u_i = H_i(C_{i1} - C_{i2}) \leq 0 \text{ on } (0, T] \times \partial\Omega_2 \times \Lambda, \tag{3.6.61}$$

$$\frac{\partial U_i}{\partial t} - \mathcal{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \mathcal{A} U_i = F_i(t, z, C_{j1}) - F_i(t, z, C_{j2}) + H_i \int_{\partial\Omega_2} c_{i1} - c_{i2} \geq 0 \text{ in } (0, T] \times \Lambda, \tag{3.6.62}$$

and from the same argument as before, using the maximum principle for the parabolic operator or comparison theorems for ordinary differential equations or first order partial differential equations, we see that $\mathcal{T}(c_{j1}, C_{j2}) \leq \mathcal{T}(c_{j2}, C_{j1})$.

It is necessary to choose a proper initial iteration to ensure that the sequences $\{(c_i^{(k)}, C_i^{(k)})\}$ are monotone sequences that converge to the unique solution of S_n, B_n and are within the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$. From Lemma 3.6.6, it is obvious that the monotonicity of these sequences obviously depend on the monotonicity of f_i and F_i and the initial iteration is taken to be either an upper or a lower solution which is required to satisfy certain inequalities on the corresponding system.

We may therefore use the initial iteration $(\bar{c}_i^{(0)}, \bar{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$ to construct the sequence $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ from the following equations

$$\frac{\partial \bar{c}_i^{(k)}}{\partial t} - D_i \nabla_x^2 \bar{c}_i^{(k)} = f_i(t, x, \bar{c}_j^{(k-1)}) \text{ in } (0, T] \times \Omega \times \Lambda,$$

$$D_i \frac{\partial \bar{c}_i^{(k)}}{\partial n} + H_i \bar{c}_i^{(k)} = H_i \bar{C}_i^{(k-1)} \ (0, T] \times \partial\Omega_2 \times \Lambda,$$

$$\frac{\partial \bar{C}_i^{(k)}}{\partial t} - \mathcal{D}_i \nabla^2 \bar{C}_i^{(k)} + u \cdot \nabla \bar{C}_i^{(k)} + H_i \mathcal{A} \bar{C}_i^{(k)} = F_i(t, z, \bar{C}_j^{(k-1)}) + H_i \int_{\partial\Omega_2} \bar{c}_i^{(k-1)} \text{ in } (0, T] \times \Lambda,$$

or the sequence $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ may be determined from the equations

$$\frac{\partial \underline{c}_i^{(k)}}{\partial t} - D_i \nabla_x^2 \underline{c}_i^{(k)} = f_i(t, x, \underline{c}_j^{(k-1)}) \text{ in } (0, T] \times \Omega \times \Lambda,$$

$$D_i \frac{\partial \underline{c}_i^{(k)}}{\partial n} + H_i \underline{c}_i^{(k)} = H_i \underline{C}_i^{(k-1)} \ (0, T] \times \partial\Omega_2 \times \Lambda,$$

$$\frac{\partial \underline{C}_i^{(k)}}{\partial t} - \mathcal{D}_i \nabla^2 \underline{C}_i^{(k)} + u \cdot \nabla \underline{C}_i^{(k)} + H_i \mathcal{A} \underline{C}_i^{(k)} = F_i(t, z, \underline{C}_j^{(k-1)}) + H_i \int_{\partial\Omega_2} \underline{c}_i^{(k-1)} \text{ in } (0, T] \times \Lambda.$$

Note that the sequences $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ and $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ may be obtained independently of each other. As in Lemma 3.6.5, uniqueness and existence of the sequences $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ and $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ follow from similar arguments for uncoupled scalar systems of nonhomogeneous linear parabolic differential equations, ordinary differential equations or first order partial differential equations by using the monotone properties of f_i and F_i.

Definition 3.6.2.
The sequences $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\bar{c}_i^{(0)}, \bar{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$, are called *minimal* and *maximal sequences*, respectively. We say that $(\underline{c}_i, \underline{C}_i)$ and $(\bar{c}_i, \bar{C}_i)$ are *minimal* and *maximal solutions* respectively in the regions $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$, if for any solution (c_i, C_i) of S_n, B_n where $\underset{\sim}{c}_i \le c_i \le \tilde{c}_i$ and $\underset{\sim}{C}_i \le C_i \le \tilde{C}_i$, then $\underline{c}_i \le c_i \le \bar{c}_i$ and $\underline{C}_i \le C_i \le \bar{C}_i$.

From Lemma 3.6.6 together with the monotonicity of $\mathcal{T}$, we shall show that the sequence $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ is monotone nondecreasing and the sequence $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ with $(\bar{c}_i^{(0)}, \bar{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$ is monotone nonincreasing.

Furthermore, $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \le (\tilde{c}_i, \tilde{C}_i)$ results in $(\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) \le (\bar{c}_i^{(k)}, \bar{C}_i^{(k)})$ for all k and pointwise limits $(\underline{c}_i, \underline{C}_i)$ and $(\bar{c}_i, \bar{C}_i)$ exist. This is all done in the following lemma for S_n, B_n.

The only difficulty arises for components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i^{(k)} \not\equiv 0$, and in this case we will have the following additional assumptions:

(H_7) $\dfrac{\partial F_i}{\partial z}$ exists and is continuous;

(H_8) $\dfrac{\partial F_i}{\partial C_j}$ exists and is continuous;

It has been shown in Lemma 3.2.2 and Lemma 3.6.4 that our assumptions (H_1) of Lipschitz continuity properties and (H_2) of Hölder continuity properties for the functions f_i and F_i imply similar Lipschitz and Hölder continuity properties for the functions $\underline{f}_i$, $\bar{f}_i$, $\underline{F}_i$ and $\bar{F}_i$. It can also be shown that similar properties hold for our assumptions (H_7)-(H_8) of differentiability properties for the functions f_i and F_i.

Lemma 3.6.7

Suppose in addition to the assumptions of Lemma 3.6.6, that $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ *are minimal sequences and* $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ *are maximal sequences. Also, assume that for components* $i \in J$, *where* $\mathcal{D}_i = 0$, $u\cdot\nabla\bar{C}_i^{(k)}$, $u\cdot\nabla\underline{C}_i^{(k)} \not\equiv 0$, *that assumptions* ($H_7$)-($H_8$) *hold. Then*

$$\underset{\sim}{c}_i \le \underline{c}_i^{(0)} \le \underline{c}_i^{(1)} \le \ldots \le \underline{c}_i^{(k)} \le \bar{c}_i^{(k)} \le \ldots \le \bar{c}_i^{(1)} \le \bar{c}_i^{(0)} \le \tilde{c}_i \ \textit{for}\ (t, x, z) \in (0, T]\times\bar{\Omega}\times\Lambda,$$

$$\underset{\sim}{C}_i \le \underline{C}_i^{(0)} \le \underline{C}_i^{(1)} \le \ldots \le \underline{C}_i^{(k)} \le \bar{C}_i^{(k)} \le \ldots \le \bar{C}_i^{(1)} \le \bar{C}_i^{(0)} \le \tilde{C}_i \ \textit{for}\ (t, z) \in (0, T]\times\bar{\Lambda},$$

for all $k = 1,2,\ldots$ *and the pointwise limits*

$$\lim_{k\to\infty} (\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) = (\underline{c}_i, \underline{C}_i),$$

$$\lim_{k\to\infty} (\bar{c}_i^{(k)}, \bar{C}_i^{(k)}) = (\bar{c}_i, \bar{C}_i),$$

exist, implying that

$$\underset{\sim}{c}_i \le \underline{c}_i^{(0)} \le \underline{c}_i^{(1)} \le \ldots \le \underline{c}_i^{(k)} \ldots \le \underline{c}_i \le \bar{c}_i \ldots \le \bar{c}_i^{(k)} \le \ldots \le \bar{c}_i^{(1)} \le \bar{c}_i^{(0)} \le \tilde{c}_i \ \textit{for}\ (t, x, z) \in (0, T]\times\bar{\Omega}\times\Lambda,$$

$$\underset{\sim}{C}_i \le \underline{C}_i^{(0)} \le \underline{C}_i^{(1)} \le \ldots \le \underline{C}_i^{(k)} \le \ldots \le \underline{C}_i \le \bar{C}_i \le \ldots \le \bar{C}_i^{(k)} \le \ldots \le \bar{C}_i^{(1)} \le \bar{C}_i^{(0)} \le \tilde{C}_i \ \textit{for}\ (t, z) \in (0, T]\times\bar{\Lambda},$$

for all $k = 1,2,\ldots$

Proof

Let $(u_i, U_i) = (\bar{c}_i^{(0)} - \bar{c}_i^{(1)}, \bar{C}_i^{(0)} - \bar{C}_i^{(1)}) = (\tilde{c}_i - \bar{c}_i^{(1)}, \tilde{C}_i - \bar{C}_i^{(1)})$, for all i. Then by definition 3.6.1 of upper and lower solutions and definition 3.6.2 of maximal sequences, the following inequalities will hold

$$\frac{\partial u_i}{\partial t} - D_i\nabla_x^2 u_i = \frac{\partial \tilde{c}_i}{\partial t} - D_i\nabla_x^2\tilde{c}_i - f_i(t, x, \tilde{c}_j) \ge 0 \text{ in } (0, T]\times\Omega\times\Lambda,$$

$$D_i\frac{\partial u_i}{\partial n} + H_i u_i = D_i\frac{\partial}{\partial n}(\tilde{c}_i - \bar{c}_i^{(1)}) + H_i(\tilde{c}_i - \bar{c}_i^{(1)}) = D_i\frac{\partial \tilde{c}_i}{\partial n} + H_i(\tilde{c}_i - \tilde{C}_i) \ge 0 \text{ on } (0, T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial U_i}{\partial t} - \mathcal{D}_i\nabla^2 U_i + u\cdot\nabla U_i + H_i\mathcal{A}U_i = [\frac{\partial \tilde{C}_i}{\partial t} - \mathcal{D}_i\nabla^2\tilde{C}_i + u\cdot\nabla\tilde{C}_i + H_i\mathcal{A}\tilde{C}_i] - [F_i(t, z, \tilde{C}_j) + H_i\int_{\partial\Omega_2}\tilde{c}_i]$$
$$\ge 0 \text{ in } (0, T]\times\Lambda,$$

with similar inequalities holding in the boundary and initial conditions.

We first consider the case when D_j, $\mathcal{D}_j > 0$ for all j. We see that from Lemma 3.1.8 (Maximum Principle) for the parabolic operator that $(u_i, U_i) \ge 0$, i.e. $\bar{c}_i^{(0)} \ge \bar{c}_i^{(1)}$ on $(0, T]\times\bar{\Omega}\times\Lambda$ and $\bar{C}_i^{(0)} \ge \bar{C}_i^{(1)}$) on $(0, T]\times\bar{\Lambda}$.

This result also follows from the monotonicity of $\mathcal{T}$, since if $(\tilde{c}_i, \tilde{C}_i) \ge (\bar{c}_i^{(0)}, \bar{C}_i^{(0)})$, then $\mathcal{T}(\tilde{c}_i, \tilde{C}_i) \ge \mathcal{T}(\bar{c}_i^{(0)}, \bar{C}_i^{(0)}) = (\bar{c}_i^{(1)}, \bar{C}_i^{(1)})$ and $(\bar{c}_i^{(0)}, \bar{C}_i^{(0)}) \ge (\bar{c}_i^{(1)}, \bar{C}_i^{(1)})$ if we let $(\bar{c}_i^{(0)}, \bar{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$.

Therefore, from Lemma 3.6.5, we conclude that $\bar{c}_i^{(1)} \in C^{1+\alpha/2,2+\alpha,\alpha}[(0,T]\times\bar{\Omega}\times\Lambda, R^{n(I)}]$ and $\bar{C}_i^{(1)} \in C^{1+\alpha/2,2+\alpha}[(0,T]\times\bar{\Lambda}, R^{n(J)}]$.

By natural imbedding this implies that $\bar{c}_i^{(1)} \in C^{1,2,0}[(0,T]\times\bar{\Omega}\times\Lambda, R^{n(I)}]$ and $\bar{C}_i^{(1)} \in C^{1,2}[(0,T]\times\bar{\Lambda}, R^{n(J)}]$.

All the other possible cases are treated similarly so that

(i) For components $i \in I$, where $D_i = H_i = 0$, $\bar{c}_i^{(1)} \in C^{1,0,0}[(0,T]\times\bar{\Omega}\times\Lambda, R^{n(I)}]$,
(ii) For components $i \in J$, where $\mathcal{D}_i = 0$, $u\cdot\nabla\bar{C}_i^{(1)} \not\equiv 0$, $\bar{C}_i^{(1)} \in C^{1,1}[(0,T]\times\bar{\Lambda}, R^{n(J)}]$,
(iii) For components $i \in J$, where $\mathcal{D}_i = 0$, $u\cdot\nabla\bar{C}_i^{(1)} \equiv 0$, $\bar{C}_i^{(1)} \in C^{1,0}[(0,T]\times\bar{\Lambda}, R^{n(J)}]$.

In the case of (iii), we see that z is treated as a parameter. If (H_7)-(H_8) are assumed, it then follows from standard results on ordinary differential equations which depend on parameters (HARTMAN [119, p. 95-99] that $\bar{C}_i^{(1)}$ will be continuously differentiable in z. Therefore, if (H_7)-(H_8) are assumed then in all cases for components $j \in J$, $\bar{C}_j^{(1)}$ will be continuously differentiable in z. Furthermore, in all cases for components $i \in I$, where $D_i, H_i > 0$, it can be demonstrated from (3.6.10) that $\bar{c}_i^{(2)}$ will also be continuously differentiable in z.

We may similarly show using by the definitions of upper and lower solutions and of minimal sequences, that $\underline{c}_i^{(0)} \le \underline{c}_i^{(1)}$ and $\underline{C}_i^{(0)} \le \underline{C}_i^{(1)}$.

Now let $(u_i, U_i) = (\bar{c}_i^{(1)} - \underline{c}_i^{(1)}, \bar{C}_i^{(1)} - \underline{C}_i^{(1)})$. Then the monotone nondecreasing property of f_i and F_i implies that

$$\frac{\partial u_i}{\partial t} - D_i\nabla_x^2 u_i = f_i(t, x, \bar{c}_j^{(0)}) - f_i(t, x, \underline{c}_j^{(0)}) = f_i(t, x, \tilde{c}_j) - f_i(t, x, \underset{\sim}{c}_j) \ge 0 \text{ in } (0,T]\times\Omega\times\Lambda,$$

$$D_i\frac{\partial u_i}{\partial n} + H_i u_i = [D_i\frac{\partial \bar{c}_i^{(1)}}{\partial n} + H_i\bar{c}_i^{(1)}] - [D_i\frac{\partial \underline{c}_i^{(1)}}{\partial n} + H_i\underline{c}_i^{(1)}] = H_i(\bar{C}_i^{(0)} - \underline{C}_i^{(0)}) = H_i(\tilde{C}_i - \underset{\sim}{C}_i) \ge 0 \text{ on } (0,T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial U_i}{\partial t} - \mathcal{D}_i\nabla^2 U_i + u\cdot\nabla U_i + H_i\mathcal{A}U_i = F_i(t, z, \tilde{C}_j) - F_i(t, z, \underset{\sim}{C}_j) + H_i\int_{\partial\Omega_2}(\tilde{c}_i - \underset{\sim}{c}_i) \ge 0 \text{ in } (0,T]\times\Lambda,$$

and it follows from the monotonicity of $\mathcal{T}$, that

$$(\underline{c}_i^{(1)}, \underline{C}_i^{(1)}) \le (\bar{c}_i^{(1)}, \bar{C}_i^{(1)}),$$

implying that

$$\underset{\sim}{c}_i \le \underline{c}_i^{(0)} \le \underline{c}_i^{(1)} \le \bar{c}_i^{(1)} \le \bar{c}_i^{(0)} \le \tilde{c}_i \text{ for } (t, x, z) \in (0,T]\times\bar{\Omega}\times\Lambda,$$

and

$$\underset{\sim}{C}_i \le \underline{C}_i^{(0)} \le \underline{C}_i^{(1)} \le \bar{C}_i^{(1)} \le \bar{C}_i^{(0)} \le \tilde{C}_i \text{ for } (t, z) \in (0,T]\times\bar{\Lambda}.$$

Assume, by induction, that

$$\bar{c}_i^{(k)} \le \bar{c}_i^{(k-1)} \text{ and } \bar{C}_i^{(k)} \le \bar{C}_i^{(k-1)},$$

for $k=1,..,m$.

The only difficulty arises for components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla \overline{C}_i^{(k)} \neq 0$ and in this case we cannot assume that in general, that the assumption (H_6) will be satisfied. However, in this case we assume (H_7)-(H_8) hold so that $\overline{C}_j^{(k-1)}$ and $\overline{C}_j^{(k-2)}$ will be continuously differentiable in z for all j by earlier arguments. Thus for components $i \in I$, where $D_i, H_i > 0$, it can be shown that $c_i^{(k-1)}$ will be continuously differentiable in z from (3.6.10), so that by assumptions (H_7)-(H_8), $F_i(t, z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)}$ will be continuously differentiable in z. For components $i \in I$, where $D_i = H_i = 0$, we see that in this case by assumptions (H_7)-(H_8), $F_i(t, z, C_j^{(k-1)})$ will be continuously differentiable in z. It then follows that (HARTMAN [119, pp. 95-99]) assumption (H_6) will be satisfied in the general case.

The functions $(u_i, U_i) = (\overline{c}_i^{(m)} - \overline{c}_i^{(m+1)}, \overline{C}_i^{(m)} - \overline{C}_i^{(m+1)})$ and the monotone nondecreasing property of f_i and F_i implies that

$$\frac{\partial u_i}{\partial t} - D_i \nabla_x^2 u_i = f_i(t, x, \overline{c}_j^{(m-1)}) - f_i(t, x, \overline{c}_j^{(m)}) \geq 0 \text{ in } (0, T]\times\Omega\times\Lambda,$$

$$D_i \frac{\partial u_i}{\partial n} + H_i u_i = [D_i \frac{\partial \overline{c}_i^{(m)}}{\partial n} + H_i \overline{c}_i^{(m)}] - [D_i \frac{\partial \overline{c}_i^{(m+1)}}{\partial n} + H_i \overline{c}_i^{(m+1)}] = H_i(\overline{C}_i^{(m-1)} - \overline{C}_i^{(m)}) \geq 0 \text{ on } (0, T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial U_i}{\partial t} - \mathcal{D}_i \nabla^2 U_i + u\cdot\nabla U_i + H_i \mathcal{A} U_i = F_i(t, z, \overline{C}_j^{(m)}) - F_i(t, z, \overline{C}_j^{(m)}) + H_i \int_{\partial\Omega_2} (\overline{c}_i^{(m)} - \overline{c}_i^{(m)}) \geq 0 \text{ in } (0, T]\times\Lambda,$$

with similar inequalities in the boundary and initial conditions. This ensures that

$$\overline{c}_i^{(m)} \geq \overline{c}_i^{(m+1)} \text{ and } \overline{C}_i^{(m)} \geq \overline{C}_i^{(m+1)},$$

from the monotonicity of $\mathcal{T}$ and proves that $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ with $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$ is a monotonic nonincreasing sequence.

It follows from a similar induction argument that $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ is a monotonic nondecreasing sequence and by a similar induction argument $\overline{c}_i^{(k-1)} \geq \underline{c}_i^{(k-1)}$ and $\overline{C}_i^{(k-1)} \geq \underline{C}_i^{(k-1)}$ for k=1,...,m ensures that $\overline{c}_i^{(m+1)} \geq \underline{c}_i^{(m+1)}$ and $\overline{C}_i^{(m+1)} \geq \underline{C}_i^{(m+1)}$. The following inequalities then hold

$$\underset{\sim}{c}_i \leq \underline{c}_i^{(0)} \leq \underline{c}_i^{(1)} \leq ... \leq \underline{c}_i^{(k)} \leq \overline{c}_i^{(k)} \leq ... \leq \overline{c}_i^{(1)} \leq \overline{c}_i^{(0)} \leq \tilde{c}_i \text{ for } (t, x, z) \in (0, T]\times\overline{\Omega}\times\Lambda,$$

$$\underset{\sim}{C}_i \leq \underline{C}_i^{(0)} \leq \underline{C}_i^{(1)} \leq ... \leq \underline{C}_i^{(k)} \leq \overline{C}_i^{(k)} \leq ... \leq \overline{C}_i^{(1)} \leq \overline{C}_i^{(0)} \leq \tilde{C}_i \text{ for } (t, z) \in (0, T]\times\overline{\Lambda},$$

for all k = 1,2,...

It follows from the monotonic property of our maximal and minimal sequences, its boundedness by $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ and the monotone convergence theorem that the pointwise limits

$$\lim_{k\to\infty} (\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) = (\underline{c}_i, \underline{C}_i),$$

$$\lim_{k\to\infty} (\overline{c}_i^{(k)}, \overline{C}_i^{(k)}) = (\overline{c}_i, \overline{C}_i),$$

exist, implying that

$$\underset{\sim}{c}_i \leq \underline{c}_i^{(0)} \leq \underline{c}_i^{(1)} \leq ... \leq \underline{c}_i^{(k)} ... \leq \underline{c}_i \leq \overline{c}_i ... \leq \overline{c}_i^{(k)} \leq ... \leq \overline{c}_i^{(1)} \leq \overline{c}_i^{(0)} \leq \tilde{c}_i \textit{ for } (t, x, z) \in (0, T]\times\overline{\Omega}\times\Lambda,$$

$$\underset{\sim}{C}_i \leq \underline{C}_i^{(0)} \leq \underline{C}_i^{(1)} \leq ... \leq \underline{C}_i^{(k)} \leq ... \leq \underline{C}_i \leq \overline{C}_i \leq ... \leq \overline{C}_i^{(k)} \leq ... \leq \overline{C}_i^{(1)} \leq \overline{C}_i^{(0)} \leq \tilde{C}_i \textit{ for } (t, z) \in (0, T]\times\overline{\Lambda},$$

for all k = 1,2,...□

3.6.3 Existence of Solutions

It can be shown that our minimal and maximal sequences $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ converge not only pointwise but converge uniformly (in appropriate function spaces) as well. The following theorem is an existence theorem for solutions to the system S_n, B_n.

Theorem 3.6.1 (Generalised Existence Theorem)

Let the assumptions of Lemma 3.6.7 hold. Then the minimal and maximal sequences $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ converge monotonically and uniformly from below and above to $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ respectively, where $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are solutions of S_n, B_n. Moreover $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are minimal and maximal solutions respectively of S_n, B_n in the regions $[\underline{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$ and by uniqueness $(\underline{c}_i, \underline{C}_i)\equiv(\overline{c}_i, \overline{C}_i)$.

Proof

We first consider the case with D_i, $\mathfrak{D}_i > 0$ for all i.

Let $\underline{c}_i^{(k)}, \overline{c}_i^{(k)} \in C^{1+\alpha/2,2+\alpha,\alpha}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\underline{C}_i^{(k)}, \overline{C}_i^{(k)} \in C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ for $k = 1,2,...$ and let us consider the maximal sequence $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$.

We note that $C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Omega}, R^{n(I)}]\subseteq W_{p_1}^{1,2}[(0, T]\times\overline{\Omega}, R^{n(I)}]$ and $C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]\subseteq W_{p_2}^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ for $p_1 \geq (m_1+2)/(1-\alpha)$ and $p_2 \geq (m_2+2)/(1-\alpha)$.

From Lemma 3.1.1, this implies that $C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Omega}, R^{n(I)}]\subseteq W_q^{1,2}[(0, T]\times\overline{\Omega}, R^{n(I)}]$ and $C^{1+\alpha/2,2+\alpha}[(0, T]\times\overline{\Lambda}, R^{n(J)}]\subseteq W_q^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$, where $q = \min\{p_1, p_2\}$.

By Theorem 3.1.4, we see that $\overline{c}_i^{(k)}$ (with Λ treated as a parameter space) and $\overline{C}_i^{(k)}$ satisfy the following Agmon-Douglis-Nirenberg estimates (see Theorem 3.1.5):

$$\begin{aligned}\|\overline{c}_i^{(k)}\|_{W_q^{1,2}[(0,T]\times\overline{\Omega},R^{n(I)}]} \leq C(&\|f_i(t, x, \overline{c}_j^{(k-1)})\|_{L^q[(0,T]\times\overline{\Omega},R^{n(I)}]}\\ &+ \|\overline{C}_i^{(k-1)}\|_{W_q^{1/2-1/2q,1-1/q}[(0,T]\times\partial\Omega_1,R^{n(I)}]}\\ &+ \|c_{i,0}\|_{W_q^{2-2/q}[\overline{\Omega},R^{n(I)}]}),\end{aligned} \tag{3.6.63}$$

and

$$\begin{aligned}\|\overline{C}_i^{(k)}\|_{W_q^{1,2}[(0,T]\times\overline{\Lambda},R^{n(J)}]} \leq C(&\|F_i(t, z, \overline{C}_j^{(k-1)}) + \int_{\partial\Omega_2}\overline{c}_i^{(k-1)}\|_{L^q[(0,T]\times\overline{\Lambda},R^{n(J)}]}\\ &+ \|C_{i,1}\|_{W_q^{1/2-1/2q,1-1/q}[(0,T]\times\partial\Lambda_1,R^{n(J)}]}\\ &+ \|C_{i,0}\|_{W_q^{2-2/q}[\overline{\Lambda},R^{n(J)}]}).\end{aligned} \tag{3.6.64}$$

The fact that $\overline{c}_j^{(k-1)}\in [\underline{c}_j, \tilde{c}_j]$ and $\overline{C}_j^{(k-1)}\in [\underset{\sim}{C}_j, \tilde{C}_j]$, i.e., $\overline{c}_j^{(k-1)}$ and $\overline{C}_j^{(k-1)}$ are bounded, the continuity of f_i and of F_i imply by the continuity and boundedness of the Nemytskii operator (Lemma 3.1.6) that the sequences $\{f_i(t, x, \overline{c}_j^{(k-1)})\}$ and $\{F_i(t, z, \overline{C}_j^{(k-1)})+\int_{\partial\Omega_2}\overline{c}_i^{(k-1)}\}$ are uniformly bounded in $C[(0, T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ respectively.

Since $C[(0, T]\times\overline{\Omega}, R^{n(I)}]$ and $C[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ are dense in $L^q[(0, T]\times\overline{\Omega}, R^{n(I)}]$ and $L^q[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ respectively, it follows by the continuity and boundedness of the Nemytskii operator (Lemma 3.1.7) that $\{f_i(t, x, \overline{c}_j^{(k-1)})\}$ and $\{F_i(t, z, \overline{C}_j^{(k-1)})+\int_{\partial\Omega_2}\overline{c}_i^{(k-1)}\}$ are bounded sequences in $L^q[(0, T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $L^q[(0, T]\times\overline{\Lambda}, R^{n(J)}]$, respectively.

This, together with the above estimates (3.6.63) and (3.6.64) shows that the sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ are uniformly bounded in $W_q^{1,2}[(0, T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and

$W_q^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ respectively. Therefore by application of Theorem 3.1.1 (Imbedding Theorem), we obtain

$$\|\overline{c}_i^{(k)}\|_{C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]} \le C\|\overline{c}_i^{(k)}\|_{W_q^{1,2}[(0,T]\times\overline{\Omega}, R^{n(I)}]}, \tag{3.6.65}$$

and

$$\|\overline{C}_i^{(k)}\|_{C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]} \le C\|\overline{C}_i^{(k)}\|_{W_q^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]}, \tag{3.6.66}$$

for all $k = 1,2,..,$ where C in both estimates are independent of any element of $W_q^{1,2}[(0,T]\times\overline{\Omega}, R^{n(I)}]$ or $W_q^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$.

From (3.6.65) and (3.6.66), we can conclude that every uniformly bounded sequence in $W_q^{1,2}[(0,T]\times\overline{\Omega}, R^{n(I)}]$ and $W_q^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ is also uniformly bounded in $C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$, respectively. From Lemma 3.1.3, we may take α in both cases to be identical.

Thus the sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ are uniformly bounded in $C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ respectively. Therefore, by applying Lemma 3.1.6, $\{f_i(t,x,\overline{c}_j^{(k-1)})\}$ and $\{F_i(t,z,\overline{C}_j^{(k-1)})+\int_{\partial\Omega_2}\overline{c}_i^{(k-1)}\}$ are also bounded sequences in $C^{\alpha/2,\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{\alpha/2,\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$, respectively. Hence by the Schauder type estimates (Theorem 3.1.3), we have

$$\|\overline{c}_i^{(k)}\|_{C^{1+\alpha/2,2+\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]} \le C(\|f_i(t,x,\overline{c}_j^{(k-1)})\|_{C^{\alpha/2,\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]} + \|\overline{C}_i^{(k-1)}\|_{C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\partial\Omega_1, R^{n(I)}]} + \|c_{i,0}\|_{C^{2+\alpha}[\overline{\Omega}, R^{n(I)}]}) \tag{3.6.67}$$

and

$$\|\overline{C}_i^{(k)}\|_{C^{1+\alpha/2,2+\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]} \le C(\|F_i(t,z,\overline{C}_j^{(k-1)})+\int_{\partial\Omega_2}\overline{c}_i^{(k-1)}\|_{C^{\alpha/2,\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]} + \|C_{i,1}\|_{C^{(1+\alpha)/2,1+\alpha}[(0,T]\times\partial\Lambda_1, R^{n(J)}]} + \|C_{i,0}\|_{C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]}) \tag{3.6.68}$$

for all $k = 1,2,..,$ which implies the uniform boundedness of sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ in $C^{1+\alpha/2,2+\alpha}[(0,T]\times\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{1+\alpha/2,2+\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$, respectively.

We may use arguments given in Lemma 3.6.5 to show that sequences $\{\overline{c}_i^{(k)}\}$ are Hölder continuous in z with exponent α and may be shown to be uniformly bounded in Λ.

Therefore, by the natural compact imbedding of $C^{1+\alpha/2,2+\alpha,\alpha}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1+\alpha/2,2+\alpha}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ into $C^{1,2,0}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$, the sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ are relatively compact in $C^{1,2,0}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ respectively.

This implies that there exists subsequences of $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ which converge in $C^{1,2,0}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ respectively.

Let $(\overline{\overline{c}}_i, \overline{\overline{C}}_i)$ where $\overline{\overline{c}}_i\in C^{1,2,0}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\overline{\overline{C}}_i\in C^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ be the limit of this subsequence.

On the other hand, we have shown that the sequence $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ converges pointwise to $(\overline{c}_i, \overline{C}_i)$. Therefore, $\overline{\overline{c}}_i = \overline{c}_i$ on $[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\overline{\overline{C}}_i = \overline{C}_i$ on $[(0,T]\times\overline{\Lambda}, R^{n(J)}]$. This shows that the whole sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ converge in $C^{1,2,0}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ to $\overline{c}_i$ and $\overline{C}_i$ respectively, that is $\lim_{k\to\infty}\overline{c}_i^{(k)} = \overline{c}_i$ in $C^{1,2,0}[(0,T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\lim_{k\to\infty}\overline{C}_i^{(k)} = \overline{C}_i$ in $C^{1,2}[(0,T]\times\overline{\Lambda}, R^{n(J)}]$ and $\underset{\sim}{c}_i \le \overline{c}_i \le \tilde{c}_i$ on $[0,T]\times\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_i \le \overline{C}_i \le \tilde{C}_i$ on $[0,T]\times\overline{\Lambda}$.

Similarly, by imitating the preceding argument relative to the minimal sequence $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$, one can conclude that the sequences $\{\underline{c}_i^{(k)}\}$ and $\{\underline{C}_i^{(k)}\}$ converge monotonically in $C^{1,2,0}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ respectively; their limits are denoted by $\underline{c}_i$ and $\underline{C}_i$ which belongs to $C^{1,2,0}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$ respectively and satisfy the relation $\hat{c}_i \le \underline{c}_i \le \tilde{c}_i$ on $[0, T]\times\overline{\Omega}\times\Lambda$ and $\hat{C}_i \le \underline{C}_i \le \tilde{C}_i$ on $[0, T]\times\overline{\Lambda}$. Thus the limits

$$\lim_{k\to\infty}\left[\frac{\partial \underline{c}_i^{(k)}}{\partial t} - D_i\nabla_x^2\underline{c}_i^{(k)}\right] = \frac{\partial \underline{c}_i}{\partial t} - D_i\nabla_x^2\underline{c}_i, \quad \lim_{k\to\infty}[f_i(t, x, \underline{c}_j^{(k-1)})] = f_i(t, x, \underline{c}_j),$$

$$\lim_{k\to\infty}\left[D_i\frac{\partial \underline{c}_i^{(k)}}{\partial n} + H_i\underline{c}_i^{(k)}\right] = D_i\frac{\partial \underline{c}_i}{\partial n} + H_i\underline{c}_i, \quad \lim_{k\to\infty}[H_i\underline{C}_i^{(k-1)}] = H_i\underline{C}_i,$$

$$\lim_{k\to\infty}\left[\frac{\partial \underline{C}_i^{(k)}}{\partial t} - \mathcal{D}_i\nabla^2\underline{C}_i^{(k)} + u\cdot\nabla\underline{C}_i^{(k)} + H_i\mathcal{A}\underline{C}_i^{(k)}\right] = \frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2\underline{C}_i + u\cdot\nabla\underline{C}_i + H_i\mathcal{A}\underline{C}_i,$$

$$\lim_{k\to\infty}\left[F_i(t, z, \underline{C}_j^{(k-1)}) + H_i\int_{\partial\Omega_2}\underline{c}_i^{(k-1)}\right] = F_i(t, z, \underline{C}_j) + H_i\int_{\partial\Omega_2}\underline{c}_i$$

and

$$\lim_{k\to\infty}\left[\frac{\partial \overline{c}_i^{(k)}}{\partial t} - D_i\nabla_x^2\overline{c}_i^{(k)}\right] = \frac{\partial \overline{c}_i}{\partial t} - D_i\nabla_x^2\overline{c}_i, \quad \lim_{k\to\infty}[f_i(t, x, \overline{c}_j^{(k-1)})] = f_i(t, x, \overline{c}_j),$$

$$\lim_{k\to\infty}\left[D_i\frac{\partial \overline{c}_i^{(k)}}{\partial n} + H_i\overline{c}_i^{(k)}\right] = D_i\frac{\partial \overline{c}_i}{\partial n} + H_i\overline{c}_i, \quad \lim_{k\to\infty}[H_i\overline{C}_i^{(k-1)}] = H_i\overline{C}_i,$$

$$\lim_{k\to\infty}\left[\frac{\partial \overline{C}_i^{(k)}}{\partial t} - \mathcal{D}_i\nabla^2\overline{C}_i^{(k)} + u\cdot\nabla\overline{C}_i^{(k)} + H_i\mathcal{A}\overline{C}_i^{(k)}\right] = \frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2\overline{C}_i + u\cdot\nabla\overline{C}_i + H_i\mathcal{A}\overline{C}_i,$$

$$\lim_{k\to\infty}\left[F_i(t, z, \overline{C}_j^{(k-1)}) + H_i\int_{\partial\Omega_2}\overline{c}_i^{(k-1)}\right] = F_i(t, z, \overline{C}_j) + H_i\int_{\partial\Omega_2}\overline{c}_i,$$

etc. exist uniformly on $C^{1,2,0}[(0, T]\times\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{1,2}[(0, T]\times\overline{\Lambda}, R^{n(J)}]$, respectively. Thus we conclude that $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are solutions of the IBVP

$$\frac{\partial \underline{c}_i}{\partial t} - D_i\nabla_x^2\underline{c}_i = f_i(t, x, \underline{c}_j),$$

$$D_i\frac{\partial \underline{c}_i}{\partial n} + H_i\underline{c}_i = H_i\underline{C}_i,$$

$$\frac{\partial \underline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2\underline{C}_i + u\cdot\nabla\underline{C}_i + H_i\mathcal{A}\underline{C}_i = F_i(t, z, \underline{C}_j) + H_i\int_{\partial\Omega_2}\underline{c}_i,$$

and

$$\frac{\partial \overline{c}_i}{\partial t} - D_i\nabla_x^2\overline{c}_i = f_i(t, x, \overline{c}_j),$$

$$D_i\frac{\partial \overline{c}_i}{\partial n} + H_i\overline{c}_i = H_i\overline{C}_i,$$

$$\frac{\partial \overline{C}_i}{\partial t} - \mathcal{D}_i\nabla^2\overline{C}_i + u\cdot\nabla\overline{C}_i + H_i\mathcal{A}\overline{C}_i = F_i(t, z, \overline{C}_j) + H_i\int_{\partial\Omega_2}\overline{c}_i,$$

respectively.

We therefore have that $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are solutions of S_n, B_n.

For components $i \in I$, where $D_i = H_i = 0$, the uniform convergence of sequences $\{c_i^{(k)}\}$ to solutions $\underline{c}_i$ and $\bar{c}_i$ is standard (HARTMAN [119], LAKSHIMIKANTHAM [157]). The sequence of approximations (3.6.8) are uniformly bounded and equicontinuous and hence possesses uniformly convergent subsequences. The rest of the argument follows along similar lines to that already discussed. The case for components $i \in J$, where $\mathcal{D}_i = 0$ and $u \cdot \nabla C_i^{(k)} \equiv 0$ is similar as is the case for components $i \in J$, where $\mathcal{D}_i = 0$ and $u \cdot \nabla C_i^{(k)} \not\equiv 0$.

Now we show that $(\underline{c}_i, \underline{C}_i)$ and $(\bar{c}_i, \bar{C}_i)$ are minimal and maximal solutions of S_n, B_n. Let (c_i, C_i) be any solution of S_n, B_n such that $\underline{c}_i \leq c_i \leq \tilde{c}_i$ and $\underset{\sim}{C}_i \leq C_i \leq \tilde{C}_i$.

Since $(c_i, C_i) = \mathcal{K}(c_i, C_i)$, it follows by Lemma 3.6.6 and from the definitions of $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$, that

$$(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i) \leq (c_i, C_i) \leq (\tilde{c}_i,\ \tilde{C}_i),$$

implies that

$$(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i) \leq \mathcal{T}(\underline{c}_i^{(0)},\ \underline{C}_i^{(0)}) \leq (c_i, C_i) = \mathcal{K}(c_i, C_i) \leq \mathcal{T}(\bar{c}_i^{(0)},\ \bar{C}_i^{(0)}) \leq (\tilde{c}_i,\ \tilde{C}_i).$$

Let us assume that for some $m > 1$,

$$(\underline{c}_i^{(m)},\ \underline{C}_i^{(m)}) \leq (c_i, C_i) = (\bar{c}_i^{(m)},\ \bar{C}_i^{(m)}).$$

Then we shall show that

$$(\underline{c}_i^{(m+1)},\ \underline{C}_i^{(m+1)}) \leq (c_i, C_i) = (\bar{c}_i^{(m+1)},\ \bar{C}_i^{(m+1)}).$$

From Lemma 3.6.6 (II) and from the definitions of $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$, we arrive at

$$(\underline{c}_i^{(m+1)},\ \underline{C}_i^{(m+1)}) = \mathcal{T}(\underline{c}_i^{(m)},\ \underline{C}_i^{(m)}) \leq (c_i, C_i) = \mathcal{K}(c_i, C_i) \leq \mathcal{T}(\bar{c}_i^{(m)},\ \bar{C}_i^{(m)}) = (\bar{c}_i^{(m+1)},\ \bar{C}_i^{(m+1)}).$$

Thus, it follows by mathematical induction that

$$(\underline{c}_i^{(k)},\ \underline{C}_i^{(k)}) \leq (c_i, C_i) = (\bar{c}_i^{(k)},\ \bar{C}_i^{(k)}),$$

for all $k = 1,2,\ldots$

Hence, we have

$$(\underline{c}_i,\ \underline{C}_i) \leq (c_i, C_i) \leq (\bar{c}_i,\ \bar{C}_i),$$

proving that $(\underline{c}_i, \underline{C}_i)$ and $(\bar{c}_i, \bar{C}_i)$ are minimal and maximal solutions of S_n, B_n.

Finally, by uniqueness results demonstrated in section 3.3, $(\underline{c}_i, \underline{C}_i) \equiv (\bar{c}_i, \bar{C}_i)$.□

For the general system S_n, B_n, which may possess no monotone properties, the following theorem follows from Theorem 3.4.1 and summarises how we may set up monotone sequences for this general system which converges to a solution of a new system which relates in some way to the solution of the original system S_n, B_n.

Theorem 3.6.2

The general system S_n, B_n for which f_i and F_i satisfies Lipschitz continuity properties (H_1) and Hölder continuity properties (H_2), may be imbedded in a system S_{2n}^*, B_{2n}^* of twice the order which is coupled by monotone functions f_i^* and F_i^* of the new dependent variables v_i and V_i. Moreover, all the solutions (c_i, C_i) of the general system S_n, B_n are solutions of the new system, where

$$v_i = c_i, \quad v_{n(I)+i} = -c_i \quad \text{for } i=1,..,n(I) \tag{3.6.69}$$

and

$$V_i = C_i,\ V_{n(J)+i} = -C_i \quad \text{for } i=1,..,n(J). \tag{3.6.70}$$

Let $(\underset{\sim}{v}_i, \underset{\sim}{V}_i)$ and $(\tilde{v}_i, \tilde{V}_i)$ *be lower and upper solutions for the system S_{2n}^*, B_{2n}^* with continuity properties given in the assumptions of Lemma 3.6.6. Let also the assumptions of Lemma 3.6.7 hold for the system S_{2n}^*, B_{2n}^*. Then the minimal and maximal sequences $\{(\underline{v}_i^{(k)}, \underline{V}_i^{(k)})\}$ and $\{(\overline{v}_i^{(k)}, \overline{V}_i^{(k)})\}$ of S_{2n}^*, B_{2n}^* given by Theorem 3.6.1 converge monotonically and uniformly from below and above to $(\underline{v}_i, \underline{V}_i)$ and $(\overline{v}_i, \overline{V}_i)$ respectively, where $(\underline{v}_i, \underline{V}_i)$ and $(\overline{v}_i, \overline{V}_i)$ are solutions of S_{2n}^*, B_{2n}^* satisfying the following inequalitites*

$$\underset{\sim}{v}_i \le \underline{v}_i^{(0)} \le \underline{v}_i^{(1)} \le \ldots \le \underline{v}_i^{(k)} \ldots \le \underline{v}_i \le \overline{v}_i \ldots \le \overline{v}_i^{(k)} \le \ldots \le \overline{v}_i^{(1)} \le \overline{v}_i^{(0)} \le \tilde{v}_i \quad \text{for } (t, x, z) \in (0, T] \times \overline{\Omega} \times \Lambda, \tag{3.6.71}$$

$$\underset{\sim}{V}_i \le \underline{V}_i^{(0)} \le \underline{V}_i^{(1)} \le \ldots \le \underline{V}_i^{(k)} \le \ldots \le \underline{V}_i \le \overline{V}_i \le \ldots \le \overline{V}_i^{(k)} \le \ldots \le \overline{V}_i^{(1)} \le \overline{V}_i^{(0)} \le \tilde{V}_i \quad \text{for } (t, z) \in (0, T] \times \overline{\Lambda}, \tag{3.6.72}$$

for all k = 1,2,...

Moreover, $(\underline{v}_i, \underline{V}_i) \equiv (\overline{v}_i, \overline{V}_i) \equiv (v_i, V_i)$ by uniqueness and all solutions (v_i, V_i) of S_{2n}^*, B_{2n}^* for which

$$w_i = v_i + v_{n(I)+i} = 0 \ \text{in } \Omega \times \Lambda, \text{ at } t = 0, \tag{3.6.73}$$

$$W_i = V_i + V_{n(J)+i} = 0 \ \text{in } \Lambda, \text{ at } t=0, \tag{3.6.74}$$

$$\frac{\partial w_i}{\partial t} - D_i \nabla_x^2 w_i = f_i^*(t, x, v_j) + f_{n(I)+i}^*(t, x, v_k) \ \text{in } (0, T] \times \Omega \times \Lambda, \tag{3.6.75}$$

$$\frac{\partial w_i}{\partial n} = 0 \ \text{on } (0, T] \times \partial\Omega_1 \times \Lambda, \tag{3.6.76}$$

$$D_i \frac{\partial w_i}{\partial n} - H_i (W_i - w_i) = 0 \ \text{on } (0, T] \times \partial\Omega_2 \times \Lambda, \tag{3.6.77}$$

$$\frac{\partial W_i}{\partial t} - \mathcal{D}_i \nabla_x^2 W_i + u \cdot \nabla W_i = F_i^*(t, z, V_j) + F_{n(J)+i}^*(t, z, V_k) - H_i \int_{\partial\Omega_2} (W_i - w_i) \ \text{in } (0, T] \times \Lambda, \tag{3.6.78}$$

$$\upsilon_1 W_i + \mathcal{D}_i \frac{\partial W_i}{\partial n_1} = 0 \ \text{on } (0, T] \times \partial\Lambda_1, \tag{3.6.79}$$

$$\frac{\partial W_i}{\partial n_\alpha} = 0 \ \text{on } (0, T] \times \partial\Lambda_\alpha,\ \alpha = 2, 3, \tag{3.6.80}$$

for $(w_i, W_i) = (v_i + v_{n(I)+i}, W_i + W_{n(J)+i})$ generates the unique solution $(\underline{c}_i, \underline{C}_i) \equiv (\overline{c}_i, \overline{C}_i) \equiv (c_i, C_i)$ of the general system S_n, B_n, where

$$\underset{\sim}{v}_i \le \underline{v}_i^{(0)} \le \underline{v}_i^{(1)} \le \ldots \le \underline{v}_i^{(k)} \ldots \le \underline{v}_i \le c_i \le \overline{v}_i \ldots \le \overline{v}_i^{(k)} \le \ldots \le \overline{v}_i^{(1)} \le \overline{v}_i^{(0)} \le \tilde{v}_i\,,$$

$$\underset{\sim}{v}_{n(I)+i} \le \underline{v}_{n(I)+i}^{(0)} \le \underline{v}_{n(I)+i}^{(1)} \le \ldots \le \underline{v}_{n(I)+i}^{(k)} \ldots \le \underline{v}_{n(I)+i} \le -c_i \le \overline{v}_{n(I)+i} \ldots \le \overline{v}_{n(I)+i}^{(k)} \le \ldots \le \overline{v}_{n(I)+i}^{(1)} \le \overline{v}_{n(I)+i}^{(0)} \le \tilde{v}_{n(I)+i}\,,$$

for $(t, x, z) \in (0, T] \times \overline{\Omega} \times \Lambda$,

$$\underset{\sim}{V}_i \le \underline{V}_i^{(0)} \le \underline{V}_i^{(1)} \le \ldots \le \underline{V}_i^{(k)} \le \ldots \le \underline{V}_i \le C_i \le \overline{V}_i \le \ldots \le \overline{V}_i^{(k)} \le \ldots \le \overline{V}_i^{(1)} \le \overline{V}_i^{(0)} \le \tilde{V}_i\,,$$

$$\underset{\sim}{V}_{n(J)+i} \le \underline{V}_{n(J)+i}^{(0)} \le \underline{V}_{n(J)+i}^{(1)} \le \ldots \le \underline{V}_{n(J)+i}^{(k)} \le \ldots \le \underline{V}_{n(J)+i} \le -C_i \le \overline{V}_{n(J)+i} \le \ldots \le \overline{V}_{n(J)+i}^{(k)} \le \ldots \le \overline{V}_{n(J)+i}^{(1)} \le \overline{V}_{n(J)+i}^{(0)} \le \tilde{V}_{n(J)+i}\,,$$

for $(t, z) \in (0, T] \times \overline{\Lambda}$, *for all* $k = 1,2,\ldots$

We have shown in this section that if the reaction functions obey a monotone property, our sequence of approximate solutions is a monotone sequence that converges uniformly and thus our limit function is actually a solution of the given problem.

Although a number of existence-comparison theorems for weakly coupled parabolic systems have also been known and can be established by various other methods such as the functional analytic approach of KUIPER [149] and in connection with invariant sets (BEBERNES *et al.* [35-37]), the monotone argument is more constructive and provides a simpler and straightforward proof than the other methods. The definition of upper and lower solutions with the monotone argument is however more restrictive (BEBERNES and SCHMITT [37]). It must be noted that it is also not the only way of obtaining a constructive existence proof. Our existence theorem in this section relies on solving quasilinear parabolic differential equations by monotone iteration. The iteration could alternatively have been done by successively applying a monotone integral operator with an appropriate Green's function as its kernel. This procedure also starts with a lower and an upper solution (BANGE [33]). Furthermore, these same approaches can be used to obtain a similar existence-comparison theorem for the time independent problem simply by dropping the time derivatives and the initial conditions. This will be discussed in a chapter four when dealing with the existence of a steady state solution.

Remark 3.6.7

In many cases, we will require for practical reasons that the functions f_i and F_i be redefined for $c_j, C_j < 0$ so that if

$$f_i^+(t, x, c_j) = \begin{cases} f_i(t, x, c_j) & \text{for } c_j \ge 0 \\ f_i(t, x, 0) & \text{for } c_j < 0, \end{cases}$$

and

$$F_i^+(t, z, C_j) = \begin{cases} F_i(t, z, C_j) & \text{for } C_j \ge 0 \\ F_i(t, z, 0) & \text{for } C_j < 0, \end{cases}$$

then it can be shown that these new functions have the same Lipschitz and Hölder continuity properties as our original functions f_i and F_i.

Remark 3.6.8

In this section we have shown that the imbedding results of section 3.4 may be used to obtain existence theorems for systems of equations with nonmonotone reaction functions. The imbedding results do not need boundedness nor does it need the additional Hölder continuity properties that we have assumed for our system. This additional continuity property was only needed in order to establish the existence of solutions of a corresponding linear system.

Suppose we prove that any solution of the system S_n, B_n must be bounded by some constant K. Change then the definitions of $f_i(t, x, c_j)$ and $F_i(t, z, C_j)$ for $|c_j|, |C_j| > K$, for instance by defining

$$\hat{f}_i(t, x, c_j) = \begin{cases} f_i(t, x, c_j) & \text{for } |c_j| \leq K \\ f_i(t, x, \pm K) & \text{for } \pm c_j > K, \end{cases}$$

and

$$\hat{F}_i(t, z, C_j) = \begin{cases} F_i(t, z, C_j) & \text{for } |C_j| \leq K \\ F_i(t, z, \pm K) & \text{for } \pm C_j > K. \end{cases}$$

If we are then able to prove the existence of a solution (c_i, C_j) for the problem S_n, B_n with $\hat{f}_i(t, x, c_j)$ and $\hat{F}_i(t, z, C_j)$ given above, then (c_i, C_j) is also a solution of the original problem S_n, B_n. The same is true of uniqueness. We also note that these new functions satisfy the same Hölder continuity properties that are required in section 3.6, as our original functions. It is common to use functions such as these new functions for proving uniqueness and existence theorems given that we have upper and lower bounds particularly for functional analytic existence proofs (FRIEDMAN [94, p.203], BEBERNES and SCHMITT [35], LADDE *et. al.* [153]). These bounds do not necessarily have to be constants K as in the above equations but may be arbitrary functions with the appropriate continuity conditions.

Remark 3.6.9

We can choose

$$\underset{\sim}{c}_i = \underset{\sim}{C}_i = -Ae^{Rt}$$

and

$$\tilde{c}_i = \tilde{C}_i = Ae^{Rt},$$

where A is a constant determined from the boundary conditions and R is, as yet an unspecified constant so that

$$-ARe^{Rt} - f_i(t, x, -Ae^{Rt}) \leq 0,$$

$$ARe^{Rt} - f_i(t, x, -Ae^{Rt}) \geq 0,$$

$$-ARe^{Rt} - F_i(t, z, -Ae^{Rt}) \leq 0,$$

$$ARe^{Rt} - F_i(t, z, -Ae^{Rt}) \geq 0,$$

and we can easily satisfy the above inequality since f_i and F_i are Lipschitz in c_j and C_j, respectively by choosing R sufficiently large. This demonstrates the existence of suitable lower and upper solutions $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ respectively.

Remark 3.6.10

The constructive methods of proving existence results for problems in this section can also provide numerical procedures for the computation of solutions which are of greater practical value than the theoretical existence results. By replacing the differential system by a suitable finite difference system (which is a discrete version of the continuous problem) and using an analogous definition of upper and lower solutions, it is possible to construct monotone sequences which converge monotonically to a solution of the finite difference problem (GROSSMAN [111], GROSSMAN and ROOS [110], PAO [219-222]).

The asymptotic stability and multiple steady states may also be studied in the framework of this finite difference system (PAO [222]) as well as error estimates between the true solution and the computed mth iteration (PAO[221]). It is obvious that these numerical procedures may be applied to the system S_n, B_n which may obey no monotone property. The discretised functional term in (3.6.12) is expressed as a summation.

From the type of nonlinearities f_i and F_i, an iterative scheme may be considered which accelerates the rate of convergence of the sequences of iterates defined in (3.6.8)-(3.6.15). This involves solving coupled systems of linear equations and thus fewer equations (LADDE [153, p.171]). It is useful in speeding up numerical convergence. An example of another process which is useful in speeding up numerical convergence will be seen in section 6.3.

Remark 3.6.11
Equations S_n, B_n have been chosen with bioreactor applications in mind, but the theory can be readily generalised in a number of ways. Our proofs are still valid for $D_i\nabla_x^2 c_i$ replaced by $\nabla_x \cdot (D_i(x, c_i)\nabla_x c_i)$ and $\mathcal{D}_i\nabla^2 C_i$ replaced by $\nabla \cdot (\mathcal{D}_i(z, C_i)\nabla C_i)$, provided that we have uniform ellipticity conditions for these more general equations. Furthermore, the mass transfer coefficients H_i could be functions of x and t, provided that these functions are still positive and satisfy appropriate continuity properties, and a wider class of coupling functions is permissible, since f_i and F_i may be permitted to depend on ∇c_i and ∇C_i, respectively. However, it is necessary to require a Nagumo type growth condition with respect to these variables.

Remark 3.6.12
In this section we have assumed that the boundary conditions (2.1.4) and (2.1.7) are of the Robin type. We may treat the Neumann and Dirichlet type boundary conditions similarly by using appropriate theorems for linear parabolic equations with Neumann and Dirichlet type boundary conditions (see Remark 3.1.2 and Remark 3.1.3).

3.7 Notes and Comments

Sections 3.3-3.5 are adapted from PARSHOTAM, MCNABB and WAKE [228] and MCNABB and PARSHOTAM [188]. However, most of the proofs for Comparison Theorems in these papers are obtained in a different manner and order.

We see from the imbedding results of section 3.4, that many results for monotone systems may be applied to systems which obey no monotone property. Since existence of solutions in our imbedded system (which obeys a monotone property) implies existence of solutions in our original system (which may not obey any monotone property) and vice versa, so does many qualitative properties of solutions. We have seen from section 3.4 and 3.5 that uniqueness and global stability may be such properties. There are also many other qualitative properties such as bounds, gradient bounds and asymptotic stability which give rise to these properties from one system to the other. We have seen from Theorem 3.6.2 that bounds on the solution in our imbedded system can give rise to bounds in our original system (it is noted however, that upper and lower bounds need not exist in order for the imbedding results to apply). From these bounds it can be shown that asymptotic stability of the solution in our imbedded system also implies asymptotic stability for solutions of our original system. Other properties of solutions which give rise to these same properties from one system to another are perturbation solutions. It is often easier to obtain a perturbation solution for systems where the nonlinearities obey a monotone property (see section 6.5). This could be useful in parameter sensitivity analysis in systems of equations which do not obey a monotone property.

There are many useful qualitative properties of scalar parabolic and elliptic equations which rely on the monotonicity of the nonlinear reaction functions. Some of these properties may be generalised to monotone systems. The imbedding results of this chapter are useful in generalising these properties to arbitrary systems which do not possess any monotone property. Some of these results could be to show the existence or nonexistence of dead cores, radially symmetric solutions which can occur if the nonlinearities are singular (GATICA *et al.* [103], CASTRO and SHIVAJI [51]), degenerate solutions, nonnegative solutions (CHABROWSKI [52]) and certain properties of unstable solutions. The imbedding results of section 3.4 also applies to weak (or generalised) solutions (CHABROWSKI [52-63]) and the qualitative properties of such solutions.

The imbedding results of section 3.4 may also be applied to a much larger class of differential equations. It is known that these imbedding results do not hold for certain hyperbolic equations but it is not clear whether it would hold for larger classes of differential equations such as differential equations of the type we have seen which are coupled in their derivatives. It is however known that comparison theorems do exist for such problems (TRUDINGER [286]) and these comparison would be useful if these imbedding results were able to be extended to such a class of equations. It would appear as if we would have to imbed such a nonmonotone system that is coupled in its derivatives several times in order to obtain a monotone system with reaction functions monotone in all its dependent variables and derivatives. It is also not clear whether these imbedding results may be extended to higher order differential equations or even functional differential equations, stocastic differential equations and a more general class of equations. It is known however that comparison theorems do hold for certain classes of causal functional differential equations (MCNABB and WEIR [187]) and higher order differential equations (SPERB [271]) and these comparison theorems would also be useful if these imbedding results were able to be extended to this class of equations.

In section 3.5, we established some useful conditions for the global stability of the general system S_n, B_n where we assumed at the outset that the system S_n, B_n was a quasimonotone system, i.e. f_i and F_i are monotone nondecreasing in c_j and C_j respectively for $j \neq i$. These results could also have been obtained by assuming that S_n, B_n was a monotone system, i.e. f_i and F_i are monotone nondecreasing in c_j and C_j respectively for all j. This is not a restriction on the stability results since if this monotone property is not satisfied, we may make the substitution $c_i = e^{-Kx_1} w_i$ and $C_i = e^{-Kz_1} W_i$, (where x_1 and z_1 are chosen without loss of generality to be the first components of x and z) to obtain a system of the same type but with new functions that are monotone nondecreasing in c_i and C_i. Note that it is more appropriate in this case to make this substitution rather than $c_i = e^{-Kt} w_i$ and $C_i = e^{-Kt} W_i$ in studying the stability of our general system.

In many cases, the nonlinear functions f_i and F_i need only satisfy a one-sided Lipschitz condition when obtaining comparison theorems and in proving monotone convergent sequences to a solution of the system S_n, B_n (KELLER [141], AMANN [5], LADDE *et al.* [153], PAO [211, 219]).

In section 3.6, it can be shown that if f_i and F_i satisfies a Hölder condition then locally upper and lower solutions can be constructed and any problem of the system S_n, B_n which has nonuniqueness locally has distinct maximal and minimal solutions (BEBERNES and SCHMITT [35]).

4

The Steady State Problem

4.0 Introduction

For the study of the stability of the solutions of parabolic initial boundary value problems, one has to have a good knowledge of the steady states, that is of solutions to the time independent problem. In this chapter, we shall look at the steady state system $\hat{S}_n, \hat{B}_n$, that corresponds to the unsteady state system S_n, B_n. We shall obtain theorems that guarantee existence of solutions to the steady state system $\hat{S}_n, \hat{B}_n$ and establish relationships between the unsteady state system S_n, B_n and the steady state system $\hat{S}_n, \hat{B}_n$.

In section 4.1, we shall collect some notational conventions and basic definitions and give some general results and relationships of the spaces that are needed in order to obtain the exact result on the solvability of linear elliptic equations. The Maximum Principle for elliptic equations which will be used throughout this thesis will also be defined.

In section 4.2, we see that for the purposes of uniqueness, stability and existence theorems, we may assume at the outset that the system $\hat{S}_n, \hat{B}_n$ is a quasimonotone system, i.e. f_i and F_i are monotone nondecreasing in c_j and C_j respectively for $j \neq i$. This is not a restriction on these theorems since if this monotone property is not satisfied, then $\hat{S}_n, \hat{B}_n$ with general functions f_i and F_i can be imbedded in a system $\hat{S}_{2n}, \hat{B}_{2n}$ of the same form. It can be shown that solutions of this new system generate solutions of the original system and therefore uniqueness, stability and existence can be implied in the original system but only if uniqueness is guaranteed in the system $\hat{S}_{2n}, \hat{B}_{2n}$.

In section 4.3, that solutions of problem $\hat{S}_n, \hat{B}_n$ specified by $C_{i,1}$ exist. This is done by constructing a sequence of approximate solutions which converges monotonically and uniformly to a limit function which is a solution of the system $\hat{S}_n, \hat{B}_n$.

In secton 4.4 we use relationships concerning the asymptotic behaviour of linear parabolic equations as $t \to \infty$ and their corresponding linear elliptic equations to make a statement about the relationships between solutions of the steady state problem $\hat{S}_n, \hat{B}_n$ and the unsteady state problem S_n, B_n.

Finally, in section 4.5 we shall discuss some relevant literature and future work.

4.1 Definitions, Notation and General Results for Linear Elliptic Equations

In this section, we shall collect some notational conventions and basic definitions. We shall also give some general results and relationships of the spaces that are needed in order to obtain the exact result on the solvability of linear elliptic equations. The Maximum Principle for elliptic equations which will be used throughout this thesis will also be defined. Finally, we shall look at some relationships between solutions of linear parabolic and linear elliptic equations.

4.1.1 Definitions and Notation

The following notation will be used throughout this section

$x = (x_1, x_2, ..., x_m)$ denotes a point in R^m,
$\mathcal{G}$ is a bounded, open, connected domain in R^m,
$\partial\mathcal{G}$ denotes the boundary of $\mathcal{G}$,
$\overline{\mathcal{G}}$ denotes the closure of $\mathcal{G}$,
$u \in R$,
$D_x u = (\partial u/\partial x_1, ..., \partial u/\partial x_m)$,
$\|\cdot\|$ will denote the Euclidean norm in R^m.

Definition 4.1.1

A vector field $\boldsymbol{v}(x) = (\boldsymbol{v}_1(x), ..., \boldsymbol{v}_m(x))$ is said to be a *unit outerward normal* (outward normal or outernormal) at $x \in \Omega$ if $x - h\boldsymbol{v} \in \Omega$ for small $h > 0$. The *outernormal derivative* is then given by

and $\nu(x)$ is a unit vector normal to Ω

$$\frac{\partial u}{\partial \boldsymbol{v}} = \lim_{h \to 0} \frac{u(x) - u(x - h\boldsymbol{v})}{h}.$$

4.1.2 General Results and the Relationships between Hölder, L^q and Sobolev Spaces

The following definitions of Hölder, L^q and Sobolev spaces are adapted from LADYZHENSKAYA [154, p.4-5] and GILBARG and TRUDINGER [106, p.144].

Hölder Spaces

For $A \subseteq \Omega$, a function f: $A \to R$ is said to be *Hölder continuous* of exponent α, where $0 < \alpha \leq 1$, if there exists a constant $H = H(A)$ such that

$$|f(x) - f(y)| \leq H\|x - y\|^{\alpha}.$$

We note that the quantity

$$H_{\alpha}^{A}(f) = \sup_{\substack{x,y \in A \\ x \neq y}} \frac{|f(x) - f(y)|}{\|x - y\|^{\alpha}},$$

is the smallest number H.

We shall say that $f \in C^{k+\alpha}[A, R]$ if $f: A \to R$ is continuous, the partial derivatives of f, up to order k are continuous on A and the kth partial derivatives are Hölder continuous with exponent α. For $f \in C^{2+\alpha}[A, R]$, we shall use the following notation:

$$\|f\|_{\alpha}^{A} = \sup_{x \in A} |f(t,x)| + H_{\alpha}^{A}(f),$$

$$\|f\|_{1+\alpha}^{A} = \|f\|_{\alpha}^{A} + \sum_{i=1}^{m} \left\| \frac{\partial f}{\partial x_i} \right\|_{\alpha}^{A},$$

$$\|f\|_{2+\alpha}^{A} = \|f\|_{1+\alpha}^{A} + \sum_{i=1}^{m} \sum_{j=1}^{m} \left\| \frac{\partial^2 f}{\partial x_i \partial x_j} \right\|_{\alpha}^{A},$$

where

$$\left\|\frac{\partial f}{\partial x_i}\right\|_{\alpha}^{A} = \sup_{x\in A}\left|\frac{\partial f}{\partial x_i}\right| + H_{\alpha}^{A}(\frac{\partial f}{\partial x_i}),$$

and

$$\left\|\frac{\partial^2 f}{\partial x_i \partial x_j}\right\|_{\alpha}^{A} = \sup_{x\in A}\left|\frac{\partial^2 f}{\partial x_i \partial x_j}\right| + H_{\alpha}^{A}(\frac{\partial^2 f}{\partial x_i \partial x_j}).$$

Since $\overline{\mathcal{G}}$ is closed, it is required that the derivatives up to order k can be continuously continued from the interior of $\mathcal{G}$ to all of $\overline{\mathcal{G}}$. If $\alpha = 1$, we also say that f is Lipschitz continuous.

The superscript in the foregoing notions may be deleted if there is no ambiguity on which set the above norms are to be determined.

L^q Spaces

$L^q[\mathcal{G}, R]$ is the Banach space consisting of all equivalent clases of Lebesgue measurable functions u defined on Ω into R with a finite norm

$$\|u\|_{L^q[\mathcal{G}, R]} = \left(\int_{\overline{\mathcal{G}}} |u(x)|^q \, dx\right)^{1/q},$$

where $q \geq 1$.

Sobolev Spaces

For nonnegative integer l, $W_q^l[\mathcal{G}, R]$ is the Banach space consisting of the elements $L^q[\overline{\mathcal{G}}, R]$ having generalised (weak or distributional) derivatives of the form D^α for all $|\alpha| \leq l$. The norm in it is defined by

$$\|u\|_{W_q^l[\mathcal{G}, R]} = \sum_{|\alpha|\leq l} \|D^\alpha u\|_{L^q[\mathcal{G}, R]},$$

where the summation $\sum_{|\alpha|\leq l}$ is taken over all nonnegative integers α satisfying the condition $\alpha \leq l$.

Note that the space $W_q^l[\mathcal{G}, R]$ is in a certain sense analogous to the $C^{l+\alpha}[\overline{\mathcal{G}}, R]$ spaces. In the $W_q^l[\mathcal{G}, R]$ spaces, continuous differentiability is replaced by weak differentiability and Hölder continuity by q-integrability, so that $W_q^l[\mathcal{G}, R] = \{u \in W^l[\mathcal{G}, R];\ D^\alpha u \in L^q[\mathcal{G}, R] \text{ for all } |\alpha| \leq l\}$, where $W^l[\mathcal{G}, R]$ is the linear space of l times weakly differential functions.

General Results in Hölder, $L^{r,q}$ and Sobolev Spaces

We now give some general results in Hölder, $L^{r,q}$ and Sobolev spaces. Most of these results are special cases of those proved in section 3.1 and are only included here for easy reference.

Lemma 4.1.1

If $f, g \in C^\alpha[A, R]$, then $f+g \in C^\alpha[A, R]$ and $\|f+g\|_\alpha^A \leq \|f\|_\alpha^A + \|g\|_\alpha^A$.

Lemma 4.1.2

If $f, g \in C^\alpha[A, R]$, then $fg \in C^\alpha[A, R]$ and $\|fg\|_\alpha^A \leq \|f\|_\alpha^A \ \|g\|_\alpha^A$.

The next three lemmas and their corollaries are analogous in Hölder, $L^{r,q}$ and Sobolev spaces.

Lemma 4.1.3
Suppose $0 < \beta \le \alpha \le 1$. *Then* $C^{\alpha}(A) \subseteq C^{\beta}(A)$.

Corollary 4.1.1
Suppose $0 < \alpha, \beta \le 1$. *Then* $C^{\alpha}(A) \cap C^{\beta}(A) = C^{\gamma}(A)$ *where* $\gamma = \min\{\alpha, \beta\}$.

The following lemma is stated without proof in BURKILL [44]

Lemma 4.1.4
Suppose $1 \le p_1 \le p_2$. *Then* $L^{p_2}[A, R] \subseteq L^{p_1}[A, R]$.

Corollary 4.1.2
Suppose $1 \le p_1, p_2$. *Then* $L^{p_2}[A, R] \cap L^{p_1}[A, R] = L^{p}[A, R]$ *where* $p = \min\{p_1, p_2\}$.

The following lemma and its corollary follows from Lemma 4.1.4 and the definition of Sobolev Spaces.

Lemma 4.1.5
Suppose $1 \le p_1 \le p_2$. *Then* $W^{l}_{p_2}[A, R] \subseteq W^{l}_{p_1}[A, R]$.

Corollary 4.1.3
Suppose $1 \le p_1, p_2$. *Then* $W^{l}_{p_2}[A, R] \cap W^{l}_{p_1}[A, R] = W^{l}_{p}[A, R]$ *where* $p = \min\{p_1, p_2\}$.

As with section 3.1, we define the following operator which takes a space into itself.

Definition 4.1.1
The Nemytskii operator $\mathcal{N}(u)$ is defined by

$$\mathcal{N}(u)(x) = h(x, u), \; x \in \overline{\mathcal{G}},$$

for $u \in C^{1+\alpha}[\overline{\mathcal{G}}, R]$.

We now present a result concerning the Nemytskii operator $\mathcal{N}(u)$ which is a special case of Lemma 3.1.6.

Lemma 4.1.6
Let $h \in C^{\alpha}[\overline{\mathcal{G}} \times R, R]$, *and let* $\mathcal{N}(u)$ *be the Nemytskii operator* $\mathcal{N}(u)$. *Then*
(i) $\mathcal{N} \in C[C^{1+\alpha}[\overline{\mathcal{G}}, R], C^{\alpha}[\overline{\mathcal{G}}, R]]$;
(ii) $\mathcal{N}$ *takes bounded sets in* $C^{1+\alpha}[\overline{\mathcal{G}}, R]$ *into bounded sets in* $C^{\alpha}[\overline{\mathcal{G}}, R]$.

Remark 4.1.1
From the fact that the space $C^{1+\alpha}[\overline{\mathcal{G}}, R]$ is compactly imbedded in $C^{1}[\overline{\mathcal{G}}, R]$ the Nemytskii operator belongs to $C[C^{1}[\overline{\mathcal{G}}, R], C[\overline{\mathcal{G}}, R]]$.

We present another result concerning the Nemytskii operator $\mathcal{N}(u)$. This lemma is a special case of Lemma 3.1.7

Lemma 4.1.7

Let $h \in C^{\alpha}[\overline{\mathcal{G}} \times R, R]$, and let $\mathcal{N}(u)$ be the Nemytskii operator $\mathcal{N}(u)$. Then

(i) $\mathcal{N} \in C[L^q[\overline{\mathcal{G}}, R], L^q[\overline{\mathcal{G}}, R]]$;

(ii) *$\mathcal{N}$ takes bounded sets in $L^q[\overline{\mathcal{G}}, R]$ into bounded sets in $L^q[\overline{\mathcal{G}}, R]$.*

The Relationships between these Spaces

The spaces defined above are needed to obtain the exact result on the solvability of boundary value problems for linear elliptic equations in spaces $W_q^2[\overline{\mathcal{G}}, R]$. Note that an analogous lemma to Lemma 3.1.8 holds for elliptic equations which relates the differential properties of the boundary values of functions from the classes $W_q^2[\overline{\mathcal{G}}, R]$ and of their derivatives in terms of the spaces $W_p^1[\partial\mathcal{G}, R]$ (see LADYSHENSKAYA [154, pp.43-44]).

We say how smooth fuctions in a Sobolev space are, by imbedding Sobolev spaces continuously into Hölder spaces. This is often called the Sobolev Lemma or the Imbedding Theorem. We firstly require the following defintion

Definition 3.1.5

Let $\mathcal{G}$ be an m-dimensional domain with boundary $\partial\mathcal{G}$. We say that $\partial\mathcal{G}$ belongs to class $C^{2+\alpha}$, if for every $x \in \partial\mathcal{G}$, there exists a neighbourhood U of x such that $\partial\mathcal{G} \cap U$ can be represented in the form

$$x_i = h(x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_m),$$

for some i, $1 \le i \le m$, where $h \in C^{2+\alpha}[\partial\mathcal{G}, R]$.

We now state the following imbedding theorem. For the proof of this theorem, see LADYZHENSKAYA [154, p.60], GILBARG and TRUDINGER [106, p.155] or ADAMS [1]. A similar theorem is given in TEMME [282, p.42] for convex domains with C^∞ boundaries.

Theorem 4.1.1 *(Imbedding Theorem or Sobolev Lemma)*

Let $\mathcal{G} \subseteq R^m$ and let $\partial\mathcal{G}$ be of class $C^{2+\alpha}$.

(i) *Suppose $2q > m > q$. Then $W_q^2[\overline{\mathcal{G}}, R]$ is imbedded in $C^{1+\mu}[\overline{\mathcal{G}}, R]$, where $0 < \mu \le 1-2/q$;*

(ii) *Suppose $m = q$. Then $W_q^2[\overline{\mathcal{G}}, R]$ is imbedded in $C^{1+\mu}[\overline{\mathcal{G}}, R]$, where $0 < \mu < 1$; moreover suppose $m = q = 1$; then $W_q^2[\overline{\mathcal{G}}, R]$ is imbedded in $C^{1+\mu}[\overline{\mathcal{G}}, R]$ for $\mu = 1$.*

4.1.3 Solvability of Linear Elliptic Equations

We will discuss in this section a specific example of a elliptic equation that occurs in this thesis. For the definitions of more general linear and quasilinear second order equations of elliptic type, as well as their uniformly elliptic conditions, see LADYZHENSKAYA [154, p.11].

Let a_{ij}, b_i and c belong to $C^{\alpha}[\overline{\mathcal{G}}, R]$ and let $c \le 0$. Let L be a second order differential operator defined by

$$L = \sum_{i,j=1}^{m} a_{ij}(x)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{m} b_i(x)\frac{\partial}{\partial x_i} + c(x). \tag{4.1.1}$$

Definition 4.1.3

The differential operator L defined by (4.1.1) is said to be *elliptic* at a point $x \in \mathcal{G}$, if the coefficient matrix $a_{ij}(x)$ is positive definite, that is there exist two functions $\underline{\lambda}$ and $\overline{\lambda}$ such that

$$0 < \underline{\lambda}(x)\|\xi\|^2 \le \sum_{i,j=1}^{m} a_{ij}(x)\xi_i\xi_j \le \overline{\lambda}(x)\|\xi\|^2, \tag{4.1.2}$$

for all $\xi \in R^m - \{0\}$. If

$$\underline{\lambda}(x) > 0 \text{ in } Q_T,$$

then $\mathcal{L}$ is called *elliptic* in $\mathcal{G}$. If

$$\underline{\lambda}(x) \ge \lambda_0 > 0,$$

for a positive number λ_0 then $\mathcal{L}$ is called *almost strictly elliptic* in $\mathcal{G}$. If

$$\frac{\overline{\lambda}(x)}{\underline{\lambda}(x)} \le K,$$

for some positive number K, then $\mathcal{L}$ is called *strictly uniformly elliptic* in $\mathcal{G}$, that is (4.1.2) can be written as

$$\frac{1}{K}\|\xi\|^2 \le \sum_{i,j=1}^{m} a_{ij}(x)\xi_i\xi_j \le K\|\xi\|^2,$$

for all $\xi \in R^m$, $x \in \mathcal{G}$.

Let $\mathcal{G}$ be a bounded domain in R^n. Let $p, q \in C^{1+\alpha}[\partial\mathcal{G}, R]$ be nonnegative functions which do not vanish simultaneously and let $\nu(x)$ be the unit outward normal vector field on $\partial\mathcal{G}$ (which belongs to the class $C^{2+\alpha}$).

Consider the linear second order elliptic boundary value problem (*BVP* for short):

$$\left.\begin{aligned} Lu &= h(x) \text{ in } \mathcal{G}, \\ Bu &= \phi(x) \text{ on } \partial\mathcal{G}, \end{aligned}\right\} \tag{4.1.3}$$

where,

$$Bu = p(x)u + q(x)\frac{\mathrm{d}u}{\mathrm{d}\nu} \text{ for } u \in C^1[\overline{\mathcal{G}}, R]. \tag{4.1.4}$$

Let us now state the classical existence and uniquenss theorem whose proof can be found in LADYSHENSKAYA [154, p.137] and GILBARG AND TRUDINGER [106, Ch 6].

Theorem 4.1.2 *Assume that*

(i) $a_{ij}, b_i, c \in C^{\alpha}[\overline{\mathcal{G}}, R]$, $c(x) \le 0$ *and* L *is strictly uniformly elliptic in* $\mathcal{G}$;

(ii) $p, q \in C^{1+\alpha}[\partial\Omega, R]$ *for* p *and* q *nonnegative functions and there exists* $\mu_1 > 0$ *such that* $p \ge \mu_1$ *for all* $x \in \partial\mathcal{G}$;

(iii) $\partial\mathcal{G}$ *belongs to class* $C^{2+\alpha}$;

(iv) $h \in C^{\alpha}[\overline{\mathcal{G}}, R]$;

(v) $\phi \in C^{1+\alpha}[\partial\mathcal{G}, R]$.

Then the linear elliptic BVP (4.1.3)-(4.1.4) *has a unique solution u such that* $u \in C^{2+\alpha}[\overline{\mathcal{G}}, R]$.

We note that u and all its first and second partial derivatives are bounded in $\overline{\mathcal{G}}$.

The following result provides the global *a priori* Schauder-type estimates for classical solutions of linear elliptic *BVP* (4.1.3)-(4.1.4). For the proof, see AGMON-DOUGLIS-NIRENBERG [3, p.668]).

Theorem 4.1.3 *Assume that the hypotheses of Theorem 4.1.2 hold. Then for any* $u \in C^{2+\alpha}[\overline{\mathcal{G}}, R]$, *there exists a positive constant*

$$C = C(\mathcal{G}, \alpha, K, \|p\|_{\alpha}^{\partial\mathcal{G}}, \|v\|_{1}^{\partial\mathcal{G}}, \max_{\substack{1\le i\le m\\ 1\le j\le m}} \|a_{ij}\|_{\alpha}^{\overline{\mathcal{G}}}, m), \tag{4.1.5}$$

which is independent of u such that

$$\|u\|_{2+\alpha}^{\overline{\mathcal{G}}} \le C(\|Lu\|_{\alpha}^{\overline{\mathcal{G}}} + \|Bu\|_{1+\alpha}^{\partial\mathcal{G}}). \tag{4.1.6}$$

Moreover, if u is the classical solution of the linear elliptic BVP (4.1.3)-(4.1.4), *then* (4.1.6) *reduces to*

$$\|u\|_{2+\alpha}^{\overline{\mathcal{G}}} \le C(\|h\|_{\alpha}^{\overline{\mathcal{G}}} + \|\phi\|_{1+\alpha}^{\partial\mathcal{G}}). \tag{4.1.7}$$

Remark 4.1.2

If either if the conditions $p \ge \mu_1 > 0$ or $c \le 0$ is not satisfied in Theorem 4.1.2, unique solvability is no longer assured. However, unique solvability holds under conditions $p \ge 0$, $c \le 0$ and either $p \not\equiv 0$ or $c \not\equiv 0$ (GILBARG and TRUDINGER [106, p.130].

Remark 4.1.3

Analogous theorems to Theorem 4.1.2 hold for the linear elliptic *BVP* (4.1.3)-(4.1.4) with Dirichlet conditions (GILBARG and TRUDINGER [106, p.107]). In this case, it is required that $\phi \in C^{2+\alpha}[\partial\mathcal{G}, R]$

We shall state some results for solutions in the Sobolev spaces $W_q^2[\overline{\mathcal{G}}, R]$, $q > 1$ analogous to the Schauder results in the Hölder spaces $C^{2+\alpha}[\overline{\mathcal{G}}, R]$. Let us state the following uniqueness and existence theorem that provides us with generalised (weak) solutions of the linear elliptic *BVP* (4.1.3)-(4.1.4). Its proof may be found in LADYZHENSAYA [154, p.160].

Theorem 4.1.4 *Assume that*

(i) $a_{ij}, b_i, c \in C[\overline{\mathcal{G}}, R]$, $c(x) \le 0$ *and L is strictly uniformly elliptic in* $\mathcal{G}$;

(ii) $p, q \in C^1[\overline{\mathcal{G}}, R]$ *for p and q nonnegative functions and there exists* $\mu_1 > 0$ *such that* $p \ge \mu_1$ *for all* $x \in \partial\mathcal{G}$;

(iii) $\partial\mathcal{G}$ *belongs to class* $C^{2+\alpha}$;

(iv) $h \in L^q[\overline{\mathcal{G}}, R]$ for $q > 1$;

(v) $\phi \in C^1[\overline{\mathcal{G}}, R]$.

Then the linear elliptic BVP (4.1.3)-(4.1.4) *has a unique solution u such that* $u \in W_q^2[\overline{\mathcal{G}}, R]$.

The following result gives the global *a priori* Agmon-Douglis-Nirenberg estimates (or L^q estimates) for generalised solutions of the linear elliptic *BVP* (4.1.3)-(4.1.4). The proof may be found in AGMON-DOUGLIS-NIRENBERG [3, p.704] and LADYZHENSAYA [154, p.162]

Theorem 4.1.5 *Assume that the hypotheses of Theorem 4.1.4 hold. Then for any* $u \in W_q^2[\overline{\mathcal{G}}, R]$, *there is a constant*

$$C = C(m, K, q, \partial\mathcal{G}, \text{the modulus of continuity of } a_{ij} \text{ and norms } b_i \text{ and } c), \tag{4.1.8}$$

which is independent of u such that

$$\|u\|_{W_q^2[\overline{\mathcal{G}}, R]} \le C(\| Lu\|_{L^q[\overline{\mathcal{G}}, R]} + \|Bu\|_{W_q^1[\partial\mathcal{G}, R]}). \tag{4.1.9}$$

Moreover, if u is a generalized solution belonging to $W_q^2[\overline{\mathcal{G}}, R]$, *then*

$$\|u\|_{W_q^2[\overline{\mathcal{G}}, R]} \le C(\| h\|_{L^q[\overline{\mathcal{G}}, R]} + \|\phi\|_{W_q^1[\partial\mathcal{G}, R]}). \tag{4.1.10}$$

Remark 4.1.4

Note that the assumptions (i), (ii), (iii) and (v) of Theorem 4.1.4 are satisfied by the assumptions (i), (ii), (iii) and (v) of Theorem 4.1.2. The uniqueness, existence and Agmon-Douglis-Nirenberg estimates of generalised (weak) solutions of the linear elliptic *BVP* (4.1.3)-(4.1.4) are often given with the assumptions of Theorem 4.1.4 and $h \in L^q[\overline{\mathcal{G}}, R]$ for $q > 1$ (TEMME [282, p.65]).

Remark 4.1.5

Analogous theorems to Theorem 4.1.4 and Theorem 4.1.5 hold for the linear elliptic *BVP* (4.1.3)-(4.1.4) with Dirichlet conditions (LADYZHENSAYA [154, p.149], GILBARG and TRUDINGER [106, p.241]).

We shall now look at the maximum principle for elliptic equations

4.1.4 The Maximum Principle for Elliptic Equations

Throughout this thesis, we will use various forms of the maximum principle for the elliptic operator to obtain information about the solutions of our equations. A simple form of the maximum principle that we will find useful is the following

Lemma 4.1.8 (Maximum Principle)

Let $\psi \in C^2[\overline{\mathcal{G}}, R]$ *be such that* $-L\psi \le 0$ in $\mathcal{G}$ *and* $B\psi \le 0$ *on* $\partial\mathcal{G}$. *Then* $\psi \le 0$ *on* $\overline{\mathcal{G}}$.

Other forms of the maximum principle for the elliptic operator are given by PROTTER and WEINBERGER [234] and SPERB [271].

4.1.5 Relationships between Solutions of Linear Elliptic and Linear Parabolic Equations

In order to show the relationships between unsteady state solutions and steady state solutions, we shall require some theorems concerning the asymptotic behaviour of linear parabolic equations as $t \to \infty$. The following theorem is proved by FRIEDMAN [94, Ch. 6] and CARTER [50]. The notation used is from section 3.1.

Theorem 4.1.6 *Suppose that*

(i) a_{ij}, b_i, c *in* $\mathcal{L}u$ *are uniformly continuous and bounded in* $\overline{Q}_T$ *and* $\mathcal{L}$ *is strictly uniformly parabolic;*

(ii) p *and* q *in* $\mathcal{B}u$ *are nonnegative functions which are uniformly continuous and bounded in* $\overline{\Gamma}_T$ *and for some* $\mu_1 > 0$, $p(t, x) \geq \mu_1$ *for all* $(t, x) \in \overline{\Gamma}_T$;

(iii) $u(t, x)$ *satisfies the differential equation*

$$\mathcal{L}u = h(t, x) \text{ in } Q_T,$$

together with the boundary condition

$$\mathcal{B}u = \phi(t, x) \text{ on } \Gamma_T,$$

where h *is continuous on* $\overline{Q}_T$ *and* ϕ *is continuous on* $\overline{\Gamma}_T$.

If $\lim_{t\to\infty} h(t, x) = 0$ *uniformly on* $\overline{Q}_T$, $\lim_{t\to\infty} \phi(t, x) = 0$ *uniformly on* $\overline{\Gamma}_T$ *and* $\lim_{t\to\infty} c(t, x) \leq 0$ *uniformly on* $\overline{Q}_T$, *then* $\lim_{t\to\infty} u(t, x) = 0$ *uniformly on* $\overline{Q}_T$.

The following theorem shows the relationships concerning the asymptotic behaviour of linear parabolic equations as $t \to \infty$ and their corresponding linear elliptic equations.

Theorem 4.1.7 *Suppose that*

(i) a_{ij}, b_i, c *in* $\mathcal{L}u$ *are uniformly continuous and bounded in* $\overline{Q}_T$ *and* $\mathcal{L}$ *is strictly uniformly parabolic;*

(ii) p *and* q *in* $\mathcal{B}u$ *are nonnegative functions which are uniformly continuous and bounded in* $\overline{\Gamma}_T$ *and for some* $\mu_1 > 0$, $p(t, x) \geq \mu_1$ *for all* $(t, x) \in \overline{\Gamma}_T$;

(iii) $\hat{a}_{ij}$, $\hat{b}_i$, $\hat{c} \in C^{\alpha}[\overline{\mathcal{G}}, R]$ *in* Lu *and* L *is strictly uniformly elliptic;*

(iv) $\hat{p}$ *and* $\hat{q}$ *in* Bu *are nonnegative functions in* $C^{1+\alpha}[\partial\mathcal{G}, R]$ *and for some* $\hat{\mu}_1 > 0$, $\hat{p}(x) \geq \hat{\mu}_1$ *for all* $x \in \partial\mathcal{G}$;

(iv) $a_{ij}(t, x) \to \hat{a}_{ij}(x)$, $b_{ij}(t, x) \to \hat{b}_i(x)$, $c(t, x) \to \hat{c}(x)$ *as* $t \to \infty$, *uniformly in* $\overline{Q}_T$;
$p(t, x) \to \hat{p}(x)$, *and* $q(t, x) \to \hat{q}(x)$ *as* $t \to \infty$, *uniformly in* $\overline{\Gamma}_T$;
$h(t, x) \to \hat{h}(x)$ *as* $t \to \infty$, *uniformly in* $\overline{Q}_T$;
$\phi(t, x) \to \hat{\phi}(x)$ *as* $t \to \infty$, *uniformly in* $\overline{\Gamma}_T$;

If $u(t, x)$ *satisfies the differential equation*

$$\mathcal{L}u = h(t, x) \text{ in } Q_T,$$

together with the boundary condition

$$\mathcal{B}u = \phi(t, x) \text{ on } \Gamma_T,$$

where h *is continuous on* $\overline{Q}_T$ *and* ϕ *is continuous on* $\overline{\Gamma}_T$ *and if* $\hat{u}(x)$ *is the unique solution of the boundary value problem*

$$L\hat{u} = \hat{h}(x) \text{ in } \mathcal{G},$$

$$Bu = \hat{\phi}(x) \text{ on } \partial\mathcal{G},$$

where $\hat{h} \in C^{\alpha}[\mathcal{G}, R]$ *and* $\hat{\phi} \in C^{1+\alpha}[\mathcal{G}, R]$, *then*

$$u(t, x) \to \hat{u}(x) \text{ as } t \to \infty \text{ uniformly on } \overline{Q}_T.$$

Proof

Put $w(t, x) = u(t, x) - \hat{u}(x)$, for $(t, x) \in \overline{Q}_T$. Then:

$$\begin{aligned}\mathscr{L}w &= \mathscr{L}u - \mathscr{L}\hat{u} + L\hat{u} - L\hat{u}\\ &= h(t, x) - \hat{h}(x) + (L - \mathscr{L})\hat{u} \text{ in } Q_T,\end{aligned}$$

$$\begin{aligned}\mathscr{B}w &= \mathscr{B}u - \mathscr{B}\hat{u} + B\hat{u} - B\hat{u}\\ &= \phi(t, x) - \hat{\phi}(x) + (B - \mathscr{B})\hat{u} \text{ on } \Gamma_T.\end{aligned}$$

From the assumptions of this theorem, the boundedness of $\hat{u}(x)$ and its first and second partial derivatives on $\overline{\mathscr{G}}$ (see Theorem 3.1.2), we may apply Theorem 4.1.6 and conclude that $\lim_{t\to\infty} w(t, x) = 0$, uniformly on $\overline{Q}_T$, implying that $u(t, x) \to \hat{u}(x)$ as $t \to \infty$ uniformly on $\overline{Q}_T$.□

Remark 4.1.6

Analogous theorems to Theorem 4.1.6 hold for the linear *BVP* (4.1.3)-(4.1.4) with Dirichlet and Neumann type boundary conditions (FRIEDMAN [94, Ch.6]).

In section 4.2, we shall present some imbedding results for the system $\hat{S}_n$, $\hat{B}_n$.

4.2 Imbedding Results

For the purposes of uniqueness, stability and existence theorems of the steady state system, we may consider the quasimonotone system $\hat{S}_n$, $\hat{B}_n$ where f_i and F_i are monotone nondecreasing in c_j and C_j respectively for $j \neq i$. This is not a restriction on these theorems of this chapter since if this monotone property is not satisfied, then the system $\hat{S}_n$, $\hat{B}_n$ with general functions f_i and F_i can be imbedded in a system $\hat{S}_{2n}$, $\hat{B}_{2n}$ of the same form where $f_i(x, c_j)$ is replaced by $\overline{f}_i(x, \underline{c}_k, \overline{c}_l)$ for the first $n(I)$ dependent variables $\overline{c}_i$ and by $\underline{f}_i(x, \underline{c}_k, \overline{c}_l)$ for the next $n(I)$ dependent variables $\underline{c}_i$. Also, $F_i(z, C_j)$ is replaced by $\overline{F}_i(z, \underline{C}_k, \overline{C}_l)$ for the first $n(J)$ dependent variables $\overline{C}_i$ and by $\underline{F}_i(z, \underline{C}_k, \overline{C}_l)$ for the next $n(J)$ dependent variables $\underline{C}_i$. It can be shown that solutions of this new system may generate solutions of the original system and therefore uniqueness, stability and existence can be implied in the original system.

We consider the new system $\hat{S}_{2n}$, $\hat{B}_{2n}$ of up to twice the order satisfied by $\underline{c}_i$, $\overline{c}_i$, $\underline{C}_i$ and $\overline{C}_i$ in the following equations:

$$-D_i\nabla_x^2\underline{c}_i = \underline{f}_i(x, \underline{c}_k, \overline{c}_l),\ -D_i\nabla_x^2\overline{c}_i = \overline{f}_i(x, \underline{c}_k, \overline{c}_l) \text{ in } \Omega\times\Lambda;$$

$$\frac{\partial\underline{c}_i}{\partial n} = 0,\ \frac{\partial\overline{c}_i}{\partial n} = 0 \text{ on } \partial\Omega_1\times\Lambda;$$

$$D_i\frac{\partial\underline{c}_i}{\partial n} = H_i(\underline{C}_i - \underline{c}_i),\ D_i\frac{\partial\overline{c}_i}{\partial n} = H_i(\overline{C}_i - \overline{c}_i) \text{ on } \partial\Omega_2\times\Lambda;$$

$$-\mathscr{D}_i\nabla^2\underline{C}_i + u\cdot\nabla\underline{C}_i + H_i\int_{\partial\Omega_2}(\underline{C}_i - \underline{c}_i) = \underline{F}_i(z, \underline{C}_k, \overline{C}_l) \text{ in } \Lambda;$$

$$-\mathscr{D}_i\nabla^2\overline{C}_i + u\cdot\nabla\overline{C}_i + H_i\int_{\partial\Omega_2}(\overline{C}_i - \overline{c}_i) = \overline{F}_i(z, \underline{C}_k, \overline{C}_l) \text{ in } \Lambda;$$

$$\upsilon_1\underline{C}_i + \mathscr{D}_i\frac{\partial\underline{C}_i}{\partial n_1} = \upsilon_1\underline{C}_{i,1},\ \upsilon_1\overline{C}_i + \mathscr{D}_i\frac{\partial\overline{C}_i}{\partial n_1} = \upsilon_1\overline{C}_{i,1} \text{ on } \partial\Lambda_1;$$

$$\frac{\partial \underline{C}_i}{\partial n_\alpha}=0,\ \frac{\partial \overline{C}_i}{\partial n_\alpha}=0 \text{ on } \partial\Lambda_\alpha,\ \alpha=2,3,$$

where $\underline{f}_i$, $\bar{f}_i$ $\underline{F}_i$ and $\overline{F}_i$ are defined in (3.2.9)-(3.2.12).

Note that the functions $\{\bar{f}_i, -\underline{f}_i\}$ and $\{\overline{F}_i, -\underline{F}_i\}$ obey a mixed quasimonotone property (mqmp) in the sense of LADDE *et al.*[153, p.107], i.e, the functions $\bar{f}_i$ and $-\underline{f}_i$ are monotone nondecreasing in $\bar{c}_l$ and monotone nonincreasing in $\underline{c}_k$ for all $i \neq k, l$ and the functions $\overline{F}_i$ and $-\underline{F}_i$ are monotone nondecreasing in $\overline{C}_l$ and monotone nonincreasing in $\underline{C}_k$ for all $i \neq k, l$.

If we therefore slightly modify the system $\hat{S}_{2n}$, $\hat{B}_{2n}$ as suggested by MCNABB [186], by introducing new variables $v_i=\bar{c}_i$, $v_{n(I)+i}=-\underline{c}_i$ for $i=1,.., n(I)$ and $V_i=\overline{C}_i$, $V_{n(J)+i}-\underline{C}_i$ for $i=1,.., n(J)$ and if we set $f_i^*=\bar{f}_i$, $f^*_{n(I)+i}=-\underline{f}_i$ for $i=1,.., n(I)$ and $F_i^*=\overline{F}_i$, $F^*_{n(J)+i}=-\underline{F}_i$ for $i=1,.., n(J)$ then we obtain a new system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ for which f_i^* and F_i^* are nondecreasing functions of v_j and V_j, respectively, for all $j \neq i$. It can be shown by Lemma 3.2.2, that these new functions have the Lipschitz properties that were imposed on the original functions f_i and F_i.

Every solution (c_i, C_i) of $\hat{S}_n$, $\hat{B}_n$ generates a solution $v_i=c_i$, $v_{n(I)+i}=-\underline{c}_i$ and $V_i=C_i$, $V_{n(J)+i}=-\underline{C}_i$ of the new system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ with the special property that for $i \le n(I)$, $v_i+v_{n(I)+i}\equiv 0$ in $\overline{\Omega}\times\Lambda$ and for $i \le n(J)$, $V_i+V_{n(J)+i}\equiv 0$ in $\overline{\Lambda}$. Conversely, any solution (v_i, V_i) of the new system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ with the special property that for $i \le n(J)$ we have $V_{i,1}+V_{n(J)+i,1}\equiv 0$ on $\partial\Lambda_1$, may in some cases be shown by the following theorem to give rise to a solution of the system $\hat{S}_n$, $\hat{B}_n$.

Theorem 4.2.1.

The general system $\hat{S}_n$, $\hat{B}_n$ for which f_i and F_i are Lipschitz continuous in c_j and C_j respectively, may be imbedded in a system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ of twice the order which is coupled by monotone functions f_i^* and F_i^* of the new dependent variables v_i and V_i. Moreover, all the solutions (c_i, C_i) of the system $\hat{S}_n$, $\hat{B}_n$ are solutions of the new system, where

$$v_i=c_i,\ v_{n(I)+i}=-c_i \text{ for } i=1,..,n(I) \tag{4.2.1}$$

and

$$V_i=C_i,\ V_{n(J)+i}=-C_i \text{ for } i=1,..,n(J) \tag{4.2.2}$$

and all the solutions (v_i, V_i) of $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ for which

$$-D_i\nabla_x^2 w_i = f_i^*(x, v_j)+f^*_{n(I)+i}(x, v_k) \text{ in } \Omega\times\Lambda, \tag{4.2.3}$$

$$\frac{\partial w_i}{\partial n}=0 \text{ on } \partial\Omega_1\times\Lambda; \tag{4.2.4}$$

$$D_i\frac{\partial w_i}{\partial n}-H_i(W_i-w_i)=0 \text{ on } \partial\Omega_2\times\Lambda; \tag{4.2.5}$$

$$-\mathcal{D}_i\nabla_x^2 W_i+u\cdot\nabla W_i = F_i^*(z, V_j)+F^*_{n(J)+i}(z, V_k)-H_i\int_{\partial\Omega_2}(W_i-w_i) \text{ in } \Lambda; \tag{4.2.6}$$

$$v_1 W_i+\mathcal{D}_i\frac{\partial W_i}{\partial n_1}=0 \text{ on } \partial\Lambda_1; \tag{4.2.7}$$

$$\frac{\partial W_i}{\partial n_\alpha}=0 \text{ on } \partial\Lambda_\alpha,\ \alpha=2,3; \tag{4.2.8}$$

with $w_i = v_i + v_{n(I)+i}$ *for* $i = 1,..,n(I)$ *and* $W_i = V_i + V_{n(J)+i}$ *for* $i = 1,..,n(J)$, *generate solutions* (c_i, C_i) *of the system* $\hat{S}_n$, $\hat{B}_n$, *provided that solutions* (v_i, V_i) *of* $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ *are unique.*

Proof

We first note that if we set $\underline{c}_i \equiv \overline{c}_i \equiv c_i$ and $\underline{C}_i \equiv \overline{C}_i \equiv C_i$ where (c_i, C_i) is a solution of $\hat{S}_n$, $\hat{B}_n$, then we have a solution of the new system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$, so that the solution set of this new system contains all of the solutions of the original system $\hat{S}_n$, $\hat{B}_n$. In this system, we make the variable change

$$v_i = \overline{c}_i, \quad v_{n(I)+i} = -\underline{c}_i, \quad \text{for } i=1,..,n(I), \tag{4.2.9}$$

$$V_i = \overline{C}_i, \quad V_{n(J)+i} = -\underline{C}_i, \quad \text{for } i=1,..,n(J), \tag{4.2.10}$$

so that the coupling functions f_i^* and F_i^* are nondecreasing functions of all the new dependent variables v_j and V_j, respectively, for all $j \neq i$. Denote this system by $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$.

The solutions of $\hat{S}_n$, $\hat{B}_n$ generate solutions in $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ for which $w_i = v_i + v_{n(I)+i} = 0$ in $\overline{\Omega} \times \Lambda$ and $W_i = V_i + V_{n(J)+i} = 0$ in $\overline{\Lambda}$.

Suppose we have a solution (v_i, V_i) of $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ for which $(w_i, W_i) = (v_i + v_{n(I)+i}, V_i + V_{n(J)+i})$ satisfies (4.2.3)-(4.2.8). We then obtain the following system of equations, $\hat{S}^*_n$ for (w_i, W_i):

$$\begin{aligned} -D_i\nabla_x^2 w_i &= f_i^*(x, v_j) + f^*_{n(I)+i}(x, v_k) \\ &= \bar{f}_i(x, \underline{c}_j, \overline{c}_k) - \underline{f}_i(x, \underline{c}_j, \overline{c}_k) \\ &= \bar{f}_i(x, \overline{c}_j - w_j, \overline{c}_k) - \underline{f}_i(x, \overline{c}_j - w_j, \overline{c}_k) \text{ in } \Omega\times\Lambda, \end{aligned} \tag{4.2.11}$$

$$\begin{aligned} -\mathcal{D}_i\nabla_x^2 W_i + u\cdot\nabla W_i &= F_i^*(z, V_j) + F^*_{n(J)+i}(z, V_k) - H_i\int_{\partial\Omega_2}(W_i - w_i) \\ &= \overline{F}_i(z, \underline{C}_j, \overline{C}_k) - \underline{F}_i(z, \underline{C}_j, \overline{C}_k) - H_i\int_{\partial\Omega_2}(W_i - w_i) \\ &= \overline{F}_i(z, \overline{C}_j - W_j, \overline{C}_k) - \underline{F}_i(z, \overline{C}_j - W_j, \overline{C}_k) - H_i\int_{\partial\Omega_2}(W_i - w_i) \text{ in } \Lambda, \end{aligned} \tag{4.2.12}$$

$$D_i\frac{\partial w_i}{\partial n} = H_i(W_i - w_i) \text{ on } \partial\Omega_2 \times \Lambda. \tag{4.2.13}$$

In addition, (w_i, W_i) satisfies the boundary conditions $\hat{B}^*_n$ given by B_n with $W_{i,1} = V_{i,1} + V_{n(J)+i,1} = 0$.

But $\bar{f}_i(x, \overline{c}_j - w_j, \overline{c}_k) - \underline{f}_i(x, \overline{c}_j - w_j, \overline{c}_k)$ and $\overline{F}_i(z, \overline{C}_j - W_j, \overline{C}_k) - \underline{F}_i(z, \overline{C}_j - W_j, \overline{C}_k) - H_i\int_{\partial\Omega_2}(W_i - w_i)$ vanish when $W_j \equiv w_j \equiv 0$ for all j, and since $(w_i, W_i) \equiv 0$ is a solution of this boundary value problem and by uniqueness it is the only solution, we conclude that $w_i \equiv 0$ in $\overline{\Omega} \times \Lambda$ and $W_i \equiv 0$ in $\overline{\Lambda}$. The conclusion of our theorem must follow.❑

An immediate consequence of these imbedding results is that existence, uniqueness and stability results for the system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ imply existence, uniqueness and stability for the corresponding solution of $\hat{S}_n$, $\hat{B}_n$. Of course, solutions of $\hat{S}_n$, $\hat{B}_n$ may be stable in $\hat{S}_n$, $\hat{B}_n$, but unstable in the larger setting $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$. This of course can imply that there may be uniqueness of solutions in $\hat{S}_n$, $\hat{B}_n$ and nonuniqueness of solutions in the larger setting $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ and if there are multiple solutions in the larger setting $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$, this implies that there can be no greater number of solutions in the original system $\hat{S}_n$, $\hat{B}_n$. The implications of this is that nonexistence of solutions in the system $\hat{S}^*_{2n}$, $\hat{B}^*_{2n}$ must imply nonexistence of solutions in $\hat{S}_n$, $\hat{B}_n$. As with the time dependent problem, there are many other implications of these imbedding results (see section 3.7).

Remark 4.2.1
Note that the functions

$$\bar{f}_i(x, \bar{c}_j - w_j, \bar{c}_k) - \underline{f}_i(x, \bar{c}_j - w_j, \bar{c}_k)$$

and

$$\bar{F}_i(z, \bar{C}_j - W_j, \bar{C}_k) - \underline{F}_i(z, \bar{C}_j - W_j, \bar{C}_k) - H_i \int_{\partial\Omega_2} (W_i - w_i)$$

in the right hand sides of (4.2.11) and (4.2.12) are monotone nondecreasing in w_j and W_j, respectively.

In section 4.3 we shall study the existence of solutions to the steady state system $\hat{S}_n$, $\hat{B}_n$.

4.3 Existence of Solutions to the Steady State Problem

In this section we shall be looking for steady state solutions of S_n, B_n which are solutions of the time independent problem $\hat{S}_n$, $\hat{B}_n$. We demonstrate in this section that solutions of problem $\hat{S}_n$, $\hat{B}_n$ specified by $C_{i,1}$ exist. By a solution, we shall understand a *classical* solution (c_i, C_i) of $\hat{S}_n$, $\hat{B}_n$, where

(i) For components $i \in I$ where $D_i, H_i > 0$, c_i are continuous in $\bar{\Omega} \times \Lambda$, have continuous first order x_j derivatives in $\bar{\Omega} \times \Lambda$ and continuous second order x_j derivatives in $\Omega \times \Lambda$. In this case, we shall look for *classical solutions* of the form $c_i(x, z) \in C^{2,0}[\bar{\Omega} \times \Lambda, R^{n(I)}]$.

(ii) For components $i \in I$ where $D_i = H_i = 0$, c_i are continuous in $\bar{\Omega} \times \Lambda$. In this case, we shall look for *classical solutions* of the form $c_i(x, z) \in C^{0,0}[\bar{\Omega} \times \Lambda, R^{n(I)}]$.

(iii) For components $i \in J$ where $\mathcal{D}_i > 0$, C_i are continuous in $\bar{\Lambda}$, have continuous first order z_j derivatives in $\bar{\Lambda}$ and continuous second order z_j derivatives in Λ. In this case we shall look for *classical solutions* of the form $C_i(z) \in C^2[\bar{\Lambda}, R^{n(J)}]$.

(iv) For components $i \in J$ where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, C_i are continuous in $\bar{\Lambda}$ and have continuous first order z_j derivatives in Λ. In this case we shall look for *classical solutions* of the form $C_i(z) \in C^1[\bar{\Lambda}, R^{n(J)}]$.

(v) For components $i \in J$ where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, C_i are continuous in $\bar{\Lambda}$. In this case we shall look for *classical solutions* of the form $C_i(z) \in C^0[\bar{\Lambda}, R^{n(J)}]$.

Comparison theorems are used in this section in conjunction with theorems on *a priori* estimates and existence of linear elliptic equations to derive estimates of the system $\hat{S}_n$, $\hat{B}_n$ and to prove the existence of solutions to this system. There may be some cases where D_i or $\mathcal{D}_i$ may be zero and these cases are treated by using standard results.

As for the system S_n, B_n, we shall need some additional continuity properties to establish existence of the corresponding linear system and make the following assumptions on $f_i(x, c_j)$ and $F_i(z, C_j)$.

(H_2') (i) $f_i(x, c_j) \in C^\alpha[\bar{\Omega} \times R^{n(I)}, R^{n(I)}]$, i.e., $f_i(x, c_j)$ is Hölder continuous in x with exponent α, for each fixed value of c_j.

(ii) $F_i(z, C_j) \in C^{\alpha}[\overline{\Lambda} \times R^{n(J)}, R^{n(J)}]$, i.e., $F_i(z, C_j)$ is Hölder continuous in z with exponent α, for each fixed value of C_j.

Note that these assumptions are satisfied by assumption (H_2) if f_i and F_i are independent of t. By Lemma 4.1.3, we see that the exponent α in both cases may be assumed to be identical.

4.3.1 The Monotone System $\hat{S}_n$, $\hat{B}_n$

We may assume at the outset that the system $\hat{S}_n$, $\hat{B}_n$ is a monotone system, in the sense that $f_i(x, c_j)$ is monotone nondecreasing in c_i and $F_i(z, C_j)$ is monotone nondecreasing in C_i for all i. This is not a restriction on the theorems of this section since if this monotone property is not satisfied we may make the following substitution to obtain a system of the same type but with new functions that are monotone nondecreasing in c_i and C_i. We first observe that if (c_i, C_i) is a solution of $\hat{S}_n$, $\hat{B}_n$ and x_1, z_1 and $u_1(z)$ are chosen without loss of generality to be the first components of x, z and $u(z)$ respectively, then (w_i, W_i) defined to be where

$$c_i = e^{-Kx_1} w_i \tag{4.3.1}$$

and

$$C_i = e^{-Kz_1} W_i, \tag{4.3.2}$$

satisfies the following system of equations:

$$-D_i(\nabla_x^2 w_i - 2K\frac{\partial w_i}{\partial x_1}) = K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j) \text{ in } \Omega\times\Lambda, \tag{4.3.3}$$

$$\frac{\partial}{\partial n} e^{-Kx_1} w_i = 0 \text{ on } \partial\Omega_1\times\Lambda, \tag{4.3.4}$$

$$D_i \frac{\partial}{\partial n} e^{-Kx_1} w_i = H_i(e^{-Kz_1} W_i - e^{-Kx_1} w_i) \text{ on } \partial\Omega_2\times\Lambda, \tag{4.3.5}$$

$$-\mathcal{D}_i(\nabla^2 W_i - 2K\frac{\partial W_i}{\partial z_1}) + u\cdot\nabla W_i + H_i \mathcal{A} W_i = \mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j)$$
$$+ H_i \int_{\partial\Omega_2} e^{-Kx_1} w_i \text{ in } \Lambda, \tag{4.3.6}$$

$$\upsilon_1 e^{-Kz_1} W_i + \mathcal{D}_i \frac{\partial}{\partial n_1} e^{-Kz_1} W_i = \upsilon_1 e^{-Kz_1} C_{i,1} \text{ on } \partial\Lambda_1, \tag{4.3.7}$$

$$\frac{\partial}{\partial n_\alpha} e^{-Kz_1} W_i = 0 \text{ on } \partial\Lambda_\alpha,\ \alpha = 2, 3. \tag{4.3.8}$$

The system is similar to the original system $\hat{S}_n$, $\hat{B}_n$ in that uniform ellipticity conditions are still preserved in (4.3.3) and (4.3.6). The nonlinear coupling function $f_i(x, c_j)$ for c_j components in these equations is replaced by

$$K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j), \tag{4.3.9}$$

the nonlinear coupling function $F_i(z, C_j)$ for C_j components in these equations is replaced by

$$\mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j), \tag{4.3.10}$$

and the functional term

$$H_i \int_{\partial\Omega_2} c_i, \tag{4.3.11}$$

is replaced by

$$H_i \int_{\partial\Omega_2} e^{-Kx_1} w_i. \tag{4.3.12}$$

The functions $K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)$ and $\mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j)$ satisfy a monotone property given by the following lemma:

Lemma 4.3.1
Our assumptions (H_1) of Lipschitz continuity properties for the functions f_i and F_i with respect to c_j and C_j imply that the functions $K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)$ and $\mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j)$ with $c_i = e^{-Kx_1} w_i$ and $C_i = e^{-Kz_1} W_i$, are monotone nondecreasing in w_i and W_i, respectively.

Proof
Assume that $w_j \le w_j^*$ so that $c_j \le c_j^*$.
From (H_1), we see that

$$K_i(c_j - c_j^*) \le f_i(x, c_j) - f_i(x, c_j^*) \le -K_i(c_j - c_j^*).$$

and therefore,

$$\begin{aligned}
&[K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)] - [K^2 D_i w_i^* + e^{Kx_1} f_i(x, e^{-Kx_1} w_j^*)] \\
&\qquad = K^2 D_i e^{Kx_1}(c_i - c_i^*) + e^{Kx_1}[f_i(x, c_j) - f_i(x, c_j^*)] \\
&\qquad \le -e^{Kx_1}[K^2 D_i(c_i^* - c_i) + K_i(c_j^* - c_j)] \\
&\qquad \le 0,
\end{aligned}$$

if K is chosen to be large enough. This shows that

$$K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j) \le K^2 D_i w_i^* + e^{Kx_1} f_i(x, e^{-Kx_1} w_j^*),$$

so that this new coupling function $K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)$ is monotone nondecreasing in w_i. A similar argument holds if we have to show that $\mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j)$ is monotone nondecreasing in W_i. This may be shown irrespective of the sign of $u_1(z)$.❑

It can also be shown that these new functions also satisfy the same Lipschitz and Hölder continuity properties as our original functions.

Lemma 4.3.2
Our assumptions (H_1) of Lipschitz continuity properties for the functions f_i and F_i with respect to the variables c_j and C_j imply similar Lipschitz continuity properties for the functions $K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)$ and $\mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j)$ with respect to the variables w_j and W_j, for $c_i = e^{-Kx_1} w_i$ and $C_i = e^{-Kz_1} W_i$.

Proof
We need to only show that

$$\begin{aligned}
&|[K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)] - [K^2 D_i w_i^* + e^{Kx_1} f_i(x, e^{-Kx_1} w_j^*)]| \\
&\qquad \le K^2 D_i |w_i - w_i^*| + e^{Kx_1} |f_i(x, e^{-Kx_1} w_j) - f_i(x, e^{-Kx_1} w_j^*)|
\end{aligned}$$

$$\le K^2 D_i |w_i - w_i^*| + e^{Kx_1} k_i |e^{-Kx_1}| w_j - w_j^*|$$
$$\le K^2 D_i |w_i - w_i^*| + k_i |w_j - w_j^*|$$
$$\le k \sup_j |w_j - w_j^*|,$$

where,

$$k = \max_j (K^2 D_i, k_i).$$

and the first part of the proof follows. The rest of the proof follows similarly.❑

Lemma 4.3.2

Our assumptions (H_1) *of Lipschitz continuity properties for the functions* f_i, *with respect to the variables* c_j *and assumptions* (H_2') *of Hölder continuity properties for the functions* f_i, *with respect to* x *with* c_j *fixed imply similar Hölder continuity properties for the functions* $K^2 D_i w_i + e^{Kx_1} f_i(x, e^{-Kx_1} w_j)$ *with respect to* x *with* w_j *fixed, where* $c_i = e^{-Kx_1} w_i$. *Similarly, our assumptions* (H_1) *of Lipschitz continuity properties for the functions* F_i, *with respect to the variables* C_j *and assumptions* (H_2') *of Hölder continuity properties for the functions* F_i, *with respect to* z *with* C_j *fixed imply similar Hölder continuity properties for the functions* $\mathcal{D}_i K^2 W_i + u_1(z) K W_i + e^{Kz_1} F_i(z, e^{-Kz_1} W_j)$ *with respect to* z *with* W_j *fixed, where* $C_i = e^{-Kz_1} W_i$.

Proof

We shall only show that $f_i(x, e^{-Kx_1} w_j)$ is Hölder continuous in x. The rest of the proof is similar and follows from Lemma 4.1.1 and Lemma 4.1.2.

$$|f_i(x, e^{-Kx_1} w_j) - f_i(x^*, e^{-Kx_1^*} w_j)|$$
$$= |f_i(x, e^{-Kx_1} w_j) - f_i(x^*, e^{-Kx_1} w_j) + f_i(x^*, e^{-Kx_1} w_j) - f_i(x^*, e^{-Kx_1^*} w_j)|$$
$$\le |f_i(x, e^{-Kx_1} w_j) - f_i(x^*, e^{-Kx_1} w_j)| + |f_i(x^*, e^{-Kx_1} w_j) - f_i(x^*, e^{-Kx_1^*} w_j)|$$
$$\le k_x(f_i) \| x - x^* \|^\alpha + k_i |e^{-Kx_1} w_j - e^{-Kx_1^*} w_j|$$
$$\le k_x(f_i) \| x - x^* \|^\alpha + k_i |w_j| |e^{-Kx_1} - e^{-Kx_1^*}|$$
$$\le k_x(f_i) \| x - x^* \|^\alpha + k_i |w_j| K \| x_1 - x_1^* \|^{1-\alpha} \| x_1 - x_1^* \|^\alpha$$
$$\le k_x(f_i(x, e^{-Kx_1} w_j)) \| x - x^* \|^\alpha,$$

where

$$k_x(f_i(x, e^{-Kx_1} w_j)) = \max(k_x(f_i), k_i |w_j| K d(\overline{\Omega})^{1-\alpha}).❑$$

We may assume that the substitution (4.3.1)-(4.3.2) has been made and that $f_i(x, c_j)$ is monotone nondecreasing in c_i and $F_i(z, C_j)$ is monotone nondecreasing in C_i. If, on the other hand the monotone property is not satisfied by all the other variables, then the system $\hat{S}_n, \hat{B}_n$ with general functions f_i and F_i can be imbedded in a system $\hat{S}_{2n}, \hat{B}_{2n}$ of the same form where $f_i(x, c_j)$ is replaced by $\bar{f}_i(x, \underline{c}_k, \bar{c}_l)$ for the first $n(I)$ dependent variables $\bar{c}_i$ and by $\underline{f}_i(x, \underline{c}_k, \bar{c}_l)$ for the next $n(I)$ dependent variables $\underline{c}_i$. Also, $F_i(z, C_j)$ is replaced by $\overline{F}_i(z, \underline{C}_k, \overline{C}_l)$ for the first $n(J)$ dependent variables $\overline{C}_i$ and by $\underline{F}_i(z, \underline{C}_k, \overline{C}_l)$ for the next $n(J)$ dependent variables $\underline{C}_i$. The existence results obtained for this new system of twice the order satisfied by

$(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\bar{c}_i, \overline{C}_i)$ then implies a solution of our original system S_n, B_n by the imbedding results of section 4.2 if uniqueness is guaranteed in the monotone system $\hat{S}_{2n}, \hat{B}_{2n}$.

It has been shown in section 3.2 that the functions $\underline{f}_i$, $\bar{f}_i$, $\underline{F}_i$ and $\overline{F}_i$ satisfy the same Lipschitz continuity properties as our original functions f_i and F_i in the system $\hat{S}_n, \hat{B}_n$. It can also be shown that these new functions satisfy the same Hölder continuity properties as our original functions and the following lemma is a special case of Lemma 3.6.4.

Lemma 4.3.3

Our assumptions (H_2') of Hölder continuity properties for the functions f_i, with respect to x with c_j fixed imply similar Hölder continuity properties for $\underline{f}_i$ and $\bar{f}_i$, with respect to x with $\underset{\sim}{c}_k$ and $\bar{c}_l$ fixed and so there are constants k_x such that

$$\left.\begin{aligned} |\underline{f}_i(x, \underset{\sim}{c}_k, \bar{c}_l) - \underline{f}_i(x^*, \underset{\sim}{c}_k, \bar{c}_l)| &\le k_x(\underline{f}_i)\|x - x^*\|^\alpha, \\ |\bar{f}_i(x, \underset{\sim}{c}_k, \bar{c}_l) - \bar{f}_i(x^*, \underset{\sim}{c}_k, \bar{c}_l)| &\le k_x(\bar{f}_i)\|x - x^*\|^\alpha. \end{aligned}\right\} \tag{4.3.13}$$

Similarly, our assumptions (H_2') of Hölder continuity properties for the functions F_i with respect to z with C_j fixed, imply similar Hölder continuity properties for $\underline{F}_i$ and $\overline{F}_i$ with respect to z with $\underset{\sim}{C}_k$ and $\overline{C}_l$ fixed and so there are constants K_z, such that

$$\left.\begin{aligned} |\underline{F}_i(z, \underset{\sim}{C}_k, \overline{C}_l) - \underline{F}_i(z^*, \underset{\sim}{C}_k, \overline{C}_l)| &\le K_z(\underline{F}_i)\|z - z^*\|^\alpha, \\ |\overline{F}_i(t, z, \underset{\sim}{C}_k, \overline{C}_l) - \overline{F}_i(t, z^*, \underset{\sim}{C}_k, \overline{C}_l)| &\le K_z(\overline{F}_i)\|z - z^*\|^\alpha. \end{aligned}\right\} \tag{4.3.14}$$

For the purposes of our existence proof, we firstly look at the monotone system $\hat{S}_n, \hat{B}_n$ where we assume our coupling functions f_i and F_i are monotone nondecreasing in c_j and C_j, respectively for all j.

4.3.1 Upper and Lower Solutions and Monotone Iteration

We shall now introduce the concepts of upper and lower solutions relative to the monotone system $\hat{S}_n, \hat{B}_n$.

Definition 4.3.1.

Assume that

(i) For components $i \in I$, where $D_i > 0$, $\underset{\sim}{c}_i$ and $\tilde{c}_i$ are continuous functions in $\overline{\Omega} \times \Lambda$ with continuous first order x_j derivatives in $\overline{\Omega} \times \Lambda$ and continuous second order x_j derivatives in $\Omega \times \Lambda$;

(ii) For components $i \in I$, where $D_i = H_i = 0$, $\underset{\sim}{c}_i$ and $\tilde{c}_i$ are continuous functions in $\overline{\Omega} \times \Lambda$;

(iii) For components $i \in J$, where $\mathcal{D}_i > 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $\overline{\Lambda}$, with continuous first order z_j derivatives in $\overline{\Lambda}$ and continuous second order z_j derivatives in Λ;

(iv) For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $\overline{\Lambda}$, with continuous first order z_j derivatives in Λ;

(v) For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $\overline{\Lambda}$;

The ordered pair of functions $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ with $\underset{\sim}{c}_i \le \tilde{c}_i$ on $\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_i \le \tilde{C}_i$ on $\overline{\Lambda}$ are said to be *lower* and *upper solutions* of $\hat{S}_n$, $\hat{B}_n$ respectively, if they satisfy:

$$
\begin{aligned}
&-D_i\nabla_x^2 \underset{\sim}{c}_i \le f_i(x,\ \underset{\sim}{c}_j) \text{ in } \Omega\times\Lambda,\\
&\frac{\partial \underset{\sim}{c}_i}{\partial n} \le 0 \text{ on } \partial\Omega_1\times\Lambda,\\
&D_i\frac{\partial \underset{\sim}{c}_i}{\partial n} \le H_i(\underset{\sim}{C}_i-\underset{\sim}{c}_i) \text{ on } \partial\Omega_2\times\Lambda,\\
&-\mathcal{D}_i\nabla^2 \underset{\sim}{C}_i+u\cdot\nabla \underset{\sim}{C}_i+H_i\int_{\partial\Omega_2}(\underset{\sim}{C}_i-\underset{\sim}{c}_i) \le F_i(z,\ \underset{\sim}{C}_j) \text{ in } \Lambda,\\
&v_1 \underset{\sim}{C}_i+\mathcal{D}_i\frac{\partial \underset{\sim}{C}_i}{\partial n_1} \le v_1 C_{i,1} \text{ on } \partial\Lambda_1,\\
&\frac{\partial \underset{\sim}{C}_i}{\partial n_\alpha} \le 0 \text{ on } \partial\Lambda_\alpha,\ \alpha = 2, 3,
\end{aligned}
$$

and

$$
\begin{aligned}
&-D_i\nabla_x^2 \tilde{c}_i \ge f_i(x,\ \tilde{c}_j) \text{ in } \Omega\times\Lambda,\\
&\frac{\partial \tilde{c}_i}{\partial n} \ge 0 \text{ on } \partial\Omega_1\times\Lambda,\\
&D_i\frac{\partial \tilde{c}_i}{\partial n} \ge H_i(\tilde{C}_i-\tilde{c}_i) \text{ on } \partial\Omega_2\times\Lambda,\\
&-\mathcal{D}_i\nabla^2 \tilde{C}_i+u\cdot\nabla \tilde{C}_i+H_i\int_{\partial\Omega_2}(\tilde{C}_i-\tilde{c}_i) \ge F_i(z,\ \tilde{C}_j) \text{ in } \Lambda,\\
&v_1 \tilde{C}_i+\mathcal{D}_i\frac{\partial \tilde{C}_i}{\partial n_1} \ge v_1 C_{i,1} \text{ on } \partial\Lambda_1,\\
&\frac{\partial \tilde{C}_i}{\partial n_\alpha} \ge 0 \text{ on } \partial\Lambda_\alpha,\ \alpha = 2, 3,
\end{aligned}
$$

respectively.

We note from the counterexample at the end of section 3.1, that comparison theorems analogous to Theorems 3.2.11 and 3.2.12 do not hold in general in the case of the corresponding steady state or time independent problem $\hat{S}_n, \hat{B}_n$. Hence, if there exist $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ which are *lower* and *upper* solutions of the steady state problem $\hat{S}_n, \hat{B}_n$ and (c_i, C_i) is a solution of $\hat{S}_n, \hat{B}_n$, then in contrast to the unsteady state problem S_n, B_n, we cannot assert that $\underset{\sim}{c}_i \le c_i \le \tilde{c}_i$ and $\underset{\sim}{C}_i \le C_i \le \tilde{C}_i$.

However, the method of monotone iteration is still applicable and shows the existence of at least one solution (c_i, C_i) of $\hat{S}_n, \hat{B}_n$ lying between $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$.

Lower and upper solutions may not always exist for elliptic equations. Therefore, as a result of this, certain unstable solutions cannot be obtained by monotone iteration (PARTER [230], KELLER and COHEN [139], AMANN [9]). However, it must be noted that as with parabolic equations (PAO [222]), there are geometric conditions which the nonlinear reaction functions f_i and F_i may satisfy which guarantee the existence of either lower or upper solutions for elliptic equations (AMANN [9]). These lower and upper solutions may not necessarily exist simultaneously.

As for the system S_n, B_n, it is important to note that the lower and upper solutions provide lower and upper bounds for solutions of $\hat{S}_n, \hat{B}_n$ which can be improved by monotone iterative procedures.

In order to establish an existence theorem for $\hat{S}_n$, $\hat{B}_n$ in terms of upper and lower solutions, we define a transformation $\mathscr{T}$, by

$$(c_i^{(k)},\ C_i^{(k)}) = \mathscr{T}(c_j^{(k-1)},\ C_j^{(k-1)}), \tag{4.6.15}$$

and consider the sequences $\{(c_i^{(k)},\ C_i^{(k)})\}$ where $c_i^{(k)}$ is obtained from the linear system

$$-D_i\nabla_x^2 c_i^{(k)} = f_i(x,\ c_j^{(k-1)}) \text{ in } \Omega\times\Lambda, \tag{4.3.16}$$

$$\frac{\partial c_i^{(k)}}{\partial n} = 0 \text{ on } \partial\Omega_1\times\Lambda, \tag{4.3.17}$$

$$D_i\frac{\partial c_i^{(k)}}{\partial n} + H_i c_i^{(k)} = H_i C_i^{(k-1)} \text{ on } \partial\Omega_2\times\Lambda, \tag{4.3.18}$$

and $C_i^{(k)}$ is obtained from the linear system

$$-\mathscr{D}_i\nabla^2 C_i^{(k)} + u\cdot\nabla C_i^{(k)} + H_i\mathscr{A}C_i^{(k)} = F_i(z,\ C_j^{(k-1)}) + H_i\int_{\partial\Omega_2} c_i^{(k-1)} \text{ in } \Lambda, \tag{4.3.19}$$

$$\upsilon_1 C_i^{(k)} + \mathscr{D}_i\frac{\partial C_i^{(k)}}{\partial n_1} = \upsilon_1 C_{i,1} \text{ on } \partial\Lambda_1, \tag{4.3.20}$$

$$\frac{\partial C_i^{(k)}}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha,\ \alpha=2,\ 3, \tag{4.3.21}$$

with $\underset{\sim}{c}_j \le c_j^{(k-1)} \le \tilde{c}_j$ on $\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_j \le C_j^{(k-1)} \le \tilde{C}_j$ on $\overline{\Lambda}$ for k = 1,....

For each k, the system (4.3.16) consists of $n(I)$ linear, completely uncoupled boundary value problems with boundary conditions given by (4.3.17)-(4.3.18) and this system is uncoupled from the system (4.3.19) which also consists of $n(J)$ linear, completely uncoupled boundary value problems with boundary conditions given by (4.3.20)-(4.3.21).

Since $c_i^{(k)}(x,\ z)$ is not differentiated with respect to z in (4.3.16), Λ may be considered to be a parameter space in (4.3.16)-(4.3.18). For functions $c_i^{(k)}(x,\ z)$ where $D_i = H_i = 0$, Ω may also be considered to be a parameter space and for functions $C_i^{(k)}(z)$, where $\mathscr{D}_i = 0$, $u\cdot\nabla C_i^{(k-1)} \equiv 0$, we may similarly treat Λ as a parameter space. The existence and uniqueness of sequences $\{(c_i^{(k)},\ C_i^{(k)})\}$ may therefore follow from solving standard scalar systems of linear elliptic equations (LADYSHENKAYA [154] or GILBARG and TRUDINGER [106]) which may or may not depend on parameters, systems of first order partial differential equations which may depend on parameters (LAKSHMIKANTHAM *et al.*[160]) and systems of algebraic equations in many variables.

The nonlinear algebraic equations $f_i(x,\ c_j) = 0$ obtained when $D_i = H_i = 0$ may be expressed as $c_i = f_i(x,\ c_j) + c_i$ in order to perform functional iterations to find c_i in terms of c_j. We shall develop a general theory for a broad class of monotone iterations involving such algebraic equations. This class of iterations includes Newton's method as well as a family of methods, which are Newton-Gauss-Seidel processes (ORTEGA and RHEINBOLT [206, 207], LADDE *et al.* [153, p. 36]). It is the Lipschitz property that may be used instead of differentiability in many other iterative methods. Note that $f_i(x,\ c_j) + c_i$ satisfy the Lipschitz and Hölder continuity properties that are assumed on our original $f_i(x,\ c_j)$ as well as the monotonicity in c_j (see Lemma 4.1.1). We may therefore rewrite (4.3.16) as $c_i^{(k)} = f_i(x,\ c_j^{(k-1)}) + c_i^{(k-1)}$ when $D_i = H_i = 0$. The existence and uniqueness of sequences $\{c_i^{(k)}\}$ follows from the uniquely defined solutions to algebraic equations.

The rest of these theorems will require Hölder continuity properties on the functions $f_i(x, c_j^{(k-1)})$ and $F_i(z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)}$ which are satisfied if either $c_j^{(k-1)} \in C^{1+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$, $c_j^{(k-1)} \in C^{\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$, $C_j^{(k-1)} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$ or $C_j^{(k-1)} \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$.

These theorems will also require Hölder continuity properties in the boundary conditions and so we make the following assumptions on $C_{i,1}$. We will assume that $\partial\Omega$ and $\partial\Lambda$ belong to class $C^{2+\alpha}$.

(H$_3'$) $C_{i,1} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$.

The velocity distribution vector function $u(z)$ is also required to satisfy the following Hölder continuity property

(H$_4'$) $\dfrac{u(z)}{u_1(z)} \in C^{\alpha}[\overline{\Lambda}, R^n]$,

where $u_1(z)$ is chosen without loss of generality to be the first component that is nonzero. For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \neq 0$, we shall also need the following additional assumptions

(H$_5'$) Assume that $\overline{\Lambda} = \overline{\Lambda}_1 \times \overline{\Lambda}_{n-1}$, where $\overline{\Lambda}_1 \in R$.

(i) For each $(z_{10}, z_0) \in \overline{\Lambda}_1 \times \overline{\Lambda}_{n-1}$, there exists a unique solution $z(z_1, z_{10}, z_0)$ of

$$\frac{dz}{dz_1} = \frac{u(z)}{u_1(z)}, \quad z(z_{10}) = z_0, \text{ on } \overline{\Lambda}_1, \tag{4.3.22}$$

where z_1 correspondes to the nonzero component $u_1(z)$;

(ii) $z(z_1, z_{10}, z_0)$ is continuously differentiable with respect to (z_{10}, z_0);

(iii) The relationship

$$\frac{\partial z}{\partial z_{10}}(z_1, z_{10}, z_0) + \frac{\partial z}{\partial z_0}(z_1, z_{10}, z_0) u(z_{10}, z_0) \neq 0, \tag{4.3.23}$$

holds.

(H$_6'$) Assume that $\overline{\Lambda}_1$ is the interval $[a, b]$

(i) For each $z_0 \in \overline{\Lambda}_{n-1}$ and $Y_{i0} \in R^{n(J)}$, there exists a unique solution $Y_i(z_1, a, Y_{i0}; z_0)$ of

$$\left.\begin{aligned} \frac{\partial Y_i}{\partial z_1} &= \frac{F_i(z_1, z(z_1, z_{10}, z_0), C_j^{(k-1)}) - H_i \mathcal{S} Y_i + H_i \int_{\partial\Omega_2} c_i^{(k-1)}(z_1, x, z(z_1, z_{10}, z_0))}{u_1(z)}, \\ Y_i(a) &= Y_{i0}, \end{aligned}\right\} \tag{4.3.24}$$

on $\overline{\Lambda}_1$, where $z(z_1, z_{10}, z_0)$ is the unique solution of (4.3.22);

(ii) $Y_i(z_1, a, Y_{i0}; z_0)$ is continuously differentiable with respect to (Y_{i0}, z_0).

Note that assumptions (H$_3'$)-(H$_6'$) will hold in either our original system $\hat{S}_n$, $\hat{B}_n$ or the monotone system $\hat{S}_{2n}$, $\hat{B}_{2n}$ and (H$_6'$) can be shown to hold in the monotone system $\hat{S}_{2n}$, $\hat{B}_{2n}$ if it holds in our original system $\hat{S}_n$, $\hat{B}_n$.

Lemma 4.3.5

Consider the BVP (4.3.16)–(4.3.21) and suppose that the assumptions (H_1), (H_2')-(H_4') *hold. Let there exist* $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ *and* $(\tilde{c}_i, \tilde{C}_i)$ *which are lower and upper solutions respectively of* $\hat{S}_n, \hat{B}_n$ *with* $\underset{\sim}{c}_j \le c_j^{(k-1)} \le \tilde{c}_j$ *on* $\overline{\Omega}\times\Lambda$ *and* $\underset{\sim}{C}_j \le C_j^{(k-1)} \le \tilde{C}_j$ *on* $\overline{\Lambda}$.

Assume that

(i) *For components* $j \in I$, *where* $D_j, H_j > 0$, $c_j^{(k-1)} \in C^{1+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$;

(ii) *For components* $j \in I$, *where* $D_j = H_j = 0$, $c_j^{(k-1)} \in C^{\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$;

(iii) *For components* $j \in J$, *where* $\mathcal{D}_j > 0$, $C_j^{(k-1)} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$;

(iv) *For components* $j \in J$, *where* $\mathcal{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \not\equiv 0$, $C_j^{(k-1)} \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$ *and assumptions* (H_5')-(H_6') *hold;*

(v) *For components* $j \in J$, *where* $\mathcal{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \equiv 0$, $C_j^{(k-1)} \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$.

Then the BVP (4.3.16)-(4.3.21) possesses a unique solution $(c_i^{(k)}, C_i^{(k)})$, *where*

(I) *For components* $i \in I$, *where* $D_i, H_i > 0$, $c_i^{(k)} \in C^{2+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$;

(II) *For components* $i \in I$, *where* $D_i = H_i = 0$, $c_i^{(k)} \in C^{1+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$;

(III) *For components* $i \in J$, *where* $\mathcal{D}_i > 0$, $C_i^{(k)} \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$;

(IV) *For components* $i \in J$, *where* $\mathcal{D}_i = 0$, $u\cdot\nabla C_i^{(k)} \not\equiv 0$, $C_i^{(k)} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$;

(V) *For components* $i \in J$, *where* $\mathcal{D}_i = 0$, $u\cdot\nabla C_i^{(k)} \equiv 0$, $C_i^{(k)} \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$.

Furthermore, in all cases $c_i^{(k)}$ *and* $C_i^{(k)}$ *satisfy the inequalities* $\underset{\sim}{c}_i \le c_i^{(k)} \le \tilde{c}_i$ *in* $\overline{\Omega}\times\Lambda$ *and* $\underset{\sim}{C}_i \le C_i^{(k)} \le \tilde{C}_i$ *in* $\overline{\Lambda}$.

Proof

We first consider the case when D_j, $\mathcal{D}_j > 0$ for all j. It is obvious that for equations (4.3.16)-(4.3.18), all conditions of Theorem 4.1.2 except for those listed in assumption (iv) are satisfied. Note that the function $C_j^{(k-1)}$ in the boundary condition of $c_i^{(k)}$ are functions of z but are independent of x. The function $C_j^{(k-1)}$ therefore satisfies the Hölder continuity property required by assumption (v) of Theorem 4.1.2 and z may be treated as a parameter. It is therefore enough to show that $f_i(x, c_j^{(k-1)}) \in C^{\alpha,\alpha}[\overline{\Omega}\times\Lambda\times R^{n(I)}, R^{n(I)}]$ and this will follow as a special case of (3.6.21).

For a given z in Λ, it follows from Theorem 4.1.2 that (4.3.16)-(4.3.18) has a unique solution $c_i^{(k)}$, where $c_i^{(k)}(x; z) \in C^{2+\alpha}[\overline{\Omega}, R^{n(I)}]$.

To show that $c_i^{(k)}$ is Hölder continuous in z with exponent α, we consider equations (4.3.16)-(4.3.18) with z and $z*$ and look at the difference of these equations. Note that from the assumptions,

$$|f_i(x, c_j^{(k-1)}(x, z)) - f_i(x, c_j^{(k-1)}(x, z^*))| \le k_z(f_i(x, c_j^{(k-1)}))\|z - z^*\|^\alpha,$$

$$|C_j^{(k-1)}(z) - C_j^{(k-1)}(z^*)| \le K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z - z^*\|^\alpha,$$

so that

$$-k_z(f_i(x, c_j^{(k-1)}))\|z - z^*\|^\alpha \le f_i(x, c_j^{(k-1)}(x, z)) - f_i(x, c_j^{(k-1)}(x, z^*)) \le k_z(f_i(x, c_j^{(k-1)}))\|z - z^*\|^\alpha,$$

$$-K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z - z^*\|^\alpha \le C_j^{(k-1)}(z) - C_j^{(k-1)}(z^*)$$
$$\le K_z(C_j^{(k-1)})|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z - z^*\|^\alpha.$$

It then follows that

$$-k_z(f_i(x, c_j^{(k-1)}))\|z - z^*\|^\alpha \le \frac{\partial}{\partial t}(c_i^{(k)}(x, z) - c_i^{(k)}(x, z^*)) - D_i\nabla_x^2(c_i^{(k)}(x, z) - c_i^{(k)}(x, z^*))$$
$$\le k_z(f_i(x, c_j^{(k-1)}))\|z - z^*\|^\alpha, \qquad (4.3.25)$$

$$-K_z(C_j^{(k-1)})H_i|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z - z^*\|^\alpha$$
$$\le D_i\frac{\partial}{\partial n}(c_i^{(k)}(x, z) - c_i^{(k)}(x, z^*)) + H_i(c_i^{(k)}(x, z) - c_i^{(k)}(x, z^*))$$
$$\le K_z(C_j^{(k-1)})H_i|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\|z - z^*\|^\alpha. \qquad (4.3.26)$$

Letting

$$w_{i1} = \frac{c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x, z^*) - k_z(f_i(t, x, c_j^{(k-1)}))\|z - z^*\|^\alpha \frac{1}{2D_i}x_1^2}{K\|z - z^*\|^\alpha}, \qquad (4.3.27)$$

and

$$w_{i2} = \frac{c_i^{(k)}(t, x, z) - c_i^{(k)}(t, x, z^*) + k_z(f_i(t, x, c_j^{(k-1)}))\|z - z^*\|^\alpha \frac{1}{2D_i}x_1^2}{K\|z - z^*\|^\alpha}, \qquad (4.3.28)$$

where

$$K = max\{k_z(f_i(t, x, c_j^{(k-1)})),\ K_z(C_j^{(k-1)})H_i|C_j^{(k-1)}|_{C^1}(d(\overline{\Lambda}))^{1-\alpha}\}, \qquad (4.3.29)$$

we obtain the problems

$$-D_i\nabla_x^2 w_1 \ge 0,\ D_i\frac{\partial w_1}{\partial n} + H_i w_1 \ge -(1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2), \qquad (4.3.30)$$

and

$$-D_i\nabla_x^2 w_2 \le 0,\ D_i\frac{\partial w_2}{\partial n} + H_i w_2 \le 1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2. \qquad (4.3.31)$$

The problems (4.3.30) and (4.3.31) are equivalent and it follows by well known results (see KEADY and MCNABB [137]) that

$$w_1 \geq -(1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2), \tag{4.3.32}$$

and

$$w_2 \leq 1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2. \tag{4.3.33}$$

Therefore

$$-K(1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2)\|z - z^*\|^\alpha \leq (c_i^{(k)}(x, z) - c_i^{(k)}(x, z^*))$$
$$\leq K(1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2)\|z - z^*\|^\alpha, \tag{4.3.34}$$

so that

$$|(c_i^{(k)}(x, z) - c_i^{(k)}(x, z^*))| \leq K(1 + d(\overline{\Omega}) + \frac{H_i}{2D_i}(d(\overline{\Omega}))^2)\|z - z^*\|^\alpha, \tag{4.3.35}$$

i.e., $c_i^{(k)}$ is Hölder continuous in z.

We see that (4.3.16)-(4.3.18) has a unique solution $c_i^{(k)}$, where

$$c_i^{(k)}(x, z) \in C^{2+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]. \tag{4.3.36}$$

Note that the equation (4.3.34) could also have been obtained by integrating (4.3.25) with boundary conditions (4.3.26) and noting that the corresponding Green's function is integrable.

It is obvious that for equations (4.3.19)-(4.3.21), $v_1 \in C^\alpha[\overline{\Lambda}, R^n]$ and all conditions of Theorem 4.1.2 except for those listed in assumption (iv) are satisfied. Therefore, it is enough to show that $F_i(z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)} \in C^\alpha[\overline{\Lambda} \times R^{n(J)}, R^{n(J)}]$ and this follows as a special case of (3.6.37). It follows from Theorem 4.1.2 that (4.6.19)-(4.6.21) has a unique solution $C_i^{(k)}$, where $C_i^{(k)} \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$.

To prove (I) and (II) in the general case, we need only observe that $f_i(x, c_j^{(k-1)}) \in C^{\alpha,\alpha}[\overline{\Omega} \times \Lambda \times R^{n(I)}, R^{n(I)}]$ from (i) and (ii). The proof is similar to that shown earlier.

In the case of (I), we note that for components i, where $D_i, H_i > 0$,

$$c_i^{(k)} \in C^{2+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}], \tag{4.3.37}$$

by the same argument as above using Theorem 4.1.2.

In the case of (II), we note that for components i, where $D_i = H_i = 0$,

$$c_i^{(k)} = f_i(x, c_j^{(k-1)}) + c_i^{(k-1)}$$

exists and is unique since it is uniquely defined. Furthermore, it follows directly that if $f_i(x, c_j^{(k-1)})$ and

$c_i^{(k-1)}$ is Hölder continuous in x and z with exponent α, then $c_i^{(k)}$ is also Hölder continuous in x and z with exponent α, implying that $c_i^{(k)} \in C^{\alpha,\alpha}[\overline{\Omega}\times \Lambda, R^{n(I)}]$.

To prove (III)–(V) in the general case, we need only observe that $F_i(z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)} \in C^{\alpha}[\overline{\Lambda}\times R^{n(J)}, R^{n(J)}]$ from (i)–(v).

In the case of (III), we note that for components i, where $\mathscr{D}_i > 0$,

$$C_i^{(k)} \in C^{2+\alpha}[\overline{\Lambda}\times R^{n(J)}, R^{n(J)}] \tag{4.3.38}$$

by the same arguments as above using Theorem 4.1.2.

In the case of (IV), we note that for components i, where $\mathscr{D}_i = 0$, $u\cdot\nabla C_i^{(k)} \equiv 0$,

$$C_i^{(k)} = \frac{F_i(z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)}}{H_i \mathscr{A}}, \tag{4.3.39}$$

exists and is unique since it is uniquely defined. By the same argument as for the proof of (II), we see that

$$C_i^{(k)} \in C^{\alpha}[\overline{\Lambda}\times R^{n(J)}, R^{n(J)}]. \tag{4.3.40}$$

In the case of (V), we see that by (H_5') and (H_6'), $z(z_1, z_{10}, z_0)$ and $Y_i(z_1, a, Y_{i0}; z_0)$ are unique solutions of (4.3.22) and (4.3.24), respectively, on $\overline{\Lambda}_1$. Choose $Y_{i0} = C_{i,1}(z_0)$ and note that if $z = z(z_1, a, z_0)$, then because of uniqueness, $z_0 = z(a, z_1, z)$. Also, the solution $(z(z_1, a, z_0), Y_i(z_1, a, Y_{i0}; z_0))$ of the systems (4.3.22) and (4.3.24) is a characteristic equation of (4.3.19). Hence, for each solution of (4.3.22) and (4.3.24), we have

$$C_i^{(k)}(z_1, z(z_1, a, z_0)) = Y_i(z_1, a, C_{i,1}(z_0); z_0), \tag{4.3.41}$$

and consequently,

$$C_i^{(k)}(z) = Y_i(z_1, a, C_{i,1}(z(a, z_1, z)); z(a, z_1, z)). \tag{4.3.42}$$

Now by using assumptions (H_5') and (H_6'), it is easy to show that $C_i^{(k)}(z)$ defined by (4.3.42) satisfies (4.3.19).

To show uniqueness of solutions of (4.3.19), we suppose, that $C_{i1}^{(k)}$ and $C_{i2}^{(k)}$ are two solutions of (4.3.19) on $\overline{\Lambda} = \overline{\Lambda}_1 \times \overline{\Lambda}_{n-1}$. By Theorem 3.2.9 (Strong Comparison Theorem) for first order partial differential equations, we see that $C_{i1}^{(k)} \le C_{i2}^{(k)} \le C_{i1}^{(k)}$ and therefore $C_{i1}^{(k)}$ coincides with $C_{i2}^{(k)}$.

The Hölder continuity of $C_i^{(k)}(t,z)$ is obtained by examining the characteristic equations (4.3.22) and (4.3.24), so that

$$C_i^{(k)} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]. \tag{4.3.43}$$

Finally, we show that $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ are lower and upper solutions of $(c_i^{(k)}, C_i^{(k)})$. To show that $(\tilde{c}_i, \tilde{C}_i)$ is an upper solution of $(c_i^{(k)}, C_i^{(k)})$, we need to only observe that

$$-D_i\nabla_x^2(\tilde{c}_i - c_i^{(k)}) \ge f_i(x, \tilde{c}_j) - f_i(x, c_j^{(k-1)}) \ge 0 \text{ in } \Omega\times\Lambda,$$

$$D_i\frac{\partial}{\partial n}(\tilde{c}_i - c_i^{(k)}) + H_i(\tilde{c}_i - c_i^{(k)}) = H_i(\tilde{C}_i - C_i^{(k-1)}) \geq 0 \text{ on } \partial\Omega_2 \times \Lambda,$$

$$\begin{aligned} -\mathcal{D}_i\nabla^2(\tilde{C}_i - C_i^{(k)}) &+ u\cdot\nabla(\tilde{C}_i - C_i^{(k)}) + H_i\mathcal{A}(\tilde{C}_i - C_i^{(k)}) \\ &\geq F_i(z,\ \tilde{C}_j) - F_i(z,\ C_i^{(k-1)}) + H_i\int_{\partial\Omega_2}(\tilde{c}_i - c_i^{(k-1)}) \\ &\geq 0 \text{ in } \Lambda, \end{aligned}$$

since f_i and F_i are monotone in c_j and C_j, respectively.

We may therefore apply Lemma 4.1.8 (Maximum Principle) for the elliptic operator or Theorem 3.2.6 (Strong Comparison Theorem) for first order partial differential equations or algebraic inequalities to conclude that $(\tilde{c}_i,\ \tilde{C}_i) \geq (c_i^{(k)},\ C_i^{(k)})$. Note that in the case for components $i \in I$, where $D_i = H_i = 0$, we have

$$\tilde{c}_i - c_i^{(k)} \geq f_i(x,\ \tilde{c}_j) - f_i(x,\ c_j^{(k-1)}) + \tilde{c}_i - c_i^{(k-1)} \geq 0 \text{ in } \Omega\times\Lambda,$$

and in the case for components $i \in J$, where $\mathcal{D}_i = u\cdot\nabla(\tilde{C}_i - C_i^{(k)}) = 0$, we need only observe that

$$H_i\mathcal{A}(\tilde{C}_i - C_i^{(k)}) \geq F_i(z,\ \tilde{C}_j) - F_i(z,\ C_j^{(k-1)}) + H_i\int_{\partial\Omega_2}(\tilde{c}_i - c_i^{(k-1)}) \geq 0 \text{ in } \Lambda,$$

since f_i and F_i are monotone in c_j and C_j, respectively and therefore $(\tilde{c}_i,\ \tilde{C}_i) \geq (c_i^{(k)},\ C_i^{(k)})$. Similarly, $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ may be shown to be a lower solution of $(c_i^{(k)},\ C_i^{(k)})$ and the theorem is complete.❑

To start off the iterative procedure, we need some continuity properties of $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$. The properties of the mapping $\mathcal{T}$, from $(c_i^{(k-1)},\ C_i^{(k-1)})$ to $(c_i^{(k)},\ C_i^{(k)})$ are then given by the following lemma.

Lemma 4.3.6.

Consider the BVP (4.3.16)-(4.3.21) and suppose that the assumptions (H_1), (H_2')-(H_4') hold. Let there exist $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ which are lower and upper solutions of $\hat{S}_n$, $\hat{B}_n$.

Assume that

(i) *For components $j \in I$, where $D_j, H_j > 0$, $\underset{\sim}{c}_j,\ \tilde{c}_j \in C^{2+\alpha,\alpha}[\overline{\Omega}\times\Lambda,\ R^{n(I)}]$;*

(ii) *For components $j \in I$, where $D_j = H_j = 0$, $\underset{\sim}{c}_j,\ \tilde{c}_j \in C^{\alpha,\alpha}[\overline{\Omega}\times\Lambda,\ R^{n(I)}]$;*

(iii) *For components $j \in J$, where $\mathcal{D}_j > 0$, $\underset{\sim}{C}_j,\ \tilde{C}_j \in C^{2+\alpha}[\overline{\Lambda},\ R^{n(J)}]$;*

(iv) *For components $j \in J$, where $\mathcal{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \not\equiv 0$, $\underset{\sim}{C}_j,\ \tilde{C}_j \in C^{1+\alpha}[\overline{\Lambda},\ R^{n(J)}]$, and assumptions (H_5')-(H_6') hold;*

(v) *For components $j \in J$, where $\mathcal{D}_j = 0$, $u\cdot\nabla C_j^{(k-1)} \equiv 0$, $\underset{\sim}{C}_j,\ \tilde{C}_j \in C^{\alpha}[\overline{\Lambda},\ R^{n(J)}]$.*

Then the mapping $\mathcal{T}$, from $(c_j^{(k-1)},\ C_j^{(k-1)})$ to $(c_i^{(k)},\ C_i^{(k)})$ possesses the following properties:

(I) $(\tilde{c}_i,\ \tilde{C}_i) \geq \mathcal{T}(\tilde{c}_j,\ \tilde{C}_j)$, $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i) \leq \mathcal{T}(\underset{\sim}{c}_j,\ \underset{\sim}{C}_j)$.

(II) *$\mathcal{T}$ is a monotone operator on the intervals $[\underset{\sim}{c}_i,\ \tilde{c}_i]$ and $[\underset{\sim}{C}_i,\ \tilde{C}_i]$.*

Proof

We first consider the case when D_j, $\mathcal{D}_j > 0$ for all components j. The natural imbedding of $C^{2+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ into $C^{2,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$ into $C^2[\overline{\Lambda}, R^{n(J)}]$ implies that $\underset{\sim}{c}_j$, $\tilde{c}_j \in C^{2,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\underset{\sim}{C}_j$, $\tilde{C}_j \in C^2[\overline{\Lambda}, R^{n(J)}]$.

The boundedness of Ω and Λ, together with the fact that their boundaries belong to $C^{2+\alpha}$, shows that, if $c_j^{(k-1)}(x; z) \in C^2[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C_j^{(k-1)}(z) \in C^2[\overline{\Lambda}, R^{n(J)}]$, then $c_j^{(k-1)}(x; z) \in W_q^2[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C_j^{(k-1)}(z) \in W_q^2[\overline{\Lambda}, R^{n(J)}]$ for $q > 1$. From Lemma 4.1.5, we may take q to be identical in both cases.

This, in view of Theorem 4.1.1 (Imbedding Theorem), yields that $c_j^{(k-1)}(x; z) \in C^{1+\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C_j^{(k-1)}(z) \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$. From Lemma 4.1.3, α may be chosen to be identical in both cases. From arguments similar to that shown in the proof of Lemma 4.3.5, we see that $c_j^{(k-1)}(x, z) \in C^{1+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$.

It is immediate that the proof of (I) follows from the choices $(c_j^{(k-1)}, C_j^{(k-1)}) = (\underset{\sim}{c}_j, \underset{\sim}{C}_j)$ and $(c_j^{(k-1)}, C_j^{(k-1)}) = (\tilde{c}_j, \tilde{C}_j)$ in Lemma 4.3.5.

All the other possible cases are treated similarly.

We have shown that if $(c_j^{(0)}, C_j^{(0)}) = (\tilde{c}_j, \tilde{C}_j)$ then $(c_i^{(0)}, C_i^{(0)}) \geq \mathcal{T}(c_j^{(0)}, C_j^{(0)}) = (c_i^{(1)}, C_i^{(1)})$ and if $(c_j^{(0)}, C_j^{(0)}) = (\underset{\sim}{c}_j, \underset{\sim}{C}_j)$ then $(c_i^{(0)}, C_i^{(0)}) \leq \mathcal{T}(c_j^{(0)}, C_j^{(0)}) = (c_i^{(1)}, C_i^{(1)})$. We have, in fact proved that the mapping $\mathcal{T}$ maps intervals $|\underset{\sim}{c}_j, \tilde{c}_j|$ and $|\underset{\sim}{C}_j, \tilde{C}_j|$ onto themselves.

To prove (II), let $c_{j1}, c_{j2} \in [\underset{\sim}{c}_j, \tilde{c}_j]$ and $C_{j1}, C_{j2} \in [\underset{\sim}{C}_j, \tilde{C}_j]$ where $(c_{j1}, C_{j1}) \geq (c_{j2}, C_{j2})$ for all components j. We want to show that $\mathcal{T}(c_{j1}, C_{j1}) \geq \mathcal{T}(c_{j2}, C_{j2})$.

Let $(u_i, U_i) = \mathcal{T}(c_{j1}, C_{j1}) - \mathcal{T}(c_{j2}, C_{j2})$. Then the monotone nondecreasing property of f_i and F_i implies that

$$-D_i\nabla_x^2 u_i = f_i(x, c_{j1}) - f_i(x, c_{j2}) \geq 0 \text{ in } \Omega\times\Lambda, \tag{4.3.44}$$

$$D_i\frac{\partial u_i}{\partial n} + H_i u_i = H_i(C_{i1} - C_{i2}) \geq 0 \text{ on } \partial\Omega_2\times\Lambda, \tag{4.3.45}$$

$$-\mathcal{D}_i\nabla^2 U_i + u\cdot\nabla U_i + H_i\mathcal{A}U_i = F_i(z, C_{j1}) - F_i(z, C_{j2}) + H_i\int_{\partial\Omega_2} c_{i1} - c_{i2} \geq 0 \text{ in } \Lambda, \tag{4.3.46}$$

and from Lemma 4.1.8 (Maximum Principle) for the elliptic operator, or Theorem 3.2.6 (Strong Comparison Theorem) for first order partial differential equations or from algebraic inequalities, we see that $(u_i, U_i) \geq 0$ or $\mathcal{T}(c_{i1}, C_{i1}) \geq \mathcal{T}(c_{i2}, C_{i2})$. This shows that $\mathcal{T}$ is a monotone operator on the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$.□

The monotone operator $\mathcal{T}$ will play a central role in the iteration scheme.

Remark 4.3.1

As with the unsteady state system S_n, B_n, we see that if f_i and F_i are strictly monotone increasing in c_j and C_j, respectively, then by Theorem 3.2.13 (Generalised Strong Comparison (Contact) Theorem), we see that $\mathcal{T}(c_{j1}, C_{j1}) > \mathcal{T}(c_{j2}, C_{j2})$, (unless $\mathcal{T}(c_{j1}, C_{j1}) \equiv \mathcal{T}(c_{j2}, C_{j2})$ in which case the right hand sides of (4.3.44) and (4.3.46) are identically zero; but this happens only if $(c_{j1}, C_{j1}) = (c_{j2}, C_{j2})$, from the strict monotone property of f_i and F_i). We say that the monotone operator $\mathcal{T}$ is monotone operator in the sense of COLLATZ [76], i.e., $(c_{j1}, C_{j1}) \geq (c_{j2}, C_{j2})$ implies that $\mathcal{T}(c_{j1}, C_{j1}) > \mathcal{T}(c_{j2}, C_{j2})$.

Remark 4.3.2

As with the unsteady state problem, S_n, B_n, we see that if f_i and F_i are monotone nonincreasing in c_j and C_j, respectively, the operator $\mathcal{T}$ is alternating on the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$ in the sense that $(c_{j1}, C_{j2}) \geq (c_{j2}, C_{j1})$ implies that $\mathcal{T}(c_{j1}, C_{j2}) \leq \mathcal{T}(c_{j2}, C_{j1})$. To prove this, let $(u_i, U_i) = \mathcal{T}(c_{j1}, C_{j2}) - \mathcal{T}(c_{j2}, C_{j1})$. Then the monotone nonincreasing property of f_i and F_i implies that

$$-D_i\nabla_x^2 u_i = f_i(x, c_{j1}) - f_i(x, c_{j2}) \leq 0 \text{ in } \Omega\times\Lambda,$$

$$D_i\frac{\partial u_i}{\partial n} + H_i u_i = H_i(C_{i1} - C_{i2}) \leq 0 \text{ on } \partial\Omega_2\times\Lambda,$$

$$-\mathcal{D}_i\nabla^2 U_i + u\cdot\nabla U_i + H_i\mathcal{A}U_i = F_i(z, C_{j1}) - F_i(z, C_{j2}) + H_i\int_{\partial\Omega_2}(c_{i1} - c_{i2}) \geq 0 \text{ in } \Lambda,$$

and from the same arguments as in Lemma 4.3.6, $\mathcal{T}c_{j1} \leq \mathcal{T}c_{j2}$ and $\mathcal{T}C_{j1} \geq \mathcal{T}C_{j2}$.

It is necessary to choose a proper initial iteration to ensure that the sequences $\{(c_i^{(k)}, C_i^{(k)})\}$ are monotone sequences that converge to a solution of $\hat{S}_n, \hat{B}_n$ and are within the intervals $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$. From Lemma 4.3.6, it is obvious that the monotonicity of these sequences obviously depend on the monotonicity of f_i and F_i and the initial iteration is taken to be either an upper or a lower solution which is required to satisfy certain inequalities on the corresponding system.

We may therefore use the initial iteration $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$ to construct the sequence $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ from the following equations

$$-D_i\nabla_x^2\overline{c}_i^{(k)} = f_i(x, \overline{c}_j^{(k-1)}) \text{ in } \Omega\times\Lambda,$$

$$D_i\frac{\partial\overline{c}_i^{(k)}}{\partial n} + H_i\overline{c}_i^{(k)} = H_i\overline{C}_i^{(k-1)} \text{ on } \partial\Omega_2\times\Lambda,$$

$$-\mathcal{D}_i\nabla^2\overline{C}_i^{(k)} + u\cdot\nabla\overline{C}_i^{(k)} + H_i\mathcal{A}\overline{C}_i^{(k)} = F_i(z, \overline{C}_j^{(k-1)}) + H_i\int_{\partial\Omega_2}\overline{c}_i^{(k-1)} \text{ in } \Lambda,$$

or the sequence $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ may be determined from the equations

$$-D_i\nabla_x^2\underline{c}_i^{(k)} = f_i(x, \underline{c}_j^{(k-1)}) \text{in } \Omega\times\Lambda,$$

$$D_i\frac{\partial\underline{c}_i^{(k)}}{\partial n} + H_i\underline{c}_i^{(k)} = H_i\underline{C}_i^{(k-1)} \text{ on } \partial\Omega_2\times\Lambda,$$

$$-\mathcal{D}_i\nabla^2\underline{C}_i^{(k)} + u\cdot\nabla\underline{C}_i^{(k)} + H_i\mathcal{A}\underline{C}_i^{(k)} = F_i(z, \underline{C}_j^{(k-1)}) + H_i\int_{\partial\Omega_2}\underline{c}_i^{(k-1)} \text{ in } \Lambda.$$

Note that the sequences $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ and $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ may be obtained independently of each other. As for before, uniqueness and existence of sequences $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ and $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ follow from similar arguments for uncoupled scalar systems of nonhomogeneous linear elliptic differential equations, first order partial differential equations or algebraic equations by using the monotonicity properties of f_i and F_i.

Definition 4.3.2.

The sequences $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$, are called *minimal* and *maximal sequences*, respectively. We say that $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are *minimal* and *maximal solutions* respectively in the regions $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$, if for any solution (c_i, C_i) of $\hat{S}_n, \hat{B}_n$ where $\underset{\sim}{c}_i \leq c_i \leq \tilde{c}_i$ and $\underset{\sim}{C}_i \leq C_i \leq \tilde{C}_i$, then $\underline{c}_i \leq c_i \leq \overline{c}_i$ and $\underline{C}_i \leq C_i \leq \overline{C}_i$.

From Lemma 4.3.6 together with the monotonicity of $\mathscr{T}$, we shall show that the sequence $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ is monotone nondecreasing and the sequence $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ with $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$ is monotone nonincreasing.

Furthermore, $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \leq (\tilde{c}_i, \tilde{C}_i)$ results in $(\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) \leq (\overline{c}_i^{(k)}, \overline{C}_i^{(k)})$ for all k and pointwise limits $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ exist. This is all done in the following lemma for $\hat{S}_n, \hat{B}_n$.

The only difficulty arises for components $i \in J$, where $\mathscr{D}_i = 0$, $u \cdot \nabla C_i^{(k)} \not\equiv 0$, and in this case we will assume in addition that the assumptions (H_7) and (H_8) hold.

Lemma 4.3.7.

Suppose in addition to the assumptions of Lemma 4.3.6, that $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ are minimal sequences and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ are maximal sequences of $\hat{S}_n, \hat{B}_n$. Also, assume that for components $i \in J$, where $\mathscr{D}_i = 0$, $u \cdot \nabla \overline{C}_i^{(k)}$, $u \cdot \nabla \underline{C}_i^{(k)} \not\equiv 0$, that the assumptions ($H_7$)-($H_8$) hold. Then

$$\underset{\sim}{c}_i \leq \underline{c}_i^{(0)} \leq \underline{c}_i^{(1)} \leq \ldots \leq \underline{c}_i^{(k)} \leq \overline{c}_i^{(k)} \leq \ldots \leq \overline{c}_i^{(1)} \leq \overline{c}_i^{(0)} \leq \tilde{c}_i \ \textit{for}\ (x, z) \in \overline{\Omega} \times \Lambda,$$

$$\underset{\sim}{C}_i \leq \underline{C}_i^{(0)} \leq \underline{C}_i^{(1)} \leq \ldots \leq \underline{C}_i^{(k)} \leq \overline{C}_i^{(k)} \leq \ldots \leq \overline{C}_i^{(1)} \leq \overline{C}_i^{(0)} \leq \tilde{C}_i \ \textit{for}\ z \in \overline{\Lambda},$$

for all $k = 1,2,\ldots$ and the pointwise limits

$$\lim_{k \to \infty} (\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) = (\underline{c}_i, \underline{C}_i),$$

$$\lim_{k \to \infty} (\overline{c}_i^{(k)}, \overline{C}_i^{(k)}) = (\overline{c}_i, \overline{C}_i),$$

exist, implying that

$$\underset{\sim}{c}_i \leq \underline{c}_i^{(0)} \leq \underline{c}_i^{(1)} \leq \ldots \leq \underline{c}_i^{(k)} \ldots \leq \underline{c}_i \leq \overline{c}_i \ldots \leq \overline{c}_i^{(k)} \leq \ldots \leq \overline{c}_i^{(1)} \leq \overline{c}_i^{(0)} \leq \tilde{c}_i \ \textit{for}\ (x, z) \in \overline{\Omega} \times \Lambda,$$

$$\underset{\sim}{C}_i \leq \underline{C}_i^{(0)} \leq \underline{C}_i^{(1)} \leq \ldots \leq \underline{C}_i^{(k)} \leq \ldots \leq \underline{C}_i \leq \overline{C}_i \leq \ldots \leq \overline{C}_i^{(k)} \leq \ldots \leq \overline{C}_i^{(1)} \leq \overline{C}_i^{(0)} \leq \tilde{C}_i \ \textit{for}\ z \in \overline{\Lambda},$$

for all $k = 1,2,\ldots$

Proof

Let $(u_i, U_i) = (\overline{c}_i^{(0)} - \overline{c}_i^{(1)}, \overline{C}_i^{(0)} - \overline{C}_i^{(1)}) = (\tilde{c}_i - \overline{c}_i^{(1)}, \tilde{C}_i - \overline{C}_i^{(1)})$, for all i. Then by definition 4.6.1 of upper and lower solutions and definition 4.6.2 of maximal sequences, the following inequalities will hold

$$-D_i \nabla_x^2 u_i = -D_i \nabla_x^2 \tilde{c}_i - f_i(x, \tilde{c}_j) \geq 0 \text{ in } \Omega \times \Lambda,$$

$$D_i \frac{\partial u_i}{\partial n} + H_i u_i = D_i \frac{\partial}{\partial n}(\tilde{c}_i - \overline{c}_i^{(1)}) + H_i(\tilde{c}_i - \overline{c}_i^{(1)}) = D_i \frac{\partial \tilde{c}_i}{\partial n} + H_i(\tilde{c}_i - \tilde{C}_i) \geq 0 \text{ on } \partial\Omega_2 \times \Lambda,$$

$$-\mathscr{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \mathscr{A} U_i = [-\mathscr{D}_i \nabla^2 \tilde{C}_i + u \cdot \nabla \tilde{C}_i + H_i \mathscr{A} \tilde{C}_i] - [F_i(z, \tilde{C}_j) + H_i \int_{\partial\Omega_2} \tilde{c}_i] \geq 0 \text{ in } \Lambda,$$

with similar inequalities holding in the boundary conditions.

We first consider the case when D_j, $\mathscr{D}_j > 0$ for all j. We see that from Lemma 4.1.8 (Maximum Principle) for the elliptic operator that $(u_i, U_i) \geq 0$, i.e. $\overline{c}_i^{(0)} \geq \overline{c}_i^{(1}$ on $\overline{\Omega} \times \Lambda$ and $\overline{C}_i^{(0)} \geq \overline{C}_i^{(1)})$ on $\overline{\Lambda}$.

This result also follows from the monotonicity of $\mathscr{T}$, since if $(\tilde{c}_i, \tilde{C}_i) \geq (\overline{c}_i^{(0)}, \overline{C}_i^{(0)})$, then $\mathscr{T}(\tilde{c}_i, \tilde{C}_i) \geq \mathscr{T}(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\overline{c}_i^{(1)}, \overline{C}_i^{(1)})$ and $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) \geq (\overline{c}_i^{(1)}, \overline{C}_i^{(1)})$ if we let $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$.

Therefore, from Lemma 4.6.5, we conclude that $\bar{c}_i^{(1)} \in C^{2+\alpha,\alpha}[\bar{\Omega} \times \Lambda, R^{n(I)}]$ and $\bar{C}_i^{(1)} \in C^{2+\alpha}[\bar{\Lambda}, R^{n(J)}]$. By natural imbedding this implies that $\bar{c}_i^{(1)} \in C^{2,0}[\bar{\Omega} \times \Lambda, R^{n(I)}]$ and $\bar{C}_i^{(1)} \in C^2[\bar{\Lambda}, R^{n(J)}]$.

All the other possible cases are treated similarly so that

(i) For components $i \in I$, where $D_i = H_i = 0$, $\bar{c}_i^{(1)} \in C^{0,0}[\bar{\Omega} \times \Lambda, R^{n(I)}]$,
(ii) For components $i \in J$, where $\mathscr{D}_i = 0$, $u \cdot \nabla \bar{C}_i^{(1)} \not\equiv 0$, $\bar{C}_i^{(1)} \in C^1[\bar{\Lambda}, R^{n(J)}]$
(iii) For components $i \in J$, where $\mathscr{D}_i = 0$, $u \cdot \nabla \bar{C}_i^{(1)} \equiv 0$, $\bar{C}_i^{(1)} \in C^0[\bar{\Lambda}, R^{n(J)}]$.

In the case of (iii), we see that if (H_7)-(H_8) are assumed, then from properties of aglebraic equations we see that $\bar{C}_i^{(1)}$ will be continuously differentiable in z. Therefore, if (H_7)-(H_8) are assumed then in all cases for components $j \in J$, $\bar{C}_j^{(1)}$ will be continuously differentiable in z. Furthermore, in all cases for components $i \in I$, where $D_i, H_i > 0$, it can be demonstrated from (4.3.18) that $\bar{c}_i^{(2)}$ will also be continuously differentiable in z.

We may similarly show using by the definitions of upper and lower solutions and of minimal sequences, that $\underline{c}_i^{(0)} \le \underline{c}_i^{(1)}$ and $\underline{C}_i^{(0)} \le \underline{C}_i^{(1)}$.

Now let $(u_i, U_i) = (\bar{c}_i^{(1)} - \underline{c}_i^{(1)}, \bar{C}_i^{(1)} - \underline{C}_i^{(1)})$. Then the monotone nondecreasing property of f_i and F_i implies that

$$-D_i \nabla_x^2 u_i = f_i(x, \bar{c}_j^{(0)}) - f_i(x, \underline{c}_j^{(0)}) = f_i(x, \tilde{c}_j) - f_i(x, \underset{\sim}{c}_j) \ge 0 \text{ in } \Omega \times \Lambda,$$

$$D_i \frac{\partial u_i}{\partial n} + H_i u_i = [D_i \frac{\partial \bar{c}_i^{(1)}}{\partial n} + H_i \bar{c}_i^{(1)}] - [D_i \frac{\partial \underline{c}_i^{(1)}}{\partial n} + H_i \underline{c}_i^{(1)}] = H_i(\bar{C}_i^{(0)} - \underline{C}_i^{(0)}) = H_i(\tilde{C}_i - \underset{\sim}{C}_i) \ge 0 \text{ on } \partial\Omega_2 \times \Lambda,$$

$$-\mathscr{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \mathscr{A} U_i = F_i(z, \tilde{C}_j) - F_i(z, \underset{\sim}{C}_j) + H_i \int_{\partial\Omega_2} (\tilde{c}_i - \underset{\sim}{c}_i) \ge 0 \text{ in } \Lambda,$$

and it follows from the monotonicity of $\mathscr{T}$, that

$$(\underline{c}_i^{(1)}, \underline{C}_i^{(1)}) \le (\bar{c}_i^{(1)}, \bar{C}_i^{(1)}),$$

implying that

$$\underset{\sim}{c}_i \le \underline{c}_i^{(0)} \le \underline{c}_i^{(1)} \le \bar{c}_i^{(1)} \le \bar{c}_i^{(0)} \le \tilde{c}_i \text{ for } (x, z) \in \bar{\Omega} \times \Lambda,$$

and

$$\underset{\sim}{C}_i \le \underline{C}_i^{(0)} \le \underline{C}_i^{(1)} \le \bar{C}_i^{(1)} \le \bar{C}_i^{(0)} \le \tilde{C}_i \text{ for } z \in \bar{\Lambda}.$$

Assume, by induction, that

$$\bar{c}_i^{(k)} \le \bar{c}_i^{(k-1)} \text{ and } \bar{C}_i^{(k)} \le \bar{C}_i^{(k-1)},$$

for $k=1,..,m$.

The only difficulty arises for components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla \overline{C}_i^{(k)} \not\equiv 0$ and in this case we cannot assume that in general, that the assumption (H_6') will be satisfied. However, in this case we can assume that (H_7)-(H_8) hold so that $\overline{C}_j^{(k-1)}$ and $\overline{C}_j^{(k-2)}$ will be continuously differentiable in z for all j by earlier arguments. Thus for components $i \in I$, where $D_i, H_i > 0$, it can be shown that $c_i^{(k-1)}$ will be continuously differentiable in z from (4.3.18), so that by assumptions (H_7)-(H_8), $F_i(z, C_j^{(k-1)}) + H_i \int_{\partial\Omega_2} c_i^{(k-1)}$ will be continuously differentiable in z. For components $i \in I$, where $D_i = H_i = 0$, we see that in this case by assumptions (H_7)-(H_8), $F_i(z, C_j^{(k-1)})$ will be continuously differentiable in z. It then follows that (HARTMAN [119, pp. 95-99]) assumption (H_6') will be satisfied in the general case.

The functions $(u_i, U_i) = (\overline{c}_i^{(m)} - \overline{c}_i^{(m+1)}, \overline{C}_i^{(m)} - \overline{C}_i^{(m+1)})$ and the monotone nondecreasing property of f_i and F_i implies that

$$-D_i \nabla_x^2 u_i = f_i(x, \overline{c}_j^{(m-1)}) - f_i(x, \overline{c}_j^{(m)}) \geq 0 \text{ in } \Omega \times \Lambda,$$

$$D_i \frac{\partial u_i}{\partial n} + H_i u_i = [D_i \frac{\partial \overline{c}_i^{(m)}}{\partial n} + H_i \overline{c}_i^{(m)}] - [D_i \frac{\partial \overline{c}_i^{(m+1)}}{\partial n} + H_i \overline{c}_i^{(m+1)}] = H_i(\overline{C}_i^{(m-1)} - \overline{C}_i^{(m)}) \geq 0 \text{ on } \partial\Omega_2 \times \Lambda,$$

$$-\mathcal{D}_i \nabla^2 U_i + u \cdot \nabla U_i + H_i \mathcal{A} U_i = F_i(z, \overline{C}_i^{(m)}) - F_i(z, \overline{C}_i^{(m)}) + H_i \int_{\partial\Omega_2} (\overline{c}_i^{(m)} - \overline{c}_i^{(m)}) \geq 0 \text{ in } \Lambda,$$

with similar inequalities in the boundary conditions. This ensures that

$$\overline{c}_i^{(m)} \geq \overline{c}_i^{(m+1)} \text{ and } \overline{C}_i^{(m)} \geq \overline{C}_i^{(m+1)},$$

from the monotonicity of $\mathcal{T}$ and proves that $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ with $(\overline{c}_i^{(0)}, \overline{C}_i^{(0)}) = (\tilde{c}_i, \tilde{C}_i)$ is a monotonic nonincreasing sequence.

It follows from a similar induction argument that $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ with $(\underline{c}_i^{(0)}, \underline{C}_i^{(0)}) = (\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ is a monotonic nondecreasing sequence and by a similar induction argument $\overline{c}_i^{(k-1)} \geq \underline{c}_i^{(k-1)}$ and $\overline{C}_i^{(k-1)} \geq \underline{C}_i^{(k-1)}$ for $k=1,...,m$ ensures that $\overline{c}_i^{(m+1)} \geq \underline{c}_i^{(m+1)}$ and $\overline{C}_i^{(m+1)} \geq \underline{C}_i^{(m+1)}$. The following inequalities then hold

$$\underset{\sim}{c}_i \leq \underline{c}_i^{(0)} \leq \underline{c}_i^{(1)} \leq ... \leq \underline{c}_i^{(k)} \leq \overline{c}_i^{(k)} \leq ... \leq \overline{c}_i^{(1)} \leq \overline{c}_i^{(0)} \leq \tilde{c}_i \text{ for } (x, z) \in \overline{\Omega} \times \Lambda,$$

$$\underset{\sim}{C}_i \leq \underline{C}_i^{(0)} \leq \underline{C}_i^{(1)} \leq ... \leq \underline{C}_i^{(k)} \leq \overline{C}_i^{(k)} \leq ... \leq \overline{C}_i^{(1)} \leq \overline{C}_i^{(0)} \leq \tilde{C}_i \text{ for } z \in \overline{\Lambda},$$

for all $k = 1, 2,...$

It follows from the monotonic property of our maximal and minimal sequences, its boundedness by $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ and the monotone convergence theorem that the pointwise limits

$$\lim_{k \to \infty} (\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) = (\underline{c}_i, \underline{C}_i),$$

$$\lim_{k \to \infty} (\overline{c}_i^{(k)}, \overline{C}_i^{(k)}) = (\overline{c}_i, \overline{C}_i),$$

exist. Therefore,

$$\underset{\sim}{c}_i \leq \underline{c}_i^{(0)} \leq \underline{c}_i^{(1)} \leq ... \leq \underline{c}_i^{(k)} ... \leq \underline{c}_i \leq \overline{c}_i ... \leq \overline{c}_i^{(k)} \leq ... \leq \overline{c}_i^{(1)} \leq \overline{c}_i^{(0)} \leq \tilde{c}_i \; for \; (x, z) \in \overline{\Omega} \times \Lambda,$$

$$\underset{\sim}{C}_i \leq \underline{C}_i^{(0)} \leq \underline{C}_i^{(1)} \leq ... \leq \underline{C}_i^{(k)} \leq ... \leq \underline{C}_i \leq \overline{C}_i \leq ... \leq \overline{C}_i^{(k)} \leq ... \leq \overline{C}_i^{(1)} \leq \overline{C}_i^{(0)} \leq \tilde{C}_i \; for \; z \in \overline{\Lambda},$$

for all $k = 1,2,...$ □

4.3.3 Existence of Solutions of the monotone system $\hat{S}_n$, $\hat{B}_n$

It can be shown that our minimal and maximal sequences $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ converge not only pointwise but converge uniformly (in appropriate function spaces) as well. The following theorem is an existence theorem for solutions to the monotone system $\hat{S}_n$, $\hat{B}_n$. This theorem shows the existence of at least one solution (c_i, C_i) of $\hat{S}_n$, $\hat{B}_n$ lying between $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$

Theorem 4.3.1 (Generalised Existence Theorem)

Let the assumptions of Lemma 4.3.7 hold. Then the minimal and maximal sequences $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ converge monotonically and uniformly from below and above to $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ respectively, where $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are solutions of $\hat{S}_n$, $\hat{B}_n$. Moreover $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are minimal and maximal solutions respectively of S_n, B_n in the regions $[\underset{\sim}{c}_i, \tilde{c}_i]$ and $[\underset{\sim}{C}_i, \tilde{C}_i]$.

Proof

We first consider the case with D_i, $\mathcal{D}_i > 0$ for all i.

Let $\underline{c}_i^{(k)}$, $\overline{c}_i^{(k)} \in C^{2+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$ and $\underline{C}_i^{(k)}$, $\overline{C}_i^{(k)} \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$ for $k = 1,2,...$ and let us consider the maximal sequence $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$.

We note that $C^{2+\alpha}[\overline{\Omega}, R^{n(I)}] \subseteq W_{p_1}^2[\overline{\Omega}, R^{n(I)}]$ and $C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}] \subseteq W_{p_2}^2[\overline{\Lambda}, R^{n(J)}]$ for $p_1 \geq (m_1+2)/(1-\alpha)$ and $p_2 \geq (m_2+2)/(1-\alpha)$.

From Lemma 4.1.5, this implies that $C^{2+\alpha}[\overline{\Omega}, R^{n(I)}] \subseteq W_q^2[\overline{\Omega}, R^{n(I)}]$ and $C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}] \subseteq W_q^2[\overline{\Lambda}, R^{n(J)}]$, where $q = \min\{p_1, p_2\}$.

By Theorem 4.1.4, we see that $\overline{c}_i^{(k)}$ (with Λ treated as a parameter space) and $\overline{C}_i^{(k)}$ satisfy the following Agmon-Douglis-Nirenberg estimates (see Theorem 4.1.5):

$$\|\overline{c}_i^{(k)}\|_{W_q^2[\overline{\Omega}, R^{n(I)}]} \leq C(\|f_i(x, \overline{c}_j^{(k-1)})\|_{L^q[\overline{\Omega}, R^{n(I)}]} + \|\overline{C}_i^{(k-1)}\|_{W_q^1[\partial\Omega_1, R^{n(I)}]}) \tag{4.3.47}$$

and

$$\|\overline{C}_i^{(k)}\|_{W_q^2[\overline{\Lambda}, R^{n(J)}]} \leq C(\|F_i(z, \overline{C}_j^{(k-1)}) + \int_{\partial\Omega_2} \overline{c}_i^{(k-1)}\|_{L^q[\overline{\Lambda}, R^{n(J)}]} + \|C_{i,1}\|_{W_q^1[\partial\Lambda_1, R^{n(J)}]}). \tag{4.3.48}$$

The fact that $\overline{c}_j^{(k-1)} \in [\underset{\sim}{c}_j, \tilde{c}_j]$ and $\overline{C}_j^{(k-1)} \in [\underset{\sim}{C}_j, \tilde{C}_j]$, i.e., $\overline{c}_j^{(k-1)}$ and $\overline{C}_j^{(k-1)}$ are bounded, the continuity of f_i and of F_i imply by the continuity and boundedness of the Nemytskii operator (Lemma 4.1.6) that the sequences $\{f_i(x, \overline{c}_j^{(k-1)})\}$ and $\{F_i(z, \overline{C}_j^{(k-1)}) + \int_{\partial\Omega_2} \overline{c}_i^{(k-1)}\}$ are uniformly bounded in $C[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C[\overline{\Lambda}, R^{n(J)}]$ respectively.

Since $C[\overline{\Omega}, R^{n(I)}]$ and $C[\overline{\Lambda}, R^{n(J)}]$ are dense in $L^q[\overline{\Omega}, R^{n(I)}]$ and $L^q[\overline{\Lambda}, R^{n(J)}]$, it follows by the continuity and boundedness of the Nemytskii operator (Lemma 4.1.7) that $\{f_i(x, \overline{c}_j^{(k-1)})\}$ and $\{F_i(z, \overline{C}_j^{(k-1)}) + \int_{\partial\Omega_2} \overline{c}_i^{(k-1)}\}$ are bounded sequences in $L^q[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $L^q[\overline{\Lambda}, R^{n(J)}]$, respectively. ,

This, together with the above estimates (4.3.47) and (4.3.48) shows that the sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ are uniformly bounded in $W_q^2[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $W_q^2[\overline{\Lambda}, R^{n(J)}]$ respectively. Therefore by application of Theorem 4.1.1 (Imbedding Theorem), we obtain

$$\|\overline{c}_i^{(k)}\|_{C^{1+\alpha}[\overline{\Omega}, R^{n(I)}]} \leq C\|\overline{c}_i^{(k)}\|_{W_q^2[\overline{\Omega}, R^{n(I)}]}, \tag{4.3.49}$$

and

$$\|\overline{C}_i^{(k)}\|_{C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]} \leq C\|\overline{C}_i^{(k)}\|_{W_q^2[\overline{\Lambda}, R^{n(J)}]}, \tag{4.3.50}$$

for all $k = 1,2,..$, where C in both estimates are independent of any element of $W_q^2[\overline{\Omega}, R^{n(I)}]$ or $W_q^2[\overline{\Lambda}, R^{n(J)}]$.

From (4.3.49) and (4.3.50), we can conclude that every uniformly bounded sequence in $W_q^2[\overline{\Omega}, R^{n(I)}]$ and $W_q^2[\overline{\Lambda}, R^{n(J)}]$ is also uniformly bounded in $C^{1+\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$, respectively. From Lemma 4.1.3, we may take α in both cases to be identical.

Thus the sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ are uniformly bounded in $C^{1+\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$. Therefore, by applying Lemma 4.1.6 $\{f_i(x, \overline{c}_j^{(k-1)})\}$ and $\{F_i(z, \overline{C}_j^{(k-1)})+\int_{\partial\Omega_2} \overline{c}_i^{(k-1)}\}$ are also bounded sequences in $C^{\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$, respectively. Hence by the Schauder type estimates (Theorem 4.1.3), we have

$$\|\overline{c}_i^{(k)}\|_{C^{2+\alpha}[\overline{\Omega},\, R^{n(I)}]} \le C(\|f_i(x, \overline{c}_j^{(k-1)})\|_{C^{\alpha}[\overline{\Omega},\, R^{n(I)}]} + \|\overline{C}_i^{(k-1)}\|_{C^{1+\alpha}[\partial\Omega_1,\, R^{n(I)}]}) \tag{4.3.51}$$

and

$$\|\overline{C}_i^{(k)}\|_{C^{2+\alpha}[\overline{\Lambda},\, R^{n(J)}]} \le C(\|F_i(z, \overline{C}_j^{(k-1)}) + \int_{\partial\Omega_2} \overline{c}_i^{(k-1)}\|_{C^{\alpha}[\overline{\Lambda},\, R^{n(J)}]} + \|C_{i,1}\|_{C^{1+\alpha}[\partial\Lambda_1,\, R^{n(J)}]}) \tag{4.3.52}$$

for all $k = 1,2,..$, which implies the uniform boundedness of sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ in $C^{2+\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$, respectively.

We may use arguments given in Lemma 4.3.5 to show that sequences $\{\overline{c}_i^{(k)}\}$ are Hölder continuous in z with exponent α and may be shown to be uniformly bounded in Λ.

Therefore, by the natural compact imbedding of $C^{2+\alpha,\alpha}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$ into $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2}[\overline{\Lambda}, R^{n(J)}]$, the sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ are relatively compact in $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2}[\overline{\Lambda}, R^{n(J)}]$ respectively.

This implies that there exists subsequences of $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ which converge in $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2}[\overline{\Lambda}, R^{n(J)}]$ respectively.

Let $(\overline{\overline{c}}_i, \overline{\overline{C}}_i)$ where $\overline{\overline{c}}_i \in C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\overline{\overline{C}}_i \in C^{1,2}[\overline{\Lambda}, R^{n(J)}]$ be the limit of this subsequence. On the other hand, we have shown that the sequence $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$ converges pointwise to $(\overline{c}_i, \overline{C}_i)$. Therefore, $\overline{\overline{c}}_i = \overline{c}_i$ on $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\overline{\overline{C}}_i = \overline{C}_i$ on $C^{2}[\overline{\Lambda}, R^{n(J)}]$. This shows that the whole sequences $\{\overline{c}_i^{(k)}\}$ and $\{\overline{C}_i^{(k)}\}$ converge in $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2}[\overline{\Lambda}, R^{n(J)}]$ to $\overline{c}_i$ and $\overline{C}_i$ respectively, that is $\lim_{k\to\infty} \overline{c}_i^{(k)} = \overline{c}_i$ in $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $\lim_{k\to\infty} \overline{C}_i^{(k)} = \overline{C}_i$ in $C^{2}[\overline{\Lambda}, R^{n(J)}]$ and $\underset{\sim}{c}_i \le \overline{c}_i \le \tilde{c}_i$ on $\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_i \le \overline{C}_i \le \tilde{C}_i$ on $\overline{\Lambda}$.

Similarly, by imitating the preceding argument relative to the minimal sequence $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$, one can conclude that the sequences $\{\underline{c}_i^{(k)}\}$ and $\{\underline{C}_i^{(k)}\}$ converge monotonically in $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2}[\overline{\Lambda}, R^{n(J)}]$ respectively; their limits are denoted by $\underline{c}_i$ and $\underline{C}_i$ which belong to $C^{2,0}[\overline{\Omega}\times\Lambda, R^{n(I)}]$ and $C^{2}[\overline{\Lambda}, R^{n(J)}]$ respectively and satisfy the relation $\underset{\sim}{c}_i \le \underline{c}_i \le \tilde{c}_i$ on $\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_i \le \underline{C}_i \le \tilde{C}_i$ on $\overline{\Lambda}$. Thus the limits

$$\lim_{k\to\infty} [-D_i\nabla_x^2 \underline{c}_i^{(k)}] = -D_i\nabla_x^2 \underline{c}_i, \quad \lim_{k\to\infty} [f_i(x, \underline{c}_j^{(k-1)})] = f_i(x, \underline{c}_j),$$

$$\lim_{k\to\infty} [D_i \frac{\partial \underline{c}_i^{(k)}}{\partial n} + H_i \underline{c}_i^{(k)}] = D_i \frac{\partial \underline{c}_i}{\partial n} + H_i \underline{c}_i, \quad \lim_{k\to\infty} [H_i \underline{C}_i^{(k-1)}] = H_i \underline{C}_i,$$

$$\lim_{k\to\infty} [-\mathscr{D}_i\nabla^2 \underline{C}_i^{(k)} + u\cdot\nabla \underline{C}_i^{(k)} + H_i\mathscr{A}\underline{C}_i^{(k)}] = -\mathscr{D}_i\nabla^2 \underline{C}_i + u\cdot\nabla \underline{C}_i + H_i\mathscr{A}\underline{C}_i,$$

$$\lim_{k\to\infty} [F_i(z, \underline{C}_j^{(k-1)}) + H_i\int_{\partial\Omega_2} \underline{c}_i^{(k-1)}] = F_i(z, \underline{C}_j) + H_i\int_{\partial\Omega_2} \underline{c}_i$$

and

$$\lim_{k\to\infty}[-D_i\nabla_x^2\bar{c}_i^{(k)}]=-D_i\nabla_x^2\bar{c}_i,\quad \lim_{k\to\infty}[f_i(x,\,\bar{c}_j^{(k-1)})]=f_i(x,\,\bar{c}_j),$$

$$\lim_{k\to\infty}[D_i\frac{\partial\bar{c}_i^{(k)}}{\partial n}+H_i\bar{c}_i^{(k)}]=D_i\frac{\partial\bar{c}_i}{\partial n}+H_i\bar{c}_i,\quad \lim_{k\to\infty}[H_i\bar{C}_i^{(k-1)}]=H_i\bar{C}_i,$$

$$\lim_{k\to\infty}[-\mathcal{D}_i\nabla^2\bar{C}_i^{(k)}+u\cdot\nabla\bar{C}_i^{(k)}+H_i\mathcal{A}\bar{C}_i^{(k)}]=-\mathcal{D}_i\nabla^2\bar{C}_i+u\cdot\nabla\bar{C}_i+H_i\mathcal{A}\bar{C}_i,$$

$$\lim_{k\to\infty}[F_i(z,\,\bar{C}_j^{(k-1)})+H_i\int_{\partial\Omega_2}\bar{c}_i^{(k-1)}]=F_i(z,\,\bar{C}_j)+H_i\int_{\partial\Omega_2}\bar{c}_i,$$

etc. exist uniformly on $C^{2,0}[\bar{\Omega}\times\Lambda,\,R^{n(I)}]$ and $C^2[\bar{\Lambda},\,R^{n(J)}]$, respectively. Thus we conclude that $(\underline{c}_i,\,\underline{C}_i)$ and $(\bar{c}_i,\,\bar{C}_i)$ are solutions of the BVP

$$-D_i\nabla_x^2\underline{c}_i=f_i(x,\,\underline{c}_j),$$

$$D_i\frac{\partial\underline{c}_i}{\partial n}+H_i\underline{c}_i=H_i\underline{C}_i,$$

$$-\mathcal{D}_i\nabla^2\underline{C}_i+u\cdot\nabla\underline{C}_i+H_i\mathcal{A}\underline{C}_i=F_i(z,\,\underline{C}_j)+H_i\int_{\partial\Omega_2}\underline{c}_i,$$

and

$$-D_i\nabla_x^2\bar{c}_i=f_i(x,\,\bar{c}_j),$$

$$D_i\frac{\partial\bar{c}_i}{\partial n}+H_i\bar{c}_i=H_i\bar{C}_i,$$

$$-\mathcal{D}_i\nabla^2\bar{C}_i+u\cdot\nabla\bar{C}_i+H_i\mathcal{A}\bar{C}_i=F_i(z,\,\bar{C}_j)+H_i\int_{\partial\Omega_2}\bar{c}_i,$$

respectively.

We therefore have that $(\underline{c}_i,\,\underline{C}_i)$ and $(\bar{c}_i,\,\bar{C}_i)$ are solutions of $\hat{S}_n,\,\hat{B}_n$.

For components i, where $D_i = H_i = 0$, the uniform convergence of sequences $\{c_i^{(k)}\}$ to solutions $\underline{c}_i$ and $\bar{c}_i$ follows from standard theory on nonlinear algebraic equations. The sequence of approximations (4.3.16) are uniformly bounded and equicontinuous and hence possesses uniformly convergent subsequences. The rest of the argument follows along similar lines to that already discussed. The case for components i, where $\mathcal{D}_i = 0$, $u\cdot\nabla C_i^{(k)}\equiv 0$ is similar as is the case for components i, where $\mathcal{D}_i = 0$, $u\cdot\nabla C_i^{(k)}\not\equiv 0$.

Now we show that $(\underline{c}_i,\,\underline{C}_i)$ and $(\bar{c}_i,\,\bar{C}_i)$ are minimal and maximal solutions of $\hat{S}_n,\,\hat{B}_n$. Let $(c_i,\,C_i)$ be any solution of $\hat{S}_n,\,\hat{B}_n$ such that $\underline{c}_i\le c_i\le\bar{c}_i$ and $\underline{C}_i\le C_i\le\bar{C}_i$.

Since $(c_i,\,C_i)=\mathcal{T}(c_i,\,C_i)$, it follows by Lemma 4.3.6 and from the definitions of $\{(\underline{c}_i^{(k)},\ \underline{C}_i^{(k)})\}$ and $\{(\bar{c}_i^{(k)},\ \bar{C}_i^{(k)})\}$, that

$$(\underset{\sim}{c}_i,\,\underset{\sim}{C}_i)\le(c_i,\,C_i)\le(\tilde{c}_i,\,\tilde{C}_i),$$

implies that

$$(\underset{\sim}{c}_i,\,\underset{\sim}{C}_i)\le\mathcal{T}(\underline{c}_i^{(0)},\,\underline{C}_i^{(0)})\le(c_i,\,C_i)=\mathcal{T}(c_i,\,C_i)\le\mathcal{T}(\bar{c}_i^{(0)},\,\bar{C}_i^{(0)})\le(\tilde{c}_i,\,\tilde{C}_i).$$

Let us assume that for some $m>1$,

$$(\underline{c}_i^{(m)}, \underline{C}_i^{(m)}) \leq (c_i, C_i) = (\overline{c}_i^{(m)}, \overline{C}_i^{(m)}).$$

Then we shall show that

$$(\underline{c}_i^{(m+1)}, \underline{C}_i^{(m+1)}) \leq (c_i, C_i) = (\overline{c}_i^{(m+1)}, \overline{C}_i^{(m+1)}).$$

From Lemma 4.3.6 (II) and from the definitions of $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\overline{c}_i^{(k)}, \overline{C}_i^{(k)})\}$, we arrive at

$$(\underline{c}_i^{(m+1)}, \underline{C}_i^{(m+1)}) = \mathcal{T}(\underline{c}_i^{(m)}, \underline{C}_i^{(m)}) \leq (c_i, C_i) = \mathcal{T}(c_i, C_i) \leq \mathcal{T}(\overline{c}_i^{(m)}, \overline{C}_i^{(m)}) = (\overline{c}_i^{(m+1)}, \overline{C}_i^{(m+1)}).$$

Thus, it follows by mathematical induction that

$$(\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) \leq (c_i, C_i) = (\overline{c}_i^{(k)}, \overline{C}_i^{(k)}),$$

for all $k = 1,2,...$

Hence, we have

$$(\underline{c}_i, \underline{C}_i) \leq (c_i, C_i) \leq (\overline{c}_i, \overline{C}_i),$$

proving that $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ are minimal and maximal solutions of $\hat{S}_n$, $\hat{B}_n$.□

Remark 4.3.3

Note that unlike the unsteady state system S_n, B_n, we cannot assume that for the steady state system $\hat{S}_n$, $\hat{B}_n$ that $(\underline{c}_i, \underline{C}_i) \equiv (\overline{c}_i, \overline{C}_i) \equiv (c_i, C_i)$ unless we have uniqueness of solutions of the system $\hat{S}_n$, $\hat{B}_n$. We have given some uniqueness criteria in section 3.3 for the system $\hat{S}_n$, $\hat{B}_n$ and these can be used to show that $(\underline{c}_i, \underline{C}_i) \equiv (\overline{c}_i, \overline{C}_i) \equiv (c_i, C_i)$. Other uniqueness conditions for systems of elliptic equations are given by LADDE *et al.*[153, p.121] and CARL and GROSSMAN [47] and may also be applied to our problem. These conditions are used to show that our minimal and maximal solutions obtained by monotone iteration satisfy the inequalities $(\underline{c}_i, \underline{C}_i) \geq (\overline{c}_i, \overline{C}_i)$ and hence uniqueness is achieved.

For the general system $\hat{S}_n$, $\hat{B}_n$, which may possess no monotone properties, the following theorem follows from Theorem 4.2.1 and summarises how we may set up monotone sequences for this general system which converge to a solution of a new system which may relate in some way to the solution of the original system $\hat{S}_n$, $\hat{B}_n$.

Theorem 4.3.2

The general system $\hat{S}_n$, $\hat{B}_n$ for which f_i and F_i satisfies Lipschitz continuity properties (H_1') and Hölder continuity properties (H_2'), may be imbedded in a system $\hat{S}_{2n}^*$, $\hat{B}_{2n}^*$ of twice the order which is coupled by monotone functions f_i^* and F_i^* of the new dependent variables v_i and V_i. Moreover, all the solutions (c_i, C_i) of the general system $\hat{S}_n$, $\hat{B}_n$ are solutions of the new system, where

$$v_i = c_i, \quad v_{n(I)+i} = -c_i \quad for\ i=1,..,n(I) \tag{4.3.53}$$

and

$$V_i = C_i, \quad V_{n(J)+i} = -C_i \quad for\ i=1,..,n(J). \tag{4.3.54}$$

Let $(\underline{v}_i, \underline{V}_i)$ and $(\tilde{v}_i, \tilde{V}_i)$ be lower and upper solutions for the system $\hat{S}_{2n}^*$, $\hat{B}_{2n}^*$ with continuity properties given in the assumptions of Lemma 4.3.6. Let also the assumptions of Lemma 4.3.7 hold for the system $\hat{S}_{2n}^*$, $\hat{B}_{2n}^*$. Then the minimal and maximal sequences $\{(\underline{v}_i^{(k)}, \underline{V}_i^{(k)})\}$ and $\{(\overline{v}_i^{(k)}, \overline{V}_i^{(k)})\}$ of S_{2n}^*, B_{2n}^* given by

Theorem 4.3.1 converge monotonically and uniformly from below and above to $(\underline{v}_i, \underline{V}_i)$ *and* $(\overline{v}_i, \overline{V}_i)$ *respectively, where* $(\underline{v}_i, \underline{V}_i)$ *and* $(\overline{v}_i, \overline{V}_i)$ *are solutions of* $\hat{S}^*_{2n}, \hat{B}^*_{2n}$ *satisfying the following inequalities*

$$\underset{\sim}{v}_i \le \underline{v}_i^{(0)} \le \underline{v}_i^{(1)} \le \ldots \le \underline{v}_i^{(k)} \ldots \le \underline{v}_i \le \overline{v}_i \ldots \le \overline{v}_i^{(k)} \le \ldots \le \overline{v}_i^{(1)} \le \overline{v}_i^{(0)} \le \tilde{v}_i \textit{ for } (x, z) \in \overline{\Omega} \times \Lambda, \tag{4.3.55}$$

$$\underset{\sim}{V}_i \le \underline{V}_i^{(0)} \le \underline{V}_i^{(1)} \le \ldots \le \underline{V}_i^{(k)} \le \ldots \le \underline{V}_i \le \overline{V}_i \le \ldots \le \overline{V}_i^{(k)} \le \ldots \le \overline{V}_i^{(1)} \le \overline{V}_i^{(0)} \le \tilde{V}_i \textit{ for } z \in \overline{\Lambda}, \tag{4.3.56}$$

for all $k = 1,2,\ldots$

If furthermore, the system $\hat{S}^*_{2n}, \hat{B}^*_{2n}$ *has a unique solution, then* $(\underline{v}_i, \underline{V}_i) \equiv (\overline{v}_i, \overline{V}_i) \equiv (v_i, V_i)$ *is the unique solution of* $\hat{S}^*_{2n}, \hat{B}^*_{2n}$ *and all solutions* (v_i, V_i) *of* $\hat{S}^*_{2n}, \hat{B}^*_{2n}$ *for which*

$$-D_i \nabla_x^2 w_i = f_i^*(x, v_j) + f^*_{n(I)+i}(x, v_k) \textit{ in } \Omega \times \Lambda, \tag{4.3.57}$$

$$\frac{\partial w_i}{\partial n} = 0 \textit{ on } \partial\Omega_1 \times \Lambda, \tag{4.3.58}$$

$$D_i \frac{\partial w_i}{\partial n} - H_i(W_i - w_i) = 0 \textit{ on } \partial\Omega_2 \times \Lambda, \tag{4.3.59}$$

$$-\mathcal{D}_i \nabla_x^2 W_i + u \cdot \nabla W_i = F_i^*(z, V_j) + F^*_{n(J)+i}(z, V_k) - H_i \int_{\partial\Omega_2} (W_i - w_i) \textit{ in } \Lambda, \tag{4.3.60}$$

$$\upsilon_1 W_i + \mathcal{D}_i \frac{\partial W_i}{\partial n_1} = 0 \textit{ on } \partial\Lambda_1, \tag{4.3.61}$$

$$\frac{\partial W_i}{\partial n_\alpha} = 0 \textit{ on } \partial\Lambda_\alpha,\ \alpha = 2, 3, \tag{4.3.62}$$

for $(w_i, W_i) = (v_i + v_{n(I)+i}, W_i + W_{n(J)+i})$ *generates the unique solution* $(\underline{c}_i, \underline{C}_i) \equiv (\overline{c}_i, \overline{C}_i) \equiv (c_i, C_i)$ *of the general system* $\hat{S}_n, \hat{B}_n$*, where*

$$\underset{\sim}{v}_i \le \underline{v}_i^{(0)} \le \underline{v}_i^{(1)} \le \ldots \le \underline{v}_i^{(k)} \ldots \le \underline{v}_i \le c_i \le \overline{v}_i \ldots \le \overline{v}_i^{(k)} \le \ldots \le \overline{v}_i^{(1)} \le \overline{v}_i^{(0)} \le \tilde{v}_i,$$

$$\underset{\sim}{v}_{n(I)+i} \le \underline{v}^{(0)}_{n(I)+i} \le \underline{v}^{(1)}_{n(I)+i} \le \ldots \le \underline{v}^{(k)}_{n(I)+i} \ldots \le \underline{v}_{n(I)+i} \le -c_i \le \overline{v}_{n(I)+i} \ldots \le \overline{v}^{(k)}_{n(I)+i} \le \ldots \le \overline{v}^{(1)}_{n(I)+i} \le \overline{v}^{(0)}_{n(I)+i} \le \tilde{v}_{n(I)+i},$$

for $(x, z) \in \overline{\Omega} \times \Lambda$,

$$\underset{\sim}{V}_i \le \underline{V}_i^{(0)} \le \underline{V}_i^{(1)} \le \ldots \le \underline{V}_i^{(k)} \le \ldots \le \underline{V}_i \le C_i \le \overline{V}_i \le \ldots \le \overline{V}_i^{(k)} \le \ldots \le \overline{V}_i^{(1)} \le \overline{V}_i^{(0)} \le \tilde{V}_i,$$

$$\underset{\sim}{V}_{n(J)+i} \le \underline{V}^{(0)}_{n(J)+i} \le \underline{V}^{(1)}_{n(J)+i} \le \ldots \le \underline{V}^{(k)}_{n(J)+i} \le \ldots \le \underline{V}_{n(J)+i} \le -C_i \le \overline{V}_{n(J)+i} \le \ldots \le \overline{V}^{(k)}_{n(J)+i} \le \ldots \le \overline{V}^{(1)}_{n(J)+i} \le \overline{V}^{(0)}_{n(J)+i} \le \tilde{V}_{n(J)+i},$$

for $z \in \overline{\Lambda}$*, for all* $k = 1,2,\ldots$

We have seen that for the purposes of our existence proof, we may look at the monotone system $\hat{S}_n, \hat{B}_n$ where we assume our coupling functions f_i and F_i are monotone nondecreasing in c_j and C_j, respectively for all j. If this monotone property is not satisfied then we may imbed our general system $\hat{S}_n, \hat{B}_n$ into a system of twice the order which is a monotone system. The existence results obtained for this new system of twice the order satisfied by $(\underline{c}_i, \underline{C}_i)$ and $(\overline{c}_i, \overline{C}_i)$ then implies a solution of our original system $\hat{S}_n, \hat{B}_n$ by the imbedding results of section 4.2 but only if uniqueness is guaranteed in the monotone system $\hat{S}_{2n}, \hat{B}_{2n}$.

If uniqueness is not guaranteed in the monotone system $\hat{S}_{2n}$, $\hat{B}_{2n}$, the following section gives a general existence theorem for the system $\hat{S}_n$, $\hat{B}_n$ where f_i and F_i may not necessarily satisfy any monotone property. Such solutions may or may not be obtained by monotone iteration.

4.3.4 Coupled Lower and Upper Solutions and General Existence of Solutions of the Nonmonotone system $\hat{S}_n$, $\hat{B}_n$

We shall now introduce the concept of coupled lower and upper solutions relative to the system $\hat{S}_n$, $\hat{B}_n$ which may not necessarily possess any monotone property.

Definition 4.3.3

Assume that

(i) For components $i \in I$, where $D_i > 0$, $\underset{\sim}{c}_i$ and $\tilde{c}_i$ are continuous functions in $\overline{\Omega} \times \Lambda$ with continuous first order x_j derivatives in $\overline{\Omega} \times \Lambda$ and continuous second order x_j derivatives in $\Omega \times \Lambda$;

(ii) For components $i \in I$, where $D_i = H_i = 0$, $\underset{\sim}{c}_i$ and $\tilde{c}_i$ are continuous functions in $\overline{\Omega} \times \Lambda$;

(iii) For components $i \in J$, where $\mathcal{D}_i > 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $\overline{\Lambda}$, with continuous first order z_j derivatives in $\overline{\Lambda}$ and continuous second order z_j derivatives in Λ;

(iv) For components $i \in J$, where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \not\equiv 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $\overline{\Lambda}$, with continuous first order z_j derivatives in Λ;

(v) For components $i \in J$ where $\mathcal{D}_i = 0$, $u \cdot \nabla C_i \equiv 0$, $\underset{\sim}{C}_i$ and $\tilde{C}_i$ are continuous functions in $\overline{\Lambda}$.

The ordered pair of functions $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ with $\underset{\sim}{c}_i \le \tilde{c}_i$ on $\overline{\Omega} \times \Lambda$ and $\underset{\sim}{C}_i \le \tilde{C}_i$ on $\overline{\Lambda}$ are said to be *coupled lower* and *upper solutions* of $\hat{S}_n$, $\hat{B}_n$ respectively, if they satisfy:

$$-D_i \nabla_x^2 \underset{\sim}{c}_i \le \underline{f}_i(x, \underset{\sim}{c}_k, \tilde{c}_l) \text{ in } \Omega{\times}\Lambda,$$

$$\frac{\partial \underset{\sim}{c}_i}{\partial n} \le 0 \text{ on } \partial\Omega_1{\times}\Lambda,$$

$$D_i \frac{\partial \underset{\sim}{c}_i}{\partial n} \le H_i(\underset{\sim}{C}_i - \underset{\sim}{c}_i) \text{ on } \partial\Omega_2{\times}\Lambda,$$

$$-\mathcal{D}_i \nabla^2 \underset{\sim}{C}_i + u \cdot \nabla \underset{\sim}{C}_i + H_i \int_{\partial\Omega_2} (\underset{\sim}{C}_i - \underset{\sim}{c}_i) \le \underline{F}_i(z, \underset{\sim}{C}_k, \tilde{C}_l) \text{ in } \Lambda,$$

$$v_1 \underset{\sim}{C}_i + \mathcal{D}_i \frac{\partial \underset{\sim}{C}_i}{\partial n_1} \le v_1 C_{i,1} \text{ on } \partial\Lambda_1,$$

$$\frac{\partial \underset{\sim}{C}_i}{\partial n_\alpha} \le 0 \text{ on } \partial\Lambda_\alpha,\ \alpha = 2, 3,$$

and

$$-D_i \nabla_x^2 \tilde{c}_i \ge \bar{f}_i(x, \underset{\sim}{c}_k, \tilde{c}_l) \text{ in } \Omega{\times}\Lambda,$$

$$\frac{\partial \tilde{c}_i}{\partial n} \ge 0 \text{ on } \partial\Omega_1{\times}\Lambda,$$

$$D_i \frac{\partial \tilde{c}_i}{\partial n} \ge H_i(\tilde{C}_i - \tilde{c}_i) \text{ on } \partial\Omega_2{\times}\Lambda,$$

$$-\mathcal{D}_i\nabla^2\tilde{C}_i+u\cdot\nabla\tilde{C}_i+H_i\int_{\partial\Omega_2}(\tilde{C}_i-\tilde{c}_i)\geq\overline{F}_i(z,\ \underset{\sim}{C}_k,\ \tilde{C}_l)\text{ in }\Lambda,$$

$$v_1\tilde{C}_i+\mathcal{D}_i\frac{\partial\tilde{C}_i}{\partial n_1}\geq v_1C_{i,1}\text{ on }\partial\Lambda_1,$$

$$\frac{\partial\tilde{C}_i}{\partial n_\alpha}\geq 0\text{ on }\partial\Lambda_\alpha,\ \alpha=2,3,$$

where $\underline{f}_i$, $\bar{f}_i$ $\underline{F}_i$ and $\overline{F}_i$ are defined in (3.2.9)-(3.2.12).

Note that these coupled lower and upper solutions may be uncoupled into lower and upper solutions by the following substitution

$$\tilde{v}_i=\tilde{c}_i,\ \tilde{v}_{n(I)+i}=-\underset{\sim}{c}_i,\ \underset{\sim}{v}_i=\underset{\sim}{c}_i,\ \underset{\sim}{v}_{n(I)+i}=-\tilde{c}_i,$$

and

$$\tilde{V}_i=\tilde{C}_i,\ \tilde{V}_{n(J)+i}=-\underset{\sim}{C}_i,\ \underset{\sim}{V}_i=\underset{\sim}{C}_i,\ \underset{\sim}{V}_{n(J)+i}=-\tilde{C}_i.$$

All the other properties of lower and upper solutions discussed earlier in this section are also valid for coupled lower and upper solutions although it must be noted that coupled upper and lower solutions must occur simultaneously.

In order to establish an existence theorem for $\hat{S}_n$, $\hat{B}_n$ in terms of coupled upper and lower solutions, we define a transformation $\mathcal{T}$, by

$$(c_i^{(k)},\ C_i^{(k)})=\mathcal{T}(c_j^{(k-1)},\ C_j^{(k-1)}),\tag{4.3.63}$$

and consider the sequences $\{(c_i^{(k)},\ C_i^{(k)})\}$ given in (4.3.16)-(4.3.21) with $c_i^{(k)}$ satisfying the inequalities $\underset{\sim}{c}_i\leq c_i^{(k)}\leq\tilde{c}_i$ in $\overline{\Omega}\times\Lambda$ and $C_i^{(k)}$ satisfying the inequalities $\underset{\sim}{C}_i\leq C_i^{(k)}\leq\tilde{C}_i$ in $\overline{\Lambda}$ for $k=1,\ldots$.

The properties of sequences $\{(c_i^{(k)},\ C_i^{(k)})\}$ are similar to that discussed earlier. However, in the present case, the transformation $\mathcal{T}$, may not be a monotone operator and so although we may obtain bounds for the solutions, these bounds may not necessarily be improved by monotone iteration.

Lemma 4.3.8

Consider the BVP (4.3.16)–(4.3.21) and suppose that the assumptions (H_1), (H_2')-(H_4') hold. Let there exist $(\underset{\sim}{c}_i,\ \underset{\sim}{C}_i)$ and $(\tilde{c}_i,\ \tilde{C}_i)$ which are coupled lower and upper solutions respectively of $\hat{S}_n$, $\hat{B}_n$ with $\underset{\sim}{c}_j\leq c_j^{(k-1)}\leq\tilde{c}_j$ on $\overline{\Omega}\times\Lambda$ and $\underset{\sim}{C}_j\leq C_j^{(k-1)}\leq\tilde{C}_j$ on $\overline{\Lambda}$.

Assume that

(i) *For components $j\in I$, where $D_j, H_j>0$, $c_j^{(k-1)}\in C^{1+\alpha,\alpha}[\overline{\Omega}\times\Lambda,\ R^{n(I)}]$;*

(ii) *For components $j\in I$, where $D_j=H_j=0$, $c_j^{(k-1)}\in C^{\alpha,\alpha}[\overline{\Omega}\times\Lambda,\ R^{n(I)}]$;*

(iii) *For components $j\in J$, where $\mathcal{D}_j>0$, $C_j^{(k-1)}\in C^{1+\alpha}[\overline{\Lambda},\ R^{n(J)}]$;*

(iv) *For components $j\in J$, where $\mathcal{D}_j=0$, $u\cdot\nabla C_j^{(k-1)}\not\equiv 0$, $C_j^{(k-1)}\in C^{\alpha}[\overline{\Lambda},\ R^{n(J)}]$ and assumptions (H_5')-(H_6') hold;*

(v) *For components $j\in J$, where $\mathcal{D}_j=0$, $u\cdot\nabla C_j^{(k-1)}\equiv 0$, $C_j^{(k-1)}\in C^{\alpha}[\overline{\Lambda},\ R^{n(J)}]$.*

Then the BVP (4.3.16)-(4.3.21) possesses a unique solution $(c_i^{(k)}, C_i^{(k)})$, *where*

(I) *For components* $i \in I$, *where* $D_i, H_i > 0$, $c_i^{(k)} \in C^{2+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$;

(II) *For components* $i \in I$, *where* $D_i = H_i = 0$, $c_i^{(k)} \in C^{1+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$;

(III) *For components* $i \in J$ *where* $\mathcal{D}_i > 0$, $C_i^{(k)} \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$;

(IV) *For components* $i \in J$, *where* $\mathcal{D}_i = 0$, $u \cdot \nabla C_i^{(k)} \not\equiv 0$, $C_i^{(k)} \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$;

(V) *For components* $i \in J$, *where* $\mathcal{D}_i = 0$, $u \cdot \nabla C_i^{(k)} \equiv 0$, $C_i^{(k)} \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$.

Furthermore, in all cases $c_i^{(k)}$ *and* $C_i^{(k)}$ *satisfy the inequalities* $\underset{\sim}{c}_i \le c_i^{(k)} \le \tilde{c}_i$ *in* $\overline{\Omega} \times \Lambda$ *and* $\underset{\sim}{C}_i \le C_i^{(k)} \le \tilde{C}_i$ *in* $\overline{\Lambda}$.

Proof

Most of this proof is identical to that given in Lemma 4.3.5. However, we need to only observe that

$$\underline{f}_i(x, \underset{\sim}{c}_k, \tilde{c}_l) \le f_i(x, c_j^{(k-1)}) \le \bar{f}_i(x, \underset{\sim}{c}_k, \tilde{c}_l),$$

and

$$\underline{F}_i(z, \underset{\sim}{C}_k, \tilde{C}_l) \le F_i(z, C_j^{(k-1)}) \le \bar{F}_i(z, \underset{\sim}{C}_k, \tilde{C}_l),$$

in order to show that $c_i^{(k)}$ and $C_i^{(k)}$ satisfy the inequalities $\underset{\sim}{c}_i \le c_i^{(k)} \le \tilde{c}_i$ in $\overline{\Omega} \times \Lambda$ and $\underset{\sim}{C}_i \le C_i^{(k)} \le \tilde{C}_i$ in $\overline{\Lambda}$.□

The following lemma follows from Lemma 4.3.6 and Lemma 4.3.8

Lemma 4.3.9

Consider the BVP (4.3.16)-(4.3.21) and suppose that the assumptions (H_1), (H_2')-(H_4') *hold. Let there exist* $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ *and* $(\tilde{c}_i, \tilde{C}_i)$ *which are coupled lower and upper solutions of* $\hat{S}_n, \hat{B}_n$.

Assume that

(i) *For components* $j \in I$, *where* $D_j, H_j > 0$, $\underset{\sim}{c}_j, \tilde{c}_j \in C^{2+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$;

(ii) *For components* $j \in I$, *where* $D_j = H_j = 0$, $\underset{\sim}{c}_j, \tilde{c}_j \in C^{\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$;

(iii) *For components* $j \in J$, *where* $\mathcal{D}_j > 0$, $\underset{\sim}{C}_j, \tilde{C}_j \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$;

(iv) *For components* $j \in J$, *where* $\mathcal{D}_j = 0$, $u \cdot \nabla C_j^{(k-1)} \not\equiv 0$, $\underset{\sim}{C}_j, \tilde{C}_j \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$, *and assumptions* (H_5')-(H_6') *hold;*

(v) *For components* $j \in J$, *where* $\mathcal{D}_j = 0$, $u \cdot \nabla C_j^{(k-1)} \equiv 0$, $\underset{\sim}{C}_j, \tilde{C}_j \in C^{\alpha}[\overline{\Lambda}, R^{n(J)}]$.

Then the mapping $\mathcal{T}$, *from* $(c_j^{(k-1)}, C_j^{(k-1)})$ *to* $(c_i^{(k)}, C_i^{(k)})$ *possesses the following properties:*

(I) $(\tilde{c}_i, \tilde{C}_i) \ge \mathcal{T}(\tilde{c}_j, \tilde{C}_j)$, $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \le \mathcal{T}(\underset{\sim}{c}_j, \underset{\sim}{C}_j)$.

(II) $\mathcal{T}$ *is an operator which maps the intervals* $[\underset{\sim}{c}_i, \tilde{c}_i]$ *and* $[\underset{\sim}{C}_i, \tilde{C}_i]$ *onto themselves.*

The following theorem is an existence theorem for solutions to the general system $\hat{S}_n, \hat{B}_n$.

Theorem 4.3.3 (Generalised Existence Theorem)
Let there exist $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ *and* $(\tilde{c}_i, \tilde{C}_i)$ *which are coupled lower and upper solutions of* $\hat{S}_n, \hat{B}_n$ *with continuity properties given in Lemma 4.3.9. Then there exists a solution* (c_i, C_i) *of* $\hat{S}_n, \hat{B}_n$ *satisfying the inequalities* $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \le (c_i, C_i) \le (\tilde{c}_i, \tilde{C}_i)$.

Proof
We first consider the case with $D_i, \mathcal{D}_i > 0$.

It has been shown by standard continuity arguments in Theorem 4.3.1 and by the Agmon-Doulis-Nirenberg and Schauder estimates that $\{c_i^{(k)}\}$ and $\{C_i^{(k)}\}$ are uniformly bounded sequences and hence are relatively compact in $C^{2,0}[\overline{\Omega} \times \Lambda, R^{n(I)}]$ and $C^2[\overline{\Lambda}, R^{n(J)}]$ respectively.

This implies that there exists subsequences of $\{c_i^{(k)}\}$ and $\{C_i^{(k)}\}$ which converge in $C^{2,0}[\overline{\Omega} \times \Lambda, R^{n(I)}]$ and $C^2[\overline{\Lambda}, R^{n(J)}]$, respectively.

The other cases follow similarly along the lines of Theorem 4.3.1.□

We note from the counterexample at the end of section 3.1, that comparison thoerems analogous to Theorems 3.2.11 and 3.2.12 do not hold in general in the case of the corresponding steady state or time independent problem $\hat{S}_n, \hat{B}_n$. Hence, if there exist $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ which are *lower* and *upper* solutions of the steady state monotone system $\hat{S}_n, \hat{B}_n$ or if there exist $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ which are *coupled lower* and *upper* solutions of the steady state system $\hat{S}_n, \hat{B}_n$ which may possess no monotone property and (c_i, C_i) is a solution of $\hat{S}_n, \hat{B}_n$, then in contrast to the unsteady state problem S_n, B_n, we cannot assert that $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \le (c_i, C_i) \le (\tilde{c}_i, \tilde{C}_i)$.

We have shown in Theorem 4.3.1 that if $\hat{S}_n, \hat{B}_n$ is a monotone system, the method of monotone iteration is still applicable and shows the existence of at least one solution (c_i, C_i) of $\hat{S}_n, \hat{B}_n$ lying between $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$. We have also shown in Theorem 4.3.3 that if $\hat{S}_n, \hat{B}_n$ does not possess any monotone property, then we can still show the existence of at least one solution (c_i, C_i) of $\hat{S}_n, \hat{B}_n$ lying between $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$.

However, if (c_i, C_i) is a unique solution of $\hat{S}_n, \hat{B}_n$, then comparison thoerems analogous to Theorems 3.2.11 and 3.2.12 may hold in general in the case of the corresponding steady state or time independent problem $\hat{S}_n, \hat{B}_n$. Hence, if there exist $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ which are *lower* and *upper* solutions of a steady state monotone system $\hat{S}_n, \hat{B}_n$ or if there exist $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ which are are *coupled lower* and *upper* solutions of a steady state system $\hat{S}_n, \hat{B}_n$ which may possess no monotone property and (c_i, C_i) is a solution of $\hat{S}_n, \hat{B}_n$, then we can assert that $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \le (c_i, C_i) \le (\tilde{c}_i, \tilde{C}_i)$.

Note that in practice, it may only be necessary to find the existence of *coupled lower* and *upper* solutions when proving uniqueness and existence. Note also that we may similarly define *coupled lower* and *upper* solutions to the time dependent problem S_n, B_n and prove existence along the lines of Theorem 4.3.3 (Generalised Existence Theorem) for nonmonotone systems. An example of this will be seen in section 6.6.

Remark 4.3.4
In this section we have assumed that the boundary conditions (2.1.4) and (2.1.7) are of the Robin type. We may treat the Neumann and Dirichlet type boundary conditions similarly by using appropriate theorems for linear elliptic equations with Neumann and Dirichlet type boundary conditions (see Remark 4.1.1, Remark 4.1.2 and Remark 4.1.4).

In section 4.4 we shall discuss the relationships between the unsteady state and steady state problems and study the stability of solutions obtained by monotone iteration.

4.4 Relationships between Solutions of the Steady State and Unsteady State Problems

In this section we use relationships concerning the asymptotic behaviour of linear parabolic equations as $t \to \infty$ and their corresponding linear elliptic equations to make a statement about the relationships between solutions of the steady state problem $\hat{S}_n$, $\hat{B}_n$ and the unsteady state problem S_n, B_n.

We may assume at the outset that the systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ are monotone systems, in the sense that $f_i(t, x, c_j)$ and $f_i(x, c_j)$ are monotone nondecreasing in c_i and $F_i(t, z, C_j)$ and $F_i(z, C_j)$ are monotone nondecreasing in C_i for all i. This is not a restriction on the theorems of this section since if this monotone property is not satisfied then the functions (w_i, W_i) defined by $c_i = e^{-Kx_1} w_i$ and $C_i = e^{-Kz_1} W_i$ in (4.3.1)-(4.3.2), satisfies new systems of the same type but with new functions that are monotone nondecreasing in w_i and W_i.

If, on the other hand the monotone property is not satisfied by all the other variables, then the systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ with general functions f_i and F_i may be imbedded in systems S_{2n}, B_{2n} and $\hat{S}_{2n}$, $\hat{B}_{2n}$, respectively of the same form where $f_i(t, x, c_j)$ and $f_i(x, c_j)$ are replaced by $\bar{f}_i(t, x, \underline{c}_k, \bar{c}_l)$ and $\bar{f}_i(x, \underline{c}_k, \bar{c}_l)$, respectively for the first $n(I)$ dependent variables $\bar{c}_i$ and by $\underline{f}_j(t, x, \underline{c}_k, \bar{c}_l)$ and $\underline{f}_j(x, \underline{c}_k, \bar{c}_l)$, respectively for the next $n(I)$ dependent variables $\underline{c}_i$. Also, $F_i(t, z, C_j)$ and $F_i(z, C_j)$ are replaced by $\bar{F}_i(t, z, \underline{C}_k, \bar{C}_l)$ and $\bar{F}_i(z, \underline{C}_k, \bar{C}_l)$, respectively for the first $n(J)$ dependent variables $\bar{C}_i$ and by $\underline{F}_i(t, z, \underline{C}_k, \bar{C}_l)$ and $\underline{F}_i(z, \underline{C}_k, \bar{C}_l)$, respectively for the next $n(J)$ dependent variables $\underline{C}_i$

It has been shown by the imbedding results of section 3.2 and section 4.2 that solutions of these new monotone systems may generate solutions of the original systems and therefore uniqueness, stability and existence may be implied in the original systems. We shall furthermore show in this section that such monotone systems are also useful in establishing relationships between solutions of the general steady state problem $\hat{S}_n$, $\hat{B}_n$ and the general unsteady state problem S_n, B_n which may possess no monotone property.

4.4.1 Asymptotic Behaviour of the System S_n, B_n as $t \to \infty$.

Firstly, we shall assume that the systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ are monotone. Suppose that we have lower and upper solutions $(\underset{\sim}{c}_i, \underset{\sim}{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ with $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \le (\tilde{c}_i, \tilde{C}_i)$ for the unsteady state problem S_n, B_n, for all $T > 0$, and lower and upper solutions $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ and $(\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$, respectively with $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i) \le (\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$ for the steady state problem $\hat{S}_n$, $\hat{B}_n$, such that $(\underset{\sim}{c}_i, \underset{\sim}{C}_i) \to (\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ and $(\tilde{c}_i, \tilde{C}_i) \to (\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$ as $t \to \infty$, uniformly for $(x, z) \in \bar{\Omega} \times \Lambda$ and $z \in \bar{\Lambda}$. Suppose also, that $\{(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})\}$ and $\{(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})\}$ are minimal and maximal sequences respectively of the system S_n, B_n and $\{(\hat{\underline{c}}_i^{(k)}, \hat{\underline{C}}_i^{(k)})\}$ and $\{(\hat{\bar{c}}_i^{(k)}, \hat{\bar{C}}_i^{(k)})\}$ are minimal and maximal sequences respectively of the system $\hat{S}_n$, $\hat{B}_n$. Also, assume that relevant continuity properties are satisfied.

It is very clear that from Theorem 3.6.2 and Theorem 4.3.2, we can by using induction, apply Theorem 4.1.6 concerning asymptotic behaviours of parabolic equations as $t \to \infty$ (or results for asymptotic behaviour of ordinary differential equations as $t \to \infty$ (LAKSHMIHANTHAM and LEELA [157, pp.108, 229]) if $D_i = H_i = 0$ or $\mathcal{D}_i = 0$) to the function pairs $(\underline{c}_i^{(k)}, \underline{C}_i^{(k)})$, $(\hat{\underline{c}}_i^{(k)}, \hat{\underline{C}}_i^{(k)})$ and $(\bar{c}_i^{(k)}, \bar{C}_i^{(k)})$, $(\hat{\bar{c}}_i^{(k)}, \hat{\bar{C}}_i^{(k)})$, and deduce that for all positive integers k:

$$(\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) \to (\hat{\underline{c}}_i^{(k)}, \hat{\underline{C}}_i^{(k)})$$

and

$$(\bar{c}_i^{(k)}, \bar{C}_i^{(k)}) \to (\hat{\bar{c}}_i^{(k)}, \hat{\bar{C}}_i^{(k)}),$$

as $t \to \infty$, uniformly for $(x, z) \in \bar{\Omega} \times \Lambda$ and $z \in \bar{\Lambda}$.

Suppose further, that $(\hat{\bar{c}}_i, \hat{\bar{C}}_i)$ is the only solution of $\hat{S}_n$, $\hat{B}_n$ lying between $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ and $(\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$. Since $(\hat{\bar{c}}_i, \hat{\bar{C}}_i)$ is the only solution of $\hat{S}_n$, $\hat{B}_n$ between $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ and $(\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$, and the sequences $\{(\hat{\underline{c}}_i^{(k)}, \hat{\underline{C}}_i^{(k)})\}$ and

$\{(\bar{\hat{c}}_i^{(k)}, \bar{\hat{C}}_i^{(k)})\}$, both converge uniformly to solutions of $\hat{S}_n$, $\hat{B}_n$ lying between $(\underset{\sim}{\hat{c}}_i, \underset{\sim}{\hat{C}}_i)$ and $(\tilde{\bar{c}}_i, \tilde{\bar{C}}_i)$, we see that by Theorem 4.1.7 (or results for the asymptotic behaviour of ordinary differential equations as $t \longrightarrow \infty$ if $D_i = H_i = 0$ or $\mathscr{D}_i = 0$), it follows that

$$(\underline{c}_i^{(k)}, \underline{C}_i^{(k)}) \rightarrow (\bar{\hat{c}}_i, \bar{\hat{C}}_i)$$

and

$$(\overline{c}_i^{(k)}, \overline{C}_i^{(k)}) \rightarrow (\bar{\hat{c}}_i, \bar{\hat{C}}_i),$$

as $k \rightarrow \infty$, uniformly for all $(x, z) \in \overline{\Omega} \times \Lambda$ and $z \in \overline{\Lambda}$, and we know that

$$\underline{\hat{c}}_i^{(k)} \leq \bar{\hat{c}}_i \leq \bar{\hat{c}}_i^{(k)},$$

$$\underline{\hat{C}}_i^{(k)} \leq \bar{\hat{C}}_i \leq \bar{\hat{C}}_i^{(k)},$$

for all $(x, z) \in \overline{\Omega} \times \Lambda$ and $z \in \overline{\Lambda}$ and all positive integers k.

Thus, given any $\varepsilon > 0$, there exists positive integers $n(\varepsilon)$ and $N(\varepsilon)$, independent of $(x, z) \in \overline{\Omega} \times \Lambda$ and $z \in \overline{\Lambda}$, such that

$$|\underline{\hat{c}}_i^{(k)}(x, z) - \underline{\hat{c}}_i(x, z)| < \frac{\varepsilon}{2},$$
$$|\underline{\hat{C}}_i^{(k)}(z) - \underline{\hat{C}}_i(z)| < \frac{\varepsilon}{2},$$
$$|\bar{\hat{c}}_i^{(k)}(x, z) - \bar{\hat{c}}_i(x, z)| < \frac{\varepsilon}{2},$$
$$|\bar{\hat{C}}_i^{(k)}(z) - \bar{\hat{C}}_i(z)| < \frac{\varepsilon}{2},$$

whenever $k \geq n(\varepsilon), N(\varepsilon)$.

Further, there exists $\tau(\varepsilon, n(\varepsilon))$ independent of $(x, z) \in \overline{\Omega} \times \Lambda$ and $\mathcal{T}(\varepsilon, N(\varepsilon))$ independent of $z \in \overline{\Lambda}$, such that

$$|\underline{c}_i^{(n)}(t, x, z) - \underline{\hat{c}}_i^{(n)}(x, z)| < \frac{\varepsilon}{2},$$
$$|\underline{C}_i^{(N)}(t, z) - \underline{\hat{C}}_i^{(N)}(z)| < \frac{\varepsilon}{2},$$
$$|\overline{c}_i^{(n)}(t, x, z) - \bar{\hat{c}}_i^{(n)}(x, z)| < \frac{\varepsilon}{2},$$
$$|\overline{C}_i^{(N)}(t, z) - \bar{\hat{C}}_i^{(N)}(z)| < \frac{\varepsilon}{2},$$

whenever $t > \tau(\varepsilon, n(\varepsilon)), \mathcal{T}(\varepsilon, N(\varepsilon))$.

Therefore,

$$|\underline{c}_i^{(n)}(t, x, z) - \bar{\hat{c}}_i(x, z)| < \varepsilon,$$

$$|\underline{C}_i^{(N)}(t, z) - \bar{\hat{C}}_i(z)| < \varepsilon,$$

$$|\overline{c}_i^{(n)}(t, x, z) - \bar{\hat{c}}_i(x, z)| < \varepsilon,$$

$$|\overline{C}_i^{(N)}(t, z) - \bar{\hat{C}}_i(z)| < \varepsilon,$$

whenever $t > \tau(\varepsilon, n(\varepsilon)), \mathcal{T}(\varepsilon, N(\varepsilon))$, which implies that

$$-\varepsilon+\bar{\hat{c}}_i(x, z)<\underline{c}_i^{(n)}(t, x, z)\le\bar{c}_i(t, x, z)\le\bar{c}_i^{(n)}(t, x, z)<\varepsilon+\bar{\hat{c}}_i(x, z),$$

$$-\varepsilon+\bar{\hat{C}}_i(z)<\underline{C}_i^{(N)}(t, z)\le\bar{C}_i(t, z)\le\bar{C}_i^{(N)}(t, z)<\varepsilon+\bar{\hat{C}}(z),$$

whenever $t > \tau(\varepsilon, n(\varepsilon))$, $\mathcal{T}(\varepsilon, N(\varepsilon))$, where $(\bar{c}_i, \bar{C}_i)$ is the solution of the system S_n, B_n obtained by monotone iteration in Theorem 3.6.1 (Generalised Existence Theorem).

By applying Theorem 3.6.1 for arbitrarily large T, we can show that $(\bar{c}_i, \bar{C}_i)$ exists for all $t \ge 0$. Therefore

$$(\bar{c}_i, \bar{C}_i)\to(\bar{\hat{c}}_i, \bar{\hat{C}}_i),$$

as $t\to\infty$, uniformly for $(x, z)\in\bar{\Omega}\times\Lambda$ and $z\in\bar{\Lambda}$.

Thus, under the given conditions, the existence of exactly one solution to the steady state problem $\hat{S}_n$, $\hat{B}_n$ lying between $(\hat{\underline{c}}_i, \hat{\underline{C}}_i)$ and $(\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$ implies that, for any initial value $(c_{i,0}, C_{i,0})$ lying between $(\underline{c}_i, \underline{C}_i)$ and $(\tilde{c}_i, \tilde{C}_i)$ at $t = 0$, the unique solution (c_i, C_i) of S_n, B_n (for arbitrarily large T) will tend to the steady state solution $(\hat{c}_i, \hat{C}_i)$ of $\hat{S}_n$, $\hat{B}_n$ as $t\to\infty$, uniformly for $(x, z)\in\bar{\Omega}\times\Lambda$ and $z\in\bar{\Lambda}$.

From the uniqueness of the steady state problem we see that the imbedding results of section 3.4 and section 4.2 apply and this shows that this relationship will hold for the general systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ which may possess no monotone property.

4.4.2 The Stability of Solutions Obtained by Monotone Iteration

We shall consider the stability properties of the solutions of the system $\hat{S}_n$, $\hat{B}_n$ obtained by monotone iteration. Let us consider the following system in the general system S_n, B_n, where the fluid velocity distribution $u(z)$ and the inlet fluid concentration $C_{i,1}$ are independent of time.

$$\frac{\partial c_i}{\partial t}-D_i\nabla_x^2c_i=f_i(x, c_j) \text{ in } (0, T]\times\Omega\times\Lambda, \tag{4.4.1}$$

$$\frac{\partial c_i}{\partial n}=0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda, \tag{4.4.2}$$

$$D_i\frac{\partial c_i}{\partial n}=H_i(C_i-c_i) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda, \tag{4.4.3}$$

$$\frac{\partial C_i}{\partial t}-\mathcal{D}_i\nabla^2C_i+u\cdot\nabla C_i+\int_{\partial\Omega_2}D_i\frac{\partial c_i}{\partial n}=F_i(z, C_j) \text{ in } (0, T]\times\Lambda, \tag{4.4.4}$$

$$\upsilon_1C_i+\mathcal{D}_i\frac{\partial C_i}{\partial n_1}=\upsilon_1C_{i,1} \text{ on } (0, T]\times\partial\Lambda_1, \tag{4.4.5}$$

$$\frac{\partial C_i}{\partial n_\alpha}=0 \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha=2, 3, \tag{4.4.6}$$

$$c_i=c_{i,0} \text{ in } \Omega\times\Lambda, \text{ at } t=0, \tag{4.4.7}$$

$$C_i=C_{i,0} \text{ in } \Lambda, \text{ at } t=0. \tag{4.4.8}$$

Note that the solutions of $\hat{S}_n$, $\hat{B}_n$ are time independent solutions of the system (4.4.1)-(4.4.8). We shall show that with the monotone iteration methods given in section 4.3, it is not possible to obtain unstable solutions. On the other hand, each solution obtained by monotone iteration is asymptotically stable at least from above or below and if solutions of $\hat{S}_n$, $\hat{B}_n$ are unique, the solution obtained by monotone iteration is asymptotically stable both from above and from below. As earlier, we shall assume that the systems $\hat{S}_n$, $\hat{B}_n$ and (4.4.1)-(4.4.8) are monotone systems.

We have seen in section 3.6, that there may be geometric conditions on f_i and F_i which guarantee the existence of lower and upper solutions to the general system S_n, B_n. We have also seen in section 4.3 that there are geometric conditions on f_i and F_i which guarantee the existence of lower and upper solutions to the system $\hat{S}_n$, $\hat{B}_n$. We now show that the existence of lower and upper solutions to the system $\hat{S}_n$, $\hat{B}_n$ can imply the existence of lower and upper solutions to the special system (4.4.1)-(4.4.8) in S_n, B_n.

Suppose that $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i)$ is a lower solution and $(\hat{\tilde{c}}_i,\ \hat{\tilde{C}}_i)$ is an upper solution with $\hat{\underset{\sim}{c}}_i \le \hat{\tilde{c}}_i$ on $\overline{\Omega}\times\Lambda$ and $\hat{\underset{\sim}{C}}_i \le \hat{\tilde{C}}_i$ on $\overline{\Lambda}$ of the system $\hat{S}_n$, $\hat{B}_n$ and $(c_i,\ C_i)$ is a solution of the system (4.4.1)-(4.4.8), where $\hat{\underset{\sim}{c}}_i \le c_{i,0} \le \hat{\tilde{c}}_i$ and $\hat{\underset{\sim}{C}}_i \le C_{i,0} \le \hat{\tilde{C}}_i$. The functions

$$(\underset{\sim}{c}_i(t,\ x,\ z),\ \underset{\sim}{C}_i(t,\ z)) \equiv (\hat{\underset{\sim}{c}}_i(x,\ z),\ \hat{\underset{\sim}{C}}_i(z))$$

and

$$(\tilde{c}_i(t,\ x,\ z),\ \tilde{C}_i(t,\ z)) \equiv (\hat{\tilde{c}}_i(x,\ z),\ \hat{\tilde{C}}_i(z)),$$

satisfy:

$$\frac{\partial \underset{\sim}{c}_i}{\partial t} - D_i\nabla_x^2 \underset{\sim}{c}_i \le f_i(x,\ \underset{\sim}{c}_j) \text{ in } (0,\ T]\times\Omega\times\Lambda,$$

$$\frac{\partial \underset{\sim}{c}_i}{\partial n} \le 0 \text{ on } (0,\ T]\times\partial\Omega_1\times\Lambda,$$

$$D_i\frac{\partial \underset{\sim}{c}_i}{\partial n} \le H_i(\underset{\sim}{C}_i - \underset{\sim}{c}_i) \text{ on } (0,\ T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial \underset{\sim}{C}_i}{\partial t} - \mathcal{D}_i\nabla^2 \underset{\sim}{C}_i + u\cdot\nabla \underset{\sim}{C}_i + H_i\int_{\partial\Omega_2}(\underset{\sim}{C}_i - c_i) \le F_i(z,\ \underset{\sim}{C}_j) \text{ in } (0,\ T]\times\Lambda,$$

$$\upsilon_1 \underset{\sim}{C}_i + \mathcal{D}_i\frac{\partial \underset{\sim}{C}_i}{\partial n_1} \le \upsilon_1 C_{i,1} \text{ on } (0,\ T]\times\partial\Lambda_1,$$

$$\frac{\partial \underset{\sim}{C}_i}{\partial n_\alpha} \le 0 \text{ on } (0,\ T]\times\partial\Lambda_\alpha,\ \alpha = 2,\ 3,$$

$$\underset{\sim}{c}_i(0,\ x,\ z) \le c_{i,0} \text{ in } \Omega\times\Lambda,$$

$$\underset{\sim}{C}_i(0,\ z) \le C_{i,0} \text{ in } \Lambda,$$

and

$$\frac{\partial \tilde{c}_i}{\partial t} - D_i\nabla_x^2 \tilde{c}_i \ge f_i(x,\ \tilde{c}_j) \text{ in } (0,\ T]\times\Omega\times\Lambda,$$

$$\frac{\partial \tilde{c}_i}{\partial n} \ge 0 \text{ on } (0,\ T]\times\partial\Omega_1\times\Lambda,$$

$$D_i\frac{\partial \tilde{c}_i}{\partial n} \ge H_i(\tilde{C}_i - \tilde{c}_i) \text{ on } (0,\ T]\times\partial\Omega_2\times\Lambda,$$

$$\frac{\partial \tilde{C}_i}{\partial t} - \mathcal{D}_i\nabla^2 \tilde{C}_i + u\cdot\nabla \tilde{C}_i + H_i\int_{\partial\Omega_2}(\tilde{C}_i - \tilde{c}_i) \ge F_i(z,\ \tilde{C}_j) \text{ in } (0,\ T]\times\Lambda,$$

$$\upsilon_1 \tilde{C}_i + \mathcal{D}_i\frac{\partial \tilde{C}_i}{\partial n_1} \ge \upsilon_1 C_{i,1} \text{ on } (0,\ T]\times\partial\Lambda_1,$$

$$\frac{\partial \tilde{C}_i}{\partial n_\alpha} \geq 0 \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha = 2, 3,$$

$$\tilde{c}_i(0, x, z) \geq c_{i,0} \text{ in } \Omega\times\Lambda,$$

$$\tilde{C}_i(0, z) \geq C_{i,0} \text{ in } \Lambda,$$

respectively, so by Theorem 3.2.12 (Generalised Strong Comparison Theorem), since $\hat{\underset{\sim}{c}}_i$, $\hat{\underset{\sim}{C}}_i$, $\tilde{\hat{c}}_i$ and $\tilde{\hat{C}}_i$ are independent of t,

$$\frac{\partial \hat{\underset{\sim}{c}}_i}{\partial t} = \frac{\partial \hat{\underset{\sim}{C}}_i}{\partial t} = \frac{\partial \tilde{\hat{c}}_i}{\partial t} = \frac{\partial \tilde{\hat{C}}_i}{\partial t} = 0, \tag{4.4.9}$$

and the inequalities

$$(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i) \leq (c_i,\ C_i) \leq (\tilde{\hat{c}}_i,\ \tilde{\hat{C}}_i), \tag{4.4.10}$$

hold for all $t > 0$.

Note that in general, the existence of both lower and upper solutions to the special system (4.4.1)-(4.4.8) in S_n, B_n does not imply the existence of both lower and upper solutions to the system $\hat{S}_n$, $\hat{B}_n$.

In particular, if $c_{i,0} = \hat{\underset{\sim}{c}}_i$ in $\Omega\times\Lambda$ at $t = 0$ and $C_{i,0} = \hat{\underset{\sim}{C}}_i$ in Λ at $t = 0$ or if $c_{i,0} = \tilde{\hat{c}}_i$ in $\Omega\times\Lambda$ at $t = 0$ and $C_{i,0} = \tilde{\hat{C}}_i$ in Λ at $t = 0$, we have the following theorem.

Theorem 4.4.1

If $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i)$ is a lower solution of the system $\hat{S}_n$, $\hat{B}_n$, then the solution (c_i, C_i) of the system (4.4.1)-(4.4.8) with initial data $c_{i,0} = \hat{\underset{\sim}{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \hat{\underset{\sim}{C}}_i$ in Λ is monotone nondecreasing in t. If $(\tilde{\hat{c}}_i,\ \tilde{\hat{C}}_i)$ is a upper solution of the system $\hat{S}_n$, $\hat{B}_n$, then the solution (c_i, C_i) of the system (4.4.1)-(4.4.8) with initial data $c_{i,0} = \tilde{\hat{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \tilde{\hat{C}}_i$ in Λ is monotone nonincreasing in t. If $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i)$ is a lower solution and $(\tilde{\hat{c}}_i,\ \tilde{\hat{C}}_i)$ is a upper solution of the system $\hat{S}_n$, $\hat{B}_n$ and (c_i, C_i) is the solution of the system (4.4.1)-(4.4.8) with initial data either $c_{i,0} = \hat{\underset{\sim}{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \hat{\underset{\sim}{C}}_i$ in Λ or $c_{i,0} = \tilde{\hat{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \tilde{\hat{C}}_i$ in Λ, then the inequalities $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i) \leq (c_i,\ C_i) \leq (\tilde{\hat{c}}_i,\ \tilde{\hat{C}}_i)$ hold for all t.

Proof

Firstly consider the case where $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i)$ is a lower solution of the system $\hat{S}_n$, $\hat{B}_n$, and (c_i, C_i) is a solution of the system (4.4.1)-(4.4.8) with initial data $c_{i,0} = \hat{\underset{\sim}{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \hat{\underset{\sim}{C}}_i$ in Λ. We see that if (c_i, C_i) exists then it satisfies

$$\frac{\partial c_i}{\partial t} - D_i\nabla_x^2 c_i = f_i(x, c_j) \text{ in } (0, T]\times\Omega\times\Lambda, \tag{4.4.11}$$

$$\frac{\partial c_i}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda, \tag{4.4.12}$$

$$D_i\frac{\partial c_i}{\partial n} = H_i(C_i - c_i) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda, \tag{4.4.13}$$

$$\frac{\partial C_i}{\partial t} - \mathcal{D}_i\nabla^2 C_i + u\cdot\nabla C_i + \int_{\partial\Omega_2} D_i\frac{\partial c_i}{\partial n} = F_i(z, C_j) \text{ in } (0, T]\times\Lambda, \tag{4.4.14}$$

$$\upsilon_1 C_i + \mathcal{D}_i\frac{\partial C_i}{\partial n_1} = \upsilon_1 C_{i,1} \text{ on } (0, T]\times\partial\Lambda_1, \tag{4.4.15}$$

$$\frac{\partial C_i}{\partial n_\alpha} = 0 \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha = 2, 3, \tag{4.4.16}$$

$$c_i = \hat{\underset{\sim}{c}}_i \text{ in } \Omega\times\Lambda, \text{ at } t = 0, \tag{4.4.17}$$

$$C_i = \hat{\underset{\sim}{C}}_i \text{ in } \Lambda, \text{ at } t = 0. \tag{4.4.18}$$

From (4.4.10), we have $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i) \le (c_i,\ C_i)$.

The equations (4.4.11)-(4.4.18) are invariant under the transformation $t \to t + h$, so let us consider the functions $c_{ih}(t, x, z) = c_i(t + h, x, z)$ and $C_{ih}(t, z) = C_i(t + h, z)$ with initial data $c_{ih}(0, x, z) = c_i(h, x, z) \ge \hat{\underset{\sim}{c}}_i$ and $C_{ih}(0, z) = C_i(h, z) \ge \hat{\underset{\sim}{C}}_i$. We therefore have the following equations

$$\frac{\partial c_{ih}}{\partial t} - D_i\nabla_x^2 c_{ih} = f_i(x, c_{jh}) \text{ in } (0, T]\times\Omega\times\Lambda, \tag{4.4.19}$$

$$\frac{\partial c_{ih}}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda, \tag{4.4.20}$$

$$D_i\frac{\partial c_{ih}}{\partial n} = H_i(C_{ih} - c_{ih}) \text{ on } (0, T]\times\partial\Omega_2\times\Lambda, \tag{4.4.21}$$

$$\frac{\partial C_{ih}}{\partial t} - \mathscr{D}_i\nabla^2 C_{ih} + u\cdot\nabla C_{ih} + \int_{\partial\Omega_2} D_i\frac{\partial c_{ih}}{\partial n} = F_i(z, C_{jh}) \text{ in } (0, T]\times\Lambda, \tag{4.4.22}$$

$$\upsilon_1 C_{ih} + \mathscr{D}_i\frac{\partial C_{ih}}{\partial n_1} = \upsilon_1 C_{i,1} \text{ on } (0, T]\times\partial\Lambda_1, \tag{4.4.23}$$

$$\frac{\partial C_{ih}}{\partial n_\alpha} = 0 \text{ on } (0, T]\times\partial\Lambda_\alpha,\ \alpha = 2, 3, \tag{4.4.24}$$

$$c_{ih}(0, x, z) \ge \hat{\underset{\sim}{c}}_i \text{ in } \Omega\times\Lambda, \tag{4.4.25}$$

$$C_{ih}(0, z) \ge \hat{\underset{\sim}{C}}_i \text{ in } \Lambda. \tag{4.4.26}$$

If we can show that $c_{ih}(t, x, z) \ge c_i(t, x, z)$ in $\overline{\Omega}\times\Lambda$ and $C_{ih}(t, z) \ge C_i(t, z)$ in $\overline{\Lambda}$ at or near $t = 0$, then the inequality holds for all greater t by Theorem 3.2.12 (Generalised Strong Comparison Theorem) noting that f_i is assumed to be monotone and therefore need not be redefined. The continuity properties of the functions $c_{ih}(t, x, z)$ and $C_{ih}(t, z)$ near $t = 0$ are satisfied by studying the behaviour of the solution near $t = 0$.

Therefore $c_i(t + h, x, z) \ge c_i(t, x, z)$ in $\overline{\Omega}\times\Lambda$ and $C_i(t + h, z) \ge C_i(t, z)$ in $\overline{\Lambda}$ and hence c_i is monotonically nondecreasing in t and C_i is monotonically nondecreasing in t.

The case where $(\tilde{\tilde{c}}_i,\ \tilde{\tilde{C}}_i)$ is an upper solution of the system $\hat{S}_n$, $\hat{B}_n$, and (c_i, C_i) is the solution of the system (4.4.1)-(4.4.8) with initial data $c_{i,0} = \tilde{\tilde{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \tilde{\tilde{C}}_i$ in Λ is treated similarly.

We see from (4.4.10) that if $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i)$ is a lower solution and $(\tilde{\tilde{c}}_i,\ \tilde{\tilde{C}}_i)$ is a upper solution of the system $\hat{S}_n$, $\hat{B}_n$ and (c_i, C_i) is the solution of the system (4.4.1)-(4.4.8) with initial data either $c_{i,0} = \hat{\underset{\sim}{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \hat{\underset{\sim}{C}}_i$ in Λ or $c_{i,0} = \tilde{\tilde{c}}_i$ in $\Omega\times\Lambda$ and $C_{i,0} = \tilde{\tilde{C}}_i$ in Λ, then the inequalities $(\hat{\underset{\sim}{c}}_i,\ \hat{\underset{\sim}{C}}_i) \le (c_i,\ C_i) \le (\tilde{\tilde{c}}_i,\ \tilde{\tilde{C}}_i)$ hold for all t.❑

We shall now prove the following theorem. There are analogous proofs given in TEMME [282, p.67] and SATTINGER [258, p.36] for scalar parabolic and elliptic equations.

Theorem 4.4.2

Consider the system (4.4.1)-(4.4.8). *If* $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ *is a lower solution and* $(\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$ *is a upper solution of the system* $\hat{S}_n$, $\hat{B}_n$, *then under the assumptions of Theorem 3.6.1,*

$$\lim_{t\to\infty} c_i(t, x, z) = \hat{c}_i(x, z) \text{ and } \lim_{t\to\infty} C_i(t, z) = \hat{C}_i(z) \text{ exist,}$$

where

$$\hat{\underset{\sim}{c}}_i \le \hat{c}_i \le \hat{\tilde{c}}_i \text{ and } \hat{\underset{\sim}{C}}_i \le \hat{C}_i \le \hat{\tilde{C}}_i .$$

Furthermore, $(\hat{c}_i, \hat{C}_i)$ *is equal a.e. to a classical solution of the steady state system* $\hat{S}_n$, $\hat{B}_n$.

Proof

By the monotone iteration procedure we can construct, for any $T > 0$, a regular solution to the system (4.4.1)-(4.4.8) for $0 \le t \le T$, so the solution exists for all $t > 0$ and satisfies (4.4.10). We may start the iterations with a lower solution $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ and from Theorem 4.4.1, since $c_i(t, x, z)$ and $C_i(t, z)$ are monotone nondecreasing with t and are bounded below and above by $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$ and $(\hat{\tilde{c}}_i, \hat{\tilde{C}}_i)$ respectively,

$$\lim_{t\to\infty} c_i(t, x, z) = \hat{c}_i(x, z)$$

and

$$\lim_{t\to\infty} C_i(t, z) = \hat{C}_i(z),$$

exist, where

$$\hat{\underset{\sim}{c}}_i \le \hat{c}_i \le \hat{\tilde{c}}_i \text{ and } \hat{\underset{\sim}{C}}_i \le \hat{C}_i \le \hat{\tilde{C}}_i .$$

For the rest of this proof, we shall only look at the case when D_i, $\mathcal{D}_i > 0$ for all i. The other cases follow from standard results on ordinary differential equations and first order partial differential equations.

First we prove that $(\hat{c}_i, \hat{C}_i)$ is a weak solution of the system $\hat{S}_n$, $\hat{B}_n$, i.e.,

$$\hat{c}_i \in L^2[\Omega\times\Lambda, R^{n(I)}],\ \nabla_x^2\hat{c}_i \in L^2[\Omega\times\Lambda, R^{n(I)}], \tag{4.4.27}$$

$$\hat{C}_i \in L^2[\Lambda, R^{n(J)}],\ \nabla^2\hat{C}_i - u\cdot\nabla\hat{C}_i \in L^2[\Lambda, R^{n(J)}], \tag{4.4.28}$$

and

$$(-\nabla_x^2\hat{c}_i, \xi_i) - (f_i(x, \hat{c}_j), \xi_i) = 0,\ \forall \xi_i \in C_0^\infty[\Omega\times\Lambda, R^{n(I)}], \tag{4.4.29}$$

$$(-\nabla^2\hat{C}_i + u\cdot\nabla\hat{C}_i + H_i\mathcal{A}\hat{C}_i, \Xi_i) - (F_i(z, \hat{C}_j) + H_i\int_{\partial\Omega_2}\hat{c}_i, \Xi_i) = 0,\ \forall \Xi_i \in C_0^\infty[\Lambda, R^{n(J)}], \tag{4.4.30}$$

where we shall assume that Λ is considered to be a parameter space in (4.4.27) and (4.4.29) and where we use the inner product notation $(\cdot,\cdot)$ to denote the usual $L^2(D)$ inner product for real functions, i.e.,

$$(u,v) = \int_D uv\,dx.$$

Equations (4.4.29) and (4.4.30) are equivalent to

$$(\hat{c}_i, -\nabla_x^{2*}\xi_i) - (f_i(x, \hat{c}_j), \xi_i) = 0,$$

$$(\hat{C}_i, (-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^* \Xi_i - (F_i(z, \hat{C}_j) + H_i\int_{\partial\Omega_2} \hat{c}_i, \Xi_i) = 0,$$

where $-\nabla_x^{2*}$ is the adjoint operator of $-\nabla_x^2$ and $(-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^*$ is the adjoint operator of $-\nabla^2 + u\cdot\nabla + H_i\mathscr{A}$. Note that the Laplacian operators $-\nabla_x^2$ and $-\nabla^2$ are self adjoint.

The function (c_i, C_i) satisfies the system S_n, B_n. Taking the inner product with the functions $\xi_i \in C_0^\infty[\Omega\times\Lambda, R^{n(I)}]$ and $\Xi_i \in C_0^\infty[\Lambda, R^{n(J)}]$, we obtain

$$(\frac{\partial c_i}{\partial t}, \xi_i) + (-\nabla_x^2 c_i, \xi_i) - (f_i(x, c_j), \xi_i) = 0,$$

$$(\frac{\partial C_i}{\partial t}, \Xi_i) + (-\nabla^2 C_i + u\cdot\nabla C_i + H_i\mathscr{A}C_i, \Xi_i) - (F_i(z, C_j) + H_i\int_{\partial\Omega_2} c_i, \Xi_i) = 0,$$

and partial integration of the second terms results in

$$(\frac{\partial c_i}{\partial t}, \xi_i) + (c_i, -\nabla_x^{2*}\xi_i) - (f_i(x, c_j), \xi_i) = 0,$$

$$(\frac{\partial C_i}{\partial t}, \Xi_i) + (C_i, (-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^*\Xi_i) - (F_i(z, C_j) + H_i\int_{\partial\Omega_2} c_i, \Xi_i) = 0,$$

This inequality holds for all $t > 0$. So we have

$$\frac{1}{T}\int_0^T (\frac{\partial c_i}{\partial t}, \xi_i)dt - \frac{1}{T}\int_0^T (c_i, -\nabla_x^{2*}\xi_i)dt - \frac{1}{T}\int_0^T (f_i(x, c_j), \xi_i)dt = 0,$$

$$\frac{1}{T}\int_0^T (\frac{\partial C_i}{\partial t}, \Xi_i)dt + \frac{1}{T}\int_0^T (C_i, (-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^*\Xi_i)dt = \frac{1}{T}\int_0^T (F_i(z, C_j) + H_i\int_{\partial\Omega_2} c_i, \Xi_i)dt = 0.$$

Now let $T \to \infty$; then

$$\frac{1}{T}\int_0^T (c_i, -\nabla_x^{2*}\xi_i)dt \to (\hat{c}_i, -\nabla_x^{2*}\xi_i),$$

$$\frac{1}{T}\int_0^T (C_i, (-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^*\Xi_i)dt \to (\hat{C}_i, (-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^*\Xi_i),$$

from the Lebesgue dominated convergence theorem and the uniform boundedness on the solution (c_i, C_i). Similarly,

$$\frac{1}{T}\int_0^T (f_i(x, c_i), \xi_i)dt \to (f_i(x, \hat{c}_j), \xi_i),$$

$$\frac{1}{T}\int_0^T (F_i(z, C_i) + H_i\int_{\partial\Omega_2} c_i, \Xi_i)dt \to (F_i(z, \hat{C}_j) + H_i\int_{\partial\Omega_2} \hat{c}_i, \Xi_i),$$

and

$$\frac{1}{T}\int_0^T (\frac{\partial c_i}{\partial t}, \xi_i)dt = \frac{1}{T}\int_0^T \frac{\partial}{\partial t}(c_i, \xi_i)dt = \frac{(c_i(T, x, z), \xi_i) - (c_i(0, x, z), \xi_i)}{T} \to 0,$$

$$\frac{1}{T}\int_0^T (\frac{\partial C_i}{\partial t}, \Xi_i)dt = \frac{1}{T}\int_0^T \frac{\partial}{\partial t}(C_i, \Xi_i)dt = \frac{(C_i(T, z), \Xi_i) - (C_i(0, z), \Xi_i)}{T} \to 0.$$

Therefore, we get in the limit, as $T \to \infty$, that

$$(\hat{c}_i, -\nabla_x^{2*}\xi_i) - (f_i(x, \hat{c}_j), \xi_i) = 0,$$

$$(\hat{C}_i, (-\nabla^2 + u\cdot\nabla + H_i\mathscr{A})^* \Xi_i) - (F_i(z, \hat{C}_j) + H_i\int_{\partial\Omega_2} \hat{c}_i, \Xi_i) = 0,$$

for each $\xi_i \in C_0^\infty[\Omega\times\Lambda, R^{n(I)}]$ and $\Xi_i \in C_0^\infty[\Lambda, R^{n(J)}]$.

Now we have to show that $(\hat{c}_i, \hat{C}_i)$ is a regular solution of of the system $\hat{S}_n$, $\hat{B}_n$. First, we note that $\hat{c}_i$ is uniformly bounded in $\Omega\times\Lambda$ and $\hat{C}_i$ is uniformly bounded in Λ, thus $\hat{c}_i \in L^q[\Omega\times\Lambda, R^{n(I)}]$ and $\hat{C}_i \in L^q[\Lambda, R^{n(J)}]$. Then by Lemma 4.1.7, $f_i(x, \hat{c}_i) \in L^q[\Omega\times\Lambda\times R^{n(I)}, R^{n(I)}]$ and $F_i(z, \hat{C}_i) + H_i\int_{\partial\Omega_2}\hat{c}_i \in L^q[\Lambda\times R^{n(J)}, R^{n(J)}]$. From Lemma 4.1.4, q may be chosen to be identical in both cases.

Consider the boundary value problem

$$-D_i\nabla_x^2 w_i = f_i(x, \hat{c}_j) \text{ in } \Omega\times\Lambda, \tag{4.4.31}$$

$$\frac{\partial w_i}{\partial n} = 0 \text{ on } \partial\Omega_1\times\Lambda, \tag{4.4.32}$$

$$D_i\frac{\partial w_i}{\partial n} + H_i w_i = \hat{C}_i \text{ on } \partial\Omega_2\times\Lambda, \tag{4.4.33}$$

$$-\mathscr{D}_i\nabla^2 W_i + u\cdot\nabla W_i + H_i\mathscr{A}W_i = F_i(z, \hat{C}_j) + H_i\int_{\partial\Omega_2}\hat{c}_i \text{ in } \Lambda, \tag{4.4.34}$$

$$\upsilon_1 W_i + \mathscr{D}_i\frac{\partial W_i}{\partial n_1} = \hat{C}_{i,1} \text{ on } \partial\Lambda_1, \tag{4. .35}$$

$$\frac{\partial W_i}{\partial n_\alpha} = 0 \quad \text{on } \partial\Lambda_\alpha, \alpha = 2, 3. \tag{4. .36}$$

By Theorem 4.1.4, the boundary value problem (4.4.31)-(4.4.36) has a unique solution (w_i, W_i), where $w_i \in W_q^2[\overline{\Omega}, R^{n(I)}]$ (with z treated as a parameter) and $W_i \in W_q^2[\overline{\Lambda}, R^{n(J)}]$. From Lemma 4.1.5, q may be chosen to be identical in both cases.

Let g be the mapping that associates with each right hand term of (4.4.31) the unique solution w_i and G be the mapping that associates with each right hand term of (4.4.34) the unique solution W_i. The solution of (4.3.31)-(4.4.33) may be written as

$$w_i = -gf_i(x, \hat{c}_j) \tag{4.4.37}$$

and the solution of (4.4.34)-(4.4.36) as

$$W_i = -G(F_i(z, \hat{C}_j) + H_i\int_{\partial\Omega_2}\hat{c}_i). \tag{4.4.38}$$

For $\hat{C}_i$ fixed, the operator $g{:}L^q \to W_q^2$ associating with each admissible right-hand term f_i the uniquely determined solution w_i, is the sum of a constant operator and a bounded linear operator. Similarly, for $\hat{C}_{i,1}$ fixed, the operator $G{:}L^q \to W_q^2$ associating with each admissible right-hand term $F_i + H_i\int_{\partial\Omega_2}\hat{c}_i$, the uniquely determined solution W_i, is the sum of a constant operator and a bounded linear operator. Thus g and G are continuous.

We denote these operators by g and G because of its connection with the Green's function of (4.4.31)-(4.3.36); G is the inverse of the elliptic operator L with boundary conditions. We will simply call G the inverse of the elliptic operator L.

For $q = 2/(1-\alpha)$, $w_i \in W_q^2[\overline{\Omega}, R^{n(I)}]$ (where Λ treated as a parameter space) and $W_i \in W_q^2[\overline{\Lambda}, R^{n(J)}]$ and we may apply Theorem 4.1.1 (Imbedding Theorem) to obtain $w_i \in C^{1+\alpha}[\overline{\Omega}, R^{n(I)}]$ (where Λ is treated as a parameter space) and $\hat{C}_i = W_i \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$. From Lemma 4.1.3, α may be chosen to be identical in both cases. Thus we have

$$(w_i, -\nabla_x^{2*}\xi_i) = (gf_i(x, \hat{c}_j), -\nabla^{2*}\xi_i) = (f_i(x, \hat{c}_j), -g^*\nabla^{2*}\xi_i) = (f_i(x, \hat{c}_j), \xi_i) = (\hat{c}_i, -\nabla^{2*}\xi_i),$$

and

$$\begin{aligned}(W_i,(-\nabla^2+u\cdot\nabla+H_i\mathscr{A})^*\Xi_i) &= (G(F_i(z, \hat{C}_j)+H_i\int_{\partial\Omega_2}\hat{c}_i), (-\nabla^2+u\cdot\nabla+H_i\mathscr{A})^*\Xi_i)\\ &= ((F_i(z, \hat{C}_j)+H_i\int_{\partial\Omega_2}\hat{c}_i), G^*(-\nabla^2+u\cdot\nabla+H_i\mathscr{A})^*\Xi_i))\\ &= ((F_i(z, \hat{C}_j)+H_i\int_{\partial\Omega_2}\hat{c}_i), \Xi_i)\\ &= (\hat{C}_i, (-\nabla^2+u\cdot\nabla+H_i\mathscr{A})^*\Xi_i),\end{aligned}$$

where g^* and G^* are the inverses of $-\nabla_x^2$ and $-\nabla^2+u\cdot\nabla+H_i\mathscr{A}$ respectively (see RIESZ AND NAGY, [248, p.104]). Hence

$$(w_i-\hat{c}_i, -\nabla_x^{2*}\xi_i) = 0 \text{ for each } \xi_i \in C_0^\infty[\Omega\times\Lambda, R^{n(I)}],$$

$$(W_i-\hat{C}_i, -\nabla^{2*}\Xi_i+u\cdot\nabla^*\Xi_i+H_i\mathscr{A}\Xi_i) = 0 \text{ for each } \Xi_i \in C_0^\infty[\Lambda, R^{n(J)}],$$

and thus

$$(w_i-\hat{c}_i, -\nabla_x^{2*}g^*\eta_i) = (w_i-\hat{c}_i, -\eta_i) = 0 \ \forall \eta_i \in C_0^\infty[\Omega\times\Lambda, R^{n(I)}],$$

$$(W_i-\hat{C}_i, G^*(-\nabla^{2*}\psi_i+u\cdot\nabla^*\psi_i+H_i\mathscr{A}\psi_i)) = 0 \ \forall \psi_i \in C_0^\infty[\Lambda, R^{n(J)}],$$

because of the invertiblity of $-\nabla_x^2$ and $-\nabla^2+u\cdot\nabla+H_i\mathscr{A}$ and thus of $-\nabla_x^{2*}$ and $(-\nabla^2+u\cdot\nabla+H_i\mathscr{A})^*$.

Thus $\hat{c}_i = w_i$ and $\hat{C}_i = W_i$ almost everywhere and $(\hat{c}_i, \hat{C}_i)$ is a weak solution of the system $\hat{S}_n$, $\hat{B}_n$. But w_i and W_i are continuous, so modifying $\hat{c}_i$ and $\hat{C}_i$ on a set of measure zero if necessary, we get $\hat{c}_i = w_i \in C^{1+\alpha}[\overline{\Omega}, R^{n(I)}]$ and $\hat{C}_i = W_i \in C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}]$. Again putting

$$w_i = -gf_i(x, \hat{c}_j) \quad \textbf{(4.4.39)}$$

and

$$W_i = -G(F_i(z, \hat{C}_j)+H_i\int_{\partial\Omega_2}\hat{c}_i), \quad \textbf{(4.4.40)}$$

where $g:C^{1+\alpha}[\overline{\Omega}, R^{n(I)}] \rightarrow C^{2+\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) is the sum of a constant operator and a linear operator which is bounded by the Schauder estimates in Theorem 4.1.3, thus g is continuous. Similarly, $G:C^{1+\alpha}[\overline{\Lambda}, R^{n(J)}] \rightarrow C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$ is the sum of a constant operator and a linear operator which is bounded by the Schauder estimates in Theorem 4.1.3, thus G is continuous.

Therefore by Theorem 4.1.2, we obtain that $w_i \in C^{2+\alpha}[\overline{\Omega}, R^{n(I)}]$ and $W_i \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$ and the same argument that $\hat{c}_i = w_i$ and $\hat{C}_i = W_i$ finally results in $\hat{c}_i \in C^{2+\alpha}[\overline{\Omega}, R^{n(I)}]$ (with Λ treated as a parameter space) and $\hat{C}_i \in C^{2+\alpha}[\overline{\Lambda}, R^{n(J)}]$. By the same arguments in Lemma 4.3.5, it can be shown that $\hat{c}_i \in C^{2+\alpha,\alpha}[\overline{\Omega} \times \Lambda, R^{n(I)}]$ and thus $(\hat{c}_i, \hat{C}_i)$ is equal a.e. to a classical solution of of the system $\hat{S}_n, \hat{B}_n$ as required.

A similar proof may be obtained if we start the iterations with an upper solution $(\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$.□

We now show that the solution $(\hat{\underline{c}}_i, \hat{\underline{C}}_i)$ of $\hat{S}_n, \hat{B}_n$ obtained by starting the iteration at $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$, is asymptotically stable from below and similarly, the solution $(\bar{\hat{c}}_i, \bar{\hat{C}}_i)$ of $\hat{S}_n, \hat{B}_n$ obtained by starting the iteration at $(\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$, an upper solution of $\hat{S}_n, \hat{B}_n$, is asymptotically stable from above.

In the special case that $(\bar{\hat{c}}_i, \bar{\hat{C}}_i) \equiv (\hat{\underline{c}}_i, \hat{\underline{C}}_i)$, we will have that $(\bar{\hat{c}}_i, \bar{\hat{C}}_i)$, $(\hat{\underline{c}}_i, \hat{\underline{C}}_i)$ are asymptotically stable both from above and from below.

We have seen that each solution (c_i, C_i) of the system (4.4.1)-(4.4.8), where $\hat{\underset{\sim}{c}}_i \le c_{i,0} \le \tilde{\hat{c}}_i$ and $\hat{\underset{\sim}{C}}_i \le C_{i,0} \le \tilde{\hat{C}}_i$ satisfies $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i) \le (c_i, C_i) \le (\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$.

Let $(\bar{c}_i, \bar{C}_i)$ be the solution of the system (4.4.1)-(4.4.8) with initial data $(\bar{c}(0, x, z), \bar{C}(0, z)) = (\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$ and let $(\underline{c}_i, \underline{C}_i)$ be the solution of the system (4.4.1)-(4.4.8) with initial data $(\underline{c}(0, x, z), \underline{C}(0, z)) = (\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i)$. By Theorem 3.2.12 (Generalised Strong Comparison theorem), each solution (c_i, C_i) of the system (4.4.1)-(4.4.8) satisfies

$$(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i) \le (\underline{c}_i, \underline{C}_i) \le (c_i, C_i) \le (\bar{c}_i, \bar{C}_i) \le (\tilde{\hat{c}}_i, \tilde{\hat{C}}_i).$$

In particular, $(\underline{c}_i, \underline{C}_i)$, satisfies

$$(\hat{\underset{\sim}{c}}_i(x, z), \hat{\underset{\sim}{C}}_i(z)) \le (\underline{c}_i(t, x, z), \underline{C}_i(t, z)) \le (\hat{\underline{c}}_i(x, z), \hat{\underline{C}}_i(z)),$$

where $(\hat{\underline{c}}_i(x, z), \hat{\underline{C}}_i(z))$ is the solution of the system $\hat{S}_n, \hat{B}_n$, which is obtained by starting the monotone iteration at $(\hat{\underset{\sim}{c}}_i(x, z), \hat{\underset{\sim}{C}}_i(z))$ since $(\hat{\underline{c}}_i(x, z), \hat{\underline{C}}_i(z))$ also satisfies the system (4.4.1)-(4.4.8).

So $(\underline{c}_i, \underline{C}_i)$ is bounded above and monotonically nondecreasing in t from Theorem 4.4.1; thus $\lim_{t \to \infty} (\underline{c}_i(t,x,z), \underline{C}_i(t,z))$ exists and is a solution of the system $\hat{S}_n, \hat{B}_n$ by Theorem 4.4.2. From Theorem 4.3.1 (Generalised Existence Theorem), we see that $(\hat{\underline{c}}_i(x, z), \hat{\underline{C}}_i(z))$ is a minimal solution. Therefore, we have,

$$\lim_{t \to \infty} (\underline{c}_i, \underline{C}_i) = (\hat{\underline{c}}_i, \hat{\underline{C}}_i).$$

Each solution (c_i, C_i) with initial data $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i) \le (c_{i,0}, C_{i,0}) \le (\hat{\underline{c}}_i, \hat{\underline{C}}_i)$ satisfies $(\underline{c}_i, \underline{C}_i) \le (c_i, C_i) \le (\hat{\underline{c}}_i, \hat{\underline{C}}_i)$ and so we have proved:

Lemma 4.4.1

If (c_i, C_i) *is a solution of* (4.4.1)-(4.4.8) *with initial data* $(\hat{\underset{\sim}{c}}_i, \hat{\underset{\sim}{C}}_i) \le (c_{i,0}, C_{i,0}) \le (\hat{\underline{c}}_i, \hat{\underline{C}}_i)$, *then* $\lim_{t \to \infty} (c_i, C_i) = (\hat{\underline{c}}_i, \hat{\underline{C}}_i)$.

If (c_i, C_i) *is a solution of* (4.4.1)-(4.4.8) *with initial data* $(\bar{\hat{c}}_i, \bar{\hat{C}}_i) \le (c_{i,0}, C_{i,0}) \le (\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$, *then* $\lim_{t \to \infty} (c_i, C_i) = (\bar{\hat{c}}_i, \bar{\hat{C}}_i)$.

If $(\hat{\underline{c}}_i, \hat{\underline{C}}_i) = (\bar{\hat{c}}_i, \bar{\hat{C}}_i)$, *then* $(\hat{\underline{c}}_i, \hat{\underline{C}}_i)$, $(\bar{\hat{c}}_i, \bar{\hat{C}}_i)$ *is asymptotically stable from above and from below.*

Corollary 4.4.1

If there exists a lower solution $(\underset{\sim}{\hat{c}}_i, \underset{\sim}{\hat{C}}_i)$ *and an upper solution* $(\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$ *of the system* $\hat{S}_n, \hat{B}_n$, *and if there is only one solution* $(\underline{\hat{c}}_i, \underline{\hat{C}}_i) \equiv (\overline{\hat{c}}_i, \overline{\hat{C}}_i)$ *of the system* $\hat{S}_n, \hat{B}_n$ *such that* $(\underset{\sim}{\hat{c}}_i, \underset{\sim}{\hat{C}}_i) \leq (\underline{\hat{c}}_i, \underline{\hat{C}}_i)$ *and* $(\overline{\hat{c}}_i, \overline{\hat{C}}_i) \leq (\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$, *then this solution is an asymptotically stable equilibrium solution of the system* (4.4.1)-(4.4.8) *and each solution of* (4.4.1)-(4.4.8) *with initial data* $(\underset{\sim}{\hat{c}}_i, \underset{\sim}{\hat{C}}_i) \leq (c_{i,0}, C_{i,0}) \leq (\tilde{\hat{c}}_i, \tilde{\hat{C}}_i)$ *tends to* $(\underline{\hat{c}}_i, \underline{\hat{C}}_i)$, $(\overline{\hat{c}}_i, \overline{\hat{C}}_i)$ *as* $t \to \infty$.

So, with the monotone iteration methods given in section 4.3, it is not possible to obtain unstable solutions. On the other hand, each solution obtained by monotone iteration is asymptotically stable at least from above or below.

If $(\underline{\hat{c}}_i, \underline{\hat{C}}_i) \equiv (\overline{\hat{c}}_i, \overline{\hat{C}}_i)$, the unique solution obtained by monotone iteration is asymptotically stable both from above and from below. We have seen in section 4.3 that given an upper and a lower solution of the system $\hat{S}_n$, $\hat{B}_n$, there exists a solution of the system $\hat{S}_n$, $\hat{B}_n$ between these upper and lower solutions which can be constructed by monotone iteration. On the other hand given an upper and a lower solution and that there exists a unique solution of the system $\hat{S}_n$, $\hat{B}_n$ between these upper and lower solutions, this unique solution can be constructed by monotone iteration and this unique solution obtained by monotone iteration is asymptotically stable both from above and from below. We have shown that uniqueness implies asymptotic stability for these class of problems. Note that this will not be true in general (LACEY [150]) unless both upper and lower solutions exist. Also, from the boundedness of our solution $(\underline{\hat{c}}_i, \underline{\hat{C}}_i)$, $(\overline{\hat{c}}_i, \overline{\hat{C}}_i)$ of the system $\hat{S}_n$, $\hat{B}_n$ and the boundedness of (c_i, C_i) of solutions of (4.4.1)-(4.4.8) for all time, it follows that the asymptotic stability and uniqueness of $(\underline{\hat{c}}_i, \underline{\hat{C}}_i)$, $(\overline{\hat{c}}_i, \overline{\hat{C}}_i)$ imply the global stability of $(\underline{\hat{c}}_i, \underline{\hat{C}}_i)$, $(\overline{\hat{c}}_i, \overline{\hat{C}}_i)$ in the system $\hat{S}_n$, $\hat{B}_n$.

Remark 4.4.1

In this section we have assumed that the boundary conditions (2.1.4) and (2.1.7) are of the Robin type. We may treat the Neumann and Dirichlet type boundary conditions similarly by using appropriate theorems for linear relationships concerning the asymptotic behaviour of linear parabolic equations as $t \to \infty$ and their corresponding linear elliptic equations with Neumann and Dirichlet boundary conditions (see Remark 4.1.6).

In all the cases of this section which involve the uniqueness of the steady state problem, we see that the imbedding results of section 3.2 and section 4.2 apply and therefore all these results may be shown to hold for the general systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ which may possess no monotone property.

4.5 Notes and Comments

As with Chapter 3, the imbedding results in section 4.2 may give a lot of useful information about solutions. However as we see in this chapter this information is more restrictive and relies on proving the uniqueness of solutions to the imbedded system.

To obtain existence results in section 4.3, where the nonlinearities obeyed no monotone property, we redefined our nonlinear reaction functions so as to obtain *a priori* bounds on our solutions and classical results were employed in order to obtain existence. This is a simple way of obtaining *a priori* bounds on our solutions but it is certainly not the only way. We could alternatively have employed functions that control the growth of the nonlinear reaction functions, thereby obtaining *a priori* bounds on our solutions (FITZGIBBON and MORGAN [91]). As in our case, classical results could then also be employed in order to obtain existence.

In section 4.3, we obtained the existence of solutions to the system $\hat{S}_n$, $\hat{B}_n$ by monotone iteration. This could alternatively have been established by embedding this system as steady state solutions of the system (4.4.1)-(4.4.8) and using results of section 4.4 as $t \to \infty$ to show that solutions of the system $\hat{S}_n$, $\hat{B}_n$ also exist. This also gives an alternative to the monotone iterative methods for obtaining minimal and maximal solutions (CHAN [64]).

It is worth noting that in the definition of lower and upper solutions for scalar elliptic equations, if the nonlinearity term f is monotone decreasing in c, then the restriction $\underline{c} \le \overline{c}$ is not required but is a consequence of the differential inequalities (PROTTER and WEINBERGER [234] and VARMA and STREIDER [1985]). It is not clear how this relates to systems of elliptic equations.

Systems of nonlinear elliptic boundary value problems arise in many applications such as multiple chemical reactions that take place in an isothermal or nonisothermal catalyst pellet and simple models of tubular chemical reactors (COHEN [73, 75] and COHEN and LAETSCH [74]). Some of these systems of elliptic boundary value problems possess multiple solutions. This thesis does not examine multiple solutions. However there are many situations in particle reactors where this does occur (CHI *et al.* [70], LUSS and AMUNDSON [173]) and interesting cases occur with the problem $\hat{S}_n$, $\hat{B}_n$ if it has several distinct solutions or if the micro structures are in the presence of several distinct steady states (ARONSON and PELETIER [23]). Simple criteria for the existence of lower and upper solutions for elliptic scalar equations is discussed by AMANN [6, 9], as is nonexistence and general uniqueness theorems and this theory has also been extended in deriving multiplicity results, namely a criterion guaranteeing the existence of at least for example three distinct solutions. Some of these results may be generalised to the system $\hat{S}_n$, $\hat{B}_n$.

5

The Linear Problem

5.0 Introduction

The nonlinearities in the system S_n, B_n generally reside in the chemical reaction terms, but at dilute concentrations, linear approximations can be good enough. The validity of such linear approximations was tested against solutions derived numerically by orthogonal collocation techniques for a system governed by nonlinear Michaelis-Menten type kinetics (PARSHOTAM, *et al.* [226]).

In this chapter, it is shown that linear systems of convection reaction-diffusion equations for particle reactors described in this thesis are shown to be amenable to certain geometrical factorization techniques which dramatically reduce the dimensionality of the system. These equations are also amenable to algebraic uncoupling transformations which simplify the tasks of obtaining analytic and numerical solutions or estimates.

These same factorization and uncoupling techniques may be also applied to an associated linear system for vectors composed of the mean action time variable for each chemical component. These vector functions give the time lags for the various chemical outputs of the system during its transition from one steady output mode to another, and the mean first passage times and mean particle residence times corresponding to tracer pulse inputs of the chemicals.

In section 5.1, a general system of linear equations is described using matrix notation, dimensionless parameters and general undefined geometric configurations in order to focus attention on certain structural aspects of the equations. Section 5.2 is concerned with a dominant transitory aspect of the system described by a mean action time variable defined for each chemical component in the micro and the macro systems. These variables satisfy an associated linear system of equations coupled to the system for the ultimate steady state solution and give a measure of the time for the transitions from one steady state to another. The ultimate steady outputs are given in terms of the final steady state solutions and the time lag constants for the various outputs are given in terms of the mean action time functions.

A geometric factorization technique for these general linear systems is developed in section 5.3. For a general class of time dependent problems with factorised initial conditions, this factorization is best revealed in the Laplace transform domain but can be developed in t-space using convolution integrals.

For steady state problems and for the systems defining the mean action times, a more obvious product factorization holds. These equations are also amenable to matrix transformations which uncouple the systems algebraically when the coupling matrices are quasisymmetric in that they are the product db of a positive nonsingular diagonal matrix d with a symmetric matrix b. This is a common structural feature of linearised chemical kinetic equations (MCNABB and BASS [189]).

The macroscopic equations are assumed to be convection dominated here. This leads to two simplifications. The diffusivity $\mathscr{D}$ in the macroscopic equations is dominated by dispersion effects and so its diagonal elements are the same for all of the chemical components. In these circumstances, we may treat $\mathscr{D}$ as a scalar in the convection-diffusion equations. Secondly, the boundary conditions at output surfaces of the bioreactor may then be assumed to be of the Danckwerts type where the normal gradients of chemical concentration are all taken to be zero.

These simplifications allow the macroscopic equations for steady state concentrations and mean action times to be algebraically uncoupled by matrix transformations. All boundary conditions except one are similarly uncoupled. On the outer boundary of the particles, a linear boundary condition of the form (5.1.3) below is assumed. This equates the flux out of the particles, defined by a diagonal diffusivity matrix D and concentration gradients normal to the surface, to the flux across a fluid boundary layer. In the common situations where H is a scalar multiple of D, this equation too remains uncoupled by the matrix transformations which uncouple the rest of the system.

5.1 Matrix Notation

Our reactor occupies a region Λ, z denotes a point in this region and $u(z)$ is the solenoidal fluid velocity distribution in Λ. The $n(J)$-vector $C(t, z)$ with components $C_i(t, z)$ describes the concentration of the ith chemical component. In the neighbourhood of any point z in Λ, there is a distribution of particles of various sizes and shapes and an active layer described by a region Ω attached to these particles.

Points in Ω are denoted by x and the vector $c(t, x, z)$ has $n(I)$-components $c_i(t, x, z)$ describing the concentrations at time t at x in Ω, which is in the neighbourhood of the point z in Λ. Each c_i is associated with the same chemical component as $C_i(t, z)$ is outside Ω if $C_i(t, z)$ exists.

The diagonal matrix D has positive elements D_i in the ith row and column representing the diffusion constant for component i in Ω. The reaction-diffusion behaviour in Ω for a time span $[0, T]$ is assumed to be given by

$$\frac{\partial c}{\partial t} - D\nabla_x^2 c - ac = 0 \text{ in } (0, T]\times\Omega\times\Lambda, \tag{5.1.1a}$$

where a is an $n(I)\times n(I)$ constant matrix describing the rate of generation of chemical components c_i due to reactions with the other components.

The region Ω is assumed to have an inner boundary $\partial\Omega_1$ defining the inert particle cores of our representative sample, and on this inner boundary we suppose there to be no flux of chemical and hence

$$\frac{\partial c}{\partial n} = 0 \text{ on } (0, T]\times\partial\Omega_1\times\Lambda. \tag{5.1.2}$$

The outer boundary $\partial\Omega_2$ of Ω permits chemical exchange between the bioparticles and the reactor fluid. A boundary layer attached to $\partial\Omega_2$ is assumed to allow a chemical flux $H(C-c)$ between Λ and Ω where H is a diagonal matrix with terms describing the diffusive boundary layer flux for each component. It is not unreasonable in many cases to assume H to be proportional to D and when this is so, we write $H = \gamma D$ where γ is the scalar constant of proportionality. The linear boundary condition derived by equating these fluxes to those in Ω near $\partial\Omega_2$ is

$$D\frac{\partial c}{\partial n} = H(C-c) \text{ on } (0,T]\times\partial\Omega_2\times\Lambda. \tag{5.1.3}$$

Concentrations C in the macroscopic system are assumed to satisfy the linear matrix system

$$\frac{\partial C}{\partial t} - \mathcal{D}\nabla^2 C + u\cdot\nabla C - BC + \int_{\partial\Omega_2} D\frac{\partial c}{\partial n} = 0 \text{ in } (0, T]\times\Lambda, \tag{5.1.4}$$

where $\mathcal{D}$ is a diagonal matrix representing diffusion and dispersion effects in Λ, ∇^2 and $u\cdot\nabla$ are scalar operators on functions of z, B is an $n(J)\times n(J)$ constant matrix describing linear chemical kinetics and the integral term gives the chemical flux into Ω at (t, z).

Let $\partial\Lambda_1$, $\partial\Lambda_2$ and $\partial\Lambda_3$ denote three sections of the boundary of Λ. Fluid flows in through $\partial\Lambda_1$ carrying chemical components at given concentrations C_1, so that

$$v_1 C + \mathcal{D}\frac{\partial C}{\partial n_1} = v_1 C_1 \text{ on } (0, T]\times\partial\Lambda_1, \tag{5.1.5}$$

where $v_1 = -u\cdot n_1$ is the scalar normal fluid velocity into Λ. Over $\partial\Lambda_2$, there is no transport of fluid or chemical, so that

$$\frac{\partial C}{\partial n_2} = 0 \text{ on } (0, T]\times\partial\Lambda_2, \tag{5.1.6}$$

and the fluid flows out through the system over $\partial\Lambda_3$, where DANCKWERTS [79] type boundary conditions prevailing at high Pèclet numbers are assumed, so that

$$\frac{\partial C}{\partial n_3} = 0 \text{ on } (0, T]\times\partial\Lambda_3. \tag{5.1.7}$$

At any time t, the chemical output is $q(t, \partial\Lambda_3)$ over $\partial\Lambda_3$, where q is an n-vector whose ith term q_i, gives the flux of component i over $\partial\Lambda_3$. If $v_3 = u\cdot n_3$ is the fluid velocity on $\partial\Lambda_3$, then

$$q(t, \partial\Lambda_3) = \int_{\partial\Lambda_3} v_3 C. \tag{5.1.8}$$

At each point z in Λ, the inputs to Ω are likewise given by the flux vector $q(t, \partial\Omega_2, z)$, where

$$q(t, \partial\Omega_2, z) = \int_{\partial\Omega_2} D\frac{\partial c}{\partial n} = \int_{\partial\Omega_2} H(C-c) = H\mathcal{A}C - H\int_{\partial\Omega_2} c, \tag{5.1.9}$$

and where $\mathcal{A}$ is the surface area of $\partial\Omega_2$.

Let L_n denote the linear system of equations and couplings (5.1.1)-(5.1.4), and B_n denote the system of external boundary conditions, (5.1.5)-(5.1.7) and the initial conditions

$$c = c_0 \text{ in } \Omega\times\Lambda,\ C = C_0 \text{ in } \Lambda \text{ at } t = 0. \tag{5.1.10}$$

5.2 Mean Action Times, Time Lag Constants and Mean Residence Times

Let us consider solutions (c, C) of the system L_n, B_n which start at $t = 0$ with c_0 and C_0 zero, and for which the given boundary vector functions C_1 are independent of time. As time progresses, these solutions tend to steady state solutions $(\hat{c}, \hat{C})$, and the chemical fluxes $q(t, \partial\Lambda_3)$, $q(t, \partial\Omega_2, z)$ which start zero, gradually approach constant values $\hat{q}(\partial\Lambda_3)$, $\hat{q}(\partial\Omega_2, z)$.

Let $Q(t, \partial\Lambda_3)$, $Q(t, \partial\Omega, z)$ measure the accumulated fluxes across $\partial\Lambda_3$ and $\partial\Omega_2$ respectively, in the time t, so that

$$Q(t, \partial\Lambda_3) = \int_0^t q(s, \partial\Lambda_3)ds = \int_0^t \hat{q}(\partial\Lambda_3) - \int_0^t [\hat{q}(\partial\Lambda_3) - q(s, \partial\Lambda_3)]ds$$

$$= \hat{q}(\partial\Lambda_3)t - \int_0^t\int_{\partial\Lambda_3} v_3[\hat{C}(z) - C(s, z)]ds \tag{5.2.1}$$

$$\sim \int_{\partial\Lambda_3} v_3[\hat{C}(z)t - \mathfrak{I}(z)],$$

for large t, where

$$\mathfrak{I}(z) \equiv \int_0^\infty [\hat{C}(z) - C(s, z)]ds. \tag{5.2.2}$$

Likewise, for large t,

$$Q(t, \partial\Omega_2, z) \sim \int_{\partial\Omega_2} D\frac{\partial}{\partial n}[\hat{c}(x, z)t - \tau(x, z)], \tag{5.2.3}$$

where

$$\tau(x, z) \equiv \int_0^\infty [\hat{c}(x, z) - c(s, x, z)]ds. \tag{5.2.4}$$

These vector functions $Q(t, \partial\Lambda_3)$and $Q(t, \partial\Omega_2, z)$ have linear asymptotes for each component for increasing time, which intersect the time axis at times $t_L(\partial\Lambda_3)_i$ and $t_L(z, \partial\Omega_2)_i$ called flux time lags. The ith component of the vector $t_L(\partial\Lambda_3)$ gives the time lag

$$t_L(\partial\Lambda_3)_i = \frac{[\int_{\partial\Lambda_3} v_3\mathfrak{I}(z)]_i}{[\int_{\partial\Lambda_3} v_3\hat{C}(z)]_i}, \tag{5.2.5}$$

for the chemical flux of component i over $\partial\Lambda_3$, and the time lag

$$t_L(\partial\Omega_2)_i = \frac{[\int_{\partial\Omega_2} D\frac{\partial\tau(x, z)}{\partial n}]_i}{[\int_{\partial\Omega_2} D\frac{\partial\hat{c}(x, z)}{\partial n}]_i}, \tag{5.2.6}$$

for the chemical flux of component i over $\partial\Omega_2$.

The vectors $\tau(x, z)$ and $\mathfrak{I}(z)$ are the mean action time vectors for this problem (McNabb and Wake [190, 193]) and the following systems of equations are obtained for them from L_n, B_n.

$$-D\nabla_x^2\tau - a\tau = \int_0^\infty \frac{\partial c}{\partial t}dt = \hat{c} \text{ in } \Omega\times\Lambda, \tag{5.2.7}$$

$$\frac{\partial\tau}{\partial n} = 0 \text{ on } \partial\Omega_1\times\Lambda, \tag{5.2.8}$$

$$D\frac{\partial\tau}{\partial n} = H(\mathfrak{I} - \tau)\text{on } \partial\Omega_2\times\Lambda, \tag{5.2.9}$$

$$-\mathcal{D}\nabla^2\mathfrak{I} + u\cdot\nabla\mathfrak{I} - B\mathfrak{I} + \int_{\partial\Omega_2} D\frac{\partial\tau}{\partial n} = \hat{C} \text{ in } \Lambda, \tag{5.2.10}$$

$$v_1\mathfrak{I} + \mathcal{D}\frac{\partial\mathfrak{I}}{\partial n} = 0 \text{ on } \partial\Lambda_1, \tag{5.2.11}$$

$$\frac{\partial\mathfrak{I}}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha = 2, 3, \tag{5.2.12}$$

where $(\hat{c}, \hat{C})$ are the steady state solutions of L_n, B_n, satisfying

$$-D\nabla_x^2\hat{c}-a\hat{c}=0 \text{ in } \Omega\times\Lambda, \tag{5.2.13}$$

$$D\frac{\partial\hat{c}}{\partial n}=H(\hat{C}-\hat{c}) \text{ on } \partial\Omega_2\times\Lambda, \tag{5.2.14}$$

$$\frac{\partial\hat{c}}{\partial n}=0 \text{ on } \partial\Omega_1\times\Lambda, \tag{5.2.15}$$

$$-\mathcal{D}\nabla^2\hat{C}+u\cdot\nabla\hat{C}-B\hat{C}+\int_{\partial\Omega_2}D\frac{\partial\hat{c}}{\partial n}=0 \text{ in } \Lambda, \tag{5.2.16}$$

$$v_1\hat{C}+\mathcal{D}\frac{\partial\hat{C}}{\partial n}=v_1C_1 \text{ on } \partial\Lambda_1, \tag{5.2.17}$$

$$\frac{\partial\hat{C}}{\partial n_\alpha}=0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha=2,3. \tag{5.2.18}$$

Various physical interpretations of these average times are discussed in some detail for single component systems in MCNABB and WAKE [190, 193].

The solution c, C above, corresponding to a step function boundary condition C_1 on $\partial\Lambda_1$ and zero initial conditions gives rise to another solution g, G for L_n, B_n given by

$$G(t,z)=\frac{\partial C}{\partial t} \text{ in } (0,T]\times\Lambda, \tag{5.2.19}$$

$$g(t,x,z)=\frac{\partial c}{\partial t} \text{ in } (0,T]\times\Omega\times\Lambda. \tag{5.2.20}$$

This solution is generated by a delta function pulse of particles of strength C_1 released on $\partial\Lambda_1$ at $t=0$. This pulse input can be regarded as a tracer solution giving a picture of various transitory aspects of the system. There are a number of natural time concepts associated with g, G which like the time lags for c and C, can be expressed as functionals of $\mathfrak{I}$ and τ.

For example, the mean first passage time $t_i^*(\partial\Lambda_3)$ for the chemical component i leaving Λ via $\partial\Lambda_3$ is given by

$$[\int_0^\infty\int_{\partial\Lambda_3}v_3G_i dt]t_i^*(\partial\Lambda_3)=[\int_0^\infty t\int_{\partial\Lambda_3}v_3G_i dt]=\int_{\partial\Lambda_3}v_3\int_0^\infty t\frac{\partial C_i}{\partial t}dt=\int_{\partial\Lambda_3}v_3\mathfrak{I}_i, \tag{5.2.21}$$

so that

$$t_i^*(\partial\Lambda_3)=\frac{[\int_{\partial\Lambda_3}v_3\mathfrak{I}]_i}{[\int_{\partial\Lambda_3}v_3\hat{C}\ ]_i}=t_L(\partial\Lambda_3)_i. \tag{5.2.22}$$

The mean residence time $\tilde{t}_i(\Lambda)$ for the ith chemical component in Λ is given by

$$[\int_\Lambda\int_0^\infty G_i dt]\tilde{t}_i(\Lambda)=[\int_\Lambda\hat{C}_i]\tilde{t}_i(\Lambda)=\int_\Lambda\int_0^\infty tG_i dt=\int_\Lambda\mathfrak{I}_i. \tag{5.2.23}$$

Likewise, the mean residence time $\tilde{t}_i(\Omega)$ at a point z in Λ is given by

$$[\int_\Omega\int_0^\infty g_i dt]\tilde{t}_i(\Omega)=[\int_\Omega\hat{c}_i]\tilde{t}_i(\Omega)=\int_\Omega\int_0^\infty tg_i dt=\int_\Omega\tau_i, \tag{5.2.24}$$

and the mean residence time $\bar{\tau}_i(\Omega \cup \Lambda)$ for the ith component in the whole system is given by

$$[\int_\Lambda \hat{C} + \int_\Lambda \int_\Omega \hat{c}_i]\bar{\tau}_i(\Omega \cup \Lambda) = \int_\Lambda \mathfrak{T}_i + \int_\Lambda \int_\Omega \tau_i \,. \tag{5.2.25}$$

The time lags at $\partial\Lambda_3$ for various chemical components coincide with their mean first passage times from the system, whereas the time lags for the fluxes to be established in the region Ω at any point z in Λ, and the mean residence times of the components in the same region Ω are different functionals of the mean action time vector τ and the steady state vector $\hat{c}$.

5.3 Geometric Factorisation

The linear system of equations L_n, B_n in full geometric generality present a computational, dimensional crisis, since the solutions are defined in seven dimensions; three in x-space, three in z-space and one in time. This is marginally relieved by considering just steady state solutions. Fortunately the equations for $(\hat{c},\ \hat{C})$ can be geometrically factorized in the following way. If $n = n(I) = n(J)$, and all $\hat{c}$ are coupled to $\hat{C}$ by (5.1.3) then the vector $\hat{c}(x, z)$ can be written as the product

$$\hat{c}(x,\ z) = \theta(x)S\hat{C}(z), \tag{5.3.1}$$

where θ and S are $n \times n$ matrices, θ is a function of x only and S is constant. If $\theta(x)$ satisfies the equations,

$$-D\nabla_x^2\theta - a\theta = 0 \text{ in } \Omega, \tag{5.3.2}$$

$$\frac{\partial\theta}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{5.3.3}$$

$$D\frac{\partial\theta}{\partial n} = H(S^{-1} - \theta) \text{ on } \partial\Omega_2, \tag{5.3.4}$$

then $(\hat{c},\ \hat{C})$ are steady state solution vectors of L_n, B_n, provided $\hat{C}$ satisfies,

$$-\mathcal{D}\nabla^2\hat{C} + u\cdot\nabla\hat{C} - B\hat{C} + (\int_{\partial\Omega_2} D\frac{\partial\theta}{\partial n})S\hat{C} = 0 \text{ in } \Lambda, \tag{5.3.5}$$

$$\upsilon_1\hat{C} + \mathcal{D}\frac{\partial\hat{C}}{\partial n_1} = \upsilon_1 C_1 \text{ on } \partial\Lambda_1, \tag{5.3.6}$$

$$\frac{\partial\hat{C}}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha = 2, 3. \tag{5.3.7}$$

The linear problems (5.3.2)-(5.3.4) and (5.3.5)-(5.3.7) are each in three dimensions only, and the first can be solved independently of the second for any given nonsingular matrix S. If D is nonsingular and positive definite, then equations (5.3.2)-(5.3.4) may be uncoupled by linear matrix transformations if a is "quasisymmetric" in the sense that

$$a = db, \tag{5.3.8}$$

where d is a positive definite diagonal matrix and b is symmetric. Furthermore, if H and D are proportional in the sense that

$$H = \gamma D, \tag{5.3.9}$$

for γ a positive scalar, then the boundary conditions are uncoupled by the same transformation.

In this case, there is a nonsingular matrix T with transpose T' for which $T'd^{-1}DT = I$ the unit matrix, and $T'bT = \mu$, a diagonal matrix. If we let $\theta = T\varphi$ and $S = T^{-1}$, then

$$-\nabla_x^2\varphi - \mu\varphi = 0 \text{ in } \Omega, \tag{5.3.10}$$

$$\frac{\partial\varphi}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{5.3.11}$$

$$\frac{\partial\varphi}{\partial n} = \gamma(I - \varphi) \text{ on } \partial\Omega_2, \tag{5.3.12}$$

and hence, φ is a diagonal matrix. A similar geometric factorization works for τ and $\mathfrak{I}$, by expressing τ in the form

$$\tau(x, z) = \theta(x)S\mathfrak{I}(z) + \zeta(x)W\hat{C}(z). \tag{5.3.13}$$

Equations (5.2.7)-(5.2.9) are satisfied for $\tau(x, z)$ if θ is a solution of (5.3.2)-(5.3.4) and $\zeta(x)$ is a solution of

$$-D\nabla_x^2\zeta - a\zeta = W^{-1} \text{ in } \Omega, \tag{5.3.14}$$

$$\frac{\partial\zeta}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{5.3.15}$$

$$D\frac{\partial\zeta}{\partial n} + H\zeta = 0 \text{ on } \partial\Omega_2. \tag{5.3.16}$$

This system may also be uncoupled algebraically when the earlier conditions (5.3.8)-(5.3.9) prevail, by choosing

$$\theta = T\varphi, \tag{5.3.17}$$

$$S = T^{-1}, \tag{5.3.18}$$

$$W = T'd^{-1}, \tag{5.3.19}$$

and

$$\zeta(x) = T\xi(x). \tag{5.3.20}$$

The matrix φ given by (5.3.10)-(5.3.12) is diagonal and $\xi(x)$ given by the Helmholtz problem,

$$-\nabla_x^2\xi - \mu\xi - I = 0 \text{ in } \Omega, \tag{5.3.21}$$

$$\frac{\partial\xi}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{5.3.22}$$

$$\frac{\partial\xi}{\partial n} + \gamma\xi = 0 \text{ on } \partial\Omega_2, \tag{5.3.23}$$

is also diagonal. The coupling term $\int_{\partial\Omega_2} D\frac{\partial\tau}{\partial n}$ in equation (5.2.10) for $\mathfrak{I}(z)$ can be expressed in the form

$$\int_{\partial\Omega_2} D\frac{\partial\tau}{\partial n} = \left(\int_{\partial\Omega_2} D\frac{\partial\theta}{\partial n}\right)S\mathfrak{I}(z) + \left(\int_{\partial\Omega_2} D\frac{\partial\zeta}{\partial n}\right)W\hat{C}(z), \tag{5.3.24}$$

and $\theta(x)$ and $\zeta(x)$ are given by (5.3.2)-(5.3.4) and (5.3.14)-(5.3.16), so that $\mathfrak{I}(z)$ and $\hat{C}(z)$ are given by coupled systems in the z variables. We note that in the algebraically uncoupled system,

$$T^{-1}\hat{c} = \varphi T^{-1}\hat{C}, \tag{5.3.25}$$

$$T^{-1}\tau = \varphi T^{-1}\mathfrak{I} + \xi T' d^{-1}\hat{C}. \tag{5.3.26}$$

The vector $\hat{C}(z)$ is given by the boundary value problem (5.3.5)-(5.3.7), and in high Pèclet number situations, the diagonal matrix $\mathcal{D}$ may be considered a scalar operator since all the elements are equal along the diagonal, each being a dispersive mixing parameter due to fluid motion that is almost independent of D_i. Since $u\cdot\nabla$ is a scalar operator too, these equations are uncoupled by a similarity transformation $\mathcal{S}$ which puts the matrix B^* given by

$$B^* = B - \int_{\partial\Omega_2} D\frac{\partial\theta}{\partial n}S = B - \int_{\partial\Omega_2} DT\frac{\partial\varphi}{\partial n}T^{-1} \tag{5.3.27}$$

into Jordan normal form. Let

$$\hat{C} = \mathcal{S}\vartheta, \tag{5.3.28}$$

so that

$$\mathcal{S}^{-1}B^*\mathcal{S} = \Gamma,$$

where Γ is the Jordan canonical form for B^*. Then if $C_1 = \mathcal{S}\vartheta_1$,

$$-\mathcal{D}\nabla^2\vartheta + u\cdot\nabla\vartheta - \Gamma\vartheta = 0 \text{ in } \Lambda, \tag{5.3.29}$$

$$v_1\vartheta + \mathcal{D}\frac{\partial\vartheta}{\partial n_1} = v_1\vartheta_1 \text{ on } \partial\Lambda_1, \tag{5.3.30}$$

$$\frac{\partial\vartheta}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha = 2, 3. \tag{5.3.31}$$

In this form, each component ϑ_i of ϑ may be solved separately or iteratively. The equations for $\mathfrak{I}$ can be treated in a similar fashion, since from (5.2.10), (5.3.24),

$$-\mathcal{D}\nabla^2\mathfrak{I} + u\cdot\nabla\mathfrak{I} - B^*\mathfrak{I} = (I - \int_{\partial\Omega_2} D\frac{\partial\zeta}{\partial n}W)\hat{C} = K^*\hat{C} \text{ in } \Lambda, \tag{5.3.32}$$

$$v_1\mathfrak{I} + \mathcal{D}\frac{\partial\mathfrak{I}}{\partial n} = 0 \text{ on } \partial\Lambda_1, \tag{5.3.33}$$

$$\frac{\partial\mathfrak{I}}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha = 2, 3. \tag{5.3.34}$$

Let $\mathfrak{I}(z) = \mathcal{S}\Xi$, so that

$$-\mathcal{D}\nabla^2\Xi + u\cdot\nabla\Xi - \Gamma\Xi = \mathcal{S}^{-1}K^*\mathcal{S}\vartheta \text{ in } \Lambda, \tag{5.3.35}$$

$$v_1\Xi + \mathcal{D}\frac{\partial\Xi}{\partial n} = 0 \text{ on } \partial\Lambda_1, \tag{5.3.36}$$

$$\frac{\partial\Xi}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha = 2, 3. \tag{5.3.37}$$

Once again, the components of the vector Ξ are algebraically uncoupled and may be solved separately, or iteratively, depending on the nature of Γ.

The geometric factorization described here has counterparts in other applied problems (MCNABB [185]), and can be generalised to apply to some time dependent problems for which the initial value function $c_0(x, z)$ can be factored. Suppose

$$c_0(x, z) = \boldsymbol{u}(x)\mathcal{U}(z), \tag{5.3.38}$$

and $\bar{c}$, $\bar{C}$ denotes the Laplace transforms

$$\bar{c} = \int_0^\infty e^{-pt} c\,dt, \tag{5.3.39}$$

and

$$\bar{C} = \int_0^\infty e^{-pt} C\,dt. \tag{5.3.40}$$

In the transform variable p, the system L_n, B_n gives

$$-D\nabla_x^2 \bar{c} + (p-a)\bar{c} = c_0 = \boldsymbol{u}(x)\mathcal{U}(z) \text{ in } Z\times\Omega\times\Lambda, \tag{5.3.41}$$

$$\frac{\partial \bar{c}}{\partial n} = 0 \text{ on } Z\times\partial\Omega_1\times\Lambda, \tag{5.3.42}$$

$$D\frac{\partial \bar{c}}{\partial n} = H(\bar{C} - \bar{c}) \text{on } Z\times\partial\Omega_2\times\Lambda, \tag{5.3.43}$$

where Z is an appropriate strip of the complex p-plane. Once again we see $\bar{c}(p, x, z)$ is factorizable in the form

$$\bar{c} = \bar{\psi}(p, x)S\bar{C}(p, z) + \bar{\pi}(p, x)W\mathcal{U}(z), \tag{5.3.44}$$

provided $\bar{\psi}$ satisfies the boundary value problem,

$$-D\nabla_x^2\bar{\psi} + (p-a)\bar{\psi} = 0 \text{ in } Z\times\Omega, \tag{5.3.45}$$

$$\frac{\partial\bar{\psi}}{\partial n} = 0 \text{ on } Z\times\partial\Omega_1, \tag{5.3.46}$$

$$D\frac{\partial\bar{\psi}}{\partial n} = H(S^{-1} - \bar{\psi}) \text{ on } Z\times\partial\Omega_2, \tag{5.3.47}$$

and $\bar{\pi}$ satisfies the boundary value problem

$$-D\nabla^2\bar{\pi} + (p-a)\bar{\pi} = W^{-1}\boldsymbol{u}(x) \text{ in } Z\times\Omega, \tag{5.3.48}$$

$$\frac{\partial\bar{\pi}}{\partial n} = 0 \text{ on } Z\times\partial\Omega_1, \tag{5.3.49}$$

$$D\frac{\partial\bar{\pi}}{\partial n} + H\bar{\pi} = 0 \text{ on } Z\times\partial\Omega_2. \tag{5.3.50}$$

Algebraic uncoupling may be pursued in a similar fashion since $pI-a$ is of the form $d(pd^{-1}-b)$ and matrix transformations can diagonalise $pd^{-1}-b$ and reduce $d^{-1}D$ to the unit matrix simultaneously.

If $S(p)$ is of the form pS^* then $S^{-1}(p) = \frac{1}{p}S^{*-1}$ is the Laplace transform of a constant matrix S^*. The problems (5.3.45)-(5.3.47) and (5.3.48)-(5.3.50) can be inverted and we find $\psi(t, x)$ is given by:

$$\frac{\partial \psi}{\partial t} - D\nabla_x^2 \psi - a\psi = 0 \text{ in } (0, \infty)\times\Omega, \tag{5.3.51}$$

$$\frac{\partial \psi}{\partial n} = 0 \text{ on } (0, \infty)\times\partial\Omega_1, \tag{5.3.52}$$

$$D\frac{\partial \psi}{\partial n} = H(S^{*-1} - \psi) \text{ on } (0, \infty)\times\partial\Omega_2, \tag{5.3.53}$$

$$\psi = 0 \text{ in } \Omega \text{ at } t = 0, \tag{5.3.54}$$

and $\pi(t, z)$ by

$$\frac{\partial \pi}{\partial t} - D\nabla_x^2 \pi - a\pi = 0 \text{ in } (0, \infty)\times\Omega, \tag{5.3.55}$$

$$\frac{\partial \pi}{\partial n} = 0 \text{ on } (0, \infty)\times\partial\Omega_1, \tag{5.3.56}$$

$$D\frac{\partial \pi}{\partial n} + H\pi = 0 \text{ on } (0, \infty)\times\partial\Omega_2, \tag{5.3.57}$$

$$\pi = W^{-1}\boldsymbol{u}(x) \text{ in } \Omega \text{ at } t = 0. \tag{5.3.58}$$

From equation (5.3.44) and the observation that $p\overline{\psi}$ is the Laplace transform of $\frac{\partial \psi}{\partial t}$, we find

$$c(t, x, z) = \int_0^t \frac{\partial \psi(t-s, x)}{\partial t} S^* C(s, z)ds + \pi(t, x)W\mathcal{U}(z). \tag{5.3.59}$$

In the transform space, $\overline{C}$ satisfies a conventional convection-diffusion equation but in t space, the integral term is a convolution integral in time, so that $C(t, z)$ satisfies the nonhomogeneous partial differential causal integral equation,

$$\frac{\partial C}{\partial t} - \mathcal{D}\nabla^2 C + u\cdot\nabla C - BC + \int_{\partial\Omega_2} D\int_0^t \frac{\partial^2 \psi(t-s, x)}{\partial t\partial n} S^* C(s, z)ds = \left(-\int_{\partial\Omega_2} D\frac{\partial \pi}{\partial n}\right)W\mathcal{U}(z) \text{ in } (0, T]\times\Lambda. \tag{5.3.60}$$

Fortunately, a broad picture of the transient behaviour of the system is provided by the mean action time vectors $\mathcal{T}(x, z)$ and $\mathfrak{I}(z)$ and as observed earlier, they satisfy equations which can be geometrically factored in a simple way, and algebraically uncoupled under very general circumstances.

More detail concerning the nature of tracer distributions g_i, G_i can be obtained from higher moments. The Laplace transforms $\overline{g}(p, x, z)$ and $\overline{G}(p, z)$ of the vectors g, G describing the solution of L_n, B_n, created by a delta function pulse of strength C_1 on $\partial\Lambda_1$ at $t = 0$, are given by the system,

$$-D\nabla_x^2 \overline{g} + (pI - a)\overline{g} = 0 \text{ in } Z\times\Omega\times\Lambda, \tag{5.3.61}$$

$$\frac{\partial \overline{g}}{\partial n} = 0 \text{ on } Z\times\partial\Omega_1\times\Lambda, \tag{5.3.62}$$

$$D\frac{\partial\overline{g}}{\partial n}=H(\overline{G}-\overline{g}) \text{ on } Z\times\partial\Omega_2\times\Lambda, \tag{5.3.63}$$

$$-\mathscr{D}\nabla^2\overline{G}+u\cdot\nabla\overline{G}+(pI-B)\overline{G}+\int_{\partial\Omega_2}D\frac{\partial\overline{g}}{\partial n}=0 \text{ in } Z\times\Lambda, \tag{5.3.64}$$

$$\upsilon_1\overline{G}+\mathscr{D}\frac{\partial\overline{G}}{\partial n}=\upsilon_1C_1 \text{ on } Z\times\partial\Lambda_1, \tag{5.3.65}$$

$$\frac{\partial\overline{G}}{\partial n_\alpha}=0 \text{ on } Z\times\partial\Lambda_\alpha, \text{ for } \alpha=2,3. \tag{5.3.66}$$

The definitions of $\overline{g}$ and $\overline{G}$ lead to the following expansions for small p:

$$\overline{g}(p,x,z)=\int_0^\infty[1-pt+\frac{p^2t^2}{2!}-\frac{p^3t^3}{3!}+\ldots]\,g(t,x,z)dt=g_0(x,z)+pg_1(x,z)+\frac{p^2}{2!}g_2(x,z)+\ldots, \tag{5.3.67}$$

$$\overline{G}(p,z)dt=G_0(z)+pG_1(z)+\frac{p^2}{2!}G_2(z)+\ldots \tag{5.3.68}$$

Equations (5.2.19) and (5.2.20) give the following connections between g_n, G_n and functions defined earlier. The functions g_0 and G_0 are equal to the steady state solutions $(\hat{c},\hat{C})$ satisfying conditions (5.1.5) for C_1 since

$$g_0(x,z)=-\int_0^\infty\frac{\partial c}{\partial t}\,dt=\hat{c}(x,z). \tag{5.3.69}$$

The functions g_1 and G_1 are given by $-\tau$ and $-\mathfrak{I}$ respectively, since

$$g_1(x,z)=-\int_0^\infty t\frac{\partial c}{\partial t}\,dt=|t(\hat{c}-c)|_0^\infty-\int_0^\infty(\hat{c}-c)dt=-\tau(x,z), \tag{5.3.70}$$

and likewise

$$G_1(z)=-\mathfrak{I}(z). \tag{5.3.71}$$

Differential equations for these functions g_m, G_m can be readily derived from the equations for $\overline{g}$ and $\overline{G}$ by differentiating the system (5.3.61) and (5.3.64) above with respect to p, m times, and putting p equal to zero. For example, the equations for g_2 and G_2 are

$$-D\nabla_x^2g_2-ag_2=2\tau \text{ in } \Omega\times\Lambda, \tag{5.3.72}$$

$$\frac{\partial g_2}{\partial n}=0 \text{ on } \partial\Omega_1\times\Lambda, \tag{5.3.73}$$

$$D\frac{\partial g_2}{\partial n}=H(G_2-g_2) \text{ on } \partial\Omega_2\times\Lambda, \tag{5.3.74}$$

$$-\mathscr{D}\nabla^2G_2+u\cdot\nabla G_2-BG_2+\int_{\partial\Omega_2}D\frac{\partial g_2}{\partial n}=2\mathfrak{I} \text{ in } \Lambda, \tag{5.3.75}$$

$$\upsilon_1G_2+\mathscr{D}\frac{\partial G_2}{\partial n}=0 \text{ on } \partial\Lambda_1, \tag{5.3.76}$$

$$\frac{\partial G_2}{\partial n_\alpha} = 0 \text{ on } \partial\Lambda_\alpha, \text{ for } \alpha = 2, 3. \qquad (5.3.77)$$

These functions g_2 and G_2 lead to expressions for variances about the various mean first passage times and mean residence times discussed earlier. These equations also allow geometric factorization and algebraic decoupling.

We assumed D was nonsingular in equation (5.1.1) and throughout this section. In many applications, there will be some chemical components c_j in Ω which are immobile and for which $D_j = 0$. Such components can only interact with the fluid concentrations C via the reaction term and interacting mobile ingredients. A more general linear formulation explicitly recognising the existence of immobile components in Ω can be formulated by expressing (5.1.1) in a partitioned matrix form

$$\frac{\partial}{\partial t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} - \begin{pmatrix} D_1 & 0 \\ 0 & 0 \end{pmatrix}\nabla_x^2\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} - \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0, \qquad (5.1.1b)$$

where all the components of c_2 are immobile in Ω.

For these ingredients, H_j like D_j is also zero. In reality, the boundary conditions (5.1.2), (5.1.3) have no relevance for c_2.

The geometric factorization of this section is still valid for singular positive semidefinite matrices D and H but the algebraic uncoupling procedure needs re-examination. Is there a nonsingular matrix T with transpose T' for which

$$T'd^{-1}DT = J \qquad (5.3.78)$$

and

$$T'bT = \mu, \qquad (5.3.79)$$

where μ is a diagonal matrix and J is diagonal with elements 1 or 0?

We wish to find matrices T_i, components of a partitioned form compatible with (5.1.1b) and diagonal matrices μ_i satisfying,

$$\begin{pmatrix} T_1' & T_3' \\ T_2' & T_4' \end{pmatrix}\begin{pmatrix} d_1^{-1}D_1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} T_1 & T_2 \\ T_3 & T_4 \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} = J \qquad (5.3.80)$$

and

$$\begin{pmatrix} T_1' & T_3' \\ T_2' & T_4' \end{pmatrix}\begin{pmatrix} b_1 & b_2 \\ b_2' & b_4 \end{pmatrix}\begin{pmatrix} T_1 & T_2 \\ T_3 & T_4 \end{pmatrix} = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix}. \qquad (5.3.81)$$

If the symmetric matrix b_4 is invertible, this is possible if we choose μ_1 and T_1 such that

$$T_1(b_1 - b_2' b_4^{-1}b_2)T_1' = \mu_1, \; T_1' d_1^{-1}D_1T_1 = I, \qquad (5.3.82)$$

$$T_2 = 0, \qquad (5.3.83)$$

$$T_3 = -b_4^{-1}b_2' T_1 \qquad (5.3.84)$$

and μ_2 and T_4 such that

$$T_4' T_4 = I, \; T_4' b_4T_4 = \mu_2. \qquad (5.3.85)$$

The algebraic uncoupling can then be accomplished as before.

There may also be some chemical components C_j which are immobile in Λ and for which $\mathcal{D}_j = 0$. The geometric factorization of this section is still valid for singular semidefinite matrices $\mathcal{D}$ but the algebraic uncoupling procedure has to be re-examinied by expressing (5.1.4) in a partitioned matrix form similar to (5.1.1b). The theory can also be extended to include the case when $n(I) \neq n(J)$.

5.4 Notes and Comments

This chapter is adapted from MCNABB, PARSHOTAM and WAKE [194].

It is very common to uses tracers (a detectable fluid which has similar properties to the flowing fluid) in particle reactors. The most commonly used methods for detecting flow maldistribution (such as "dead" zones and "stagnant" zones) utilize tracers (usually responses to impulses of tracers) and tracers can also be utilized in studying many other physical characteristics of particle reactors. The tracer-determined residence time distribution (RTD) has been utilized in the analysis of many kinds of flow systems, including chemical reactors, biological systems and underground reservoirs (ROBINSON and TESTER [250], HANRATTY and DUDUKOVIC [114]. This time distribution for the fluid in a packed bed reactor for example reflects the combined history of the fluid flowing external to the porous particles in the reactor bed and the fluid which enters the porous structure. DANCKWERTS [79] popularised the tracer method by developing the mathematics necessary to interpret an inlet-outlet tracer experiment. A list of internal residence time distribution functions within particles and external residence time distribution functions within the bulk fluid in particle reactors from the time of Danckwerts to the present is given by ROBINSON and TESTER [250].

In this chapter we have shown how appropriate the definitions of mean first passsage times and mean particle residence times corresponding to such tracer pulse imputs of chemicals within such particle reactors are in order to achieve some useful results that rely only on solving uncoupled differential equations. Some of the other internal and external residence time distribution functions from literature may also be treated in a similar way.

In (5.3.78)-(5.3.79) we look for a nonsingular matrix T with transpose T' for which $T'd^{-1}DT = J$ and $T'bT = \mu$, where μ is a diagonal matrix and J is diagonal with elements 1 or 0. This problem is equivalent to the simultaneous reduction of a pair of Hermitian forms one of which is nonnegative definite. A necessary and sufficient condition for the existence of such a transformation as well as its method of construction is given by RAO and MITRA [239, p.120-134].

The geometric factorization in this chapter has its analogy in uncoupling systems of linear first order differential equations by reducing them to Jordan Canonical form. There is also considerable work on factorisation techniques for *almost linear* systems of first order differential equations. The geometric factorization in this chapter may in a similar way be generalised to *almost linear* systems of elliptic and parabolic equations.

6

Examples

6.0 Introduction

This thesis with all its theory would not be complete without some suitable examples. In this Chapter, we shall bring some of the theory developed in this thesis and look at some specific examples. The examples we shall present will generally be those that have motivated this study.

Since these sections are written as completed published or publishable papers, there may be a repetition in the model development and problem description.

In section 6.1 we look at an example where a kinetic model is proposed for a surface supported biological film (bioparticle) employed in many biological processes. The equations that govern kinetic and diffusion controlled substrate uptake by the attached organisms are invariably nonlinear and analytical solutions if any are impossible to find. It is therefore desirable to determine approximate analytical solutions, failing this, bounds for the exact numerical solution. This example represents an attempt to provide increasingly better bounds to such equations by a linearisation technique. An iterative scheme relying on the maximum principle is presented for obtaining upper and lower bounds to solutions to resulting non-linear reaction-diffusion equations. In particular, a spherical bioparticle with Michaelis-Menten type of reaction kinetics is considered. Its application to more general equations is also discussed. These bounds are in good agreement with the numerical solutions obtained by shooting and finite difference procedures. The method, which can easily be generalised to other geometries, is relatively simple to use and converges rapidly to a very good upper and lower bound.

In section 6.2, a kinetic model is proposed for substrate conversion in a fluidised bed biofilm reactor (FBBR) where substrate conversion obeys Michaelis-Menten type kinetics. This model results in a reaction-diffusion equation which is coupled in the boundary conditions to outside bulk fluid concentrations. Upper and Lower analytical bounds to the solutions are developed which agree with numerial results obtained by orthogonal collocation. In particular, it is shown that if substrate conversion follows Michaelis-Menten kinetics, the bulk fluid concentration never reaches zero concentration in the bulk liquid nor in a bioparticle.

In section 6.3, we shall develop and compare some monotone iteration methods. These methods prove not only to be powerful tools in constructive existence proofs but are also useful for numerical computation of solutions. These iteration schemes may produce either monotone or alternating sequences and under special conditions, Newton's method may be applied which accelerates the rate of convergence. The objective of this example is to help us to understand the relationship between the properties of the reaction functions and the resulting sequences.

In section 6.4, we shall look at a specific example from literature of a modified urea transfer model for predicting urea removal in a compact artificial kidney. Uniqueness and Existence theorems are developed for the steady state problem. The method of proving uniqueness and existence differs from the methods discussed in this thesis and we shall suggest how it may be useful for proving uniquenss and existence theorems for general systems discussed in this thesis.

In section 6.5, we set out the equations for a tubular fluidised bed biofilm reactor (FBBR) problem of applied interest. The bioparticle reaction kinetics involve three chemical components, a substrate s such as phenol or nitrogenous wastes which needs to be converted to harmless byproducts, oxygen o, an active ingredient which helps facilitate the reaction kinetics, and a product p which linearly inhibits the reaction kinetics. We shall look at the question of existence and uniqueness of solutions and see how these solutions relate to the steady state solution. We shall also study the stability of this system.

In section 6.6, we look at an example of a Continuous Stirred Basket Reactor (CSBR) from literature. This involves the study of a reaction inside porous pellets. The enzyme reaction kinetics involve three chemical components, a substrate s which is converted to a product p under the action of immobilised enzyme, e. The bulk fluid fluid involves only two chemical components, bulk substrate S_b which is introduced into the reactor as steady flow and bulk product P_b that is produced in the reactor. This example is slightly different from the general model developed in this thesis but we find that this does not cause any difficulties. We shall study the question of existence and uniqueness to the time dependent problem illustrating the usefulness of the concept of coupled upper and lower solutions and using methods developed for arbitrary kinetics.

We have chosen to concentrate on some specific examples throughout this chapter such as the fluidised bed biofilm reactor (FBBR) since it has motivated our study. Our development is also intended to be generally applicable to other particle reactor models. However, certain analytical approximations derived in this chapter may prove to be very useful to these specific systems but may not be favourable generally.

6.1 A Simple Method for Obtaining Good Bounds for Solutions of a Bioparticle Model

The biological growth attached to surfaces (commonly referred to as biofilms) is extensively employed in microbial processes such as fermentation and waste water treatment. Such processes give rise to reaction-diffusion problems with non-linear kinetics. The solutions to these problems are usually obtained by numerical techniques such as the shooting method (PARSHOTAM [223], MCELWAIN [180]) and finite difference procedures (KELLER [140]) and the orthogonal collocation methods (VILLADSEN and MICHELSEN [296]). These approaches all suffer from the drawback that they require extensive computation. Various asymptotic techniques such as regular and singular perturbation are suggested for more general equations with very low and very high Thiele moduli (MURRAY [203], FINLAYSON [90] and VEGA and LINÁN [290] of parameter space. FINLAYSON [89] has used construction techniques by trial functions for finding bounding solutions. Numerical calculations for examples of such problems have been carried out by ANDERSON and ARTHURS [12, 13] using variational methods based on extremum principles and these methods were compared by TOSAKA and MIYAKE [284] using integral equation methods. In all previous work, except one isolated case of an unpublished work of VILLADSEN reported by ARIS [21, Ch.3], the maximum principle has not been used to directly generate approximate solutions to such differential equations. The method appears however to be adumbrated by VILLADSEN and MICHELSEN [296]. A technique was suggested by ANDERSON and ARTHURS [14] and VARMA and STREIDER [289] based on this method to directly generate approximate solutions and this method was shown to be much simpler than variational methods to use and could be applicable to situations when a problem admits multiple solutions and where the variational method simply does not apply. This method was also discovered independently by PARSHOTAM, BHAMIDIMARRI and WAKE [225] and we shall discribe it in this section.

It is interesting to note that the method discribed in this section has the disadvantage of producing a good lower (upper) bound and a weak upper (lower) bound. This method has recently been improved to find optimum lower and upper bounds by REGALBUTO *et al.* [245, 246]. The method has also been generalised to systems of equations exibiting multiple solutions (REGALBUTO *et al.* [247]). It is also interesting to note that the methods of obtaining lower and upper bounds based on the integral representation of solutions that were introduced by TOSAKA and MIYAKE [284] have also been developed further (GARNER [98] and ASAITHAMBI and GARNER [24]). These methods result in sharp polynomial approximations to the solution, are compared to the methods of ANDERSON and ARTHURS [14] and are shown to yield sharper bounds with fewer integration steps.

In this section we will use an iterative technique to obtain successive better bounding solutions and approximations. These approximate analytical solutions and bounding solutions are obtained via a linearisation technique which yields good upper and lower bounds to the exact solution and which apply to all parameter values. It can be shown analytically that this lower bound is always strictly positive which implies the solution to these type of reaction-diffusion equations is always strictly positive. The linearisation of Michaelis-Menten type kinetics with diffusion has been reported using Taylor's series expansions, (MURRAY [203]) but has often been done at an arbitrary point. This approach invariably results in significant errors in solutions. At times, the point of linearisation can even be shown to be outside of the region in which the solution lies and even if the point of linearisation is in the region the solution lies, it could still result in a negative concentration as an approximation. In this work, a novel method is developed to determine a point for linearisation which would give minimal errors in solutions over parameter ranges of significance. It also produces good linear approximations to Michaelis-Menten kinetics over all parameter space and using these approximations, universal bounds are obtained for the solutions to resulting reaction-diffusion equations.

6.1.1 Biofilm Model Formulation

For a biofilm supported on a spherical inert particle shown in FIG. 6.1, if the mass-transfer within the biofilm is governed by Fick's first law and the biochemical reaction follows Michaelis-Menten type of kinetics, the substrate transport and reaction within the biofilm at steady state is written as

$$\frac{D}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}S}{\mathrm{d}r}\right) = R_{mm}(S), \tag{6.1.1}$$

where $R_{mm}(S)$ is the Michaelis-Menten type reaction rate defined as

$$R_{mm}(S) = \frac{kS}{K_m + S}. \tag{6.1.2}$$

The boundary conditions are

$$S'(r_{sm}) = 0 \text{ and } S(r_{bp}) = S_b. \tag{6.1.3}$$

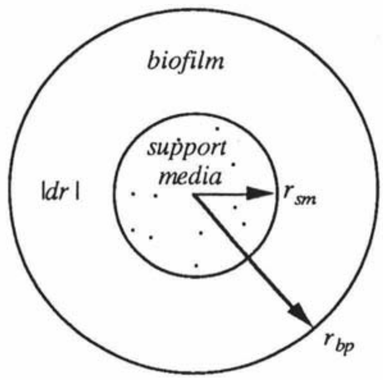


FIG. 6.1 Schematic of a bioparticle

The dimensionless mass balance of the substrate in a spherical bioparticle may be expressed as

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2\frac{\mathrm{d}y}{\mathrm{d}x}\right) = \phi^2 F(y), \tag{6.1.4}$$

with

$$F(y) = \frac{y}{1+\beta y}, \tag{6.1.5}$$

and the corresponding boundary conditions are

$$y'(\alpha) = 0 \text{ and } y(1) = 1, \tag{6.1.6}$$

where the variables are

$$y = \frac{S}{S_b}, \quad x = \frac{r}{r_{bp}}, \tag{6.1.7}$$

and the parameters are

$$\alpha = \frac{r_{sm}}{r_{bp}}, \ \beta = \frac{S_b}{K_m} \text{ and } \phi^2 = \frac{r_{bp}^2 k}{DK_m}. \tag{6.1.8}$$

6.1.2 Upper and Lower solutions and Monotonicity

Here we use the one dimensional maximum principle (PROTTER and WEINBERGER [234]) for solutions to

$$y''(x) + H(x, y, y') = 0, \; a < x < b \tag{6.1.9}$$

with boundary conditions

$$\left.\begin{aligned} -y'(a)\cos\theta + y(a)\sin\theta &= \gamma_1 \\ y'(b)\cos\omega + y(b)\sin\omega &= \gamma_2, \end{aligned}\right\} \tag{6.1.10}$$

where $0 \le \theta \le \pi/2$, $0 \le \omega \le \pi/2$ and θ and ω are not both zero. We also have the condition that $\partial H/\partial y \le 0$. This is given in Theorem 22 in PROTTER and WEINBERGER [234]. In our case,

$$H(x, y, y') = \frac{2}{x}\frac{dy}{dx} - \phi^2 \frac{y}{1+\beta y}, \tag{6.1.11}$$

and

$$\frac{\partial H}{\partial y} = -\frac{\phi^2}{(1+\beta y)^2} \le 0. \tag{6.1.12}$$

as required. Also $a = \alpha$, $b = 1$, $\theta = 0$, $\omega = \pi/2$, $\gamma_1 = 0$ and $\gamma_2 = 1$ as required.

Direct application of this theorem gives the following :

Let y be a solution of the boundary value problem

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{dy}{dx}) - \phi^2\frac{y}{1+\beta y} = 0,$$

with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$.

If $\underline{y}$ *satisfies*

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{d\underline{y}}{dx}) - \phi^2\frac{\underline{y}}{1+\beta \underline{y}} \ge 0,$$

with the boundary conditions

$$\underline{y}'(\alpha) = 0 \text{ and } \underline{y}(1) = 1,$$

and if $\bar{y}$ *satisfies the same conditions with the signs reversed then the upper and lower bounds*

$$\underline{y}(x) \le y(x) \le \bar{y}(x), \tag{6.1.13}$$

are valid.

The above result implies that a solution of (6.1.4) which satisfies boundary conditions (6.1.6) exists and must be unique, for if y and $\bar{y}$ are solutions, we can let $\underline{y} = y = \bar{y}$ to find $y \equiv \bar{y}$. We note that $\underline{y}(x) \equiv 0$ and $\bar{y}(x) \equiv 1$ are respectively lower and upper solutions, that is

$$0 \le y(x) \le 1. \tag{6.1.14}$$

It also follows directly from the maximum principle that minimum and maximum values of $y(x)$ are at the boundaries $x = \alpha$ and $x = 1$, respectively.

Monotonicity with parameters

We now show that $y(x)$ is monotonically decreasing with ϕ. Likewise a similar proof may be obtained to show that $y(x)$ is monotonically increasing with β.

Theorem

$y(x)$ is monotonically decreasing with ϕ.

Proof

(1) Assume $\phi_1 > \phi_2$, $\beta \geq 0$.

(2) Assume $y_1, y_2 > 0$ (the strict inequality is shown in equation (6.1.21)).

(3) Let y_1 be a solution of (6.1.4) with ϕ_1:

$$L[y_1] = \frac{1}{x^2}\frac{d}{dx}(x^2\frac{dy_1}{dx}) = \phi_1^2\frac{y_1}{1+\beta y_1},$$

with boundary conditions

$$y_1'(\alpha) = 0 \text{ and } y_1(1) = 1.$$

(4) Let y_2 be a solution of (6.1.4) with ϕ_2:

$$L[y_2] = \frac{1}{x^2}\frac{d}{dx}(x^2\frac{dy_2}{dx}) = \phi_2^2\frac{y_2}{1+\beta y_2},$$

with boundary conditions

$$y_2'(\alpha) = 0 \text{ and } y_2(1) = 1.$$

(5) Consider the equation

$$L[y_2] - \phi_1^2\frac{y_2}{1+\beta y_2} = (\phi_2^2 - \phi_1^2)\frac{y_2}{1+\beta y_2} < 0 = L[y_1] - \phi_1^2\frac{y_1}{1+\beta y_1}.$$

Using the theorem in Protter and Weinberger this gives $y_2 \geq y_1$ for $\alpha \leq x \leq 1$.

(6) Look at the difference $z = y_2 - y_1$. The equation below is obtained

$$L[z] = \frac{1}{x^2}\frac{d}{dx}(x^2\frac{dz}{dx}) = L[y_2 - y_1] = L[y_2] - L[y_1] = \phi_2^2\frac{y_2}{1+\beta y_2} - \phi_1^2\frac{y_1}{1+\beta y_1}$$

with homogeneous boundary conditions

$$z'(\alpha) = z(1) = 0.$$

(7) Simplifying,

$$L[z]=\frac{\phi_2^2(1+\beta y_1)y_2-\phi_1^2(1+\beta y_2)y_1}{(1+\beta y_2)(1+\beta y_1)}<\frac{\phi_1^2(1+\beta y_1)y_2-\phi_1^2(1+\beta y_2)y_1}{(1+\beta y_2)(1+\beta y_1)}\le\phi_1^2(y_2-y_1)=\phi_1^2 z,$$

since $y_2(x)\ge y_1(x)$.

(8) Therefore, we have the problem

$$L[z]-\phi_1^2 z<0, \tag{6.1.15}$$

with boundary conditions

$$z'(\alpha)=z(1)=0. \tag{6.1.16}$$

(9) It follows from the strict form of the positivity lemma (KELLER [143, p.222]) that $z>0$ for $\alpha<x<1$ iff $-\phi_1^2<\mu_1$, where μ_1 is the principal (i.e., least) eigenvalue of the problem

$$L[p]+\mu p=0,$$

with boundary conditions

$$p'(\alpha)=p(1)=0.$$

This in turn implies that $y_2>y_1$ for $\alpha<x<1$. Thus y is monotonically decreasing with ϕ, across the bioparticle.❑

The physical importance of this is seen by noting that as the Thiele modulus, ϕ^2 increases (say k increases or D decreases), the substrate concentration decreases. This is physically reasonable.

Lower bounds

Any linearisation by a Taylor's series expansion of $\phi^2F(y)$ will be strictly greater (for $\beta\ne 0$) than $\phi^2F(y)$ and will lead to a lower solution, since

$$F(y)\le F(\varepsilon)+(y-\varepsilon)F'(\varepsilon) \text{ for } y,\ \varepsilon\ge 0.$$

The linearised problem about some $\varepsilon\in[0,1]$ is

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{d\underline{y}}{dx}\right)=\underline{\psi}^2\underline{y}+\underline{\lambda}, \tag{6.1.17}$$

where

$$\underline{\psi}^2=\frac{\phi^2}{1+\beta\varepsilon} \text{ and } \underline{\lambda}=\frac{\phi^2\varepsilon^2\beta}{(1+\beta\varepsilon)^2}, \tag{6.1.18}$$

and satisfies the boundary conditions

$$\underline{y}'(\alpha)=0 \text{ and } \underline{y}(1)=1. \tag{6.1.19}$$

Solving for $\underline{y}(x)$, a lower bound is obtained to $y(x)$ where

$$\underline{y}(x) = \frac{\underline{A}\cosh\underline{\psi}(1-x)}{x} + \frac{\underline{B}\sinh\underline{\psi}(1-x)}{x} - \frac{\underline{\lambda}}{\underline{\psi}^2}, \tag{6.1.20}$$

and $\underline{A}$ and $\underline{B}$ are determined by the boundary conditions (6.1.19).

Linearising $\phi^2F(y)$ at various ε and choosing the maximum lower bound over the whole region produces a good lower bound. Alternatively, knowing that $\underline{y}(x)$ is a lower bound, the region below its minimum, $\underline{y}(\alpha)$ may be eliminated and we limit ourselves to linearising $\phi^2F(y)$ only in the interval $\varepsilon \in [\underline{y}(\alpha), 1]$.

Linearising $\phi^2F(y)$ in the interval $\underline{y}(\alpha) \le y(x) \le 1$ does not exclude the possibility that a negative concentration may be obtained as an approximation. This situation would be avoided if the first approximation of the lower bound is strictly greater than zero and subsequent iterations produce increasingly better lower bounds.

We do this as follows. The solution of the linearised problem at $\varepsilon = 0$ is taken as a first lower bound:

$$\underline{y}_1(x) = \frac{\alpha\phi\cosh\phi(x-\alpha) + \sinh\phi(x-\alpha)}{x[\alpha\phi\cosh\phi(1-\alpha) + \sinh\phi(1-\alpha)]}, \tag{6.1.21}$$

which is always strictly positive since all the terms in the above expression are positive. This is enough to guarantee that $y(x)$ is strictly positive.

A second linearisation is performed at $\varepsilon = \underline{y}_1(\alpha)$ and a third at $\varepsilon = \underline{y}_2(\alpha)$ Subsequently, an nth linearisation performed at $\varepsilon = \underline{y}_{n-1}(\alpha)$ would be an improvement on the previous iteration and would be positive.

Upper bounds

A trivial upper bound to y is $\bar{y}$ such that

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{d\bar{y}}{dx}) = \frac{\phi^2}{1+\beta}\bar{y} \tag{6.1.22}$$

and satisfies the boundary conditions

$$\bar{y}(1) = 1 \text{ and } \bar{y}'(\alpha) = 0. \tag{6.1.23}$$

This has the solution

$$\bar{y}(x) = \frac{\alpha\frac{\phi}{\sqrt{1+\beta}}\cosh\frac{\phi}{\sqrt{1+\beta}}(x-\alpha) + \sinh\frac{\phi}{\sqrt{1+\beta}}(x-\alpha)}{x[\alpha\frac{\phi}{\sqrt{1+\beta}}\cosh\frac{\phi}{\sqrt{1+\beta}}(1-\alpha) + \sinh\frac{\phi}{\sqrt{1+\beta}}(1-\alpha)]} \tag{6.1.24}$$

and is an upper solution to y since for $0 \le y \le 1$,

$$F(y) \ge \frac{y}{1+\beta},$$

and therefore $\bar{y}(x) \ge y(x)$ for $\alpha \le x \le 1$. Subsequent improved upper bounds are $\bar{y}_n$, where $\underline{y}(\alpha) \le y(x) \le \bar{y}_n(x) \le 1$ and where $\bar{y}_n$ satisfies the equation

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2\frac{\mathrm{d}\bar{y}_n}{\mathrm{d}x}\right)=\bar{\psi}_n^2\bar{y}_n+\bar{\lambda}_n\le\phi^2F(y), \tag{6.1.25}$$

where

$$\bar{\psi}_n^2=\frac{F(1)-F(\underline{y}_n(\alpha))}{1-\underline{y}_n(\alpha)} \text{ and } \bar{\lambda}_n=F(1)-\bar{\psi}_n^2, \tag{6.1.26}$$

with the boundary conditions

$$\bar{y}_n(1)=1 \text{ and } \bar{y}_n'(\alpha)=0. \tag{6.1.27}$$

Solving for $\bar{y}_n(x)$, successive upper bounds are obtained to $y(x)$ which depend on $\underline{y}_n(\alpha)$, as

$$\bar{y}_n(x)=\frac{\bar{A}\,cosh\;\bar{\psi}_n(1-x)}{x}+\frac{\bar{B}\,sinh\;\bar{\psi}_n(1-x)}{x}-\frac{\bar{\lambda}_n}{\bar{\psi}_n^2}, \tag{6.1.28}$$

and where $\bar{A}$ and $\bar{B}$ are determined by the boundary conditions (6.1.27).

6.1.3 Results and Discussion

In general, the following iteration scheme may be used to find lower and upper bounds for $y(x)$

$$\underline{y}_0(\alpha)=0 \tag{6.1.29}$$

$$\underline{y}_n(x)=\frac{\underline{A}_n\,cosh\;\underline{\psi}_n(1-x)}{x}+\frac{\underline{B}_n\,sinh\;\underline{\psi}_n(1-x)}{x}-\frac{\underline{\lambda}_n}{\underline{\psi}_n^2},\quad n=1,2,3,.. \tag{6.1.30}$$

with

$$\underline{\psi}_n^2=\frac{\phi^2}{(1+\beta\underline{y}_{n-1}(\alpha))^2} \text{ and } \underline{\lambda}_n=\frac{\phi^2\beta\underline{y}_{n-1}^2(\alpha)}{(1+\beta\underline{y}_{n-1}(\alpha))^2} \tag{6.1.31}$$

and where $\underline{A}_n$ and $\underline{B}_n$ are determined by the boundary conditions as

$$\underline{A}_n=1+\frac{\underline{\lambda}_n}{\underline{\psi}_n^2},\quad \underline{B}_n=-\underline{A}_n\frac{\underline{\psi}_n\alpha\,sinh\,\underline{\psi}_n(1-\alpha)+cosh\,\underline{\psi}_n(1-\alpha)}{\underline{\psi}_n\alpha\,cosh\,\underline{\psi}_n(1-\alpha)+sinh\,\underline{\psi}_n(1-\alpha)}. \tag{6.1.32}$$

Similarly,

$$\bar{y}_n(x)=\frac{\bar{A}_n\,cosh\;\bar{\psi}_n(1-x)}{x}+\frac{\bar{B}_n\,sinh\;\bar{\psi}_n(1-x)}{x}-\frac{\bar{\lambda}_n}{\bar{\psi}_n^2},\quad n=2,3,4,.. \tag{6.1.33}$$

with

$$\bar{\psi}_n^2=\frac{\phi^2}{(1+\beta)(1+\beta\underline{y}_{n-1}(\alpha))} \text{ and } \bar{\lambda}_n=\frac{\phi^2\beta\underline{y}_{n-1}^2(\alpha)}{(1+\beta)(1+\beta\underline{y}_{n-1}(\alpha))} \tag{6.1.34}$$

and where $\bar{A}_n$ and $\bar{B}_n$ are determined by the boundary conditions as

$$\bar{A}_n=1+\frac{\bar{\lambda}_n}{\bar{\psi}_n^2},\quad \bar{B}_n=-\bar{A}_n\frac{\bar{\psi}_n\alpha\,sinh\,\bar{\psi}_n(1-\alpha)+cosh\,\bar{\psi}_n(1-\alpha)}{\bar{\psi}_n\alpha\,cosh\,\bar{\psi}_n(1-\alpha)+sinh\,\bar{\psi}_n(1-\alpha)}. \tag{6.1.35}$$

The linearisations of $F(y)$ are shown in FIG. 6.2 where $\underline{\psi}_n^2$, $\overline{\psi}_n^2$, $\underline{\lambda}_n$ and $\overline{\lambda}_n$ are functions of $\underline{y}_{n-1}(\alpha)$.

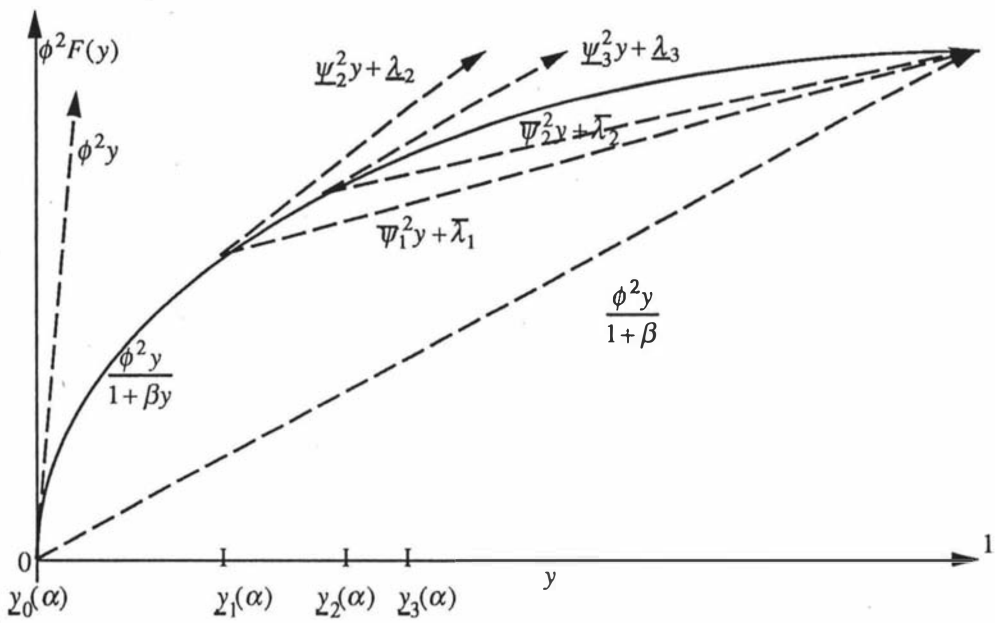


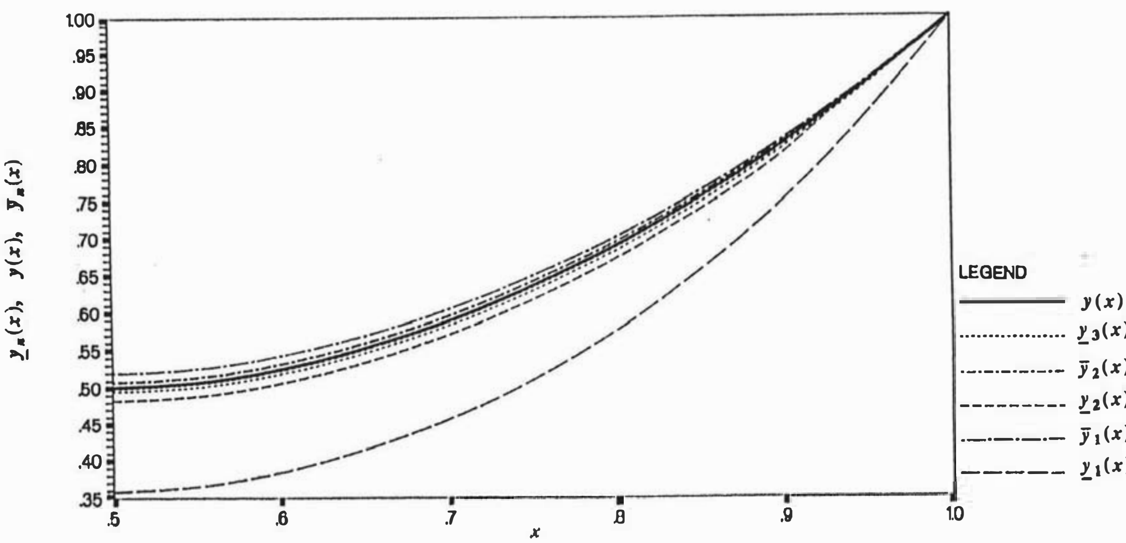
FIG. 6.2 Schematic of successive linear bounds obtained for $F(y)$.

Since a linearised solution (by a Taylor's series expansion) of equation (6.1.4) would always be a lower solution, it is not expected that this iterative scheme would converge to the exact solution every time. It does however perform very well within numerical limits as shown in FIG 6.3. FIG. 6.3(a) shows the approximations for the variable y itself for typical parameter values and FIG. 6.3(b) shows it in terms of percentage relative errors, that is

$$(\frac{\overline{y}_n}{y}-1)\% \text{ or } (\frac{\underline{y}_n}{y}-1)\%.$$

An arithmetic average of $\underline{y}_3$ and $\overline{y}_3$ is also plotted (where $y_{av}=(\underline{y}_3+\overline{y}_3)/2$). In this typical example, the maximum relative error of y_{av} to the exact solution $y(x)$ was shown to be 0.05%.The method is sensitive to an increase in the Thiele modulus, ϕ^2 when $\phi^2 F(y)$ becomes very nonlinear. This is seen in FIG. 6.4. For diffusion limited reactions in bacterial films the Thiele modului are usually higher than those for films of moulds or yeasts (ϕ^2 = 20 is still considered to be physically extremely high) and this technique results in increased error between the exact solution and upper and lower bounds for such biofilms. The method is also sensitive to a decrease in α as seen in FIG. 6.5 .The linearisation technique may not therefore be as effective for thick biofilms with very small support particles or bacterial flocs. It is however, considerably better than its first approximation which in the example of FIG. 6.5 where typical parameter values were chosen has a maximum relative error to the exact solution of -64% (not shown completely in this graph) and an average of $\overline{y}_2(\alpha)$ and $\underline{y}_3(\alpha)$ produce a maximum relative error to the exact solution of only 0.1%. The iterative method produces an increase in relative error for intermediate values of β as shown in FIG. 6.6. The approximation of Michaelis-Menten type of kinetics by either zero order or first order has been widely reported (BAILEY and OLLIS [30]). However, such an approximation results in a solution that is given by only the first iteration of the scheme presented in this work and may not be the best. On the other hand, this technique leads to a better approximation of the solution in a parameter space in addition to obtaining the universal bounds on the exact solution. For instance, an average of upper and lower bounds after 3 iterations produces an approximate analytical solution of within 3% relative error over the parameter space of interest in biological systems, namely, $\phi^2 \in [0, 20]$, $\beta \in [0, \infty)$ and $\alpha \in (0, 1]$.

a)



b)

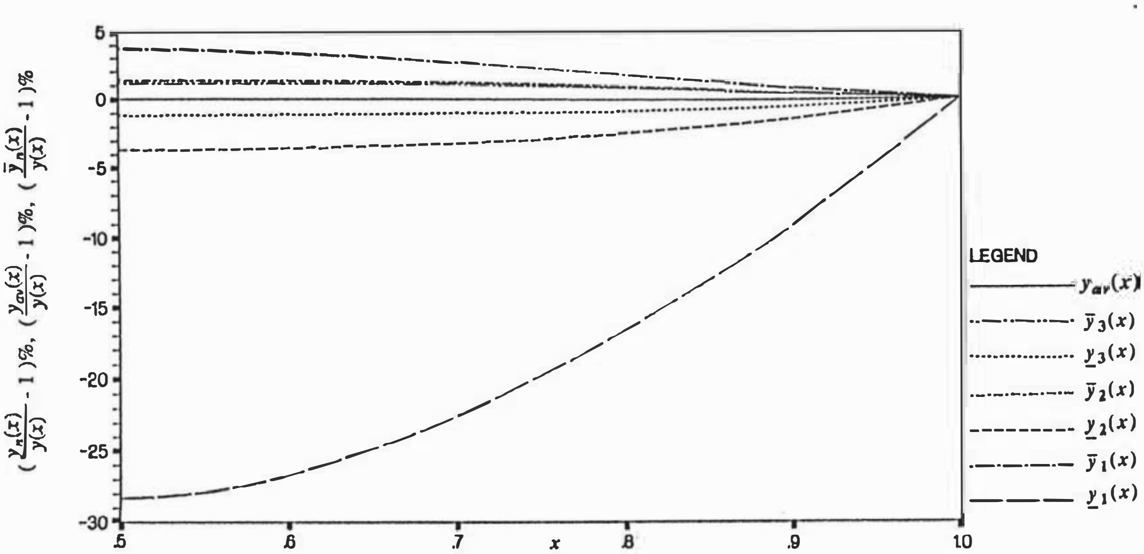


FIG. 6.3 (a) Successive upper and lower bounds to the exact solution $y(x)$ with α = 0.5, ϕ^2 = 16 and β = 1. (b) Percentage relative error to the exact solution $y(x)$ with α = 0.5, ϕ^2 = 16 and β = 1.

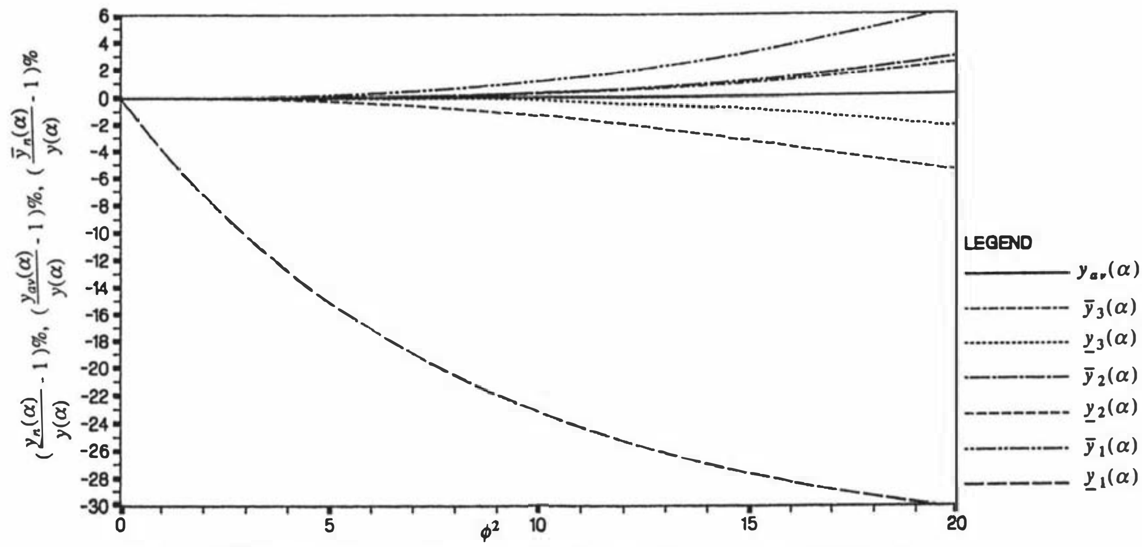


FIG 6.4 Percentage relative error to $y(\alpha)$ with $\alpha = 0.5$, $\beta = 1$ and various ϕ^2

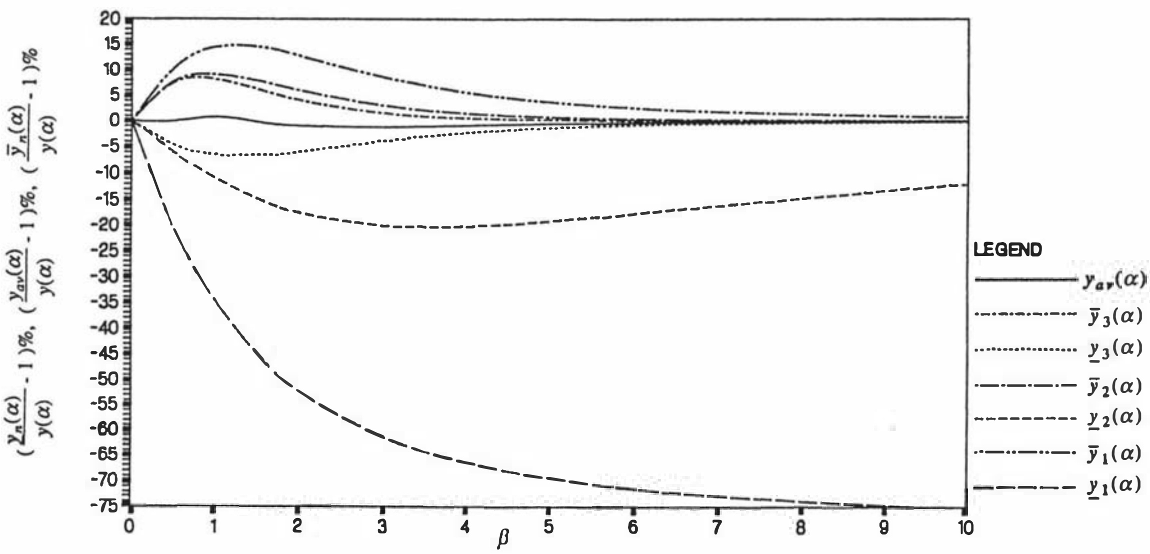


FIG 6.5 Percentage relative error to $y(\alpha)$ with $\beta = 5$, $\phi^2 = 10$ and various α

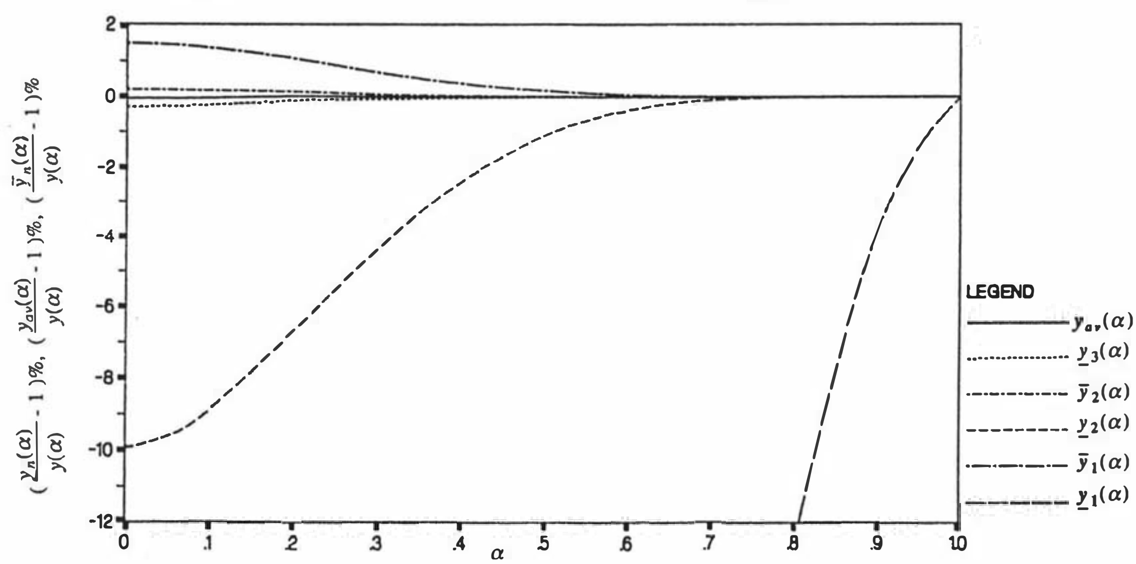


FIG 6.6 Percentage relative error to $y(\alpha)$ with $\alpha = 0.2$, $\phi^2 = 15$ and various β

6.1.3 Conclusions and remarks

The Maximum Principle may be applied to finding upper and lower bounds to a wide class of equations including reaction-diffusion type with nonlinear kinetics. The method developed in this section is that of obtaining a better linearisation of the nonlinear terms by narrowing down the region of linearisation. The method of obtaining successive bounds for these source or sink terms relies on the fact that these terms must be either concave up or down. The technique is sensitive to the diffusion parameter although the relative error of the approximate solution is significantly low. The linearisation technique offers a convenient method for obtaining the universal bounds for the exact solution which can be used for obtaining bounds for performance indicators such as effectiveness factors.

Nomenclature

$\underline{A}$	constant, determined by the boundary conditions that relates to the lower solution $\underline{y}$
$\underline{B}$	constant, determined by the boundary conditions that relates to the lower solution $\underline{y}$
$\underline{A}_n$	constant, defined in eq. (6.1.32), that relates to the lower solution $\underline{y}_n$
$\underline{B}_n$	constant, defined in eq. (6.1.32), that relates to the lower solution $\underline{y}_n$
$\overline{A}$	constant, determined by the boundary conditions that relates to upper solution $\overline{y}$
$\overline{B}$	constant, determined by the boundary conditions that relates to upper solution $\overline{y}$
$\overline{A}_n$	constant, defined in eq. (6.1.35) that relates to upper solution $\overline{y}_n$
$\overline{B}_n$	constant, defined in eq. (6.1.35) that relates to upper solution $\overline{y}_n$
D	effective diffusivity
$F(y)$	dimensionless Michaelis-Menten term, defined by eq. (6.1.5)
k	rate constant
K_m	Michaelis-Menten constant
r	radial distance
r_{bp}	bioparticle radius
r_{sm}	support media radius
R_{mm}	Michaelis-Menten type reaction rate, defined by eq. (6.1.2)
S	substrate concentration
S_b	bulk substrate concentration
x	dimensionless distance
y	dimensionless concentration
$\underline{y}$	a lower solution of y
$\underline{y}_n$	an nth lower solution of y
$\overline{y}$	an upper solution of y
$\overline{y}_n$	an nth upper solution of y
y_{av}	an average of upper and lower bounds

Greek letters

α	ratio of support media radius to bioparticle radius
β	dimensionless Michaelis-Menten constant
ε	point of linearisation
ϕ^2	Thiele modulus (ratio of the reaction rate to diffusion rate)
$\underline{\lambda}$	constant, defined in eq. (6.1.18)
$\underline{\lambda}_n$	constant, defined in eq. (6.1.31)
$\overline{\lambda}_n$	constant, defined in eq. (6.1.34)
$\underline{\psi}$	constant, defined in eq. (6.1.18)
$\underline{\psi}_n$	constant, defined in eq. (6.1.31)
$\overline{\psi}_n$	constant, defined in eq. (6.1.34)

6.2 Analytical Bounds to a Model of a Fluidised Bed Biofilm Reactor (FBBR)

A significant step in the numerical solution of packed bed reactor models was taken with the introduction of the method of orthogonal collocation to this class of problems (FINALYSON [88]). This method was shown to be much faster and more accurate than that based on finite differences.

The orthogonal collocation method for solving partial differential equations developed largely by VILLADSEN *et al.* [293-296] and FINLAYSON [88] has been found to require less computer time than standard finite difference methods. The method is now usually applied to and is particularly suited to the simulation of fluidised, fixed and packed bed reactors (HANSEN [115]; KARANTH and HUGHES [135]; RAGHAVAN and RUTHVEN [237]; HASSAN and BEG [120]), the simulation of an adsoption column (LIAPIS and RIPPIN [169]) and fixed bed catalytic reactor simulation with moving boundaries (GARDINI *et al.* [97]). This method has now been the generally accepted procedure in numerically implementing such models.

These models all involve reaction-diffusion equations involving interacting macro and microstructures where outside concentrations govern the boundary conditions for local behaviour. The equations that govern kinetic and diffusion-controlled substrate uptake by the attached organisms in a fluidised bed biofilm reactor are invariably nonlinear and analytical solutions if any are impossible to find.

This section considers such equations and demonstrates that although such equations may be diffucult to solve, it is relatively easy to provide analytical bounds on the solution. These universal bounds agree with numerical solutions for such equations with parameters found in chemical engineering literature but apply to all parameter values. It also provides us with approximate analytical solutions.

6.2.1 The Fluidised Bed Biofilm Reactor

The fluidised bed biofilm reactor (FBBR) is a novel biological process which has been applied to both wastewater treatment processes and biochemical manufacture. The application of fluidised-bed biofilm reactors for biological wastewater treatment has been attempted by several researches in recent years and include denitrification, nitrification and organic carbon removal (JERIS and OWENS [134]). The fluidised-bed biofilm reactor is a high-energy high-efficiency reactor in which the liquid to be treated is passed upward through a bed of small support particles such as activated carbon or other support media at velocities sufficient to impart motion to, or fluidise the particles. Each particle offers a large surface area for biological growth, resulting in biomass concentration of an order of magnitude greater compared to conventional dispersed growth systems. The bed is seeded with microorganisms which eventually grow to form a biological growth known as a biofilm around the core particle. The very high growth support surface afforded by these bioparticles results in denitrification of volatile solid concentrations as high as 30,000 mg l^{-1} and a bed detention times as low as 6 minutes for 99% nitrate removal.

In this work, predictive models for the fluidised bed biofilm reactor are developed. These models have existed for many years in literature and often with the axial dispersion term being neglected (e.g. MULCAHY *et al.* [199-202]) The model is similar to the modified urea transfer model presented by LIN [170] in predicting the urea removal in a compact artificial kidney by microencapsulated urease particles. In both models, a simpler plug flow equation is usually used instead of a general dispersion one is employed to describe substrate concentration changes throughout the liquid phase. This is usually justified by the rather large Peclet number for the above systems when in operation (MULCAHY *et. al.* [199-202] and LIN [170]). The example in this section however shall assume a more general dispersion model.

6.2.2 The Fluidised Bed Biofilm Reactor Model Formulation

The fluidised Bed Biofilm Reactor, the typical schematic with bioparticles is shown in FIG. 6.7, consists of a column reactor in which granular media with high specific surface area are fluidised with nutrient solution. The key process components of this system with a uniform biofilm are:

(i) reaction-diffusion within a single bioparticle
(ii) Solute transport through reactor flow

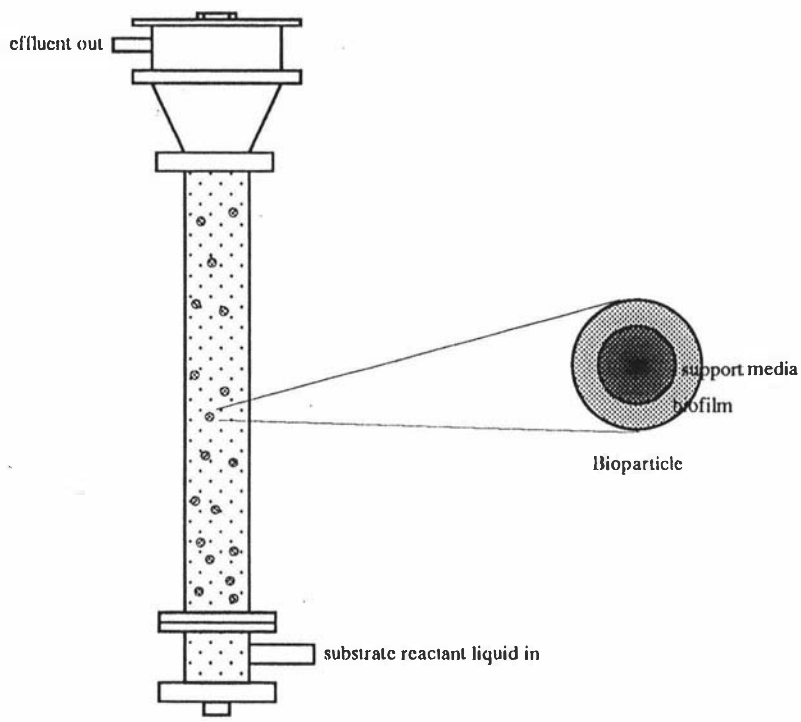


FIG. 6.7 Schematic of a FBBR with Bioparticles

Bioparticle-Reactor Model Development

The mathematical model of the FBBR substrate conversion process is divided into two submodels. The "Bioparticle Model" is concerned with the intra-biofilm diffusion and substrate conversion by micro-organisms attatched to the individual support particles which are in a fluidised state. The "Reactor Flow Model" discusses the hydraulic flow transport of substrate through a FBBR. The two models are coupled by biofilm-bulk liquid boundary conditions to yield an overall model for substrate conversion in an FBBR.

We make the following simplifying assumptions

Bioparticle Model

1. Homogeneous biofilm of constant and uniform thickness
2. Spherical support media of uniform size
3. Internal diffusion of substrate is governed by Fick's first law
4. Substrate-limited biochemical reaction described by Michaelis-Menten kinetics

Reactor Flow Model

1. Liquid phase substrate transport is by plug flow convection and axial dispersion.
2. No macroscopic radial gradients exist
3. Bioparticle characteristics are independent of position within the reactor
4. No substrate conversion occurs in the liquid phase
5. Cylindrical reactor

Under these assumptions, the following differential equation is derived from a substrate mass balance across an axial reactor element

$$\frac{\partial S_b}{\partial t} - D_{Sb}\frac{\partial^2 S_b}{\partial Z} + U_{Sb}\frac{\partial S_b}{\partial Z} + R_v = 0, \qquad (6.2.1)$$

where the observed substrate conversion rate per unit fluidised bed volume is given by

$$R_v = NAD_s \left.\frac{\partial S(r)}{\partial r}\right|_{r=r_{bp}}. \qquad (6.2.2)$$

The number of particles per unit volume of the reactor is calculated from the total initial mass of the bed and the expanded bed height for a set of operating conditions.

$$N = \frac{\text{Total mass of support material}}{\text{Mass of single particle}} = \frac{M}{\frac{4}{3}\pi r_{sm}^3 \rho_{sm}}. \qquad (6.2.3)$$

Within a bioparticle the substrate mass balance on a differential shell may be written as:

$$\frac{\partial S}{\partial t} - \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial S}{\partial r}\right) + \frac{\mu_m \rho_{bf}}{Y_{X/S}}\left(\frac{S}{S+K_s}\right) - 0 \quad \text{for } r_{sm} < r < r_{bp},\ 0 < Z < h,\ t > 0, \qquad (6.2.4)$$

with initial and boundary conditions

$$S(t, r, Z) = 0 \text{ at } t = 0 \text{ for } r_{sm} < r < r_{bp},\ 0 < Z < h, \qquad (6.2.5)$$

$$D_s\frac{\partial S}{\partial r} = 0 \text{ at } r = r_{sm},\ 0 < Z < h, \qquad (6.2.6)$$

$$D_s\frac{\partial S}{\partial r} = H_s(S_b(Z) - S) \text{ at } r = r_{bp},\ 0 < Z < h, \qquad (6.2.7)$$

and outside the bioparticle in the external fluid, we have from (6.2.1) and (6.2.2),

$$\frac{\partial S_b}{\partial t} - D_{S_b}\frac{\partial^2 S_b}{\partial Z^2} + U_{S_b}\frac{\partial S_b}{\partial Z} + NAD_s\left.\frac{\partial S}{\partial r}\right|_{r=r_{bp}} = 0, \quad t > 0,\ 0 < Z < h, \qquad (6.2.8)$$

with initial conditions

$$S_b(Z, t) = 0 \qquad \text{at } t = 0,\ 0 < Z < h \qquad (6.2.9)$$

and boundary conditions given by WEHNER and WILHELM [306] and DANCKWERTS [79], respectively.

$$D_{S_b}\frac{\partial S_b}{\partial Z} = U_{S_b}(S_b - S_{b,i}) \text{ at } Z = 0,\ t > 0, \qquad (6.2.10)$$

$$D_{S_b}\frac{\partial S_b}{\partial Z}=0 \text{ at } Z=h,\ t>0. \tag{6.2.11}$$

In dimensionless coordinates, these equations have the form

$$-\frac{\partial y}{\partial \tau}+\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial y}{\partial x})=\phi^2\frac{y}{1+\beta y} \quad \text{in } \alpha<x<1,\ 0<z<1,\ \tau>0, \tag{6.2.12}$$

$$-\chi\frac{\partial Y}{\partial \tau}+\frac{1}{\mathcal{Pe}}\frac{\partial^2 Y}{\partial z^2}-\frac{\partial Y}{\partial z}=\zeta\frac{\partial y}{\partial x} \quad \text{in } 0<z<1,\ x=1,\ \tau>0, \tag{6.2.13}$$

$$y+\frac{1}{\mathcal{Sh}}\frac{\partial y}{\partial v}=Y(t,\ z) \quad \text{at } x=1 \text{ for } 0<z<1,\ \tau>0, \tag{6.2.14}$$

$$\frac{\partial y}{\partial v}=0 \quad \text{at } x=\alpha \text{ for } 0<z<1,\ \tau>0, \tag{6.2.15}$$

$$Y-\frac{1}{\mathcal{Pe}}\frac{\partial Y}{\partial z}=1 \quad \text{at } z=0,\ \tau>0, \tag{6.2.16}$$

$$\frac{\partial Y}{\partial z}=0 \quad \text{at } z=1,\ \tau>0, \tag{6.2.17}$$

$$y(x,\ 0)=0 \quad \text{for } \alpha\le x\le 1, \tag{6.2.18}$$

$$Y(z,\ 0)=0 \quad \text{for } 0\le z\le 1, \tag{6.2.19}$$

where the dimensionless variables are

$$x=\frac{r}{r_{bp}},\ y=\frac{S}{S_{b,i}},\ Y=\frac{S_b}{S_{b,i}},\ z=\frac{Z}{h} \text{ and } \tau=\frac{D_s t}{r_{bp}^2}, \tag{6.2.20}$$

and the parameters are

$$\alpha=\frac{r_{sm}}{r_{bp}},\ \beta=\frac{S_{b,i}}{K_s},\ \phi^2=\frac{\mu_m\rho_{bf}r_{bp}^2}{Y_{X/S}D_sK_s},\ \zeta=\frac{NAD_sh}{U_{S_b}r_{bp}},\ \chi=\frac{hD_s}{U_{S_b}r_{bp}^2},\ \mathcal{Sh}=\frac{H_sr_{bp}}{D_s} \text{ and } \mathcal{Pe}=\frac{hU_{S_b}}{D_{S_b}}. \tag{6.2.21}$$

At steady-state the equations take the following form

$$\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial y}{\partial x})=\phi^2\frac{y}{1+\beta y} \quad \text{in } \alpha<x<1,\ 0<z<1, \tag{6.2.22}$$

$$\frac{1}{\mathcal{Pe}}\frac{d^2Y}{dz^2}-\frac{dY}{dz}=\zeta\frac{\partial y}{\partial x} \quad \text{in } 0<z<1,\ x=1, \tag{6.2.23}$$

$$y+\frac{1}{\mathcal{Sh}}\frac{\partial y}{\partial v}=Y(z) \quad \text{at } x=1 \text{ for } 0<z<1, \tag{6.2.24}$$

$$\frac{\partial y}{\partial v}=0 \quad \text{at } x=\alpha \text{ for } 0<z<1, \tag{6.2.25}$$

$$Y-\frac{1}{\mathcal{Pe}}\frac{dY}{dz}=1 \quad \text{at } z=0, \tag{6.2.26}$$

$$\frac{dY}{dz}=0 \quad \text{at } z=1. \tag{6.2.27}$$

3.2.3 The Numerical Solution - the Method of Orthogonal Collocation

The general form of the model (equations (6.2.12)-(6.2.19)) is solved numerically by converting the partial differential equations (pde's) to a system of ordinary differential equations (ode's). Orthogonal collocation, a method of weighted residuals, lends itself well to converting similar types of pde's to systems of ode's (RAGHAVAN and RUTHVEN [237], VILLADSEN *et al.* [293-296]). The resulting set of ode's can then be solved by a number of standard techniques.

Weighted residual methods allow separation of the time and spatial dependency of a pde by approximating the exact solution with a series of products of time-varying coefficients and spatial basis or trial functions. The collocation method requires that the residual between the numerical approximation of the pde and its exact value be orthogonal to the Dirac delta function at specified collocation points. This results in the residuals being zero at the collocation points (FINLAYSON [90]).

Orthogonal collocation uses orthogonal polynomials as basis functions and specifics that the collocation points be located at the basis function roots. In this work we chose to use Jacobi polynomials since it has this orthogonality property. The polynomials were constructed orthogonal to each other with respect to a weight function. The weight functions used in the construction of the polynomials for the different equations were chosen to make the numerical solution stable.

We shall only be interested in this section in bounds for the numerical solutions at steady state.

3.2.4 Upper and Lower Bounding Solutions

The equations (6.2.22)-(6.2.27) are interesting in that the coupling is found in the boundary condition (6.2.24) of (6.2.22). Also, (6.2.23) depends on the solution to (6.2.22). Despite these features, we are able to show that we can obtain comparison results as that found in (PARSHOTAM, BHAMIDIMARRI and WAKE [225]).

Suppose that we can find functions $\underline{y}$, $\bar{y}$, $\underline{Y}$ and $\bar{Y}$ so that the following differential inequalities are satisfied for $\underline{y}$ and $\underline{Y}$:

$$\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial \underline{y}}{\partial x}\right) \geq \phi^2\frac{\underline{y}}{1+\beta\underline{y}} \qquad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.2.28}$$

$$\frac{1}{\mathcal{Pe}}\frac{d^2\underline{Y}}{dz^2} - \frac{d\underline{Y}}{dz} \geq \zeta\frac{\partial \underline{y}}{\partial x} \qquad \text{in } 0 < z < 1,\ x = 1, \tag{6.2.29}$$

$$\underline{y} + \frac{1}{\mathcal{Sh}}\frac{\partial \underline{y}}{\partial v} \leq \underline{Y}(z) \qquad \text{at } x = 1 \text{ for } 0 < z < 1, \tag{6.2.30}$$

$$\frac{\partial \underline{y}}{\partial v} \leq 0 \qquad \text{at } x = \alpha \text{ for } 0 < z < 1, \tag{6.2.31}$$

$$\underline{Y} - \frac{1}{\mathcal{Pe}}\frac{d\underline{Y}}{dz} \leq 1 \qquad \text{at } z = 0, \tag{6.2.32}$$

$$\frac{d\underline{Y}}{dz} \leq 0 \qquad \text{at } z = 1. \tag{6.2.33}$$

and the inequalities are reversed for $\bar{y}$ and $\bar{Y}$.

We see that the functions $\underline{y}-K$, $\underline{Y}-K$, $\bar{y}+K$ and $\bar{Y}+K$ for K positive constants satisfy conditions of Theorem 3.5.2 and so all solutions of (6.2.12)-(6.2.19) (including (6.2.22)-(6.2.27)) are globally stable. This also implies uniqueness of solutions to (6.2.22)-(6.2.27) and so (see the end of section 4.3), it follows that the upper and lower bounds

$$\underline{y}(x, z) \le y(x, z) \le \overline{y}(x, z) \quad \textbf{(6.2.34)}$$

and

$$\underline{Y}(z) \le Y(z) \le \overline{Y}(z) \quad \textbf{(6.2.35)}$$

are valid.

One way to obtain upper and lower analytical bounds would therefore be to choose two functions $\underline{f}$ and $\overline{f}$ such that

$$\overline{f} \le \phi^2 \frac{y}{1+\beta y} \le \underline{f} \quad \textbf{(6.2.36)}$$

For example, we may choose $\underline{f}=\phi^2\underline{y}$ and $\overline{f}=\phi^2\frac{\overline{y}}{1+\beta}$ and let $\underline{y}(x, z)$ and $\underline{Y}(z)$ be the solution to the following system

$$\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{y}}{\partial x}) = \phi^2\underline{y} \qquad \text{in } \alpha < x < 1,\ 0 < z < 1, \quad \textbf{(6.2.37)}$$

$$\frac{1}{\mathcal{Pe}}\frac{d^2\underline{Y}}{dz^2} - \frac{d\underline{Y}}{dz} = \zeta\frac{\partial \underline{y}}{\partial x} \qquad \text{in } 0 < z < 1,\ x = 1, \quad \textbf{(6.2.38)}$$

$$\underline{y} + \frac{1}{\mathcal{Sh}}\frac{\partial \underline{y}}{\partial v} = \underline{Y}(z) \qquad \text{at } x = 1 \text{ for } 0 < z < 1, \quad \textbf{(6.2.39)}$$

$$\frac{\partial \underline{y}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 < z < 1, \quad \textbf{(6.2.40)}$$

$$\underline{Y} - \frac{1}{\mathcal{Pe}}\frac{d\underline{Y}}{dz} = 1 \qquad \text{at } z = 0, \quad \textbf{(6.2.41)}$$

$$\frac{d\underline{Y}}{dz} = 0 \qquad \text{at } z = 1. \quad \textbf{(6.2.42)}$$

These equations are solved analytically to obtain the following equations for $\underline{y}(x, z)$ and $\underline{Y}(z)$:

$$\underline{Y}(z) = exp[\frac{\mathcal{Pe}}{2}z](c_1\, exp[\frac{c_4\mathcal{Pe}}{2}z] + c_2\, exp[-\frac{c_4\mathcal{Pe}}{2}z]) \quad \textbf{(6.2.43)}$$

and

$$\underline{y}(x, z) = \frac{\underline{Y}_1(z)}{c_3 x}[\frac{\phi\alpha\, cosh\, \phi(x-\alpha) + sinh\, \phi(x-\alpha)}{\phi\alpha\, sinh\, \phi(x-\alpha) + cosh\, \phi(x-\alpha)}] \quad \textbf{(6.2.44)}$$

where

$$c_1 = \frac{2(-1+c_4)}{exp[\mathcal{Pe}c_4](1+c_4)^2 - (1-c_4)^2} \quad \textbf{(6.2.45)}$$

$$c_2 = -c_1\, exp[c_4\mathcal{Pe}](\frac{1+c_4}{1-c_4}) \quad \textbf{(6.2.46)}$$

$$c_3 = 1 - \frac{1}{\mathcal{S}h} + \frac{\phi}{\mathcal{S}h}\left[\frac{\phi\alpha \sinh \phi(1-\alpha) + \cosh \phi(1-\alpha)}{\phi\alpha \cosh \phi(1-\alpha) + \sinh \phi(1-\alpha)}\right] \tag{6.2.47}$$

$$c_4 = \sqrt{1 + \frac{4\zeta c_5}{\mathcal{P}e}} \tag{6.2.48}$$

$$c_5 = \frac{c_3 = -1 + \phi\left[\frac{\phi\alpha \sinh \phi(1-\alpha) + \cosh \phi(1-\alpha)}{\phi\alpha \cosh \phi(1-\alpha) + \sinh \phi(1-\alpha)}\right]}{c_3} \tag{6.2.49}$$

To find $\bar{y}$ and $\bar{Y}$ we solve the following equations

$$\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{y}}{\partial x}) = \frac{\phi^2}{1+\beta}\bar{y} \qquad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.2.50}$$

$$\frac{1}{\mathcal{P}e}\frac{d^2\bar{Y}}{dz^2} - \frac{d\bar{Y}}{dz} = \zeta\frac{\partial \bar{y}}{\partial x} \qquad \text{in } 0 < z < 1,\ x = 1, \tag{6.2.51}$$

$$\bar{y} + \frac{1}{\mathcal{S}h}\frac{\partial \bar{y}}{\partial v} = \bar{Y}(z) \qquad \text{at } x = 1 \text{ for } 0 < z < 1, \tag{6.2.52}$$

$$\frac{\partial \bar{y}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 < z < 1, \tag{6.2.53}$$

$$\bar{Y} - \frac{1}{\mathcal{P}e}\frac{d\bar{Y}}{dz} = 1 \qquad \text{at } z = 0, \tag{6.2.54}$$

$$\frac{d\bar{Y}}{dz} = 0 \qquad \text{at } z = 1. \tag{6.2.55}$$

where the solutions for $\bar{y}$ and $\bar{Y}$ are given as in (6.2.43)-(6.2.49) but with ϕ replaced by $\dfrac{\phi}{\sqrt{1+\beta}}$.

To show that constants c_1, $c_2 > 0$ we are only required to show that $c_5 > 0$. We note that

$$c_5 > 0 \Leftrightarrow \left[\frac{\phi\alpha \sinh \phi(1-\alpha) + \cosh \phi(1-\alpha)}{\phi\alpha \cosh \phi(1-\alpha) + \sinh \phi(1-\alpha)}\right] > 1 \tag{6.2.56}$$

$$\Leftrightarrow g(\phi) = \frac{e^{2\phi}(\phi-1)}{\phi+1} > \frac{e^{2\alpha\phi}(\alpha\phi-1)}{\alpha\phi+1} = g(\alpha\phi) \tag{6.2.57}$$

and this is clearly true since g can be shown to be a monotonically increasing function for $0 \leq \alpha < 1$ and $\phi > 0$. Finally, since $c_1, c_2 > 0$, it follows that $Y(z) > 0$ since $Y(z) > \underline{Y}(z)$ and $\underline{Y}(z)$ is exponentially decaying and is strictly bounded below by zero. This in turn implies that $y(x, z) > 0$, since $\underline{y}$ is similarly strictly bounded below by zero.

For a given set of parameter values found in literature, we plot a graph of analytical bounds $\underline{Y}(z)$ and $\bar{Y}(z)$ with $Y(z)$ obtained by orthogonal collocation (see FIG 6.8).

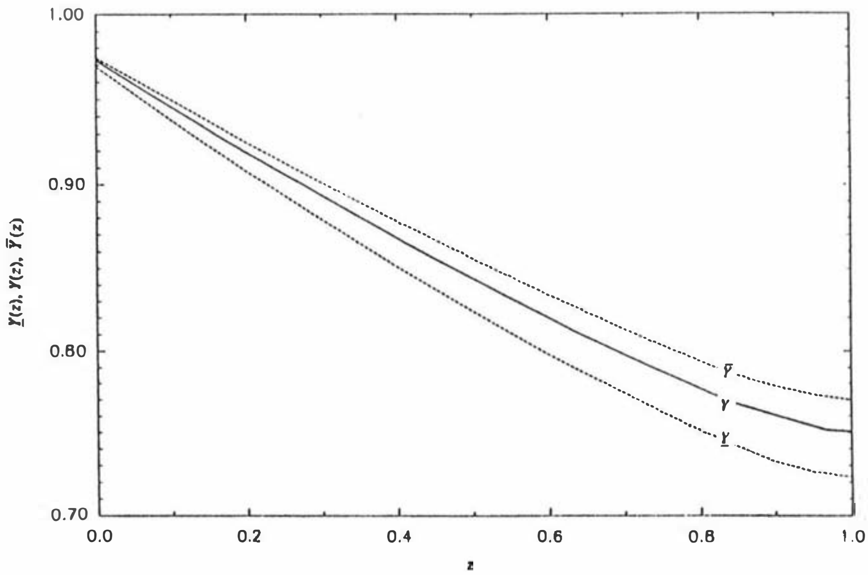


FIG. 6.8 Upper and Lower Bounds to $Y(z)$ with α=0.3, β=0.5, ϕ=5, ζ=0.1, $\mathcal{Sh}$=20 and $\mathcal{Pe}$=10

6.2.5 Conclusions and Remarks

The method demonstrated in this work may be applied to finding upper and lower bounds to a wide class of such equations with reaction terms very nonlinear. In the problem demonstrated in this section, since the Michaelis-Menten reaction term is concave down, a lower bound is always obtained when this term is linearised by a Taylor's series expansion. This lower bound is always strictly greater that zero and gives a good indication of concentrations at the outlet of the reactor. For diffusion limited reactions in microbial films where the Thiele modulus is very high, these bounds may not be so effective approximate solutions. The method is also sensitive to a decrease in α and may not therefore be as effective for biofilms with very small support particle sizes. For typical parameter values it is a very convenient method of checking numerical results as well as numerical results that involve very small concentrations. It can also be demonstrated analytically with the help of the maximum principle that dimensionless substrate concentration within a bioparticle is monotonically increasing with the parameters α, β, $\mathcal{Sh}$ and monotonically decreasing with the parameter ϕ^2. Also it can be shown that bulk concentration is monotonically decreasing with all parameters $\mathcal{Pe}$, $\mathcal{Sh}$ and ζ. These properties can all be interpreted physically.

Nomenclature

A	cross sectional area, typically 20cm^2
D_s	effective diffusivity constant, typically 1-2$\times$10^{-6}cm^{2}sec^{-1}
D_{S_b}	axial dispersion coefficient
h	dimensional height of the reactor, typically 80-90cm
H_s	Mass transfer resistance
K_s	Michaelis-Menten saturation constant (kg m^{-3})
N	number of bioparticles per unit volume 20-100cm^{-3}
$\mathcal{Pe}$	Péclet number given in (6.2.21)
U_{S_b}	superficial liquid velocity- typically 0.1-2cmsec^{-1}
r	radial distance within a bioparticle

r_{sm}	support media radius
r_{bp}	bioparticle radius- typically 0.3-0.6cm
$\mathcal{Sh}$	Sherwood number given in (6.2.21)
S	substrate concentration within a bioparticle
S_b	bulk substrate concentration which varies up the reactor (kgm^{-3})
$S_{b,i}$	input bulk substrate concentration (kgm^{-3})
t	actual time
x	dimensionless distance within a bioparticle
y	dimensionlesssubstrate concentration at position x of a bioparticle at height z
Y	dimensionless bulk substrate concentration at given height z
$Y_{X/S}$	growth yield
Z	height up the reactor
z	dimensionless height up the reactor

Greek letters

α	ratio of support media radius to bioparticle radius
β	dimensionless Michaelis Menten constant
χ	parameter given in (6.2.21)
ϕ^2	Thiele moduli given in (6.2.21), typically 0-5
μ_m	maximum specific growth rate constant
ρ_{bf}	biofilm density
τ	dimensionless time
ζ	parameter given in (6.2.21), typically 0-12

6.3 Monotone Iteration Techniques in the construction of Upper and Lower Solutions

Although upper and lower solutions are useful in the investigation of qualitive properties of solutions and do prove to be good as approximate solutions (PARSHOTAM *et al.* [225, 226]), they can also be improved by monotone iteration techniques. The method of combining upper and lower solutions with monotone iterative techniques has proved not only to be a powerful tool in proving existence of solutions but has also recently been shown to be useful for numerical computation of solutions of boundary value problems for both scalar equations and systems of weakly coupled elliptic equations (GROSSMANN [111], GROSSMANN and ROOS [110], PAO [219-222]). The objective of this example is to help us to understand the relationship between the properties of the reaction functions and the resulting sequences. We examine some monotone iterative techniques and suggest how such techniques may be useful for numerical computation of solutions of the general system S_n, B_n.

Several monotone iteration methods are given by KELLER [141] for scalar elliptic equations. These provide us with either monotone sequences, alternating sequences and in some cases monotone sequences with accelerated convergences. These sequences are all obtained with the help of the strong maximum principle for the elliptic operator. In this section, we shall look at the problem developed in section 6.2 but for more general arbitrary reaction functions and show that although this problem is non standard in that it involves elliptic equations which are coupled in the boundary conditions in a functional way, we can also obtain similar monotone sequences. These are also obtained with the help of the strong maximum principle in various ways.

An iteration scheme is set up which generally results in solving either coupled or uncoupled linear differential equations. These iteration shemes may produce either monotone or alternating sequences and under special conditions, Newton's method may be applied which accelerates the rate of convergence. A lower or an upper solution is taken as a good candidate for a first iteration.

6.3.1 Upper and Lower Solutions

Consider the boundary value problem

$$L_1 y = \phi^2 f(x,y) \qquad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.3.1}$$

$$L_2 Y = \zeta \frac{\partial y}{\partial x} = \zeta \mathcal{Sh}(Y - y) \qquad \text{in } 0 < z < 1,\ x = 1, \tag{6.3.2}$$

$$y + \frac{1}{\mathcal{Sh}} \frac{\partial y}{\partial v} = Y(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1, \tag{6.3.3}$$

$$\frac{\partial y}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1, \tag{6.3.4}$$

$$Y - \frac{1}{\mathcal{Pe}} \frac{dY}{dz} = 1 \qquad \text{at } z = 0, \tag{6.3.5}$$

$$\frac{dY}{dz} = 0 \qquad \text{at } z = 1, \tag{6.3.6}$$

where

$$L_1 \equiv \frac{1}{x^2} \frac{\partial}{\partial x} (x^2 \frac{\partial}{\partial x}), \tag{6.3.7}$$

and

$$L_2 \equiv \frac{1}{\mathcal{Pe}} \frac{d^2}{dz^2} - \frac{d}{dz}, \tag{6.3.8}$$

A lower solution to this problem is a function $(\underset{\sim}{y}, \underset{\sim}{Y})$ satisfying

$$L_1 \underset{\sim}{y} \geq \phi^2 f(x,\underset{\sim}{y}) \quad \text{in } \alpha < x < 1, 0 < z < 1, \tag{6.3.9}$$

$$L_2 \underset{\sim}{Y} \geq \zeta \mathcal{Sh}(\underset{\sim}{Y} - \underset{\sim}{y}) \quad \text{in } 0 < z < 1, x = 1, \tag{6.3.10}$$

$$\underset{\sim}{y} + \frac{1}{\mathcal{Sh}} \frac{\partial \underset{\sim}{y}}{\partial x} \leq \underset{\sim}{Y}(z) \quad \text{at } x = 1 \text{ for } 0 \leq z \leq 1, \tag{6.3.11}$$

$$\frac{\partial \underset{\sim}{y}}{\partial v} \leq 0 \quad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1, \tag{6.3.12}$$

$$\underset{\sim}{Y} - \frac{1}{\mathcal{Pe}} \frac{d\underset{\sim}{Y}}{dz} \leq 1 \quad \text{at } z = 0, \tag{6.3.13}$$

$$\frac{d\underset{\sim}{Y}}{dz} \leq 0 \quad \text{at } z = 1. \tag{6.3.14}$$

An upper solution to this problem is a function $(\tilde{y}, \tilde{Y})$ satisfying

$$L_1 \tilde{y} \leq \phi^2 f(x,\tilde{y}) \quad \text{in } \alpha < x < 1, 0 < z < 1, \tag{6.3.15}$$

$$L_2 \tilde{Y} \leq \zeta \mathcal{Sh}(\tilde{Y} - \tilde{y}) \quad \text{in } 0 < z < 1, x = 1, \tag{6.3.16}$$

$$\tilde{y} + \frac{1}{\mathcal{Sh}} \frac{\partial \tilde{y}}{\partial v} \geq \tilde{Y}(z) \quad \text{at } x = 1 \text{ for } 0 \leq z \leq 1, \tag{6.3.17}$$

$$\frac{\partial \tilde{y}}{\partial v} \geq 0 \quad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1, \tag{6.3.18}$$

$$\tilde{Y} - \frac{1}{\mathcal{Pe}} \frac{d\tilde{Y}}{dz} \geq 1 \quad \text{at } z = 0, \tag{6.3.19}$$

$$\frac{d\tilde{Y}}{dz} = 0 \quad \text{at } z = 1, \tag{6.3.20}$$

where $(\underset{\sim}{y}, \underset{\sim}{Y}) \leq (\tilde{y}, \tilde{Y})$.

6.3.2 Monotone Iteration Methods

We shall assume that y_n and y_{n+1} are restricted to the set $min\ \underset{\sim}{y} \leq y_n, y_{n+1} \leq max\ \tilde{y}$ and that Y_n and Y_{n+1} are restricted to the set $min\ \underset{\sim}{Y} \leq Y_n, Y_{n+1} \leq max\ \tilde{Y}$.

In each of the following methods, we shall define transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ from (y_n, Y_n) to (y_{n+1}, Y_{n+1}) and show that these transformations have some sort of a monotone property. In the general case, we shall mean that $\mathcal{T}_1$ and $\mathcal{T}_2$ are *monotone* in the sense of COLLATZ [76], i.e., i.e., $y_n \leq y_{n+1}$ and $Y_n \leq Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$. The monotone property of transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ are shown to usually depend on the properties of the function f. In all these methods B_1 and B_2 are relevant boundary operators.

Assume, for the first three methods that f is a smooth function on $min\ \underset{\sim}{y} \leq y \leq max\ \tilde{y}$ and that

$$\phi^2 \frac{\partial f}{\partial y}, \tag{6.3.21}$$

is bounded below for $\alpha < x < 1$ and $min\ \underset{\sim}{y} \leq y \leq max\ \tilde{y}$, so that

$$\phi^2 \frac{\partial f}{\partial y} - m < 0, \tag{6.3.22}$$

for m sufficiently large.

Define

$$F(x, y_n) = \phi^2 f(x, y_n) - m y_n. \tag{6.3.23}$$

Then by assumption,

$$F_{y_n} < 0, \tag{6.3.24}$$

implies that F is decreasing. The quantity

$$\phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) - m(y_{n+1} - y_n), \tag{6.3.25}$$

is

$$F(x, y_{n+1}) - F(x, y_n), \tag{6.3.26}$$

so that for $y_n \le y_{n+1}$,

$$\phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) - m(y_{n+1} - y_n) = F(x, y_{n+1}) - F(x, y_n) \le 0. \tag{6.3.27}$$

Method 1

We define the (nonlinear) transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ as follows:

$$\mathcal{T}_1 \colon y_{n+1} = \mathcal{T}_1 y_n$$

and

$$\mathcal{T}_2 \colon Y_{n+1} = \mathcal{T}_2 Y_n$$

if

$$(L_1 - m) y_{n+1} = \phi^2 f(x, y_n) - m y_n \qquad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta \mathcal{S}h) Y_{n+1} = -\zeta \mathcal{S}h\, y_n \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+1} + \frac{1}{\mathcal{S}h} \frac{\partial y_{n+1}}{\partial v} = Y_n(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1,$$

$$\frac{\partial y_{n+1}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$

$$Y_{n+1} - \frac{1}{\mathcal{P}e} \frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z} = 1 \qquad \text{at } z = 0,$$

$$\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z} = 0 \qquad \text{at } z = 1.$$

In this method, the equations for Y_{n+1} and y_{n+1} are uncoupled and we show that both $\mathcal{T}_1$ and $\mathcal{T}_2$ are *monotone* in the sense that $y_n \le y_{n+1}$ and $Y_n \le Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$.

We have, if $y_n \le y_{n+1}$ and $Y_n \le Y_{n+1}$

$$(L_1 - m)\mathcal{T}_1 y_n = (L_1 - m) y_{n+1} = \phi^2 f(x, y_n) - m y_n \qquad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta \mathcal{S}h)\mathcal{T}_2 Y_n = (L_2 - \zeta \mathcal{S}h) Y_{n+1} = -\zeta \mathcal{S}h\, y_n \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+1} + \frac{1}{\mathcal{S}h} \frac{\partial y_{n+1}}{\partial v} = Y_n(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1,$$

$$\frac{\partial y_{n+1}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$

$$Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 1 \qquad \text{at } z = 0,$$

$$\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 0 \qquad \text{at } z = 1,$$

and

$$(L_1 - m)\mathcal{T}_1 y_{n+1} = (L_1 - m)y_{n+2} = \phi^2 f(x, y_{n+1}) - m y_{n+1} \quad \text{in } \alpha < x < 1, 0 < z < 1,$$

$$(L_2 - \zeta\mathcal{Sh})\mathcal{T}_2 Y_{n+1} = (L_2 - \zeta\mathcal{Sh})Y_{n+2} = -\zeta\mathcal{Sh}\, y_{n+1} \quad \text{in } 0 < z < 1, x = 1,$$

$$y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v} = Y_{n+1}(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1,$$

$$\frac{\partial y_{n+2}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$

$$Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+2}}{\mathrm{dz}} = 1 \qquad \text{at } z = 0,$$

$$\frac{\mathrm{d}Y_{n+2}}{\mathrm{dz}} = 0 \qquad \text{at } z = 1.$$

Therefore,

$$(L_1 - m)(\mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n) = \phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) - m(y_{n+1} - y_n) \le 0 \quad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.3.28}$$

$$(L_2 - \zeta\mathcal{Sh})(\mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n) = -\zeta\mathcal{Sh}(y_{n+1} - y_n) \le 0 \quad \text{in } 0 < z < 1,\ x = 1, \tag{6.3.29}$$

$$[y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v}] - [y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v}] = Y_{n+1}(z) - Y_n(z) \ge 0 \quad \text{at } x = 1 \text{ for } 0 \le z \le 1, \tag{6.3.30}$$

$$\frac{\partial y_{n+2}}{\partial v} - \frac{\partial y_{n+1}}{\partial v} = 0 \ge 0, \quad \text{at } x = \alpha \text{ for } 0 \le z \le 1, \tag{6.3.31}$$

$$[Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+2}}{\mathrm{dz}}] - [Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}}] = 1 - 1 = 0 \ge 0 \quad \text{at } z = 0, \tag{6.3.32}$$

$$\frac{\mathrm{d}Y_{n+2}}{\mathrm{dz}} - \frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 0 \ge 0 \quad \text{at } z = 1. \tag{6.3.33}$$

and we therefore have the problem

$$L_1 w \le 0 \qquad \text{in } \alpha < x < 1, 0 < z < 1,$$

$$L_2 W \le 0 \qquad \text{in } 0 < z < 1, x = 1,$$

$$B_1 w \ge 0 \qquad \text{on } x = \alpha, x = 1,$$

$$B_2 W \ge 0, \qquad \text{on } z = 0, z = 1,$$

where,

$$w = \mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n \text{ and } W = \mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n.$$

By the strong maximum principle, $w > 0$ in $\alpha < x < 1$ and $W > 0$ in $0 < z < 1$ (unless w, $W \equiv 0$ in which case $\mathcal{T}y_{n+1} = \mathcal{T}y_n$ and $\mathcal{T}_2 Y_{n+1} = \mathcal{T}_2 Y_n$ and the right hand sides of (6.3.28) and (6.3.29) are identically zero; but this happens only if $y_n \equiv y_{n+1}$ and $Y_n \equiv Y_{n+1}$, since F is strictly monotonic, so $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$). It can similarly be shown that $y_n \geq y_{n+1}$ and $Y_n \geq Y_{n+1}$ implies $\mathcal{T}_1 y_n > \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n > \mathcal{T}_2 Y_{n+1}$.

Method 2

We define the (nonlinear) transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ as follows:

$$\mathcal{T}_1\colon y_{n+1} = \mathcal{T}_1 y_n$$

and

$$\mathcal{T}_2\colon Y_{n+1} = \mathcal{T}_2 Y_n$$

if

$$(L_1 - m)y_{n+1} = \phi^2 f(x, y_n) - m y_n \qquad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta\mathcal{S}h)Y_{n+1} = -\zeta\mathcal{S}h\, y_{n+1} \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+1} + \frac{1}{\mathcal{S}h}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) \qquad \text{at } x = 1 \text{ for } 0 \leq z \leq 1,$$

$$\frac{\partial y_{n+1}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1,$$

$$Y_{n+1} - \frac{1}{\mathcal{P}e}\frac{dY_{n+1}}{dz} = 1 \qquad \text{at } z = 0,$$

$$\frac{dY_{n+1}}{dz} = 0 \qquad \text{at } z = 1.$$

In this method the equations for Y_{n+1} and y_{n+1} are coupled and we show that $\mathcal{T}_1$ and $\mathcal{T}_2$ are also *monotone* in the sense that $y_n \leq y_{n+1}$ and $Y_n \leq Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$.

We have, if $y_n \leq y_{n+1}$ and $Y_n \leq Y_{n+1}$

$$(L_1 - m)\mathcal{T}_1 y_n = (L_1 - m)y_{n+1} = \phi^2 f(x, y_n) - m y_n \qquad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta\mathcal{S}h)\mathcal{T}_2 Y_{n+1} = (L_2 - \zeta\mathcal{S}h)Y_{n+1} = -\zeta\mathcal{S}h\, y_{n+1} \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$(L_2 - \zeta\mathcal{S}h)\mathcal{T}Y_n = (L_2 - \zeta\mathcal{S}h)Y_{n+1} = -\zeta\mathcal{S}h\, y_n \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+1} + \frac{1}{\mathcal{S}h}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) \qquad \text{at } x = 1 \text{ for } 0 \leq z \leq 1,$$

$$\frac{\partial y_{n+1}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1,$$

$$Y_{n+1} - \frac{1}{\mathcal{P}e}\frac{dY_{n+1}}{dz} = 1 \qquad \text{at } z = 0,$$

$$\frac{dY_{n+1}}{dz} = 0 \qquad \text{at } z = 1,$$

and

$$(L_1 - m)\mathcal{T}_1 y_{n+1} = (L_1 - m)y_{n+2} = \phi^2 f(x, y_{n+1}) - m y_{n+1} \qquad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta\mathcal{S}h)\mathcal{T}_2 Y_{n+1} = (L_2 - \zeta\mathcal{S}h)Y_{n+2} = -\zeta\mathcal{S}h\, y_{n+2} \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+2} + \frac{1}{\mathcal{S}h}\frac{\partial y_{n+2}}{\partial v} = Y_{n+1}(z) \qquad \text{at } x = 1 \text{ for } 0 \leq z \leq 1,$$

$$\frac{\partial y_{n+2}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$

$$Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+2}}{dz} = 1 \qquad \text{at } z = 0,$$

$$\frac{dY_{n+2}}{dz} = 0 \qquad \text{at } z = 1.$$

Therefore,

$$(L_1 - m)(\mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n) = \phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) - m(y_{n+1} - y_n) \le 0 \quad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.3.34}$$

$$(L_2 - \zeta\mathcal{Sh})(\mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n) = -\zeta\mathcal{Sh}(y_{n+2} - y_{n+1}) \quad \text{in } 0 < z < 1,\ x = 1, \tag{6.3.35}$$

$$[y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v}] - [y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v}] = Y_{n+1}(z) - Y_n(z) \ge 0 \quad \text{at } x = 1 \text{ for } 0 \le z \le 1, \tag{6.3.36}$$

$$\frac{\partial y_{n+2}}{\partial v} - \frac{\partial y_{n+1}}{\partial v} = 0 \ge 0, \quad \text{at } x = \alpha \text{ for } 0 \le z \le 1, \tag{6.3.37}$$

$$[Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+2}}{dz}] - [Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+1}}{dz}] = 1 - 1 = 0 \ge 0 \quad \text{at } z = 0, \tag{6.3.38}$$

$$\frac{dY_{n+2}}{dz} - \frac{dY_{n+1}}{dz} = 0 \ge 0 \quad \text{at } z = 1. \tag{6.3.39}$$

and we therefore have the problem

$$L_1 w \le 0 \qquad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$B_1 w \ge 0 \qquad \text{on } x = \alpha,\ x = 1,$$

where,

$$w = \mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n.$$

By the strong maximum principle, $w > 0$ in $\alpha < x < 1$. This implies that the right hand side of (6.3.35) is negative so that

$$L_2 W \le 0 \qquad \text{in } 0 < z < 1,\ x = 1,$$

$$B_2 W \ge 0 \qquad \text{on } z = 0,\ z = 1,$$

where,

$$W = \mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n.$$

By the strong maximum principle, $W > 0$ in $0 < z < 1$. Therefore, $y_n \le y_{n+1}$ and $Y_n \le Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$. It can similarly be shown that, $y_n \ge y_{n+1}$ and $Y_n \ge Y_{n+1}$ implies $\mathcal{T}_1 y_n > \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n > \mathcal{T}_2 Y_{n+1}$.

Method 3

We define the (nonlinear) transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ as follows:

$$\mathcal{T}_1\colon y_{n+1} = \mathcal{T}_1 y_n$$

and

$$\mathcal{T}_2\colon Y_{n+1} = \mathcal{T}_2 Y_n$$

if

$$(L_1-m)y_{n+1}=\phi^2 f(x,y_n)-my_n \qquad \text{in } \alpha<x<1,\ 0<z<1,$$

$$(L_2-\zeta\mathcal{S}\!h)Y_{n+1}=-\zeta\mathcal{S}\!h\, y_n \qquad \text{in } 0<z<1,\ x=1,$$

$$y_{n+1}+\frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+1}}{\partial v}=Y_{n+1}(z) \qquad \text{at } x=1 \text{ for } 0\le z\le 1,$$

$$\frac{\partial y_{n+1}}{\partial v}=0 \qquad \text{at } x=\alpha \text{ for } 0\le z\le 1,$$

$$Y_{n+1}-\frac{1}{\mathcal{P}\!e}\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}=1 \qquad \text{at } z=0,$$

$$\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}=0 \qquad \text{at } z=1.$$

In this method the equations for Y_{n+1} and y_{n+1} are coupled and we show that $\mathcal{T}_1$ and $\mathcal{T}_2$ are *monotone* in the sense that $y_n \le y_{n+1}$ implies that $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$ and this in turn implies that $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$. We have, if $y_n \le y_{n+1}$

$$(L_1-m)\mathcal{T}_1 y_n=(L_1-m)y_{n+1}=\phi^2 f(x,y_n)-my_n \qquad \text{in } \alpha<x<1,\ 0<z<1,$$

$$(L_2-\zeta\mathcal{S}\!h)\mathcal{T}_2 Y_n=(L_2-\zeta\mathcal{S}\!h)Y_{n+1}=-\zeta\mathcal{S}\!h\, y_n \qquad \text{in } 0<z<1,\ x=1,$$

$$y_{n+1}+\frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+1}}{\partial v}=Y_{n+1}(z) \qquad \text{at } x=1 \text{ for } 0\le z\le 1,$$

$$\frac{\partial y_{n+1}}{\partial v}=0 \qquad \text{at } x=\alpha \text{ for } 0\le z\le 1,$$

$$Y_{n+1}-\frac{1}{\mathcal{P}\!e}\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}=1 \qquad \text{at } z=0,$$

$$\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}=0 \qquad \text{at } z=1,$$

and

$$(L_1-m)\mathcal{T}_1 y_{n+1}=(L_1-m)y_{n+2}=\phi^2 f(x,y_{n+1})-my_{n+1} \qquad \text{in } \alpha<x<1,\ 0<z<1,$$

$$(L_2-\zeta\mathcal{S}\!h)\mathcal{T}_2 Y_{n+1}=(L_2-\zeta\mathcal{S}\!h)Y_{n+2}=-\zeta\mathcal{S}\!h\, y_{n+2} \qquad \text{in } 0<z<1,\ x=1,$$

$$y_{n+2}+\frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+2}}{\partial v}=Y_{n+2}(z) \qquad \text{at } x=1 \text{ for } 0\le z\le 1,$$

$$\frac{\partial y_{n+2}}{\partial v}=0 \qquad \text{at } x=\alpha \text{ for } 0\le z\le 1,$$

$$Y_{n+2}-\frac{1}{\mathcal{P}\!e}\frac{\mathrm{d}Y_{n+2}}{\mathrm{d}z}=1 \qquad \text{at } z=0,$$

$$\frac{\mathrm{d}Y_{n+2}}{\mathrm{d}z}=0 \qquad \text{at } z=1.$$

Therefore,

$$(L_1-m)(\mathcal{T}_1 y_{n+1}-\mathcal{T}_1 y_n)=\phi^2 f(x,y_{n+1})-\phi^2 f(x,y_n)-m(y_{n+1}-y_n)\le 0 \quad \text{in } \alpha<x<1,\ 0<z<1, \tag{6.3.40}$$

$$(L_2-\zeta\mathcal{S}\!h)(\mathcal{T}_2 Y_{n+1}-\mathcal{T}_2 Y_n)=-\zeta\mathcal{S}\!h(y_{n+1}-y_n)\le 0 \quad \text{in } 0<z<1,\ x=1, \tag{6.3.41}$$

$$[y_{n+2}+\frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v}]-[y_{n+1}+\frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v}]=Y_{n+2}(z)-Y_{n+1}(z) \qquad \text{at } x=1 \text{ for } 0\le z\le 1, \tag{6.3.42}$$

$$\frac{\partial y_{n+2}}{\partial v}-\frac{\partial y_{n+1}}{\partial v}=0\ge 0, \qquad \text{at } x=\alpha \text{ for } 0\le z\le 1, \tag{6.3.43}$$

$$[Y_{n+2}-\frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+2}}{\mathrm{d}z}]-[Y_{n+1}-\frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}]=1-1=0\ge 0 \qquad \text{at } z=0, \tag{6.3.44}$$

$$\frac{\mathrm{d}Y_{n+2}}{\mathrm{d}z}-\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}=0\ge 0 \qquad \text{at } z=1. \tag{6.3.45}$$

Therefore, we have the problem

$L_2W \le 0$ in $0 < z < 1$, $x=1$,

$B_2W \ge 0$, on $z = 0$, $z = 1$

where,

$$W = \mathcal{T}Y_{n+1} - \mathcal{T}Y_n,$$

and by the strong maximum principle, $W > 0$ in $0 < z < 1$. This implies that the right hand side of (6.3.42) is negative so that

$L_1w \le 0$ in $\alpha < x < 1$, $0 < z < 1$,

$B_1w \ge 0$ on $x = \alpha$, $x = 1$,

where,

$$w = \mathcal{T}y_{n+1} - \mathcal{T}y_n.$$

By the strong maximum principle, $w > 0$ in $\alpha < x < 1$. Therefore, $y_n \le y_{n+1}$ implies $\mathcal{T}_2Y_n < \mathcal{T}_2Y_{n+1}$ which in turn implies that $\mathcal{T}_1y_n < \mathcal{T}_1y_{n+1}$. It can similarly be shown that, $y_n \ge y_{n+1}$ implies $\mathcal{T}_2Y_n > \mathcal{T}_2Y_{n+1}$ which in turn implies that $\mathcal{T}_1y_n > \mathcal{T}_1y_{n+1}$.

If in addition to the assumptions on f, we assume that f is monotone increasing, the following two iteration procedures yield alternating sequences which form two monotone sequences bounding the solution from above and below. Therefore, by assumption, for $y_n \le y_{n+1}$

$$\phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) \ge 0. \tag{6.3.46}$$

Method 4

We define the (nonlinear) transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ as follows:

$$\mathcal{T}_1\!: y_{n+1} = \mathcal{T}_1 y_n$$

and

$$\mathcal{T}_2\!: Y_{n+1} = \mathcal{T}_2 Y_n$$

if

$L_1y_{n+1} = \phi^2 f(x, y_n)$ in $\alpha < x < 1$, $0 < z < 1$,

$(L_2 - \zeta\mathcal{Sh})Y_{n+1} = -\zeta\mathcal{Sh}y_n$ in $0 < z < 1$, $x = 1$,

$$y_{n+1} + \frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1,$$
$$\frac{\partial y_{n+1}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$
$$Y_{n+1} - \frac{1}{\mathcal{P}\!e}\frac{dY_{n+1}}{dz} = 1 \qquad \text{at } z = 0,$$
$$\frac{dY_{n+1}}{dz} = 0 \qquad \text{at } z = 1.$$

In this method the equations for Y_{n+1} and y_{n+1} are uncoupled and we show that $\mathcal{T}_1$ and $\mathcal{T}_2$ are monotone in the sense that $y_n \le y_{n+1}$ and $Y_n \ge Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n > \mathcal{T}_2 Y_{n+1}$.

We have, if $y_n \le y_{n+1}$ and $Y_n \le Y_{n+1}$

$$L_1\mathcal{T}_1 y_n = L_1 y_{n+1} = \phi^2 f(x, y_n) \qquad \text{in } \alpha < x < 1, 0 < z < 1,$$
$$(L_2 - \zeta\mathcal{S}\!h)\mathcal{T}_1 Y_n = (L_2 - \zeta\mathcal{S}\!h)Y_{n+1} = -\zeta\mathcal{S}\!h y_n \qquad \text{in } 0 < z < 1, x = 1,$$
$$y_{n+1} + \frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1,$$
$$\frac{\partial y_{n+1}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$
$$Y_{n+1} - \frac{1}{\mathcal{P}\!e}\frac{dY_{n+1}}{dz} = 1 \qquad \text{at } z = 0,$$
$$\frac{dY_{n+1}}{dz} = 0 \qquad \text{at } z = 1.$$

and

$$L_1\mathcal{T}_1 y_{n+1} = L_1 y_{n+2} = \phi^2 f(x, y_{n+1}) \qquad \text{in } \alpha < x < 1, 0 < z < 1,$$
$$(L_2 - \zeta\mathcal{S}\!h)\mathcal{T}_1 Y_{n+1} = (L_2 - \zeta\mathcal{S}\!h)Y_{n+2} = -\zeta\mathcal{S}\!h y_{n+1} \qquad \text{in } 0 < z < 1, x = 1,$$
$$y_{n+2} + \frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+2}}{\partial v} = Y_{n+1}(z) \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1,$$
$$\frac{\partial y_{n+2}}{\partial v} = 0 \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1,$$
$$Y_{n+2} - \frac{1}{\mathcal{P}\!e}\frac{dY_{n+2}}{dz} = 1 \qquad \text{at } z = 0,$$
$$\frac{dY_{n+2}}{dz} = 0 \qquad \text{at } z = 1.$$

Therefore,

$$L_1(\mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n) = \phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) \ge 0 \qquad \text{in } \alpha < x < 1, 0 < z < 1, \tag{6.3.47}$$
$$(L_2 - \zeta\mathcal{S}\!h)(\mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n) = -\zeta\mathcal{S}\!h(y_{n+1} - y_n) \le 0 \qquad \text{in } 0 < z < 1, x = 1, \tag{6.3.48}$$
$$[y_{n+2} + \frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+2}}{\partial v}] - [y_{n+1} + \frac{1}{\mathcal{S}\!h}\frac{\partial y_{n+1}}{\partial v}] = Y_{n+1}(z) - Y_n(z) \le 0 \qquad \text{at } x = 1 \text{ for } 0 \le z \le 1, \tag{6.3.49}$$
$$\frac{\partial y_{n+2}}{\partial v} - \frac{\partial y_{n+1}}{\partial v} = 0 \ge 0, \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1, \tag{6.3.50}$$

$$[Y_{n+2} - \frac{1}{\mathcal{P}e}\frac{\mathrm{d}Y_{n+2}}{\mathrm{d}z}] - [Y_{n+1} - \frac{1}{\mathcal{P}e}\frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z}] = 1 - 1 = 0 \geq 0 \qquad \text{at } z = 0, \tag{6.3.51}$$

$$\frac{\mathrm{d}Y_{n+2}}{\mathrm{d}z} - \frac{\mathrm{d}Y_{n+1}}{\mathrm{d}z} = 0 \geq 0 \qquad \text{at } z = 1. \tag{6.3.52}$$

Therefore, we have the problem

$$\begin{array}{ll} L_1 w \geq 0 & \text{in } \alpha < x < 1, 0 < z < 1, \\ L_2 W \leq 0 & \text{in } 0 < z < 1, x = 1, \\ B_1 w \leq 0 & \text{on } x = \alpha, x = 1, \\ B_2 W \geq 0, & \text{on } z = 0, z = 1, \end{array}$$

where,

$w = \mathcal{T}y_{n+1} - \mathcal{T}y_n$ and $W = \mathcal{T}Y_{n+1} - \mathcal{T}Y_n$ and B_1 and B_2 are boundary operators.

By the strong maximum principle, $w < 0$ in $\alpha < x < 1$ and $W > 0$ in $0 < z < 1$ (unless $w, W \equiv 0$ in which case $\mathcal{T}_1 y_{n+1} = \mathcal{T}_1 y_n$ and $\mathcal{T}_2 Y_{n+1} = \mathcal{T}_2 Y_n$ and the right hand sides of (6.3.47) and (6.3.48) are identically zero; but this happens only if $y_n \equiv y_{n+1}$ and $Y_n \equiv Y_{n+1}$, since f is strictly monotonic, so $\mathcal{T}_1 y_n > \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n <$ $\mathcal{T}_2 Y_{n+1}$). Similarly, $y_n \leq y_{n+1}$ and $Y_n \geq Y_{n+1}$ implies $\mathcal{T}_1 y_n > \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$. This also implies that $\mathcal{T}_1^2$ and $\mathcal{T}_2^2$ are *monotone* in the sense that $y_n \leq y_{n+1}$ and $Y_n \geq Y_{n+1}$ implies $\mathcal{T}_1^2 y_n < \mathcal{T}_1^2 y_{n+1}$ and $\mathcal{T}_2^2 Y_n > \mathcal{T}_2^2 Y_{n+1}$.

Method 5

We define the (nonlinear) transformations $\mathcal{T}_1$ and $\mathcal{T}_2$ as follows:

$$\mathcal{T}_1\colon y_{n+1} = \mathcal{T}_1 y_n$$

and

$$\mathcal{T}_2\colon Y_{n+1} = \mathcal{T}_2 Y_n$$

if

$$\begin{array}{ll} L_1 y_{n+1} = \phi^2 f(x, y_n) & \text{in } \alpha < x < 1, 0 < z < 1, \\ (L_2 - \zeta\mathcal{S}h)Y_{n+1} = -\zeta\mathcal{S}h\, y_{n+1} & \text{in } 0 < z < 1, x = 1, \\ y_{n+1} + \dfrac{1}{\mathcal{S}h}\dfrac{\partial y_{n+1}}{\partial v} = Y_n(z) & \text{at } x = 1 \text{ for } 0 \leq z \leq 1, \\ \dfrac{\partial y_{n+1}}{\partial v} = 0 & \text{at } x = \alpha \text{ for } 0 \leq z \leq 1, \\ Y_{n+1} - \dfrac{1}{\mathcal{P}e}\dfrac{\mathrm{d}Y_{n+1}}{\mathrm{d}z} = 1 & \text{at } z = 0, \\ \dfrac{\mathrm{d}Y_{n+1}}{\mathrm{d}z} = 0 & \text{at } z = 1. \end{array}$$

In this method the equations for Y_{n+1} and y_{n+1} are coupled and we show that $\mathcal{T}_1$ and $\mathcal{T}_2$ are monotone in the sense that $y_n \leq y_{n+1}$ and $Y_n \geq Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$.

We have, if $y_n \leq y_{n+1}$ and $Y_n \geq Y_{n+1}$

$$L_1\mathcal{T}_1 y_n = L_1 y_{n+1} = \phi^2 f(x, y_n) \quad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta\mathcal{Sh})\mathcal{T}_2 Y_n = (L_2 - \zeta\mathcal{Sh})Y_{n+1} = -\zeta\mathcal{Sh}\, y_{n+1} \quad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) \quad \text{at } x = 1 \text{ for } 0 \leq z \leq 1,$$

$$\frac{\partial y_{n+1}}{\partial v} = 0 \quad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1,$$

$$Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+1}}{dz} = 1 \quad \text{at } z = 0,$$

$$\frac{dY_{n+1}}{dz} = 0 \quad \text{at } z = 1.$$

and

$$L_1\mathcal{T}_1 y_{n+1} = L_1 y_{n+2} = \phi^2 f(x, y_{n+1}) \quad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$(L_2 - \zeta\mathcal{Sh})\mathcal{T}_2 Y_{n+1} = (L_2 - \zeta\mathcal{Sh})Y_{n+2} = -\zeta\mathcal{Sh}\, y_{n+2} \quad \text{in } 0 < z < 1,\ x = 1,$$

$$y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v} = Y_{n+1}(z) \quad \text{at } x = 1 \text{ for } 0 \leq z \leq 1,$$

$$\frac{\partial y_{n+2}}{\partial v} = 0 \quad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1,$$

$$Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+2}}{dz} = 1 \quad \text{at } z = 0,$$

$$\frac{dY_{n+2}}{dz} = 0 \quad \text{at } z = 1.$$

Therefore,

$$L_1(\mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n) = \phi^2 f(x, y_{n+1}) - \phi^2 f(x, y_n) \geq 0 \quad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.3.53}$$

$$(L_2 - \zeta\mathcal{Sh})(\mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n) = -\zeta\mathcal{Sh}(y_{n+2} - y_{n+1}) \quad \text{in } 0 < z < 1,\ x = 1, \tag{6.3.54}$$

$$[y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v}] - [y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v}] = Y_{n+1}(z) - Y_n(z) \leq 0 \quad \text{at } x = 1 \text{ for } 0 \leq z \leq 1, \tag{6.3.55}$$

$$\frac{\partial y_{n+2}}{\partial v} - \frac{\partial y_{n+1}}{\partial v} = 0 \geq 0, \quad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1, \tag{6.3.56}$$

$$[Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+2}}{dz}] - [Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+1}}{dz}] = 1 - 1 = 0 \leq 0 \quad \text{at } z = 0, \tag{6.3.57}$$

$$\frac{dY_{n+2}}{dz} - \frac{dY_{n+1}}{dz} = 0 \leq 0 \quad \text{at } z = 1. \tag{6.3.58}$$

Therefore, we have the problem

$$L_1 w \geq 0 \quad \text{in } \alpha < x < 1,\ 0 < z < 1,$$

$$B_1 w \leq 0 \quad \text{on } x = \alpha,\ x = 1,$$

where,

$$w = \mathscr{T}_1 y_{n+1} - \mathscr{T}_1 y_n$$

and by the strong maximum principle, $w < 0$ in $\alpha < x < 1$. This implies that the right hand side of (6.3.54) is positive so that

$$L_2 W \geq 0 \qquad \text{in } 0 < z < 1, x = 1,$$

$$B_2 W \leq 0, \qquad \text{on } z = 0, z = 1$$

where,

$$W = \mathscr{T}_2 Y_{n+1} - \mathscr{T}_2 Y_n.$$

By the strong maximum principle, $W < 0$ in $0 < z < 1$. Therefore, $y_n \geq y_{n+1}$ and $Y_n \leq Y_{n+1}$ implies $\mathscr{T}_1 y_n < \mathscr{T}_1 y_{n+1}$ and $\mathscr{T}_2 Y_n < \mathscr{T}_2 Y_{n+1}$. It can similarly be shown that, $y_n \geq y_{n+1}$ and $Y_n \leq Y_{n+1}$ implies $\mathscr{T}_1 y_n > \mathscr{T}_1 y_{n+1}$ and $\mathscr{T}_2 Y_n > \mathscr{T}_2 Y_{n+1}$.

If the nonlinearities $f(x, y)$ have continuous y-derivatives, then we may attempt a further iteration scheme to solve the equations (6.3.1)-(6.3.8). This is known as Newton's method. Under appropriate conditions we will show that the Newton iterates converge monotonically. This convergence is frequently quadratic (KELLER [141]) and hence we expect that the iterates give more accurate approximations to earlier methods discussed in this section. However, as we shall see, the Newton iterates converge either from above (if f_y is increasing in y) or from below (if f_y is decreasing in y). We therefore cannot obtain both monotone increasing and monotone decreasing sequences and therefore upper and lower approximations for the problem (6.3.1)-(6.3.8) as was done in earlier examples.

Assume that f satisfies all previous assumptions and in addition,

$$\frac{\partial f}{\partial y} \geq 0 \tag{6.3.59}$$

and $\dfrac{\partial f}{\partial y}$ is monotone increasing.

Define

$$F[x; y_{n+1}, y_n] \equiv \int_0^1 \frac{\partial f}{\partial y}(x; t y_{n+1} + (1-t) y_n) \mathrm{d}t. \tag{6.3.60}$$

Then it follows that

$$f(x, y_{n+1}) - f(x, y_n) = F[x; y_{n+1}, y_n](y_{n+1} - y_n). \tag{6.3.61}$$

Further, if $y_n \leq y_{n+1}$, then by the above assumptions,

$$\frac{\partial f}{\partial y}(x, y_{n+1}) - F[x; y_{n+1}, y_n] = F[x; y_{n+1}, y_{n+1}] - F[x; y_{n+1}, y_n] \geq 0 \tag{6.3.62}$$

Method 6 (Newton's Method)
We define the (nonlinear) transformations $\mathscr{T}_1$ and $\mathscr{T}_2$ as follows:

$$\mathcal{T}_1:\ y_{n+1} = \mathcal{T}_1 y_n$$

and

$$\mathcal{T}_2:\ Y_{n+1} = \mathcal{T}_2 Y_n$$

if

$$\begin{aligned}
&(L_1 - \frac{\partial f}{\partial y}(x,y_n))y_{n+1} = \phi^2 f(x,y_n) - \frac{\partial f}{\partial y}(x,y_n)y_n && \text{in } \alpha < x < 1,\ 0 < z < 1,\\
&(L_2 - \zeta \mathcal{Sh})Y_{n+1} = -\zeta \mathcal{Sh} y_n && \text{in } 0 < z < 1,\ x = 1,\\
&y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) && \text{at } x = 1 \text{ for } 0 \le z \le 1,\\
&\frac{\partial y_{n+1}}{\partial v} = 0 && \text{at } x = \alpha \text{ for } 0 \le z \le 1,\\
&Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 1 && \text{at } z = 0,\\
&\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 0 && \text{at } z = 1.
\end{aligned}$$

In this method, the equations for Y_{n+1} and y_{n+1} are uncoupled and we show that both $\mathcal{T}_1$ and $\mathcal{T}_2$ are *monotone* in the sense that $y_n \le y_{n+1}$ and $Y_n \le Y_{n+1}$ implies $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$.

We have, if $y_n \le y_{n+1}$ and $Y_n \le Y_{n+1}$

$$\begin{aligned}
&(L_1 - \frac{\partial f}{\partial y}(x,y_n))\mathcal{T}_1 y_n = (L_1 - \frac{\partial f}{\partial y}(x,y_n))y_{n+1} = \phi^2 f(x,y_n) - \frac{\partial f}{\partial y}(x,y_n)y_n && \text{in } \alpha < x < 1,\ 0 < z < 1,\\
&(L_2 - \zeta \mathcal{Sh})\mathcal{T}_2 Y_n = (L_2 - \zeta \mathcal{Sh})Y_{n+1} = -\zeta \mathcal{Sh} y_n && \text{in } 0 < z < 1,\ x = 1,\\
&y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v} = Y_n(z) && \text{at } x = 1 \text{ for } 0 \le z \le 1,\\
&\frac{\partial y_{n+1}}{\partial v} = 0 && \text{at } x = \alpha \text{ for } 0 \le z \le 1,\\
&Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 1 && \text{at } z = 0,\\
&\frac{\mathrm{d}Y_{n+1}}{\mathrm{dz}} = 0 && \text{at } z = 1.
\end{aligned}$$

and

$$\begin{aligned}
&(L_1 - \frac{\partial f}{\partial y}(x,y_{n+1}))\mathcal{T}_1 y_{n+1} = (L_1 - \frac{\partial f}{\partial y}(x,y_{n+1}))y_{n+2} = \phi^2 f(x,y_{n+1}) - \frac{\partial f}{\partial y}(x,y_{n+1})y_{n+1} && \text{in } \alpha<x<1,\ 0<z<1,\\
&(L_2 - \zeta \mathcal{Sh})\mathcal{T}_2 Y_{n+1} = (L_2 - \zeta \mathcal{Sh})Y_{n+2} = -\zeta \mathcal{Sh} y_{n+1} && \text{in } 0 < z < 1,\ x = 1,\\
&y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v} = Y_{n+1}(z) && \text{at } x = 1 \text{ for } 0 \le z \le 1,\\
&\frac{\partial y_{n+2}}{\partial v} = 0 && \text{at } x = \alpha \text{ for } 0 \le z \le 1,\\
&Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{\mathrm{d}Y_{n+2}}{\mathrm{dz}} = 1 && \text{at } z = 0,\\
&\frac{\mathrm{d}Y_{n+2}}{\mathrm{dz}} = 0 && \text{at } z = 1.
\end{aligned}$$

Therefore,

$$(L_1 - \frac{\partial f}{\partial y}(x,y_{n+1}))(\mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n) = \phi^2 f(x,y_{n+1}) - \phi^2 f(x,y_n) - \frac{\partial f}{\partial y}(x,y_n)(y_{n+1} - y_n))$$
$$= [\phi^2 F[x;y_{n+1},y_n] - \frac{\partial f}{\partial y}(x,y_{n+1})](y_{n+1} - y_n)$$
$$= \phi^2 F[x;y_{n+1},y_n] - \phi^2 F[x;y_{n+1},y_{n+1}] \leq 0 \text{ in } \alpha < x < 1, 0 < z < 1, \tag{6.3.63}$$

$$(L_2 - \zeta\mathcal{Sh})(\mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n) = -\zeta\mathcal{Sh}(y_{n+1} - y_n) \leq 0 \qquad \text{in } 0 < z < 1, x = 1, \tag{6.3.64}$$

$$[y_{n+2} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+2}}{\partial v}] - [y_{n+1} + \frac{1}{\mathcal{Sh}}\frac{\partial y_{n+1}}{\partial v}] = Y_{n+1}(z) - Y_n(z) \geq 0 \qquad \text{at } x = 1 \text{ for } 0 \leq z \leq 1, \tag{6.3.65}$$

$$\frac{\partial y_{n+2}}{\partial v} - \frac{\partial y_{n+1}}{\partial v} = 0 \geq 0, \qquad \text{at } x = \alpha \text{ for } 0 \leq z \leq 1, \tag{6.3.66}$$

$$[Y_{n+2} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+2}}{dz}] - [Y_{n+1} - \frac{1}{\mathcal{Pe}}\frac{dY_{n+1}}{dz}] = 1 - 1 = 0 \geq 0 \qquad \text{at } z = 0, \tag{6.3.67}$$

$$\frac{dY_{n+2}}{dz} - \frac{dY_{n+1}}{dz} = 0 \geq 0 \qquad \text{at } z = 1. \tag{6.3.68}$$

Therefore, we have the problem

$$\begin{aligned} L_1 w &\leq 0 && \text{in } \alpha < x < 1, 0 < z < 1, \\ L_2 W &\leq 0 && \text{in } 0 < z < 1, x = 1, \\ B_1 w &\geq 0 && \text{on } x = \alpha, x = 1, \\ B_2 W &\geq 0, && \text{on } z = 0, z = 1 \end{aligned}$$

where,

$$w = \mathcal{T}_1 y_{n+1} - \mathcal{T}_1 y_n \text{ and } W = \mathcal{T}_2 Y_{n+1} - \mathcal{T}_2 Y_n \, .$$

By the strong maximum principle, $w > 0$ in $\alpha < x < 1$ and $W > 0$ in $0 < z < 1$. (unless w, $W \equiv 0$ in which case $\mathcal{T}_1 y_{n+1} = \mathcal{T}_1 y_n$ and $\mathcal{T}_2 Y_{n+1} = \mathcal{T}_2 Y_n$ and the right hand sides of (6.3.63) and (6.3.64) are identically zero; but this happens only if $y_n \equiv y_{n+1}$ and $Y_n \equiv Y_{n+1}$, since F is strictly monotonic, so $\mathcal{T}_1 y_n < \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n < \mathcal{T}_2 Y_{n+1}$). It can similarly be shown that $y_n \geq y_{n+1}$ and $Y_n \geq Y_{n+1}$ implies $\mathcal{T}_1 y_n > \mathcal{T}_1 y_{n+1}$ and $\mathcal{T}_2 Y_n > \mathcal{T}_2 Y_{n+1}$. However, to show this we need to assume that f satisfies all previous assumptions, but $\frac{\partial f}{\partial y}$ is now monotone decreasing instead of increasing as in (6.3.59). Define, as before

$$F[x;y_{n+1},y_n] \equiv \int_0^1 \frac{\partial f}{\partial y}(x;ty_{n+1} + (1-t)y_n)dt. \tag{6.3.69}$$

Then it follows that

$$f(x,y_{n+1}) - f(x,y_n) = F[x;y_{n+1},y_n](y_{n+1} - y_n). \tag{6.3.70}$$

Further, if $y_n \geq y_{n+1}$, then by the above assumptions,

$$\frac{\partial f}{\partial y}(x,y_{n+1}) - F[x;y_{n+1},y_n] = F[x;y_{n+1},y_{n+1}] - F[x;y_{n+1},y_n] \leq 0 \tag{6.3.71}$$

The proof follows exactly, with some reversals of inequalities.

The monotone iterative methods discussed in this section have applications in constructive existence proofs. Iteration schemes are used and yield monotone convergence to the maximal solution from above, to the minimal solution from below or both for some unique solutions. Newton's method may be shown to converge from above or below to a unique solution (the uniqueness is guaranteed from the monotone property of f and applying the maximum principle). Newton's method can be shown to converge quadratically (KELLER [141]). However some additional continuity properties are needed. In our case f_y is required to be Lipschitz continuous in x.

To see how these montone iterations are useful in a constructive existence proof let us consider Method 1 and define

$$\underline{y}_1=\mathcal{T}_1\underline{y}_0,\ \underline{Y}_1=\mathcal{T}_2\underline{Y}_0,\ \bar{y}_1=\mathcal{T}_1\bar{y}_0,\ \bar{Y}_1=\mathcal{T}_2\bar{Y}_0 \tag{6.3.72}$$

where

$$\underline{y}_0=\underset{\sim}{y},\ \underline{Y}_0=\underset{\sim}{Y},\ \bar{y}_0=\tilde{y} \text{ and } \bar{Y}_0=\tilde{Y}. \tag{6.3.73}$$

We show that the following strict inequalities hold

$$\underline{Y}_1>\underline{Y}_0,\ \bar{Y}_1<\bar{Y}_0,\ \underline{y}_1>\underline{y}_0 \text{ and } \bar{y}_1<\bar{y}_0. \tag{6.3.74}$$

We have

$$(L_1-m)\underline{y}_1=\phi^2 f(x,\underline{y}_0)-m\underline{y}_0 \qquad \text{in } \alpha<x<1,\ 0<z<1,$$

$$(L_2-M)\underline{Y}_1=\zeta\mathcal{S}h(\underline{Y}_0-\underline{y}_0)-M\underline{Y}_0 \qquad \text{in } 0<z<1,\ x=1,$$

$$\underline{y}_1+\frac{1}{\mathcal{S}h}\frac{\partial\underline{y}_1}{\partial v}=\underline{Y}_0(z) \qquad \text{at } x=1 \text{ for } 0\le z\le 1,$$

$$\frac{\partial\underline{y}_1}{\partial v}=0 \qquad \text{at } x=\alpha \text{ for } 0\le z\le 1,$$

$$\underline{Y}_1-\frac{1}{\mathcal{P}e}\frac{\mathrm{d}\underline{Y}_1}{\mathrm{d}z}=1 \qquad \text{at } z=0,$$

$$\frac{\mathrm{d}\underline{Y}_1}{\mathrm{d}z}=0 \qquad \text{at } z=1.$$

So

$$(L_1-m)(\underline{y}_1-\underline{y}_0)=\phi^2 f(x,\underline{y}_0)-m\underline{y}_0-L_1\underline{y}_0+m\underline{y}_0=\phi^2 f(x,\underset{\sim}{y})-L_1\underset{\sim}{y}\le 0 \text{ in } \alpha<x<1,\ 0<z<1,$$

$$(L_2-M)(\underline{Y}_1-\underline{Y}_0)=\zeta\mathcal{S}h(\underline{Y}_0-\underline{y}_0)-M\underline{Y}_0-L_2\underline{Y}_0+M\underline{Y}_0=\zeta\mathcal{S}h(\underset{\sim}{Y}-\underset{\sim}{y})-L_2\underset{\sim}{Y}\le 0 \text{ in } 0<z<1,\ x=1,$$

$$[\underline{y}_1+\frac{1}{\mathcal{S}h}\frac{\partial\underline{y}_1}{\partial v}]-[\underline{y}_0+\frac{1}{\mathcal{S}h}\frac{\partial\underline{y}_0}{\partial v}]=\underline{Y}_0(z)-\underset{\sim}{Y}\ge 0 \qquad \text{at } x=1 \text{ for } 0\le z\le 1,$$

$$\frac{\partial\underline{y}_1}{\partial v}-\frac{\partial\underline{y}_0}{\partial v}\ge 0 \qquad \text{at } x=\alpha \text{ for } 0\le z\le 1,$$

$$[\underline{Y}_1-\frac{1}{\mathcal{P}e}\frac{\mathrm{d}\underline{Y}_1}{\mathrm{d}z}]-[\underline{Y}_0-\frac{1}{\mathcal{P}e}\frac{\mathrm{d}\underline{Y}_0}{\mathrm{d}z}]\ge 0 \qquad \text{at } z=0,$$

$$\frac{\mathrm{d}\underline{Y}_1}{\mathrm{d}z}-\frac{\mathrm{d}\underline{Y}_0}{\mathrm{d}z}\ge 0 \qquad \text{at } z=1.$$

Therefore, by the strong maximum principle, $\underline{y}_1 > \underline{y}_0$ and $\underline{Y}_1 > \underline{Y}_0$. (Assume that $L_1\underline{y}_0 \not\equiv \phi^2 f(x,\underline{y}_0)$ and $L_2\underline{Y}_0 \not\equiv \zeta\mathcal{Sh}(\underline{Y}_0 - \underline{y}_0)$). A similar argument holds if we have to show that $\bar{y}_1 < \bar{y}_0$ and $\bar{Y}_1 < \bar{Y}_0$.

Now define $\underline{y}_2 = \mathcal{T}_1\underline{y}_1, \underline{Y}_2 = \mathcal{T}_2\underline{Y}_2$. Then $\underline{Y}_1 > \underline{Y}_0$ and $\underline{y}_1 > \underline{y}_0$ implies that $\underline{y}_2 = \mathcal{T}_1\underline{y}_1 > \mathcal{T}_1\underline{y}_0 = \underline{y}_1$ and $\underline{Y}_2 = \mathcal{T}_2\underline{Y}_1 > \mathcal{T}_2\underline{Y}_0 = \underline{Y}_1$. By induction, the sequences defined by $\underline{y}_1 = \mathcal{T}_1\underline{y}_0$, $\underline{y}_n = \mathcal{T}_1\underline{y}_{n-1}$ and $\underline{Y}_1 = \mathcal{T}_2\underline{Y}_0$, $\underline{Y}_n = \mathcal{T}_2\underline{Y}_{n-1}$ are monotone increasing. Similarly, the sequences defined by $\bar{y}_1 = \mathcal{T}_1\bar{y}_0$, $\bar{y}_n = \mathcal{T}_1\bar{y}_{n-1}$ and $\bar{Y}_1 = \mathcal{T}_2\bar{Y}_0$, $\bar{Y}_n = \mathcal{T}_2\bar{Y}_{n-1}$ defines monotone increasing sequences.

Furthermore, we have $\underline{y}_n < \bar{y}_n$ and $\underline{Y}_n < \bar{Y}_n$ for all n:

$$\underline{y}_0 < \underline{y}_1 < \underline{y}_2 < \ldots \underline{y}_{n-1} < \underline{y}_n < \ldots < \bar{y}_n < \bar{y}_{n-1} < \ldots < \bar{y}_1 < \bar{y}_0$$

$$\underline{Y}_0 < \underline{Y}_1 < \underline{Y}_2 < \ldots \underline{Y}_{n-1} < \underline{Y}_n < \ldots < \bar{Y}_n < \bar{Y}_{n-1} < \ldots < \bar{Y}_1 < \bar{Y}_0$$

In fact, $\underline{y}_0 < \bar{y}_0$ and $\underline{Y}_0 < \bar{Y}_0$; suppose that $\underline{y}_{n-1} < \bar{y}_{n-1}$ and $\underline{Y}_{n-1} < \bar{Y}_{n-1}$. Then $\underline{y}_n = \mathcal{T}_1\underline{y}_{n-1} < \mathcal{T}_1\bar{y}_{n-1} = \bar{y}_n$ and $\underline{Y}_n = \mathcal{T}_2\underline{Y}_{n-1} < \mathcal{T}_2\bar{Y}_{n-1} = \bar{Y}_n$, so the proof follows from induction.

Since the sequences $\{\underline{y}_k\}$, $\{\underline{Y}_k\}$, $\{\bar{y}_k\}$ and $\{\bar{Y}_k\}$ are monotone and uniformly bounded, the pointwise limits

$$\underline{y}(x,z) = \lim_{k\to\infty} \underline{y}_k(x,z), \quad \bar{y}(x,z) = \lim_{k\to\infty} \bar{y}_k(x,z) \tag{6.3.75}$$

$$\underline{Y}(z) = \lim_{k\to\infty} \underline{Y}_k(z), \quad \bar{Y}(z) = \lim_{k\to\infty} \bar{Y}_k(z) \tag{6.3.76}$$

all exist.

To show that the sequences defined above converge uniformly and that the limits above are is in $C^{2+\alpha}$, we may use standard continuity arguments described in Chapter 4. A similar proof holds for all other iterative methods described in this section.

6.3.3 Conclusions and Remarks

The novelty of such problems discussed in this thesis is that the coupling of differential equations in the boundary conditions of the particle model and the mass transfer resistances in a particle is incorporated into the liquid phase balance equations. These equations pose no problems in applying several monotone iteration methods given in literature for scalar elliptic equations.

Such monotone iterative techniques may also useful in numerical computation. We have seen in section 6.1 and section 6.2 that upper and lower solutions are useful in the investigation of qualitive properties of solutions and do prove to be good as approximate solutions. These upper and lower solutions can be computationally improved by such monotone iteration techniques. These techniques may also be generalised to the general system S_n, B_n and its corresponding steady state system $\hat{S}_n$, $\hat{B}_n$.

We have discussed in section 3.7 how the method of upper and lower solutions for the systems S_n, B_n and its corresponding steady state system $\hat{S}_n$, $\hat{B}_n$ may be extended to a nonlinear finite difference system which is a discrete version of the continuous problems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$. It was noted that solving coupled systems involves solving fewer equations. We would thus expect convergence for the iterative methods given in this section involving solving coupled systems to give a faster rate of convergence.

This section also gives us an idea of conditions that our nonlinear reaction functions have to satisfy in order to obtain monotone sequences, alternating sequences and accelerated monotone sequences and how these results may be generalised to the systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$. We have already studied in section 3.6

some of the properties that our nonlinear functions in the system S_n, B_n have to satisfy in order to get monotone and alternating sequences (see Lemma 3.6.6 and Remark 3.6.6). We have also seen in section 4.3 that such properties also hold for the system $\hat{S}_n$, $\hat{B}_n$ (see Lemma 4.3.6 and Remark 4.3.6). It would be useful to generalise and to study some monotone sequences which give accelerated convergences to the systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ using the methods given in this section. Such a method may be a generalisation of Newton's method to systems of equations and may prove to be computationally useful.

6.4 Uniqueness and Existence Theorems for a Model of an Artificial Kidney

In this section, we shall look at a specific example found in literature (LIN [170]) of a modified urea transfer model for predicting urea removal in a compact artificial kidney. Since the transient behaviour of such models are determined by the steady-state behaviour of resulting equations, this section shall only examine the uniqueness and existence of solutions to the steady-state problem. This problem involves three elliptic equations which are all coupled together in their boundary conditions. The approach taken in proving these theorems differs from the approach discussed in the early part of this thesis and the problem differs slightly as well.

The method used in this section may be generalised to proving existence and uniqueness to the general system S_n, B_n and its corresponding steady state system $\hat{S}_n$, $\hat{B}_n$.

6.4.1 The Artificial Kidney

An artificial kidney is a compact device that is that is worn by a patient and uses a replacement unit for removal of nitrogeneous waste products from the blood. Within this device are micro-encapsulated enzyme particles which consists of a layer of membrane and an inner urease solution. This particle membrane permits the urea to diffuse through and into the urease solution but retains the urease because of the larger urease molecules. Ammonia is generated by the enzymatic conversion of urea and in turn reacts with the ion exchange resins which are suspended in the urease solution. In addition, the urease solution may also contain a small amount of activated carbon for removal of uric acid and creatinine.

We shall develop a generalised model for the artificial kidney. The model applies as well to removal of other toxic uremic molecules, which is also of main concern of the artificial kidney. Many early models (CHANG and POZNANSKY [68], VIETH *et al.* [292]) are mainly concerned with reaction and diffusion only within the micro-encapsulated enzyme particles and are not concerned with what happens outside of these particles. However a few models such as that of LEVINE and LACOURSE [168] examine the performance of the whole artificial kidney. These people also show that an artificial kidney of 10cm long is sufficient to remove 90% of the urea from the bloodstream.

In this work, predictive models for the artificial kidney are developed. This model is similar to that proposed for a fluidised bed biofilm reactor (SHIEH *et al.* [263], PARSHOTAM *et al.* [226]). However, for the present model, the boundary condition for the particles has a correction factor to account for external diffusion within the layer of membrane. This diffusion within the membrane could be quite significant (MCELWAIN [180]). Despite this feature we are still able to obtain uniquness and existence theorems. However, in this section, we shall develop methods for proving uniqueness and existence theorems that differs from earlier methods and appears to be more suitable to this range of problems.

The model is developed by assuming Michaelis-Menten kinetics but for the sake of uniqueness and existence there is no additional difficulty in assuming the general case where micro-encapsulated enzyme particle kinetics are monotone increasing and nonnegative.

6.4.2 The Artificial Kidney Model Formulation

The artificial kidney, the typical schematic is shown in FIG. 6.9, consists of a compact device in which micro-encapsulated enzyme particles (see FIG. 6.10) are in a fluidised state.

The key processes of this system with uniform membrane thickness is:

(i) Urea transport through the artificial kidney.

(ii) diffusion within the microencapsulated urease particle membrane

(iii) reaction-diffusion within a single microencapsulated urease particle

Microencapsulated urease particle-Artificial Kidney Model Development

The mathematical model of the artificial kidney urea conversion process is divided into three submodels. The "Microencapsulated urease particle Model" is concerned with diffusion within the urease solution and urea conversion by the microencapsulated urease particles. The "Microencapsulated urease particle membrane Model" is concerned with diffusion within the urease particle membrane. The "Artificial Kidney Plug Flow Model" is concerned with the hydraulic plug flow transport of urea through the artificial kidney and is external to a microencapsulated urease particle. The three models are coupled by urease particle-bulk liquid boundary conditions to yield an overall model for urea conversion in an the artificial kidney.

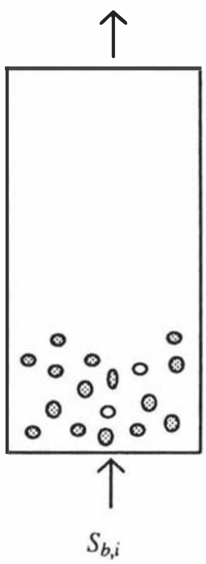


FIG. 6.9 Artificial Kidney

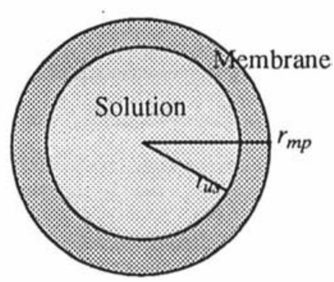


FIG. 6.10 Microencapsulated particle with urease solution

The one dimensional dispersion equation for describing the urea concentration in the blood stream passing through the artificial kidney can be represented by

$$D\frac{d^2S_b}{dZ^2}-u\frac{dS_b}{dZ}-nAk_L(S_b-s_m\big|_{r=r_{mp}}) = 0, \tag{6.4.1}$$

where S_b is the urea concentration in the blood stream passing through the artificial kidney, s_m is the urea concentration in the membrane, D is the dispersion coefficient, u is the velocity of blood flow, n is the number of microencapsulated particles per unit volume of fluid, A is the microencapsulated particle surface area, k_L is the mass transfer coefficient and Z the axial coordinate.

The Reynolds number for the present system is given by

$$\mathcal{Re} = \frac{d_p u \rho}{\mu}, \tag{6.4.2}$$

where d_p is the diameter, ρ is the density and μ is the viscosity of the microencapsulated particle and the Peclét number for this system is given by

$$\mathcal{Pe} = \frac{ul}{D}, \tag{6.4.3}$$

with l being the length of the artificial kidney. It is common to neglect the second order differential term in (6.4.1) in the present system since the Peclét number for this system is often quite high (LEVENSPIEL [166, p.275], LIN [170], SHIEH *et al.* [263]). However, we shall include this term in our model equations as there is no additional difficulty for the purposes of uniqueness and existence theorems.

The urea distribution profiles in both membrane and solution phases are expected to be different because of different urea diffusion coefficients in these phases. Therefore, the urea balance in both phases can be expressed as

$$D_m\left(\frac{\partial^2 s_m}{\partial r^2}+\frac{2}{r}\frac{\partial s_m}{\partial r}\right)=0, \tag{6.4.4}$$

$$D_s\left(\frac{\partial^2 s}{\partial r^2}+\frac{2}{r}\frac{\partial s}{\partial r}\right)=\frac{V_m s}{s+k_m}, \tag{6.4.5}$$

where s_m is the urea concentration in the membrane and s is the urea concentration in the urease solution, D_m and D_s are the corresponding urea diffusion coefficients, V_m is the maximum reaction rate, k_m is the Michaelis constant and r is the radial coordinates.

The boundary conditions are given by

$$\frac{\mathrm{d}S_b}{\mathrm{d}Z}=0 \qquad \text{at } Z = l, \tag{6.4.6}$$

$$D\frac{\mathrm{d}S_b}{\mathrm{d}Z}=u(S_b-S_{b,i}) \qquad \text{at } Z = 0, \tag{6.4.7}$$

$$D_m\frac{\partial s_m}{\partial r}=D_s\frac{\partial s}{\partial r},\ s_m = Hs \qquad \text{at } r = r_{us}, \tag{6.4.8}$$

$$D_m\frac{\partial s_m}{\partial r}=k_L(S_b-s_m) \qquad \text{at } r = r_{mp}, \tag{6.4.9}$$

where H is the partition coefficient between the membrane and the urease solution.

In dimensionless form, the equations (6.4.1) and (6.4.4)-(6.4.9) take the following form

$$\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial y_m}{\partial x}\right) = 0 \qquad \text{in } \alpha < x < 1,\ 0 < z < 1, \tag{6.4.10}$$

$$\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial y}{\partial x}\right) = \phi^2\frac{y}{1+\beta y} \qquad \text{in } 0 < x < \alpha,\ 0 < z < 1, \tag{6.4.11}$$

$$\frac{1}{\mathcal{P}e}\frac{\mathrm{d}^2Y}{\mathrm{d}z^2}-\frac{\mathrm{d}Y}{\mathrm{d}z} = \zeta\mathcal{S}h(Y-y_m) \qquad \text{in } 0 < z < 1,\ x = 1, \tag{6.4.12}$$

$$\frac{\partial y_m}{\partial x} = \gamma\frac{\partial y}{\partial x},\ \ y_m = Hy \qquad \text{in } 0 < z < 1,\ x = \alpha, \tag{6.4.13}$$

$$y_m + \frac{1}{\mathcal{S}h}\frac{\partial y_m}{\partial v} = Y(z) \qquad \text{at } x = 1 \text{ for } 0 < z < 1, \tag{6.4.14}$$

$$\frac{\partial y}{\partial v} = 0 \qquad \text{at } x = 0 \text{ for } 0 < z < 1, \tag{6.4.15}$$

$$Y-\frac{1}{\mathcal{P}e}\frac{\mathrm{d}Y}{\mathrm{d}z}=1 \qquad \text{at } z=0, \tag{6.4.16}$$

$$\frac{\mathrm{d}Y}{\mathrm{d}z}=0 \qquad \text{at } z=1, \tag{6.4.17}$$

at steady-state the equations, where the dimensionless variables are

$$x=\frac{r}{r_{mp}},\ y=\frac{s}{S_{b,i}},\ y_m=\frac{s_m}{S_{b,i}},\ Y=\frac{S_b}{S_{b,i}},\ z=\frac{Z}{h} \tag{6.4.18}$$

and the parameters are

$$\alpha=\frac{r_{us}}{r_{mp}},\ \beta=\frac{S_{b,i}}{k_m},\ \gamma=\frac{D_s}{D_m},\ \phi^2=\frac{V_m r_{bp}^2}{D_s k_m},\ \zeta=\frac{nAD_m l}{u r_{mp}},\ \mathcal{S}h=\frac{k_L r_{mp}}{D_m}\ \text{and}\ \mathcal{P}e=\frac{ul}{D}. \tag{6.4.19}$$

Equation (6.4.10) is linear and can be integrated to give

$$\frac{\mathrm{d}y_m}{\mathrm{d}x}=\frac{c_1}{x^2} \tag{6.4.20}$$

which is further integrated to give

$$y_m=-\frac{c_1}{x}+c_2, \tag{6.4.21}$$

where c_1 and c_2 are constants of integration. Substitution of equations (6.4.10) and (6.4.21) into equation (6.4.14) gives

$$y_m=c_2[1+\frac{\mathcal{S}h}{x(1-\mathcal{S}h)}]-\frac{Y}{x}\frac{\mathcal{S}h}{(1-\mathcal{S}h)}. \tag{6.4.22}$$

The integration constant c_2 can be eliminated by inserting equations (6.4.10) and (6.4.22) into equation (6.4.13) so that

$$\frac{\partial y}{\partial x}=\mathcal{S}h_m(Y-Hy) \qquad \text{at } x=\alpha, \tag{6.4.23}$$

where,

$$\mathcal{S}h_m=\frac{\mathcal{S}h}{\gamma\alpha(\mathcal{S}h+\alpha(1-\mathcal{S}h))}. \tag{6.4.24}$$

From equations (6.4.13) and (6.4.20), we can show that

$$\left.\frac{\partial y_m}{\partial x}\right|_{x=1}=\alpha^2\gamma\left.\frac{\partial y_m}{\partial x}\right|_{x=\alpha}. \tag{6.4.25}$$

Therefore equation (6.4.25) can be substituted into (6.4.14) which is substituted into equation (6.4.13) so that the original set of equations is reduced to the following set of equations

$$\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial y}{\partial x})=\phi^2\frac{y}{1+\beta y} \qquad \text{in } 0<x<\alpha,\ 0<z<1, \tag{6.4.26}$$

$$\frac{1}{\mathcal{P}e}\frac{d^2Y}{dz^2} - \frac{dY}{dz} = \alpha^2\gamma\frac{\partial y}{\partial x}\bigg|_{x=\alpha} \qquad \text{in } 0 < z < 1,\ x = \alpha, \tag{6.4.27}$$

$$\frac{\partial y}{\partial x} = \mathcal{S}h_m(Y - Hy) \qquad \text{at } x = \alpha \text{ for } 0 \le z \le 1, \tag{6.4.28}$$

$$\frac{\partial y}{\partial v} = 0 \qquad \text{at } x = 0 \text{ for } 0 \le z \le 1, \tag{6.4.29}$$

$$Y - \frac{1}{\mathcal{P}e}\frac{dY}{dz} = 1 \qquad \text{at } z = 0, \tag{6.4.30}$$

$$\frac{dY}{dz} = 0 \qquad \text{at } z = 1. \tag{6.4.31}$$

We see that the boundary condition (6.4.28) has a correction factor to account for the external diffusion within the microencapsulated urease particle membrane. We note that this problem reduces to the case discussed in sections 6.2 and 6.3 in the limit as H tends to unity and $\mathcal{S}h_m$ tends to $\mathcal{S}h$.

For purposes of uniqueness and existence, we shall substitute equation (6.4.26) for the more general equation

$$\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial y}{\partial x}) = \phi^2 f(y) \qquad \text{in } 0 < x < \alpha,\ 0 < z < 1, \tag{6.4.32}$$

where the Michaelis-Menten term in (6.4.26) is replaced by an arbitrary function $f(y)$ which is monotone increasing, nonnegative and Lipschitz continuous with respect to y.

6.4.3 Uniqueness and Existence theorems

We have reduced three coupled elliptic equations to two coupled elliptic equations by solving (6.4.10) and have obtained a system similar to that in section 6.2 and section 6.3. The system (6.4.26)-(6.4.32) is nonstandard in the way that (6.4.32) is coupled to (6.4.27) via the boundary condition (6.4.28).

Although it may be observed from well known results (e.g. HILTMAN AND LORY [126]) that for a given a unique $Y(z)$ there exists a unique $y(x, z)$, it cannot be assumed because of the coupled nature of the equations for $y(x, z)$ and $Y(z)$ that $Y(z)$ is in fact unique for a given z. We therefore consider the one-parameter family of solutions, $y_\mu(x)$ where $y_\mu(x)$ is a solution to the microencapsulated urease problem and where μ has captured the z. We shall establish a one-to-one correspondence between $y_\mu(x)$ and $y(x, z)$. In summary, we have the following

$$\forall z \in [0,\ 1],\ \exists\ !\ \mu(z) : y(x, z) = y_\mu(x). \tag{6.4.33}$$

Consider the following o.d.e. that is parametrised by height z

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{dy_\mu}{dx}) = \phi^2 f(y_\mu) \text{ in } 0 < x < \alpha, \tag{6.4.34}$$

with the boundary conditions

$$\frac{dy_\mu}{dx} = 0 \qquad \text{at } x = 0, \tag{6.4.35}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{\mathrm{d}y_\mu}{\mathrm{d}x}+Hy_\mu=\mu \quad \text{at } x=1, \tag{6.4.36}$$

and where $y_\mu(x)$ may be thought of as the family of solutions $y(x)$ with given constant μ and f is monotone increasing, nonnegative and Lipschitz with respect to y_μ with Lipschitz constant K. We have the following comparison results for y_μ.

***Lemma* 6.4.1** (*Comparison Results*)
Let $y_\mu(x)$ denote the solution of (6.4.34)-(6.4.36) *and suppose that two functions $\underline{y}_\mu$ and $\bar{y}_\mu$ can be found so that the differential inequalities*

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}(x^2\frac{\mathrm{d}\bar{y}_\mu}{\mathrm{d}x})\le\phi^2 f(\bar{y}_\mu) \text{ in } 0<x<\alpha, \tag{6.4.37}$$

hold with the boundary conditions

$$\frac{\mathrm{d}\bar{y}_\mu}{\mathrm{d}x}\ge 0 \qquad \text{at } x=0, \tag{6.4.38}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{\mathrm{d}\bar{y}_\mu}{\mathrm{d}x}+H\bar{y}_\mu\ge\mu \quad \text{at } x=\alpha, \tag{6.4.39}$$

and the differential inequalities

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}(x^2\frac{\mathrm{d}\underline{y}_\mu}{\mathrm{d}x})\ge\phi^2 f(\underline{y}_\mu) \text{ in } 0<x<\alpha, \tag{6.4.40}$$

hold with the boundary conditions

$$\frac{\mathrm{d}\underline{y}_\mu}{\mathrm{d}x}\le 0 \qquad \text{at } x=0, \tag{6.4.41}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{\mathrm{d}\underline{y}_\mu}{\mathrm{d}x}+H\underline{y}_\mu\le\mu \quad \text{at } x=\alpha. \tag{6.4.42}$$

Then

$$\underline{y}_\mu\le y_\mu\le\bar{y}_\mu. \tag{6.4.43}$$

Proof
From (6.4.34) and (6.4.37), we have

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}(x^2\frac{\mathrm{d}}{\mathrm{d}x}(\underline{y}_\mu-y_\mu))\ge\phi^2 f(\underline{y}_\mu)-\phi^2 f(y_\mu)\ge m(\underline{y}_\mu-y_\mu) \tag{6.4.44}$$

for $m\ge 0$, since f is monotone increasing. Hence,

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}(x^2\frac{\mathrm{d}}{\mathrm{d}x}(\underline{y}_\mu-y_\mu))-m(\underline{y}_\mu-y_\mu)\ge 0 \tag{6.4.45}$$

From (6.4.35)-(6.4.36) and (6.4.38)-(6.4.39), we have

$$\frac{\mathrm{d}}{\mathrm{d}x}(\underline{y}_{\mu} - y_{\mu}) \leq 0 \qquad \text{at } x = 0, \tag{6.4.46}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{\mathrm{d}}{\mathrm{d}x}(\underline{y}_{\mu} - y_{\mu})) + H(\underline{y}_{\mu} - y_{\mu}) \leq 0 \quad \text{at } x = \alpha, \tag{6.4.47}$$

implying by the maximum principle that

$$\underline{y}_{\mu} - y_{\mu} \leq 0 \text{ or } \underline{y}_{\mu} \leq y_{\mu}. \tag{6.4.48}$$

In the same way from (6.4.34)-(6.4.36) and (6.4.40)-(6.4.42), we find that $y_{\mu} \leq \bar{y}_{\mu}$. Combining these results, we therefore have shown that the upper and lower bounds

$$\underline{y}_{\mu} \leq y_{\mu} \leq \bar{y}_{\mu} \tag{6.4.49}$$

are valid.❑

The equation (6.4.49) is a special case of theorems established for elliptic equations by AMANN [5]. The functions $\underline{y}_{\mu}$ and $\bar{y}_{\mu}$ where $\underline{y}_{\mu} \leq \bar{y}_{\mu}$ are lower and upper functions of (6.4.34)-(6.4.36) respectively and so there exists a solution y_{μ} of (6.4.34)-(6.4.36) where $\underline{y}_{\mu} \leq y_{\mu} \leq \bar{y}_{\mu}$.

Lemma 6.4.1 implies a solution of (6.4.34) which satisfies boundary conditions (6.4.35)-(6.4.36) must be unique for if u and v are solutions, we can let $\underline{y}_{\mu} = u$ and $\bar{y}_{\mu} = v$, to find that $u \equiv v$.

Thus given μ is unique for a given z, then y_{μ} is unique. However, we cannot assume that μ is unique for a given z and for that we shall need the following lemma:

***Lemma* 6.4.2**
$y_{\mu}(x)$ is monotonically increasing in μ and is Lipschitz in μ.

Proof
Consider the equations y_{μ_1} and y_{μ_2} with $\mu_1 \geq \mu_2$ and where y_{μ_1} satisfies the equations

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}(x^2\frac{\mathrm{d}y_{\mu_1}}{\mathrm{d}x}) - \phi^2 f(y_{\mu_1}) = 0 \text{ in } 0 < x < \alpha, \tag{6.4.50}$$

with the boundary conditions

$$\frac{\mathrm{d}y_{\mu_1}}{\mathrm{d}x} = 0 \qquad \text{at } x = 0, \tag{6.4.51}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{\mathrm{d}y_{\mu_1}}{\mathrm{d}x} + Hy_{\mu_1} = \mu_1 \qquad \text{at } x = 1, \tag{6.4.52}$$

and y_{μ_2} satisfies the equation

$$\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}(x^2\frac{\mathrm{d}y_{\mu_2}}{\mathrm{d}x}) - \phi^2 f(y_{\mu_2}) = 0 \text{ in } 0 < x < \alpha, \tag{6.4.53}$$

with the boundary conditions

$$\frac{dy_{\mu_2}}{dx}=0 \qquad \text{at } x = 0, \tag{6.4.54}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{dy_{\mu_2}}{dx}+Hy_{\mu_2}=\mu_2 \qquad \text{at } x = 1. \tag{6.4.55}$$

These equations satisfy the differential inequalities

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{dy_{\mu_1}}{dx})-\phi^2 f(y_{\mu_1})=0\leq 0 \text{ in } 0<x<\alpha, \tag{6.4.56}$$

with the inequalities in the boundary conditions

$$\frac{dy_{\mu_1}}{dx}=0\geq 0 \qquad \text{at } x = 0, \tag{6.4.57}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{dy_{\mu_1}}{dx}+Hy_{\mu_1}=\mu_1\geq\mu_2 \qquad \text{at } x = 1, \tag{6.4.58}$$

and y_{μ_2} satisfies the differential inequalities

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{dy_{\mu_2}}{dx})-\phi^2 f(y_{\mu_2})=0\geq 0 \text{ in } 0<x<\alpha, \tag{6.4.59}$$

with the inequalities in the boundary conditions

$$\frac{dy_{\mu_2}}{dx}=0\leq 0 \qquad \text{at } x = 0, \tag{6.4.60}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{dy_{\mu_2}}{dx}+Hy_{\mu_2}=\mu_2\leq\mu_2 \qquad \text{at } x = 1. \tag{6.4.61}$$

and from Lemma 6.4.1, this implies that

$$y_{\mu_1}\geq y_{\mu_2}. \tag{6.4.62}$$

Hence y_μ is monotonically increasing in μ.

To show that $y_\mu(x)$ is Lipschitz in μ, we need to only consider the case when $\mu_1 \geq \mu_2$.

Let us consider the equations (6.4.50)-(6.4.55) and look at the difference. We then obtain the inequalities

$$\frac{1}{x^2}\frac{d}{dx}(x^2\frac{d}{dx}(y_{\mu_1}-y_{\mu_2}))-\phi^2 f(y_{\mu_1})+\phi^2 f(y_{\mu_2})\leq 0 \text{ in } 0<x<\alpha, \tag{6.4.63}$$

with the inequalities in the boundary conditions

$$\frac{d}{dx}(y_{\mu_1}-y_{\mu_2})=0 \qquad \text{at } x = 0, \tag{6.4.64}$$

$$\frac{1}{\mathcal{Sh}_m}\frac{d}{dx}(y_{\mu_1}-y_{\mu_2})+H(y_{\mu_1}-y_{\mu_2})=\mu_1-\mu_2\geq 0 \quad \text{at } x = 1, \tag{6.4.65}$$

From the maximum principle we see that the maximum value for this problem is at the boundary $x = 1$ and $\mu_1 - \mu_2 \geq 0$ implies $y_{\mu_1} - y_{\mu_2} \geq 0$ so that

$$\|y_{\mu_1} - y_{\mu_2}\| \leq \|\mu_1 - \mu_2\| \tag{6.4.66}$$

Hence $y_\mu(x)$ is Lipschitz in μ with Lipschitz constant $k = 1$.□

Let us define the following function

$$F(\mu) = \phi^2 \int_0^\alpha x^2 f(y_\mu(x))\mathrm{d}x = \alpha^2 \left.\frac{\mathrm{d}y_\mu}{\mathrm{d}x}\right|_{x=\alpha}, \tag{6.4.67}$$

which is obtained from integrating (6.4.32) and applying the boundary conditions (6.4.29).

Lemma 6.4.3
$F(\mu)$ is monotonically increasing in μ and Lipschitz in μ.

Proof
To show that $F(\mu)$ is monotonically increasing in μ, we note that y_μ is monotonically increasing in μ, $f(y_\mu(x))$ is monotonically increasing in y_μ and therefore $F(\mu)$ is monotonically increasing in μ.

To show that $F(\mu)$ is Lipschitz in μ, we note from Lemma 6.4.2 that $y_\mu(x)$ is Lipschitz in μ. Therefore

$$\begin{aligned}
\|F(\mu) - F(\mu^*)\| &= \phi^2 \left\| \int_0^\alpha x^2 f(y_\mu) - x^2 f(y_{\mu^*}) \mathrm{d}x \right\| \\
&= \phi^2 \left\| \int_0^\alpha x^2 (f(y_\mu) - f(y_{\mu^*})) \mathrm{d}x \right\| \\
&\leq \phi^2 \int_0^\alpha \|x^2 (f(y_\mu) - f(y_{\mu^*}))\| \mathrm{d}x \\
&\leq \phi^2 \int_0^\alpha \|(f(y_\mu) - f(y_{\mu^*}))\| \mathrm{d}x \\
&\leq \phi^2 K \int_0^\alpha \|y_\mu - y_{\mu^*}\| \mathrm{d}x \\
&\leq \phi^2 K \int_0^\alpha \|\mu - \mu^*\| \mathrm{d}x \\
&\leq \phi^2 \alpha K \|\mu - \mu^*\|
\end{aligned}$$

and $F(\mu)$ is Lipschitz in μ with Lipschitz constant $k = \phi^2 K\,(1-\alpha)$.□

Consider the following differential equation

$$\frac{1}{\mathcal{P}e}\frac{\mathrm{d}^2\mu}{\mathrm{d}z^2} - \frac{\mathrm{d}\mu}{\mathrm{d}z} = \gamma F(\mu) \qquad \text{in } 0 < z < 1,\ x = \alpha, \tag{6.4.68}$$

with boundary conditions

$$\mu-\frac{1}{\mathcal{P}e}\frac{d\mu}{dz}=1 \qquad \text{at } z=0, \tag{6.4.69}$$

$$\frac{d\mu}{dz}=0 \qquad \text{at } z=1. \tag{6.4.70}$$

$F(\mu)$ is given by (6.4.67).

Lemma 6.4.4
The solution of (6.4.68)-(6.4.70) exists and is unique.

Proof
The existence and uniqueness of solutions follows from applying Theorem 2.6 of AMANN [8] given that $F(\mu)$ is monotonically increasing in μ and is Lipschitz in μ from Lemma 6.4.3. This theorem will also require that upper and lower solutions to (6.4.68)-(6.4.70) exist and these can be constructed from $\underline{y}_\mu$ and $\overline{y}_\mu$ in (6.4.37)-(6.4.42) and using the monotonicity of $F(\mu)$ in (6.4.67).□

The equations (6.4.68)-(6.4.70) are obtained from (6.4.27), (6.4.30)-(6.4.31) and we may no longer treat μ as a parameter. We are now justified in stating that $Y(z)$ is unique for a given $z \in [0, 1]$ and that there exists a unique solution $y(x, z)$ given that $\underline{y}_\mu$ and $\overline{y}_\mu$ are lower and upper solutions respectively and therefore $y_\mu(x)$ in (6.4.34)-(6.4.36) exists and is unique. We have shown that there exists a solution of (6.4.27)-(6.4.32) if there exists a solution of (6.4.34)-(6.4.36) and that there is a one-to-one correspondence between the one-parameter family of solutions, $y_\mu(x)$ and $y(x, z)$. Furthermore standard results (HILTMAN and LORY [126]) may be used in this case to show uniqueness and existence to the system (6.4.26)-(6.4.31).

Conclusions and Remarks
The problem discussed in this section differs somewhat from the problems discussed in section 6.2 and in section 6.3. In this problem there is diffusion within the urease particle membrane. Literature suggests that this diffusion within the particle membrane could be quite significant. This problem involves three elliptic equations which are coupled in their boundary conditions and these equations are reduced to two equations which are coupled in their boundary conditions by solving a diffusion equation within the microencapsulated urease particle membrane.

The method of proving uniquness and existence theorems differs from earlier chapters. In this section we prove uniqueness and existence theorems by establishing a one to one correspondence between urea transport through the artificial kidney and reaction-diffusion within a single microencapsulated urease particle.

This method of proving uniqueness and existence also makes good use of the derivative term in the right hand side of (6.4.27). This term may not be expressed in a linear form by making use of boundary conditions as was done in section 6.2 and in section 6.3 and therefore our definitions of upper and lower solutions in section 6.2 and section 6.3 would not be the same for this problem. However, this method of proving uniquness and existence demonstrated in this section can still be used in proving uniquness and existence for the problems in section 6.2 and in section 6.3 and may be generalised to proving existence and uniqueness to the general system S_n, B_n and its corresponding steady state system $\hat{S}_n$, $\hat{B}_n$. It also provides us with bounding solutions.

Nomenclature

A	The microencapsulated particle surface area - typically 400cm^2
D	The dispersion coefficient, u is the velocity of blood flow -typically $10^{-5}\text{cm}^2\text{sec}^{-1}$
D_m	Urea diffusion coefficients in the membrane
d_p	The diameter of the microencapsulated particle - typically 5×10^{-5}m
D_s	Urea diffusion coefficients in the urease solution
k_L	The mass transfer coefficient
k_m	The Michaelis constant and r is the radial coordinates.
l	The length of the artificial kidney
n	The number of microencapsulated particles per unit volume of fluid - typically 10^5 cm^{-3}
$\mathscr{Pe}$	Peclét number - typically 450 for $l = 10$cm
r_{mp}	microencapsulated particle radius
r_{us}	microencapsulated particle radius with urease solution
$\mathscr{Re}$	Reynolds number - typically 0.05
S	The urea concentration in the blood stream passing through the artificial kidney,
s	The urea concentration in the urease solution
u	The velocity of blood flow - typically 0.1 cm sec^{-1}
V_m	The maximum reaction rate
Z	The axial coordinate.

Greek letters

α	ratio of microencapsulated particle radius to microencapsulated particle radius with urease solution
β	dimensionless Michaelis constant given in (6.4.19)
ϕ^2	Thiele modulus given in (6.4.19)
γ	parameter given in (6.4.19)
μ	The viscoscity of the microencapsulated particle - typically 0.012g cm sec^{-1}
ρ	The density of the microencapsulated particle - typically 1.2g cm^{-3}
ζ	parameter given in (6.4.19)

6.5 A Fluidised Bed Biofilm Reactor (FBBR) Model Involving Multicomponents

In this section, we bring theory into focus by setting out the equations for a tubular fluidised bed biofilm reactor (FBBR) problem of applied interest. The bioparticle reaction kinetics involve three chemical components, a substrate s such as phenol or nitrogenous wastes which needs to be converted to harmless byproducts, oxygen o, an active ingredient which helps facilitate the reaction kinetics and a product p which linearly inhibits the reaction kinetics. The first two components s and o have reaction functions of Michaelis-Menten character. The linear product inhibition term is discussed by LEVENSPIEL [167].

6.5.1 Model Formulation

The equations governing bioparticle kinetics are similar to those given in HOSSAIN [132] where they are expressed in dimensionless terms as follows:

$$\begin{aligned}
&\frac{\partial s}{\partial t} - d_1\nabla_x^2 s = -\phi_1^2 f(s,\, o,\, p)\\
&\frac{\partial o}{\partial t} - d_2\nabla_x^2 o = -\phi_2^2 f(s,\, o,\, p)\\
&\frac{\partial p}{\partial t} - d_3\nabla_x^2 p = \phi_3^2 f(s,\, o,\, p) \text{ in } (0,\, T]\times\Omega\times\Lambda,
\end{aligned} \tag{6.5.1}$$

where

$$f(s,\, o,\, p) = \begin{cases} \dfrac{s}{1+\beta_1 s}\,\dfrac{o}{1+\beta_2 o}(1-p) & \text{if } s,\, o \geq 0,\ p \leq 1 \\ 0 & \text{if } s,\, o < 0,\ p > 1\ , \end{cases} \tag{6.5.2}$$

with boundary conditions

$$\frac{\partial s}{\partial n} = \frac{\partial o}{\partial n} = \frac{\partial p}{\partial n} = 0 \text{ on } (0,\, T]\times\partial\Omega_1\times\Lambda, \tag{6.5.3}$$

$$\frac{\partial s}{\partial n} = \mathcal{Sh}(S-s),\ \frac{\partial o}{\partial n} = \mathcal{Sh}(O-o),\ \frac{\partial p}{\partial n} = \mathcal{Sh}(P-p) \text{ on } (0,\, T]\times\partial\Omega_2\times\Lambda, \tag{6.5.4}$$

and initial conditions

$$s(t,\, x,\, z) = o(t,\, x,\, z) = 1,\ p(t,\, x,\, z) = 0 \text{ in } \Omega\times\Lambda \text{ at } t = 0, \tag{6.5.5}$$

and where Λ is the interval (0, 1). The external or bulk fluid concentrations S, O and P are given by the following equations

$$\begin{aligned}
&\chi\frac{\partial S}{\partial t} - \frac{1}{\mathcal{Pe}}\frac{\partial^2 S}{\partial z^2} + \frac{\partial S}{\partial z} + \xi_1\int_{\partial\Omega_2}\frac{\partial s}{\partial n} = 0\\
&\chi\frac{\partial O}{\partial t} - \frac{1}{\mathcal{Pe}}\frac{\partial^2 O}{\partial z^2} + \frac{\partial O}{\partial z} + \xi_2\int_{\partial\Omega_2}\frac{\partial o}{\partial n} = 0\\
&\chi\frac{\partial P}{\partial t} - \frac{1}{\mathcal{Pe}}\frac{\partial^2 P}{\partial z^2} + \frac{\partial P}{\partial z} + \xi_3\int_{\partial\Omega_2}\frac{\partial p}{\partial n} = 0 \text{ in } (0,\, T]\times\Lambda,
\end{aligned} \tag{6.5.6}$$

with boundary conditions

$$S-\frac{1}{\mathcal{P}e}\frac{\partial S}{\partial z}=1,\ O-\frac{1}{\mathcal{P}e}\frac{\partial O}{\partial z}=1,\ P-\frac{1}{\mathcal{P}e}\frac{\partial P}{\partial z}=0 \text{ at } z=0,\ t>0, \tag{6.5.7}$$

$$\frac{\partial S}{\partial z}=\frac{\partial O}{\partial z}=\frac{\partial P}{\partial z}=0 \text{ at } z=1,\ t>0, \tag{6.5.8}$$

and initial conditions

$$S(t,z)=O(t,z)=1,\ P(t,z)=0 \text{ in } \Lambda \text{ at } t=0. \tag{6.5.9}$$

We see that $f(s, o, p)$ is monotone increasing in s and o and monotone decreasing in p. Therefore, in (6.5.1), $-\phi_1^2 f(s, o, p)$ and $-\phi_2^2 f(s, o, p)$ are monotone decreasing in s and o and monotone increasing in p and $\phi_3^2 f(s, o, p)$ is monotone increasing in s and o and monotone decreasing in p.

By letting $c_1 = s$, $C_1 = S$, $c_2 = o$, $C_2 = O$, $c_3 = 1-p$ and $C_3 = 1-P$, the associated concentrations c_1, c_2, c_3, C_1, C_2, C_3 in f_i and F_i are given by

$$f_i(c_1, c_2, c_3)=\begin{cases}-\phi_i^2\dfrac{c_1c_2c_3}{(1+\beta_1c_1)(1+\beta_2c_2)} & \text{for } c_1,\ c_2\geq 0,\ c_3\leq 1\\ 0 & \text{for } c_1,\ c_2,\ c_3<0\\ -\phi_i^2\dfrac{c_1c_2}{(1+\beta_1c_1)(1+\beta_2c_2)} & \text{for } c_3\geq 1, \text{ where } i\neq 3\\ 0 & \text{for } c_3<0, \text{ where } i=3,\end{cases} \tag{6.5.10}$$

where f_i is monotone decreasing with respect to c_1, c_2 and c_3. Also, we see that

$$F_i(C_1,C_2,C_3)\equiv 0. \tag{6.5.11}$$

In dimensionless terms, the bioreactor model equations for $t > 0$ are

$$\frac{\partial c_i}{\partial t}-d_i\nabla_x^2 c_i=f_i(c_j) \text{ in } (0,T]\times\Omega\times\Lambda, \tag{6.5.12}$$

$$\frac{\partial c_i}{\partial n}=0 \text{ on } (0,T]\times\partial\Omega_1\times\Lambda, \tag{6.5.13}$$

$$\frac{\partial c_i}{\partial n}=\mathcal{S}h(C_i-c_i) \text{ on } (0,T]\times\partial\Omega_2\times\Lambda, \tag{6.5.14}$$

$$\chi\frac{\partial C_i}{\partial t}-\frac{1}{\mathcal{P}e}\frac{\partial^2 C_i}{\partial z^2}+\frac{\partial C_i}{\partial z}+\xi_i\int_{\partial\Omega_2}\frac{\partial c_i}{\partial n}=0 \text{ in } (0,T]\times\Lambda, \tag{6.5.15}$$

$$C_i-\frac{1}{\mathcal{P}e}\frac{\partial C_i}{\partial z}=1 \text{ at } z=0,\ t>0, \tag{6.5.16}$$

$$\frac{\partial C_i}{\partial z}=0 \text{ at } z=1,\ t>0, \tag{6.5.17}$$

$$c_i(t,x,z)=1 \text{ in } \Omega\times\Lambda \text{ at } t=0, \tag{6.5.18}$$

$$C_i(t,z)=1 \text{ in } \Lambda \text{ at } t=0. \tag{6.5.19}$$

6.5.2 Uniqueness, Existence and Stability

We study the stability, uniqueness and existence of solutions of this system by following the path outlined in Chapters 3-4. The comparison functions for $c_1, c_2 \geq 0, c_3 \leq 1$ are:

$$\frac{\partial \underline{c}_1}{\partial t} - d_1 \nabla_x^2 \underline{c}_1 \leq \underline{f}_1(\underline{c}_1, \bar{c}_2, \bar{c}_3) = -\phi_1^2 \frac{\underline{c}_1 \bar{c}_2 \bar{c}_3}{(1+\beta_1 \underline{c}_1)(1+\beta_2 \bar{c}_2)}$$

$$\frac{\partial \bar{c}_1}{\partial t} - d_1 \nabla_x^2 \bar{c}_1 \geq \bar{f}_1(\bar{c}_1, \underline{c}_2, \underline{c}_3) = -\phi_1^2 \frac{\bar{c}_1 \underline{c}_2 \underline{c}_3}{(1+\beta_1 \bar{c}_1)(1+\beta_2 \underline{c}_2)}$$

$$\frac{\partial \underline{c}_2}{\partial t} - d_2 \nabla_x^2 \underline{c}_2 \leq \underline{f}_2(\bar{c}_1, \underline{c}_2, \bar{c}_3) = -\phi_2^2 \frac{\bar{c}_1 \underline{c}_2 \bar{c}_3}{(1+\beta_1 \bar{c}_1)(1+\beta_2 \underline{c}_2)}$$

$$\frac{\partial \bar{c}_2}{\partial t} - d_2 \nabla_x^2 \bar{c}_2 \geq \bar{f}_2(\underline{c}_1, \bar{c}_2, \underline{c}_3) = -\phi_2^2 \frac{\underline{c}_1 \bar{c}_2 \underline{c}_3}{(1+\beta_1 \underline{c}_1)(1+\beta_2 \bar{c}_2)}$$

$$\frac{\partial \underline{c}_3}{\partial t} - d_3 \nabla_x^2 \underline{c}_3 \leq \underline{f}_3(\bar{c}_1, \bar{c}_2, \underline{c}_3) = -\phi_3^2 \frac{\bar{c}_1 \bar{c}_2 \underline{c}_3}{(1+\beta_1 \bar{c}_1)(1+\beta_2 \bar{c}_2)}$$

$$\frac{\partial \bar{c}_3}{\partial t} - d_3 \nabla_x^2 \bar{c}_3 \geq \bar{f}_3(\underline{c}_1, \underline{c}_2, \bar{c}_3) = -\phi_3^2 \frac{\underline{c}_1 \underline{c}_2 \bar{c}_3}{(1+\beta_1 \underline{c}_1)(1+\beta_2 \underline{c}_2)}$$

with the following inequalities in the boundary conditions

$$\frac{\partial \underline{c}_i}{\partial n} \leq 0, \quad \frac{\partial \bar{c}_i}{\partial n} \geq 0 \text{ on } (0, T] \times \partial\Omega_1 \times \Lambda,$$

$$\frac{\partial \underline{c}_i}{\partial n} \leq \mathcal{S}h(\underline{C}_i - \underline{c}_i), \quad \frac{\partial \bar{c}_i}{\partial n} \geq \mathcal{S}h(\bar{C}_i - \bar{c}_i) \text{ on } (0, T] \times \partial\Omega_2 \times \Lambda,$$

and the following inequalities in the initial conditions

$$\underline{c}_i(t, x, z) \leq 1, \quad \bar{c}_i(t, x, z) \geq 1 \text{ in } \Omega \times \Lambda \text{ at } t = 0.$$

Note that $\underline{c}_i$ are uncoupled from $\bar{c}_i$ for each $i = 1, 2, 3$. The comparison functions for C_1, C_2, C_3 are:

$$\chi \frac{\partial \underline{C}_1}{\partial t} - \frac{1}{\mathcal{P}e} \frac{\partial^2 \underline{C}_1}{\partial z^2} + \frac{\partial \underline{C}_1}{\partial z} + \xi_1 \int_{\partial\Omega_2} \frac{\partial \underline{c}_1}{\partial n} \leq 0$$

$$\chi \frac{\partial \bar{C}_1}{\partial t} - \frac{1}{\mathcal{P}e} \frac{\partial^2 \bar{C}_1}{\partial z^2} + \frac{\partial \bar{C}_1}{\partial z} + \xi_1 \int_{\partial\Omega_2} \frac{\partial \bar{c}_1}{\partial n} \geq 0$$

$$\chi \frac{\partial \underline{C}_2}{\partial t} - \frac{1}{\mathcal{P}e} \frac{\partial^2 \underline{C}_2}{\partial z^2} + \frac{\partial \underline{C}_2}{\partial z} + \xi_2 \int_{\partial\Omega_2} \frac{\partial \underline{c}_2}{\partial n} \leq 0$$

$$\chi \frac{\partial \bar{C}_2}{\partial t} - \frac{1}{\mathcal{P}e} \frac{\partial^2 \bar{C}_2}{\partial z^2} + \frac{\partial \bar{C}_2}{\partial z} + \xi_2 \int_{\partial\Omega_2} \frac{\partial \bar{c}_2}{\partial n} \geq 0$$

$$\chi \frac{\partial \underline{C}_3}{\partial t} - \frac{1}{\mathcal{P}e} \frac{\partial^2 \underline{C}_3}{\partial z^2} + \frac{\partial \underline{C}_3}{\partial z} + \xi_3 \int_{\partial\Omega_2} \frac{\partial \underline{c}_3}{\partial n} \leq 0$$

$$\chi \frac{\partial \bar{C}_3}{\partial t} - \frac{1}{\mathcal{P}e} \frac{\partial^2 \bar{C}_3}{\partial z^2} + \frac{\partial \bar{C}_3}{\partial z} + \xi_3 \int_{\partial\Omega_2} \frac{\partial \bar{c}_3}{\partial n} \geq 0$$

with the following inequalities in the boundary conditions

$$\underline{C}_i - \frac{1}{\mathcal{P}e}\frac{\partial \underline{C}_i}{\partial z} \leq 1,\ \overline{C}_i - \frac{1}{\mathcal{P}e}\frac{\partial \overline{C}_i}{\partial z} \geq 1 \text{ at } z = 0,\ t > 0,$$

$$\frac{\partial \underline{C}_i}{\partial z} \leq 0,\ \frac{\partial \overline{C}_i}{\partial z} \geq 0 \text{ at } z = 1,\ t > 0,$$

and the following inequalities in the initial conditions

$$\underline{C}_i(t,\ z) \leq 1,\ \overline{C}_i(t,\ z) \geq 1 \text{ in } \Lambda \text{ at } t = 0,$$

for all $i = 1, 2, 3$. Note that these equations are all uncoupled.

From Theorem 3.2.12 (Generalised Strong Comparison Theorem) we see that for $i = 1,2,3$, $\underline{c}_i = \underline{C}_i = 0$ are lower solutions and $\overline{c}_i = \overline{C}_i = K_i \geq 1$ are upper solutions for constants K_i so that $\underline{c}_i = \underline{C}_i = 0$ and $\overline{c}_i = \overline{C}_i = K_i \geq 1$ on $\partial\Lambda_1$ provide bounds for c_i and C_i since the functions f_i are negative.

Moreover, $\underline{c}_i = \underline{C}_i = 0$ and $\overline{c}_i = \overline{C}_i = K_i \geq 1$ are also lower and upper bounds respectively, of the steady state problem and so by Theorem 4.4.1, if c_1, c_2 and c_3 are solutions of the system (6.5.12)-(6.5.19), then

$$\frac{\partial c_1}{\partial t},\ \frac{\partial c_2}{\partial t},\ \frac{\partial c_3}{\partial t},\ \frac{\partial C_1}{\partial t},\ \frac{\partial C_2}{\partial t},\ \frac{\partial C_3}{\partial t} \leq 0,$$

or

$$\frac{\partial s}{\partial t},\ \frac{\partial o}{\partial t},\ \frac{\partial S}{\partial t},\ \frac{\partial O}{\partial t} \leq 0$$

and

$$\frac{\partial p}{\partial t},\ \frac{\partial P}{\partial t} \geq 0.$$

The solutions s, o, S and O therefore decrease monotonically with time and the solutions p and P therefore increase monotonically with time towards a positive limit which must be a steady state solution of (6.5.12)-(6.5.19) by Theorem 4.4.2.

The system S_3, B_3 is imbedded in the system S_6, B_6 where inequalities in the above comparison equations are replaced by equalities.

Letting $v_i = \overline{c}_i$, $V_i = \overline{C}_i$ and $v_{3+i} = -\underline{c}_i$, $V_{3+i} = -\underline{C}_i$ for $i = 1, 2, 3$ and setting $f_i^* = \overline{f}_i$, $F_i^* = \overline{F}_i$, $f_{3+i}^* = -\underline{f}_i$ and $F_{3+i}^* = -\underline{F}_i$ for $i = 1, 2, 3$, we obtain the following monotone system S_6^*, B_6^*:

$$\frac{\partial v_1}{\partial t} - d_1\nabla_x^2 v_1 = f_1^*(v_1,..,v_6) = -\phi_1^2\frac{v_1 v_5 v_6}{(1+\beta_1 v_1)(1-\beta_2 v_5)}$$

$$\frac{\partial v_2}{\partial t} - d_2\nabla_x^2 v_2 = f_2^*(v_1,..,v_6) = -\phi_2^2\frac{v_4 v_2 v_6}{(1-\beta_1 v_4)(1+\beta_2 v_2)}$$

$$\frac{\partial v_3}{\partial t} - d_3\nabla_x^2 v_3 = f_3^*(v_1,..,v_6) = -\phi_3^2\frac{v_4 v_5 v_3}{(1-\beta_1 v_4)(1-\beta_2 v_5)}$$

$$\frac{\partial v_4}{\partial t} - d_1\nabla_x^2 v_4 = f_4^*(v_1,..,v_6) = -\phi_1^2\frac{v_4 v_2 v_3}{(1-\beta_1 v_4)(1+\beta_2 v_2)}$$

$$\frac{\partial v_5}{\partial t} - d_2\nabla_x^2 v_5 = f_5^*(v_1,..,v_6) = -\phi_2^2\frac{v_1 v_5 v_3}{(1+\beta_1 v_1)(1-\beta_2 v_5)}$$

$$\frac{\partial v_6}{\partial t} - d_3 \nabla_x^2 v_6 = f_6^*(v_1,..,v_6) = -\phi_3^2 \frac{v_1 v_2 v_6}{(1+\beta_1 v_1)(1+\beta_2 v_2)}$$

$$\chi \frac{\partial V_1}{\partial t} - \frac{1}{\mathcal{Pe}} \frac{\partial^2 V_1}{\partial z^2} + \frac{\partial V_1}{\partial z} + \xi_1 \int_{\partial\Omega_2} \frac{\partial v_1}{\partial n} = 0$$

$$\chi \frac{\partial V_2}{\partial t} - \frac{1}{\mathcal{Pe}} \frac{\partial^2 V_2}{\partial z^2} + \frac{\partial V_2}{\partial z} + \xi_2 \int_{\partial\Omega_2} \frac{\partial v_2}{\partial n} = 0$$

$$\chi \frac{\partial V_3}{\partial t} - \frac{1}{\mathcal{Pe}} \frac{\partial^2 V_3}{\partial z^2} + \frac{\partial V_3}{\partial z} + \xi_3 \int_{\partial\Omega_2} \frac{\partial v_3}{\partial n} = 0$$

$$\chi \frac{\partial V_4}{\partial t} - \frac{1}{\mathcal{Pe}} \frac{\partial^2 V_4}{\partial z^2} + \frac{\partial V_4}{\partial z} + \xi_1 \int_{\partial\Omega_2} \frac{\partial v_4}{\partial n} = 0$$

$$\chi \frac{\partial V_5}{\partial t} - \frac{1}{\mathcal{Pe}} \frac{\partial^2 V_5}{\partial z^2} + \frac{\partial V_5}{\partial z} + \xi_2 \int_{\partial\Omega_2} \frac{\partial v_5}{\partial n} = 0$$

$$\chi \frac{\partial V_6}{\partial t} - \frac{1}{\mathcal{Pe}} \frac{\partial^2 V_6}{\partial z^2} + \frac{\partial V_6}{\partial z} + \xi_3 \int_{\partial\Omega_2} \frac{\partial v_6}{\partial n} = 0$$

where v_1 is uncoupled from v_4, v_2 is uncoupled from v_5, and v_3 is uncoupled from v_6. These have the appropriate boundary and initial conditions. The matrix $\frac{\partial f_i^*}{\partial v_j}$ is given below

$$\begin{pmatrix}
\frac{-\phi_1^2 v_5 v_6}{(1+\beta_1 v_1)^2(1-\beta_2 v_5)} & 0 & 0 & 0 & \frac{-\phi_1^2 v_1 v_6}{(1+\beta_1 v_1)(1-\beta_2 v_5)^2} & \frac{-\phi_1^2 v_1 v_5}{(1+\beta_1 v_1)(1-\beta_2 v_5)} \\
0 & \frac{-\phi_2^2 v_4 v_6}{(1-\beta_1 v_4)(1+\beta_2 v_2)^2} & 0 & \frac{-\phi_2^2 v_2 v_6}{(1-\beta_1 v_4)^2(1+\beta_2 v_2)} & 0 & \frac{-\phi_2^2 v_4 v_2}{(1-\beta_1 v_4)(1+\beta_2 v_2)} \\
0 & 0 & \frac{-\phi_3^2 v_4 v_5}{(1-\beta_1 v_4)(1-\beta_2 v_5)} & \frac{-\phi_3^2 v_5 v_3}{(1-\beta_1 v_4)^2(1-\beta_2 v_5)} & \frac{-\phi_3^2 v_4 v_3}{(1-\beta_1 v_4)(1-\beta_2 v_5)^2} & 0 \\
0 & \frac{-\phi_1^2 v_4 v_3}{(1-\beta_1 v_4)(1+\beta_2 v_2)^2} & \frac{-\phi_1^2 v_4 v_2}{(1-\beta_1 v_4)(1+\beta_2 v_2)} & \frac{-\phi_1^2 v_2 v_3}{(1-\beta_1 v_4)^2(1+\beta_2 v_2)} & 0 & 0 \\
\frac{-\phi_2^2 v_5 v_3}{(1+\beta_1 v_1)^2(1-\beta_2 v_5)} & 0 & \frac{-\phi_2^2 v_1 v_5}{(1+\beta_1 v_1)(1-\beta_2 v_5)} & 0 & \frac{-\phi_2^2 v_1 v_3}{(1+\beta_1 v_1)(1-\beta_2 v_5)^2} & 0 \\
\frac{-\phi_3^2 v_2 v_6}{(1+\beta_1 v_1)^2(1+\beta_2 v_2)} & \frac{-\phi_3^2 v_1 v_6}{(1+\beta_1 v_1)(1+\beta_2 v_2)^2} & 0 & 0 & 0 & \frac{-\phi_3^2 v_1 v_2}{(1+\beta_1 v_1)(1+\beta_2 v_2)}
\end{pmatrix}$$

with matrix a_{ij} of the linear equations $P(\varepsilon)$ of the form:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\phi_1^2}{(1+\beta_1)} & \frac{\phi_1^2}{(1+\beta_1)(1+\beta_2)} \\ 0 & 0 & 0 & \frac{\phi_2^2}{(1+\beta_2)} & 0 & \frac{\phi_2^2}{(1+\beta_1)(1+\beta_2)} \\ 0 & 0 & 0 & \frac{\phi_3^2}{(1+\beta_2)} & \frac{\phi_3^2}{(1+\beta_1)} & 0 \\ 0 & \frac{\phi_1^2}{(1+\beta_1)} & \frac{\phi_1^2}{(1+\beta_1)(1+\beta_2)} & 0 & 0 & 0 \\ \frac{\phi_2^2}{(1+\beta_2)} & 0 & \frac{\phi_2^2}{(1+\beta_1)(1+\beta_2)} & 0 & 0 & 0 \\ \frac{\phi_3^2}{(1+\beta_2)} & \frac{\phi_3^2}{(1+\beta_1)} & 0 & 0 & 0 & 0 \end{pmatrix}$$

or

$$\begin{pmatrix} 0 & B \\ B & 0 \end{pmatrix}, \text{ where } B = \begin{pmatrix} 0 & \frac{\phi_1^2}{(1+\beta_1)} & \frac{\phi_1^2}{(1+\beta_1)(1+\beta_2)} \\ \frac{\phi_2^2}{(1+\beta_2)} & 0 & \frac{\phi_2^2}{(1+\beta_1)(1+\beta_2)} \\ \frac{\phi_3^2}{(1+\beta_2)} & \frac{\phi_3^2}{(1+\beta_1)} & 0 \end{pmatrix} \qquad \textbf{(6.5.20)}$$

and V_i are all uncoupled for $i = 1,.., 6$ and

$$A_{ij} = 0.$$

It is clear that $f_i(c_j)$ satisfies the Lipschitz and Hölder properties required in assumptions (H_1) and (H_2) for $c_1, c_2 \geq 0$ and $c_3 \leq 1$. By Remark 3.6.7, these continuity properties also hold by extending the function in (6.5.10) to all defined values of c_1, c_2 and c_3.

We may apply Theorem 3.3.1 (Generalised Uniqueness Theorem), Theorem 3.4.1 and Theorem 3.6.1 (Generalised Existence Theorem) to show that there exists a unique solution to the system (6.5.12)-(6.5.19).

We now study the stability of the system S_6^*, B_6^*. If we seek functions (w, W) satisfying the system $P(\varepsilon)$ for which all the w_i components are equal to $\tilde{w}$, a positive scalar, then the inequalities (3.5.12)-(3.5.14) are satisfied if we can find $\tilde{w} > 0$ satisfying

$$\nabla_x^2 \tilde{w} + \lambda \tilde{w} \leq 0 \text{ in } \Omega \times \Lambda \text{ for } \lambda \geq (\varepsilon + \sum_j a_{ij}) / d_i \text{ for all } i, \qquad \textbf{(6.5.21)}$$

$$\frac{\partial \tilde{w}}{\partial n} \geq 0 \text{ on } \partial\Omega_1 \times \Lambda, \qquad \textbf{(6.5.22)}$$

$$\frac{\partial \tilde{w}}{\partial n} \geq \gamma(\tilde{W} - \tilde{w}) \text{ on } \partial\Omega_2 \times \Lambda, \qquad \textbf{(6.5.23)}$$

where

$$\tilde{W} \geq W_i \text{ for all } i \qquad \textbf{(6.5.24)}$$

and

$$\gamma = \sup_i \frac{H_i}{d_i}. \tag{6.5.25}$$

The equations for (3.5.15)-(3.5.17) are likewise satisfied by $W_i = \tilde{W}$, if we can find $\tilde{W} > 0$, satisfying

$$\frac{1}{\mathcal{P}e}\frac{d^2\tilde{W}}{dz^2} - \frac{d\tilde{W}}{dz} + (\varepsilon - \xi\mathcal{A})\tilde{W} + \xi\int_{\partial\Omega_2} \tilde{w} \le 0 \text{ in } \Lambda, \tag{6.5.26}$$

$$\tilde{W} - \frac{1}{\mathcal{P}e}\frac{d\tilde{W}}{dz} \ge 1 \text{ at } z=0, \tag{6.5.27}$$

$$\frac{d\tilde{W}}{dz} \ge 0 \text{ at } z=1, \tag{6.5.28}$$

where

$$\xi = \sup_i \xi_i. \tag{6.5.29}$$

These scalar equations for $\tilde{w}$ and $\tilde{W}$ uncouple if we set

$$\tilde{w} = \theta(x)\tilde{W}(z) \tag{6.5.30}$$

so that

$$\nabla^2\theta + \lambda\theta \le 0 \text{ in } \Omega, \tag{6.5.31}$$

$$\frac{\partial\theta}{\partial n} \ge 0 \text{ on } \partial\Omega_1, \tag{6.5.32}$$

$$\frac{\partial\theta}{\partial n} \ge \gamma(1-\theta) \text{ on } \partial\Omega_2. \tag{6.5.33}$$

and $\tilde{W}$ satisfies the scalar equation

$$\frac{1}{\mathcal{P}e}\frac{d^2\tilde{W}}{dz^2} - \frac{d\tilde{W}}{dz} + (\varepsilon - \xi\mathcal{A})\tilde{W} + \xi\left(\int_{\partial\Omega_2} \theta\right)\tilde{W} \le 0 \text{ in } \Lambda, \tag{6.5.34}$$

$$\tilde{W} - \frac{1}{\mathcal{P}e}\frac{d\tilde{W}}{dz} \ge 1 \text{ at } z = 0, \tag{6.5.35}$$

$$\frac{d\tilde{W}}{dz} \ge 0 \text{ at } z = 1. \tag{6.5.36}$$

Now λ, given by $\sup_i (\sum a_{ij})/d_i$, depends on the square of the bioparticle size and positive θ solutions for equations (6.5.31)-(6.5.33) exist for small enough λ.

In the case of large Péclet number $\mathcal{P}e$, where the macroscopic system is convection dominated, the $\tilde{W}$ equation has a solution

$$\tilde{W} = \mathcal{C}e^{Kz}, \tag{6.5.37}$$

for some constant $\mathcal{C}$, if the following conditions are met

$$\frac{1}{\mathcal{P}e}K^2 - K + \mu \le 0, \tag{6.5.38}$$

where

$$\mu \geq \varepsilon - \xi \mathscr{A} + \xi \int_{\partial\Omega_2} \theta. \tag{6.5.39}$$

Note, K real and positive exists satisfying (6.5.38) if $\mathscr{P}_e \geq 4\mu$. At $z = 0$, $\widetilde{W}$ must also satisfy

$$\widetilde{W} - \frac{1}{\mathscr{P}_e}\frac{d\widetilde{W}}{dz} = \mathscr{C}[1 - \frac{K}{\mathscr{P}_e}] \geq 1. \tag{6.5.40}$$

This requires $\mathscr{P}_e > K$ and $\mathscr{C}$ large enough. These conditions are met with $K=2\mu$, where $\mathscr{P}_e \geq 4\mu$. We conclude that all solutions of the system (6.5.1)-(6.5.5) are stable and there is no more than one steady state solution when the following two conditions hold:

For the given geometry of Ω, the boundary value problem (6.5.31)-(6.5.33) for θ has a positive solution. This will be the case if $\lambda < \lambda_1$ where λ_1 is the smallest eigenvalue of problem

$$\nabla^2\theta^* + \lambda_1\theta^* = 0 \text{ in } \Omega, \tag{6.5.41}$$

$$\frac{\partial\theta^*}{\partial n} = 0 \text{ on } \partial\Omega_1, \tag{6.5.42}$$

$$\frac{\partial\theta^*}{\partial n} = \gamma(1-\theta^*) \text{ on } \partial\Omega_2. \tag{6.5.43}$$

The first requirement is then that

$$\lambda_1 > \sup_i \; (\sum_j a_{ij}) / d_i. \tag{6.5.44}$$

If $\lambda < \lambda_1$ and the function θ satisfies (6.5.31)-(6.5.33), and μ_0 is given by

$$\mu_0 = \xi\int_{\partial\Omega_2}(\theta - 1) = -\frac{\xi}{\gamma}\int_{\partial\Omega_2}\frac{\partial\theta}{\partial n} = \frac{\xi\lambda}{\gamma}\int_{\Omega}\theta, \tag{6.5.45}$$

the second requirement is that

$$\mathscr{P}_e > 4\mu_0 = 4\frac{\xi\lambda}{\gamma}\int_{\Omega}\theta. \tag{6.5.46}$$

We therefore have stability and uniqueness for the system (6.5.1)-(6.5.5) for small enough particles and high enough Péclet number, $\mathscr{P}_e$.

6.6 A Continuous Stirred Basket Reactor (CSBR) Model involving Multicomponents

In recent years there has been considerable interest in the possibility of using immobilised enzymes as industrial catalysts. These enzymes are usually trapped in or attatched to water-insoluble supports by a variety of methods. In the following example, a general model is developed for the study of an enzyme reaction inside such porous support pellets contained in a Continuous Stirred Basket Reactor (CSBR). The enzyme reaction kinetics we shall look at in this section involves three chemical components, a substrate s which is converted to a product p under the action of immobilised enzyme, e. The porous support pellet permits the substrate s and product p to move in and out of these pellets but retains the enzyme e because of the larger enzyme molecules. The bulk fluid therefore involves only two chemical components, bulk substrate S_b which is introduced into the reactor as a steady flow and bulk product, P_b which is produced in the reactor.

This example is found in literature (HOSSAIN [132]) and we shall study the question of uniqueness and existence to the time dependent problem using methods developed in this thesis and adapting the theory to reactors such as the CSBR. The objective is to look at the following arbitrary kinetics:

(i) Michaelis–Menten type reaction kinetics,
(ii) substrate inhibition (non competitive or anticompetitive) type reaction kinetics,
(iii) product inhibition (competitive) type reaction kinetics,
(iv) product inhibition (non competitive or anticompetitive) type reaction kinetics,
(v) zero order kinetics.

6.6.1 The Continuous Stirred Basket Reactor (CSBR)

The Continuous Stirred Basket Reactor (CSBR) consists of a cylindrical vessel in which it is essential to have perfect mixing of the contents. The effect of good mixing is that all elements of the fluid in the vessel have virtually the same composition. The liquid motion is induced by mechanical stirring. The result is that porous support pellets contained in the CSBR circulate in a somewhat haphazard manner that characterises the CSBR. A schematic of a CSBR is given in FIG. 6.11.

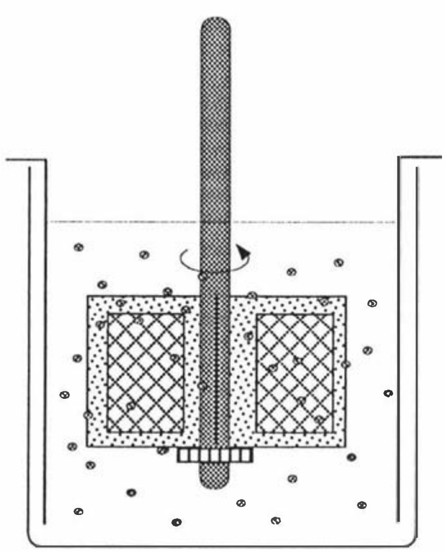


FIG. 6.11 Schematic of a Continuous Stirred Basket Reactor (CSBR)

6.6.2 The Continuous Stirred Basket Reactor (CSBR) Model Formulation

The mathematical model of the CSBR is divided into two submodels. The "Support pellet Model" is concerned with reaction and diffusion within a support pellet and the "CSBR Model" which is concerned with bulk fluid concentrations within the reactor. We make the following simplifying assumptions

Model Assumptions

1. The porous pellet is spherical and uniform in size
2. The effective diffusivities of the substrate and product within the porous pellet are constant
3. The volume and the density of the reacting medium within the porous pellet are constant
4. The reaction kinetics within the porous pellet of the main reaction is arbitrary
5. The process within the porous pellet is diffusion controlled
6. The bulk fluid is perfectly mixed

The equations describing the concentrations of intrasupport substrate and product, active enzyme concentration are

$$\varepsilon_p \frac{\partial s}{\partial t} = D_{es} \frac{1}{r^2} \frac{\partial}{\partial r}(r^2 \frac{\partial s}{\partial r}) - k\rho_p f(s, p)e(r, t) \tag{6.6.1}$$

$$\varepsilon_p \frac{\partial p}{\partial t} = D_{ep} \frac{1}{r^2} \frac{\partial}{\partial r}(r^2 \frac{\partial p}{\partial r}) + k\rho_p f(s, p)e(r, t) \tag{6.6.2}$$

$$\frac{\partial e}{\partial t} = -k_d f(s, p)e(r, t) \tag{6.6.3}$$

with boundary conditions

$$\frac{\partial s}{\partial r} = \frac{\partial p}{\partial r} = 0 \text{ at } r = 0, \tag{6.6.4}$$

$$D_{es} \frac{\partial s}{\partial r} = k_{ms}(S_b - s) \text{ at } r = r_p, \tag{6.6.5}$$

$$D_{ep} \frac{\partial p}{\partial r} = k_{mp}(P_b - p) \text{ at } r = r_p, \tag{6.6.6}$$

and initial conditions

$$s(0, r) = s_0, \tag{6.6.7}$$

$$p(0, r) = 0, \tag{6.6.8}$$

$$e(0, r) = e_0(r). \tag{6.6.9}$$

The bulk concentrations of substate and product in the CSBR are given by

$$V \frac{dS_b}{dt} = F_r(S_0 - S_b) - \frac{m_p}{\rho_p} \frac{3}{r_p} (D_{es} \left. \frac{\partial s}{\partial r} \right|_{r=r_p}), \tag{6.6.10}$$

$$V \frac{dP_b}{dt} = -F_r P_b - \frac{m_p}{\rho_p} \frac{3}{r_p} (D_{ep} \left. \frac{\partial p}{\partial r} \right|_{r=r_p}), \tag{6.6.11}$$

and initial conditions

$$S_b = S_{b,i} \text{ at } t = 0, \tag{6.6.12}$$

$$P_b = 0 \text{ at } t = 0. \tag{6.6.13}$$

For the five kinetic expressions mentioned earlier, $f(s, p)$ has the following form:

$$f(s,p) = \begin{cases} \dfrac{s}{K_m + s} & \text{Michaelis–Menten type kinetics} \\ \dfrac{s}{[(s+K_m)(1+s/K_i)]} & \text{substrate inhibition (non competitive) type kinetics} \\ \dfrac{s}{[s+K_m(1+p/K_i)]} & \text{product inhibition (competitive) type kinetics} \\ \dfrac{s}{(s+K_m)(1+p/K_i)]} & \text{product inhibition (noncompetitive) type kinetics} \\ 1 & \text{zero order kinetics} \end{cases}$$

for $s, p \geq 0$ and

$$f(s, p) = 0,$$

for $s, p < 0$.

It may be observed that in the case of Michaelis-Menten type kinetics $f(s, p)$ is monotone increasing with s and independent of p. In the case of substrate inhibition (non competitive or anticompetitive) type kinetics $f(s, p)$ is concave down, has a maximum positive value, is independent of p and is zero when s is zero and when s is very large. In the case of product inhibition (competitive) type kinetics, $f(s, p)$ is monotone increasing with s and monotone decreasing in p. In the case of product type inhibition (non competitive or anticompetitive type) kinetics, $f(s, p)$ is monotone increasing with s and monotone decreasing in p. Zero order kinetics is of course independent of both s and p.

It may also be observed that this model with constant flow rate F_r, is a limiting case of the more general model developed in Chapter 2 which involves the convection operator $u \cdot \nabla$. Consider, for example the following equation:

$$\frac{\partial S_b}{\partial t} = u \cdot \nabla S_b, \tag{6.6.14}$$

where the spatial average is defined as

$$\bar{S}_b = \frac{1}{V} \int S_b(t,z) \mathrm{d}V. \tag{6.6.15}$$

Differentiating (6.6.15) with respect to t and applying a result from Gauss's Theorem (RUTHERFORD [253, p.77], we obtain

$$\frac{\mathrm{d}\bar{S}_b}{\mathrm{d}t} = \frac{1}{V} \int \frac{\partial S_b}{\partial t} \mathrm{d}V = \frac{1}{V} \int u \cdot \nabla S_b \mathrm{d}V = \frac{u}{V} \cdot \int \nabla S_b \mathrm{d}V = \frac{u}{V} \cdot \int S_b n \mathrm{d}S = u \cdot n. \tag{6.6.16}$$

In only one variable, therefore

$$\frac{d\overline{S}_b}{dt} = uA(S_i - S_0), \tag{6.6.17}$$

where S_i is the inlet concentration and S_0 is the outlet concentration and A is the reactor inlet surface area. Here $uA = F_r$ with the units $m^3\ sec^{-1}$.

The methods developed in this thesis for proving uniqueness, existence and stability theorems for more general type equations with a convection term may therefore be adapted to problems where there is a constant flow rate of substrate into the reactor such as that found in our model of the CSBR. For the purposes of mathematical convenience, the terms $F_r(S_0-S_b)$ and $-F_rP_b$ may be considered to be reaction terms in the bulk fluid as there is no convection term involved.

Nondimensionalisation of the above governing equations leads to the following equations

$$\frac{\partial c_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial c_1}{\partial x}) = -\phi^2 h(c_1, c_2)c_3(x, \tau) \text{ for } 0 < x < 1, \tau > 0, \tag{6.6.18}$$

$$\frac{\partial c_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial c_2}{\partial x}) = \phi^2 h(c_1, c_2)c_3(x, \tau) \text{ for } 0 < x < 1, \tau > 0, \tag{6.6.19}$$

$$\frac{\partial c_3}{\partial \tau} = -\phi^2 h(c_1, c_2)c_3(x, \tau) \text{ for } 0 < x < 1, \tau > 0, \tag{6.6.20}$$

$$\frac{dC_1}{d\tau} = \alpha(1-C_1) - N\left.\frac{\partial c_1}{\partial x}\right|_{x=1} \text{ for } \tau > 0, \tag{6.6.21}$$

$$\frac{dC_2}{d\tau} = -\alpha C_2 - \frac{N}{\delta}\left.\frac{\partial c_2}{\partial x}\right|_{x=1} \text{ for } \tau > 0, \tag{6.6.22}$$

$$\frac{\partial c_1}{\partial x} = \frac{\partial c_2}{\partial x} = 0 \text{ at } x = 0, \tau > 0, \tag{6.6.23}$$

$$\frac{\partial c_1}{\partial x} = Bi_s(C_1 - c_1) \text{ at } x = 1, \tau > 0, \tag{6.6.24}$$

$$\frac{\partial c_2}{\partial x} = Bi_p(C_2 - c_2) \text{ at } x = 1, \tau > 0, \tag{6.6.25}$$

$$c_1(0, x) = c_{1,0} \text{ for } 0 < x < 1, \tag{6.6.26}$$

$$c_2(0, x) = 0 \text{ for } 0 < x < 1, \tag{6.6.27}$$

$$c_3(0, x) = c_{3,0}(x) \text{ for } 0 < x < 1, \tag{6.6.28}$$

$$C_1(0) = C_{1,0}, \tag{6.6.29}$$

$$C_2(0) = 0, \tag{6.6.30}$$

where,

$$h(c_1, c_2) = \begin{cases} \dfrac{c_1}{1+\beta c_1} & \text{Michaelis– Menten type kinetics} \\ \dfrac{c_1}{(1+\beta c_1)(1+\gamma c_1)} & \text{substrate inhibition (non competitive) type kinetics} \\ \dfrac{c_1}{\beta c_1 + (1+\gamma c_2)} & \text{product inhibition (competitive) type kinetics} \\ \dfrac{c_1}{(1+\beta c_1)(1+\gamma c_2)} & \text{product inhibition (noncompetitive) type kinetics} \\ 1 & \text{zero order kinetics} \end{cases}$$

for $c_1, c_2 \geq 0$ and

$$h(c_1, c_2) = 0 \text{ for } c_1, c_2 < 0.$$

The parameters are

$$\alpha = \frac{r_p^2 \varepsilon_p F_r}{D_{es}},\ \beta = \frac{S_0}{K_m},\ \delta = \frac{D_{es}}{D_{ep}},\ \gamma = \frac{S_0}{K_i},\ \psi = \frac{\varepsilon_p S_0 k_d}{\rho_p k \bar{e}_0},\ N = \frac{3(m_p/\rho_p)\varepsilon_p}{V}, \tag{6.6.31}$$

$$Bi_s = \frac{k_m r_p}{D_{es}},\ Bi_p = \frac{k_m r_p}{D_{ep}}. \tag{6.6.32}$$

Also,

$$\phi^2 = \frac{k \bar{e}_0 \rho_p r_p^2}{D_{es} s_0}, \tag{6.6.33}$$

for zero order kinetics and

$$\phi^2 = \frac{k \bar{e}_0 \rho_p r_p^2}{D_{es} K_m}, \tag{6.6.34}$$

for Michaelis–Menten, substrate inhibition (non competitive or anticompetitive) and product inhibition (competitive and non competitive) type kinetics.

The variables are

$$x = \frac{r}{r_p},\ \tau = \frac{D_{es} t}{r_p^2 \varepsilon_p}, \tag{6.6.35}$$

$$c_1 = \frac{s}{S_0},\ c_2 = \frac{p}{S_0},\ c_3 = \frac{e}{\bar{e}_0},\ C_1 = \frac{S_b}{S_0},\ C_2 = \frac{P_b}{S_0},\ c_{1,0} = \frac{s_0}{S_0},\ c_{3,0} = \frac{e_0(r)}{\bar{e}_0},\ C_{1,0} = \frac{S_{b,i}}{S_0}, \tag{6.6.36}$$

where the nondimensional enzyme concentration is scaled with respect to the mean initial concentration, which is defined as

$$\bar{e}_0 = \frac{3}{r_p^3} \int_0^{r_p} r^2 e_0(r) \mathrm{d}r \tag{6.6.37}$$

and in nondimensional form it becomes

$$3\int_0^1 x^2 c_{3,0}(x) \mathrm{d}x = 1. \tag{6.6.38}$$

6.6.3 Uniqueness, Existence and Comparison Results

We study the uniqueness and existence of the system (6.6.18)-(6.6.30) by following the path outlined in chapters 3–4. The comparison functions for C_1 and C_2 are given by:

$$\frac{\mathrm{d}\underline{C}_1}{\mathrm{d}\tau} \le \alpha(1-\underline{C}_1) - N\frac{\partial \underline{c}_1}{\partial x}\bigg|_{x=1}, \tag{6.6.39}$$

$$\frac{\mathrm{d}\bar{C}_1}{\mathrm{d}\tau} \ge \alpha(1-\bar{C}_1) - N\frac{\partial \bar{c}_1}{\partial x}\bigg|_{x=1}, \tag{6.6.40}$$

$$\frac{\mathrm{d}\underline{C}_2}{\mathrm{d}\tau} \le -\alpha\underline{C}_2 - \frac{N}{\delta}\frac{\partial \underline{c}_2}{\partial x}\bigg|_{x=1}, \tag{6.6.41}$$

$$\frac{\mathrm{d}\bar{C}_2}{\mathrm{d}\tau} \ge -\alpha\bar{C}_2 - \frac{N}{\delta}\frac{\partial \bar{c}_2}{\partial x}\bigg|_{x=1}, \tag{6.6.42}$$

and the comparison functions for c_1, c_2 and c_3 depend on the arbitrary kinetics considered. In the case of Michaelis–Menten type reaction kinetics the comparison functions for c_1, c_2 and c_3 are given by:

$$\frac{\partial \underline{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_1}{\partial x}) \le -\phi^2\frac{\underline{c}_1}{1+\beta\underline{c}_1}\bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_1}{\partial x}) \ge -\phi^2\frac{\bar{c}_1}{1+\beta\bar{c}_1}\underline{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_2}{\partial x}) \le \phi^2\frac{\underline{c}_1}{1+\beta\underline{c}_1}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_2}{\partial x}) \ge \phi^2\frac{\bar{c}_1}{1+\beta\bar{c}_1}\bar{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_3}{\partial \tau} \le -\phi^2\frac{\bar{c}_1}{1+\beta\bar{c}_1}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau} \ge -\phi^2\frac{\underline{c}_1}{1+\beta\underline{c}_1}\bar{c}_3(x,\tau).$$

In the case of substrate inhibition (anticompetitive or non competitive) type reaction kinetics the comparison functions for c_1, c_2 and c_3 are given by:

$$\frac{\partial \underline{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_1}{\partial x}) \le -\phi^2\frac{\underline{c}_1}{(1+\beta\underline{c}_1)(1+\gamma\underline{c}_1)}\bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_1}{\partial x}) \ge -\phi^2\frac{\bar{c}_1}{(1+\beta\bar{c}_1)(1+\gamma\bar{c}_1)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_2}{\partial x}) \le \phi^2\underline{c}_3(x,\tau)\ min\ \{\frac{\underline{c}_1}{(1+\beta\underline{c}_1)(1+\gamma\underline{c}_1)}, \frac{\bar{c}_1}{(1+\beta\bar{c}_1)(1+\gamma\bar{c}_1)}\},$$

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_2}{\partial x}) \ge \phi^2\frac{\frac{1}{\sqrt{\beta\gamma}}}{(1+\frac{\beta}{\sqrt{\beta\gamma}})(1+\frac{\gamma}{\sqrt{\beta\gamma}})}\bar{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_3}{\partial \tau} \le -\phi^2\frac{\frac{1}{\sqrt{\beta\gamma}}}{(1+\frac{\beta}{\sqrt{\beta\gamma}})(1+\frac{\gamma}{\sqrt{\beta\gamma}})}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau} \ge -\phi^2\bar{c}_3(x,\tau)\ min\ \{\frac{\underline{c}_1}{(1+\beta\underline{c}_1)(1+\gamma\underline{c}_1)}, \frac{\bar{c}_1}{(1+\beta\bar{c}_1)(1+\gamma\bar{c}_1)}\}.$$

In the case of product inhibition (competitive) type reaction kinetics the comparison functions for c_1, c_2 and c_3 are given by:

$$\frac{\partial \underline{c}_1}{\partial \tau}-\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_1}{\partial x})\le -\phi^2\frac{\underline{c}_1}{\beta\underline{c}_1+(1+\gamma\underline{c}_2)}\bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_1}{\partial \tau}-\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_1}{\partial x})\ge -\phi^2\frac{\bar{c}_1}{\beta\bar{c}_1+(1+\gamma\bar{c}_2)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_2}{\partial \tau}-\frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_2}{\partial x})\le \phi^2\frac{\underline{c}_1}{\beta\underline{c}_1+(1+\gamma\underline{c}_2)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_2}{\partial \tau}-\frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_2}{\partial x})\ge \phi^2\frac{\bar{c}_1}{\beta\bar{c}_1+(1+\gamma\bar{c}_2)}\bar{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_3}{\partial \tau}\le -\phi^2\frac{\bar{c}_1}{\beta\bar{c}_1+(1+\gamma\underline{c}_2)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau}\ge -\phi^2\frac{\underline{c}_1}{\beta\underline{c}_1+(1+\gamma\bar{c}_2)}\bar{c}_3(x,\tau),$$

In the case of product inhibition (anticompetitive or noncompetitive) type reaction kinetics the comparison functions for c_1, c_2 and c_3 are given by:

$$\frac{\partial \underline{c}_1}{\partial \tau}-\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_1}{\partial x})\le -\phi^2\frac{\underline{c}_1}{(1+\beta\underline{c}_1)(1+\gamma\underline{c}_2)}\bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_1}{\partial \tau}-\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_1}{\partial x})\ge -\phi^2\frac{\bar{c}_1}{(1+\beta\bar{c}_1)(1+\gamma\bar{c}_2)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_2}{\partial \tau}-\frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_2}{\partial x})\le \phi^2\frac{\underline{c}_1}{(1+\beta\underline{c}_1)(1+\gamma\underline{c}_2)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_2}{\partial \tau}-\frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_2}{\partial x})\ge \phi^2\frac{\bar{c}_1}{(1+\beta\bar{c}_1)(1+\gamma\bar{c}_2)}\bar{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_3}{\partial \tau}\le -\phi^2\frac{\bar{c}_1}{(1+\beta\bar{c}_1)(1+\gamma\underline{c}_2)}\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau}\ge -\phi^2\frac{\underline{c}_1}{(1+\beta\underline{c}_1)(1+\gamma\bar{c}_2)}\bar{c}_3(x,\tau).$$

In the case of zero order kinetics the comparison functions for c_1, c_2 and c_3 are given by:

$$\frac{\partial \underline{c}_1}{\partial \tau}-\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_1}{\partial x})\le -\phi^2\bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_1}{\partial \tau}-\frac{1}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_1}{\partial x})\ge -\phi^2\underline{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_2}{\partial \tau}-\frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \underline{c}_2}{\partial x})\le \phi^2\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_2}{\partial \tau}-\frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2\frac{\partial \bar{c}_2}{\partial x})\ge \phi^2\bar{c}_3(x,\tau),$$

$$\frac{\partial \underline{c}_3}{\partial \tau}\le -\phi^2\underline{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau}\ge -\phi^2\bar{c}_3(x,\tau).$$

The inequalities in the boundary and initial conditions are

$$\frac{\partial \underline{c}_1}{\partial x}, \frac{\partial \underline{c}_2}{\partial x} \le 0 \text{ at } x=0, \tag{6.6.43}$$

$$\frac{\partial \overline{c}_1}{\partial x}, \frac{\partial \overline{c}_2}{\partial x} \ge 0 \text{ at } x=0, \tag{6.6.44}$$

$$\frac{\partial \underline{c}_1}{\partial x} \le Bi_s(\underline{C}_1-\underline{c}_1),\ \frac{\partial \underline{c}_2}{\partial x} \le Bi_p(\underline{C}_2-\underline{c}_2) \text{ at } x=1, \tag{6.6.45}$$

$$\frac{\partial \overline{c}_1}{\partial x} \ge Bi_s(\overline{C}_1-\overline{c}_1),\ \frac{\partial \overline{c}_2}{\partial x} \ge Bi_p(\overline{C}_2-\overline{c}_2) \text{ at } x=1, \tag{6.6.46}$$

$$\underline{c}_1(0,x) \le c_{1,0},\ \overline{c}_1(0,x) \ge c_{1,0} \tag{6.6.47}$$

$$\underline{c}_2(0,x) \le 0,\ \overline{c}_2(0,x) \ge 0, \tag{6.6.48}$$

$$\underline{c}_3(0,x) \le c_{3,0}(x),\ \overline{c}_3(0,x) \ge c_{3,0}(x), \tag{6.6.49}$$

$$\underline{C}_1(0) \le C_{1,0},\ \overline{C}_1(0) \ge C_{1,0}, \tag{6.6.50}$$

$$\underline{C}_2(0) \le 0,\ \overline{C}_2(0) \ge 0. \tag{6.6.51}$$

In the case of Michaelis–Menten, substrate inhibition (non competitive or anticompetitive) and product inhibition (competitive and non competitive) type kinetics, we see that the comparison functions for c_1, c_2 and c_3 are all coupled in some way.

In all cases we also see that the nonlinear reaction functions are monotone increasing in some of the variables and monotone decreasing in all other variables. From section 3.4 we see that all these systems may be made into quasimonotone nondecreasing systems (with inequalities replaced by equalities) by the substitution $v_i = \overline{c}_i$, $v_{3+i} = -\underline{c}_i$ for $i = 1, 2, 3$ and $V_i = \overline{C}_i$, $V_{2+i} = -\underline{C}_i$ for $i = 1, 2$.

However, rather than defining upper and lower solutions for this new monotone system we may still define *coupled* upper and lower solutions of our original system. These as we have seen in section 4.3 for the time independent problem can also give us uniqueness and existence results.

In the case of Michaelis–Menten, substrate inhibition (non competitive or anticompetitive) and product inhibition (competitive and non competitive) type kinetics, we shall take $\underline{c}_1 = \underline{c}_2 = \underline{c}_3 = \underline{C}_1 = \underline{C}_2 = 0$ as lower solutions and look for upper solutions in terms of these lower solutions.

In the case of Michaelis-Menten type reaction kinetics the only difficulty is to find functions $\overline{c}_1$, $\overline{c}_2$ and $\overline{c}_3$ that satisfy the inequalities

$$\frac{\partial \overline{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \frac{\partial \overline{c}_1}{\partial x}\right) \ge 0,$$

$$\frac{\partial \overline{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}\left(x^2 \frac{\partial \overline{c}_2}{\partial x}\right) \ge \phi^2 \frac{\overline{c}_1}{1+\beta \overline{c}_1}\overline{c}_3(x,\tau),$$

$$\frac{\partial \overline{c}_3}{\partial \tau} \ge 0.$$

In this case we may choose

$$\bar{c}_1 = \bar{C}_1 = K_1,\ \bar{c}_2 = \bar{C}_2 = \phi^2 \frac{K_1}{(1+\beta K_1)} K_3 t,\ \bar{c}_3 = \bar{C}_3 = K_3,$$

where K_1 and K_3 are positive constants satisfying

$$K_1 \geq max\ \{c_{1,0},\ 1,\ C_{1,0}\} \text{ and } K_3 \geq c_{3,0}.$$

In the case of substrate inhibition (non competitive or anticompetitive) type reaction kinetics the only difficulty is to find functions $\bar{c}_1$, $\bar{c}_2$ and $\bar{c}_3$ that satisfy the inequalities

$$\frac{\partial \bar{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \bar{c}_1}{\partial x}) \geq 0,$$

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \bar{c}_2}{\partial x}) \geq \phi^2 \frac{\frac{1}{\sqrt{\beta\gamma}}}{(1+\frac{\beta}{\sqrt{\beta\gamma}})(1+\frac{\gamma}{\sqrt{\beta\gamma}})} \bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau} \geq 0.$$

In this case we may choose

$$\bar{c}_1 = \bar{C}_1 = K_1,\ \bar{c}_2 = \bar{C}_2 = \phi^2 \frac{\frac{1}{\sqrt{\beta\gamma}}}{(1+\frac{\beta}{\sqrt{\beta\gamma}})(1+\frac{\gamma}{\sqrt{\beta\gamma}})} K_3 t,\ \bar{c}_3 = \bar{C}_3 = K_3,$$

where K_1 and K_3 are positive constants satisfying

$$K_1 \geq max\ \{c_{1,0},\ 1,\ C_{1,0}\} \text{ and } K_3 \geq c_{3,0}.$$

In the case of product inhibition (competitive) type reaction kinetics the only difficulty is to find functions $\bar{c}_1$, $\bar{c}_2$ and $\bar{c}_3$ that satisfy the inequalities

$$\frac{\partial \bar{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \bar{c}_1}{\partial x}) \geq 0,$$

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \bar{c}_2}{\partial x}) \geq \phi^2 \frac{\bar{c}_1}{\beta \bar{c}_1 + (1+\gamma \bar{c}_2)} \bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau} \geq 0.$$

In this case we may choose

$$\bar{c}_1 = \bar{C}_1 = K_1,\ \bar{c}_3 = \bar{C}_3 = K_3,$$

where K_1 and K_3 are positive constants satisfying

$$K_1 \geq max\ \{c_{1,0},\ 1,\ C_{1,0}\} \text{ and } K_3 \geq c_{3,0},$$

and the only difficulty now is to find $\bar{c}_2$ satisfying

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \bar{c}_2}{\partial x}) \geq \phi^2 \frac{K_1}{\beta K_1 + (1+\gamma \bar{c}_2)} K_3.$$

However, since

$$\phi^2 \frac{K_1}{\beta K_1 + (1+\gamma \bar{c}_2)} K_3,$$

and

$$\frac{\partial}{\partial \bar{c}_2}\left(\phi^2 \frac{K_1}{\beta K_1 + (1+\gamma \bar{c}_2)} K_3\right) = -\frac{\phi^2 K_1 K_3 \gamma}{(\beta K_1 + (1+\gamma \bar{c}_2))^2},$$

are uniformly bounded, we are assured that upper solutions $\bar{c}_2$ exist and may be constructed (PAO [222]). For example, we may take $\bar{c}_2 = \bar{C}_2 = Ae^{Rt}$, so that

$$Ae^{Rt} \geq \phi^2 \frac{K_1}{\beta K_1 + (1+\gamma Ae^{Rt})} K_3,$$

where A is determined from the boundary condtions and R can be chosen large enough.

In the case of product inhibition (non competitive or anticompetitive) type reaction kinetics the only difficulty is to find functions $\bar{c}_1$, $\bar{c}_2$ and $\bar{c}_3$ that satisfy the inequalities

$$\frac{\partial \bar{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \frac{\partial \bar{c}_1}{\partial x}\right) \geq 0,$$

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}\left(x^2 \frac{\partial \bar{c}_2}{\partial x}\right) \geq \phi^2 \frac{\bar{c}_1}{(1+\beta \bar{c}_1)(1+\gamma \bar{c}_2)} \bar{c}_3(x,\tau),$$

$$\frac{\partial \bar{c}_3}{\partial \tau} \geq 0.$$

In this case we may choose

$$\bar{c}_1 = \bar{C}_1 = K_1, \ \bar{c}_3 = \bar{C}_3 = K_3,$$

where K_1 and K_3 are positive constants satisfying

$$K_1 \geq max\ \{c_{1,0},\ 1,\ C_{1,0}\} \text{ and } K_3 \geq c_{3,0},$$

and the only difficulty now is to find $\bar{c}_2$ satisfying

$$\frac{\partial \bar{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}\left(x^2 \frac{\partial \bar{c}_2}{\partial x}\right) \geq \phi^2 \frac{K_1}{(1+\beta K_1)(1+\gamma \bar{c}_2)} K_3.$$

However, since

$$\phi^2 \frac{K_1}{(1+\beta K_1)(1+\gamma \bar{c}_2)} K_3,$$

and

$$\frac{\partial}{\partial \bar{c}_2}\left(\phi^2 \frac{K_1}{(1+\beta K_1)(1+\gamma \bar{c}_2)} K_3\right) = -\frac{\phi^2 K_1 K_3 \gamma (1+\beta K_1)}{(1+\beta K_1)^2 (1+\gamma \bar{c}_2)^2},$$

are uniformly bounded, we are assured that upper solutions $\bar{c}_2$ exist and may be constructed (PAO [222]). For example, we may take $\bar{c}_2 = \bar{C}_2 = Ae^{Rt}$, so that

$$Ae^{Rt} \geq \phi^2 \frac{K_1}{(1+\beta K_1)(1+\gamma Ae^{Rt})} K_3,$$

where A is determined from the boundary condtions and R can be chosen large enough.

In the case of zero order kinetics we may take $\underline{c}_2 = \underline{c}_3 = \underline{C}_2 = 0$ as lower solutions. The only difficulty is to find functions $\underline{c}_1$, $\overline{c}_1$, $\overline{c}_2$ and $\overline{c}_3$ that satisfy the inequalities

$$\frac{\partial \underline{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \underline{c}_1}{\partial x}) \le -\phi^2 \overline{c}_3(x,\tau),$$

$$\frac{\partial \overline{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \overline{c}_1}{\partial x}) \ge 0,$$

$$\frac{\partial \overline{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \overline{c}_2}{\partial x}) \ge \phi^2 \overline{c}_3(x,\tau),$$

$$\frac{\partial \overline{c}_3}{\partial \tau} \ge -\phi^2 \overline{c}_3(x,\tau).$$

In this case we may choose

$$\overline{c}_1 = \overline{C}_1 = K_1, \ \overline{c}_3 = \overline{C}_3 = K_3,$$

where K_1 and K_3 are positive constants satisfying

$$K_1 \ge max \ \{c_{1,0}, \ 1, \ C_{1,0}\} \text{ and } K_3 \ge c_{3,0},$$

and the only difficulty now is to find $\underline{c}_1$ and $\overline{c}_2$ satisfying

$$\frac{\partial \underline{c}_1}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \underline{c}_1}{\partial x}) \le -\phi^2 K_3,$$

$$\frac{\partial \overline{c}_2}{\partial \tau} - \frac{\delta}{x^2}\frac{\partial}{\partial x}(x^2 \frac{\partial \overline{c}_2}{\partial x}) \ge \phi^2 K_3.$$

In this case we may take $\overline{c}_2 = \overline{C}_2 = \phi^2 K_3 t$ and $\underline{c}_1 = \underline{C}_1 = -\phi^2 K_3 t$.

Our comparison functions provide us with valid coupled lower and upper solutions $\underline{c}_1$, $\underline{c}_2$, $\underline{c}_3$, $\underline{C}_1$, $\underline{C}_2$ and $\overline{c}_1$, $\overline{c}_2$, $\overline{c}_3$, $\overline{C}_1$, $\overline{C}_2$, respectively for the time dependent problem (6.6.18)-(6.6.30) with $\underline{c}_1 \le \overline{c}_1$, $\underline{c}_2 \le \overline{c}_2$, $\underline{c}_3 \le \overline{c}_3$, $\underline{C}_1 \le \overline{C}_1$ and $\underline{C}_2 \le \overline{C}_2$. Since our Hölder and Lipschitz continuity properties are satisfied by the nonlinear terms there exists a unique solution of the problem (6.6.18)-(6.6.30) by Theorem 3.3.1 and results from section 3.6.

6.6.4 Conclusions and Remarks

Our coupled upper and lower solutions also provide us with bounds on the solution, c_1, c_2, c_3, C_1 and C_2. These bounds can all be interpreted physically. The existence of solutions to the steady state problem is treated similary by following the methods in this section and using Theorem 4.3.3 (Generalised Existence Theorem) for nonmonotone systems. The study of stability and uniqueness of the steady state problem follows along the lines set forward in section 6.5.

Note that $\underline{c}_1 = \underline{C}_1 = 0$ is not a universal lower bound on c_1 in the case of zero order kinetics and c_1 may possess a negative solution. This of course is physically unrealistic and the problem would have to redefined to avoid this. It can be shown with the strong maximum principle that $\underline{c}_2$, $\underline{c}_3$ and $\underline{C}_2$ are strictly bounded below by zero and so therefore is c_2, c_3 and C_2. However we cannot say this of zero order kinetics, (in fact of fractional order kinetics) which may allow for incomplete penetration of substrate (PARSHOTAM

[223]) in our model. The physical implications of this is that substrate concentrations may approach and reach zero concentration somewhere in a particle and reactor but product and enzyme concentrations will never reach zero.

Nomenclature

A	reactor inlet surface area
Bi_s	Biot number for substrate mass transfer
Bi_p	Biot number for product mass transfer
c_1	nondimensional intracatalyst substrate concentration
c_2	nondimensional product concentration
c_3	nondimensional immobilised enzyme concentration
C_1	nondimensional reactor substrate concentration
C_2	nondimensional reactor product concentration
d_p	diameter of particle
D_{es}	effective diffusivity of substrate in the pellet
D_p	effective diffusivity of product in the pellet
e	active immobilised enzyme concentration in the pellet
e_0	initial distribution of active immobilised enzyme concentration
$\bar{e}_0$	mean active enzyme concentration defined in (6.6.37)
f	arbitrary kinetic expression
F_r	Volumetric flow rate of substrate to the reactor
h	arbitrary kinetic expression
k	enzymatic reaction rate constant
k_d	deactivation rate constant of immobilised enzyme concentration
K_i	Inhibition constant for the supported catalyst
K_m	Michaelis–Menten constant for the supported catalyst
k_{mp}	mass transfer coefficients of the product
k_{ms}	mass transfer coefficients of the substrate
m_p	total mass of the enzyme pellet in the reactor
N	ratio of support volume to that of reactor - defined in (6.6.31)
p	intrasupport product concentration
P_b	Bulk concentration of the product in the reactor
r	radial position in the pellet
r_p	pellet radius
s	intracatalyst substrate concentration
S_0	Inlet concentration of substrate
S_b	Bulk concentration of substrate in the reactor
$S_{b,i}$	Initial bulk concentration of substrate in the reactor
t	real time
u	variable flow rate into the reactor
V	volume of the reacting solutions or of the CSBR
x	nondimensional spatial variable

Greek letters

α parameter defined in (6.6.31)
β parameter defined in (6.6.31)
δ parameter defined in (6.6.31)
ε_p partical voidage, i.e., initial porosity of support pellet
ϕ^2 Thiele moduli defined in (6.6.33)-(6.6.34)
γ parameter defined in (6.6.31)
ρ_p pellet density
ψ parameter defined in (6.6.31)
τ dimensionless time

6.7 Notes and Comments

Section 6.1 is adapted from PARSHOTAM *et al.* [225], section 6.2 is adapted from PARSHOTAM *et al.* [226], section 6.3 is adapted from PARSHOTAM [227], section 6.4 is adapted from PARSHOTAM [229] and section 6.5 is adapted from PARSHOTAM [228].

Note that the analytical bounds demonstrated in section 6.2 can be improved by using techniques developed in section 6.1. These techniques however are not so straightforward and may also be applied in some cases to systems of such equations.

An exact analytical solution to the system S_n, B_n with porous spherical particles and a cylindrical isothermal adsorption column without reaction in either particles nor the reactor and for a single chemical component has been derived by RASMUSON and NERETNIEKS [243] and is improved by RASMUSON [244]. The fast Fourier transform (FFT) has also been used in these problems (CHEN and HSU) to predict breakthrough curves for this problem and this is compared with the orthogonal collocation results of RAGHAVAN and RUTHVEN [237].

In section 6.5 the function $f_i(c_j)$ in equation (6.5.10) is not only monotonically decreasing with respect to c_j but it is also a negative function which is concave up and $f_i(0) = 0$. Therefore a linearisation of this function by a Taylor's series expansion, uncoupling the resulting linear equations by using methods developed in Chapter 5 and solving these linear equations should give a solution which is a lower bound of the original system. Similarly, an upper bound may be constructed along the same lines by using methods developed example 6.2 and these bounds can also be improved by using the methods developed in example 6.1. In general this theory may be applied to the systems S_n, B_n and $\hat{S}_n$, $\hat{B}_n$ if a_{ij}, $A_{ij} \geq 0$ and f_{ij} or F_{ij} are either concave up or concave down for all i, j. Note that this conclusion would not be reached if the substitution $c_3 = 1 - p$ and $C_3 = 1 - P$ had not been made. In this case we may still have got a monotone system but it is not true that $a_{ij} \geq 0$ for $i = j$.

In section 6.5, we have stability and uniqueness for small enough particles and high Péclet number. This is consistent with what is well documented in literature from numerical and analytical studies for reactors and particles (MCGUIRE and LAPIDUS [181], GAVALAS [104], HLAVACEK [127-131], HELLINCKX *et al.* [122], LUSS [174, 175], LUSS and AMUNDSON [173] and WEISZ and HICKS [307]).

In section 6.6 we see that substrate concentrations may decrease and approach zero somewhere in the interior of the reactor or particle. From a physical standpoint, this concept of partial penetration or incomplete penetration of substrate through a particle is very important to operating conditions. It can be demonstrated that certain kinetics cannot allow for partial or incomplete penetration (PARSHOTAM [223, 225, 226]) in a particle in a reactor. This problem has its mathematical analogy in demonstrating the existence or nonexistence of a dead core or finding nonnegative solutions with interior zeros (BANDLE and STAKGOLD [31], BANDLE, *et al.*[31, 32], BOBISUD [39-41], FRIEDMAN and PHILIPS [95]) and these problems do not exist in positone problems (CASTRO and SHIVAJI [51]). It can be shown by the maximum principle that for some kinetics, this dead core is empty and this behaviour of solutions usually occurs with zero order and fractional order kinetics (GRAHAM-EAGLE and STAKGOLD [108]). These results may also be generalised to systems of equations by the methods developed in this thesis.

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