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Title

A thesis presented in partial fulfillment of the requirements for the degree of Master of Philosophy in Biotechnology at Massey University

Full name : Aroon A. Parshotam
Year : 1988

Topic - Mathematical Analysis of the reaction diffusion processes occuring within a biofilm

by

Aroon A. Parshotam

Submitted as a 3 paper thesis for the degree of Masters of Philosophy in Biotechnology at Massey University in New Zealand.

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Abstract

This thesis investigates the behaviour of the solutions to mass transfer type reaction-diffusion equations within a biological film around a spherical particle, around a rotating cylinder and on a slab. In general these biological films may be found in any biological system and as examples of systems with spherical, cylindrical and slab geometry we examine biofilms in a fluidised bed biofilm reactor, biological growth around a rotating cylinder and on a rotating biological disk contactor.

These equations model concentrations of substrates within a single biofilm as a function of position and time.

In dimensionless coordinates , these equations have the form

$$\frac{\partial y}{\partial t} = \frac{1}{x^{a-1}} \frac{\partial}{\partial x} \left(x^{a-1} \frac{\partial y}{\partial x}\right) - \phi^2 F(y) \qquad \text{(P)}$$

for a = 1,2,3 being geometries of a slab, cylinder and sphere respectively and where

F(y) may correspond to F_0,F_1,F_n or F_{mm} and where

$F_0 = 1$ corresponds to zero order kinetics
$F_1 = y$ corresponds to first order kinetics
$F_n = y^n$ corresponds to nth order kinetics where n is an integer and
$F_{mm} = \frac{y}{1+\beta y}$ corresponds to Michaelis-Menten reaction kinetics

The dependent variable y corresponds to concentration and the independent variables x and t correspond to distance and time respectively.

The model parameters are saturation parameter β, which describes the concentration and Thiele modulus ϕ, which is the ratio of reaction to diffusion coefficients.

The boundary conditions are

$$\frac{\partial y}{\partial x}(\alpha,t)=0 \quad \text{and } y(1,t)=1 \text{ for all time } >0$$

Here α is the internal boundary, a parameter that corresponds in spherical geometries to the ratio of the radius of a support media to the total radius of the bioparticle, in cylindrical geometries to the radius of a cylinder without biofilm to the total radius of the cylinder with biofilm and in slab geometry to be the ratio of the inactive region of diffusion to the thickness of biofilm measured from the centre of the slab. This may vary but for our purposes we shall take it to be a constant.

The major part of this thesis is concerned with the solution to the steady state associated with problem (P).

Using the maximum principle and, methods of upper and lower solutions and standard topologocal results from non-linear analysis, existence , uniqueness and monotonicity results are obtained.

In particular it is shown that the steady state problem has a unique solution for all values of the parameters when $\alpha \geq 0$, $\beta \geq 0$, $\phi^2 \geq 0$ and F(y) of the form above in the geometries slab, cylinder and sphere.

It is also shown that if $F(0) = 0$, $F(y) \geq 0$, the unique solution of the steady state problem associated with (P) is strictly greater than zero. This is indeed true for nth order and Michaelis-Menten kinetics.

For the zero order case $F(0) \neq 0$ implies that our solution to the steady state problem associated with (P) could become negative. Having a negative concentration is not a physical reality and we impose a third boundary condition that redefines α in terms of Thiele modulus, ϕ.

We also show that our solution to the steady state problem associated with problem (P) is monotonically decreasing in ϕ and monotonically increasing in β for all geometries and all orders. This may be generalised to all time for the unsteady state case.

The final part of this thesis considers the equation of the existence of solutions to problem (P) which are defined for all time . Such existence results are derived and approximate analytical solutions are obtained for some special cases ; but for general regions , only partial answers are obtained.

Dedication

Towards the last few weeks of typing up this thesis I came to the realisation that it may be far more important to study the creator of biofilms than to study these measely biofilms themselves. These biofilms seem to me now so insignificant in spite of the bother they have been causing me. I therefore humbly and sincerely dedicate this thesis to God.

Declaration

The work embodied in this thesis is to the best of my knowledge and belief, original, except as acknowledged in the text, and has not been submitted for a degree at any university either in whole or in part.

Aroon A. Parshotam 22/11/88

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Key words

Biofilm, Biofouling,Biocylinder, Bioparticle, Bioslab, fluidised bed biofilm reactor,flocreactors,glyco-proteins,Michaelis-Menten kinetics,proteoglycan, rotating biological disk contactor, substrate, Sloughing, trickling filter, Thiele modulus,

Chapter 1

Chapter 1 -Introduction, the model and the problem

1.1 Biofilms -an introduction

Definition (Biofilms)
Biofilms are multiple layers of microorganisms on a solid surface of any geometry in an aqueous environment.

Adhesion of micro-organisms to submerged or intermittently wetted surfaces is a virtually universal phenomenon which has been studied extensively by the engineering and medical fraternities, largely from the standpoint of the deleterious effects of biofilm formation (biofouling). These are manifest in engineering technology as heat transfer reduction, fluid flow resistance, corrosion and limitations imposed on mass transfer and chemical transformations - medical applications include fouling of prosthetic implants, dental decay and pathogen activity. The significance of microbial films in fermentation processes has also not been overlooked.

In natural environments, frequently nutrient deficient, observed increases in the concentration of nutrients at interfaces (gas/liquid, gas/solid, liquid/ solid) bestows obvious advantages on microbes colonizing the phase boundary. In contrast, the objective of controlled application of biofilms in bioengineering is expedited through the provision of optimal conditions for substrate transfer at the interface and within the biofilm.This has been discussed by Anderson,G.K. and Sanderson,J.A. [1].

Biofilms will form at almost any interface where there is a microbial presence, indeed, it is more than many operators can do to prevent biofilm formation. Development of a biofilm is not simply the outcome of biological activity but the net result of a complex combination of physical, chemical and biological interactions at the phase boundary.
A sequential series of events occurs during initial biofilm formation leading ultimately to an unstable equilibrium condition:

(i) transport and adsorption of organic molecules to the wetted surface forming an organic conditioning layer. This is virtually spontaneous and the conditioning layer is comprised mainly of glyco-proteins, proteoglycans or their humic residues

(ii) transport of microbial cells to the 'conditioned' surface

(iii) microbial adhesion

(iv) biofilm proliferation and metabolism

(v) detachment (sloughing) of the microbial film

The dynamic equilibrium is maintained when (iv) and (v) are occuring simultaneously.

As examples of biofilm growth in various geometries, we shall examine biological growth around spheres, cylinders and on slabs.

Examples of these geometries in various biological systems are also given .

In particular, the fluidised bed biofilm reactor (FBBR) is an example of where spherical bioparticles may be found, a rotating cylinder is an example of a cylinder and a Rotating Biological Contactor Plant , an example of many slabs close together to support biological film growth.

We shall analyse these systems in more detail in the following examples.

1.1.1 Spherical Bioparticles

The fluidized bed biofilm reactor (FBBR)-an example of a general biological system where spherical bioparticles may be found.

The fluidized bed biofilm reactor is an ingeneous biological wastewater treatment process and also a biochemical manufacturing process that makes use of small particles in a fluidized state to provide a large surface area to support biological growth .

Wastewater to be treated is pumped upwards through a column reactor that is partially filled with granular media such as sand , coal, or activated carbon at superficial velocities sufficient to impart motion to or fluidize the granular bed. Once fluidized , each medium provides a large surface area for microbial growth .

It is common to remove the non-settleable organic content of wastewater by converting its energy and carbon content into growth of these microbial organisms which can be separated more easily.[1] There are also gases being produced by these organisms in aerobic respiration such as $C0_2$ which escapes to the atmosphere.

Each particle, in time becomes covered with biofilm . Biological growth has been demonstrated to support biomass concentrations of an order of magnitude larger than that of conventional systems . This in turn , leads to a significant reduction in the required retention time for effective removal of the waste components and in the size of the treatment plant for a given volumetric load.

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.

1A list of different microorganism which break down specific wasteproducts may be found in *"Microbial Ecology"* A.Laskin & H. Lechevalier, 1974 CRC Press table 2 pp. 158-159.

A schematic diagram of the fluidised bed system is shown in figure 1-1

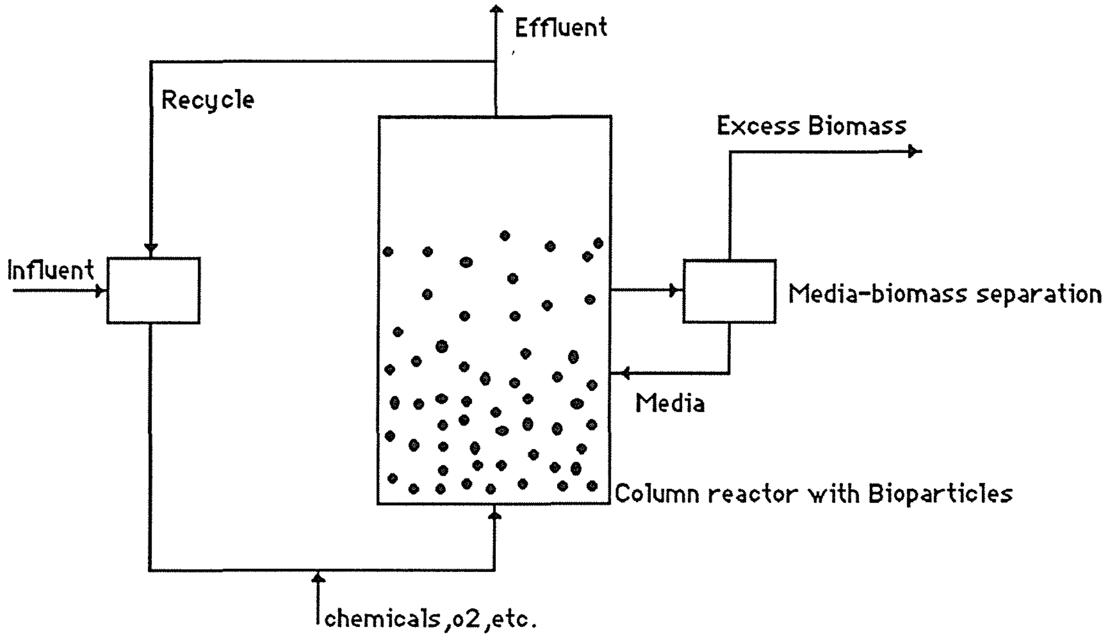

figure 1-1 A schematic diagram of the FBBR process.

As the microbial film (biofilm) forms on the media surface, the overall density of the biofilm-coated media (bioparticle) decreases. This eventually causes bioparticles to be removed from the reactor very easily.

While the treatment is similar in concept to a trickling filter, the FBBR offers distinct mechanical advantages which allow small, high surface area media to be used without the head loss and bed clogging problems which would be encountered in a fixed bed reactor. Rather than clog with new growth, the FBBR simply expands. The bed expansion is usually controlled at a given level to prevent the loss of too many bioparticles and when the bed height reaches this level, a portion of the bioparticles in the reactor is mechanically separated from the media . The cleaned medium is then returned to to the reactor and the separated biomass is wasted as the excess sludge. To provide a uniform fluidisation and an adequate substrate loading rate, a recycling of reactor effulent is often employed. The FBBR can be operated as either an aerobic or an anaerobic process , depending on the application , and often gases or chemicals are added to speed up the process.
What would take up to 2 hours to remove wastes in an ordinary trickling filter could take as little as 6 minutes in a FBBR .

1.1.2. Cylinders covered by a biofilm

The rotating Cylinder -an example of a general 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 rotating biological disk contractor is also an ingeneous method of removing non-settleable organic content of wastewater. It is however more ideal on a smale scale.

The principle involved is lowering of a rotating cylinder into wastewater which is being pumped in and out. This 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.

In time this cylinder gets covered with a biofilm and substrate diffuses through this biofilm. A schematic diagram of a biological rotating cylinder is given in figure 1-2

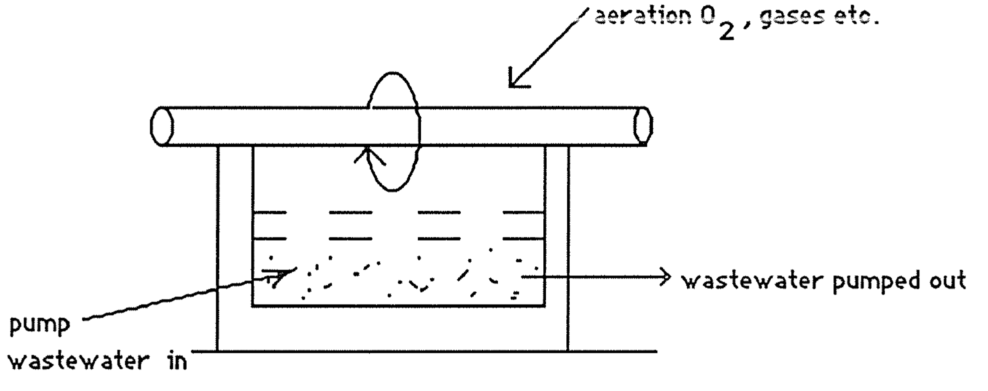

figure 1-2 A Schematic diagram of a biological rotating cylinder

As with the FBBR, the cylinder may be temporarily removed and cleaned and the separated biomass wasted as excess sludge.

1.1.3. The Rotating Biological Disk Contactor Plant- an example of a general biological system where 'slabs' are covered by a thin biofilm consisting of layers of microorganisms held in place by extracellular material.

As with the rotaing cylinder and FBBR, the concepts of waste treatment using a rotating biological contactor plant, are quite similar.It is used in almost an identical way to a rotating cylinder, but provides more surface area for biological film growth.

A schematic of the Biological Contactor Plant is given in figure where individual compartments are individual disks.

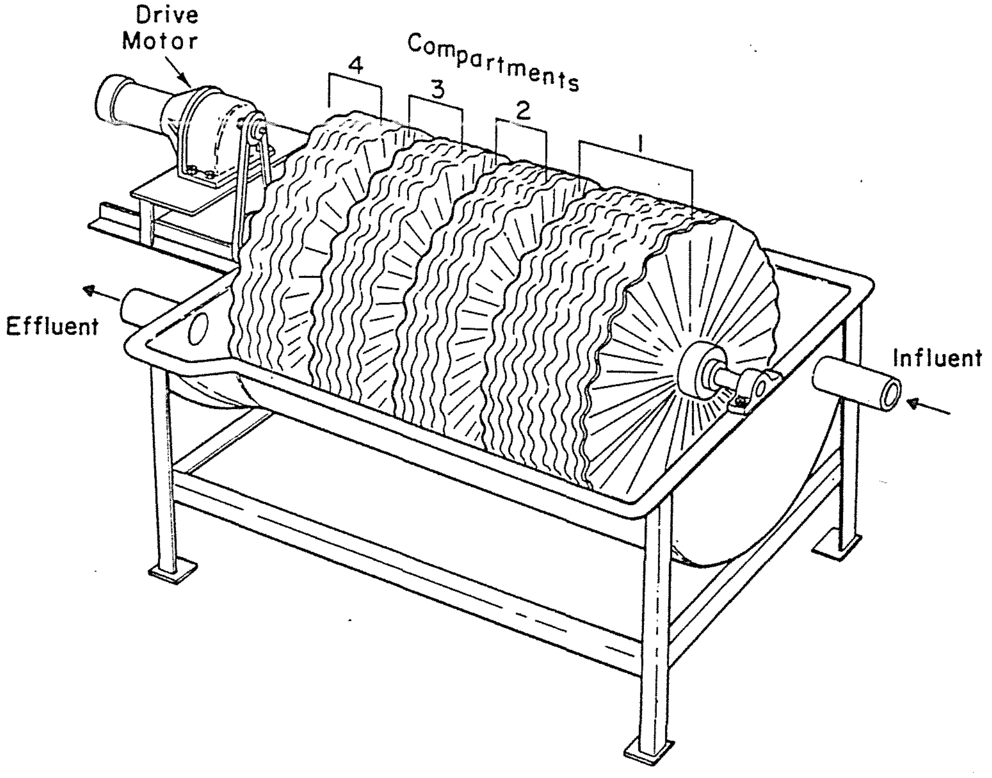

figure 1-3 A Shematic diagram of the rotating Biological Contactor Plant

Uses of this Thesis

The factors affecting process performance should be identified to provide a rational basis for process design and control purposes. This thesis examines the first part of the model , the model of the intrinsic reactions occuring within a biofilm . It also examines the substrate conversion rate by biofilms with various different kinetic rate laws. and thereby gives an intrinsic understanding of growth and overall order.

We shall, in this thesis only be concerned with reactions of zero, first and Michaelis-Menten reaction kinetics for physical, practical and research purposes.

This thesis shall be useful in gaining a much better understanding of the mathematical processes that occur with various kinetic reactions within a biofilm . It shall be made clear why certain things have not been well understood in the past and although the resultant model is non-linear and requires computer solutions which are inconvenient for design and routine purposes , it shall attempt to approximate mathematical solutions to these models .

This model does, however demonstrate the significance of mass transfer resistances on observed kinetics and also provides an insight into a control strategy which can be used to optimise system operating variables.

Presented herein, is a kinetic model for a biofilm system found in many biological systems.

1.2 Fundamentals of Chemical Kinetics [2]

We shall discuss fundamentals of chemical kinetics which shall be very useful in the development of this thesis. Most results and definitions are standard and may be found in any standard text on chemical kinetics.

1.2.1 Rate constant

The rate constant is a measure of the rate of a given chemical reaction under specified conditions. It is the rate of change in concentration of reactant or product with time for a reaction in which all the reactants are unit concentration. It is constant at a given temperature and pressure and increases rapidly with temperature.

1.2.2 Reaction rate or Reaction velocity

The rate of a reaction is the decrease in concentration per unit time of one of the reactants .
If [A] represents the concentration of the reactant A, measured at time t, then the rate is defined as

$$\text{rate} = -\frac{d[A]}{dt} \qquad \textbf{(1-1)}$$

(This is negative because the concentration of the reactant decreases with increasing time.)

An alternative definition of the rate of a reaction is in terms of the product, P
If a represents the initial concentration of A and x represents the concentration of product at time t then

$$\text{rate} = +\frac{dx}{dt} \qquad \textbf{(1-2)}$$

(This is positive because the concentration of product increases with time.)

This could also be represented as

$$\text{rate} = -\frac{d(a-x)}{dt} \qquad \textbf{(1-3)}$$

The rate of reaction therefore becomes

rate of reaction = a constant multiplied by a function of the concentrations of reactants or

---

[2] We shall use this to develop Michaelis-Menten Kinetics.

$$\text{rate of reaction} = \frac{dx}{dt} = k \times F(a,b,c,.......) \qquad \textbf{(1-4)}$$

where k is the rate constant and a,b,c, ... represent the concentrations of the reactants A,B,C,..... at time t.

The function F(a,b,c,....) represents some mathematical expression that is a characteristic of the reaction and involves the products of the concentrations, each raised to a certain power, and so becomes unity when all the concentrations are unit concentrations.

A typical curve of percentage reaction against time is shown in figure 1-4.

Note that the amount of reaction in a given time decreases as the reaction proceeds. i.e. the rate of reaction is given by the slope of the curve, clearly decreases with increasing time.

Note also that there is no definite instant of time at which the reaaction is completed as the curve approaches 100% reaction asymptotically

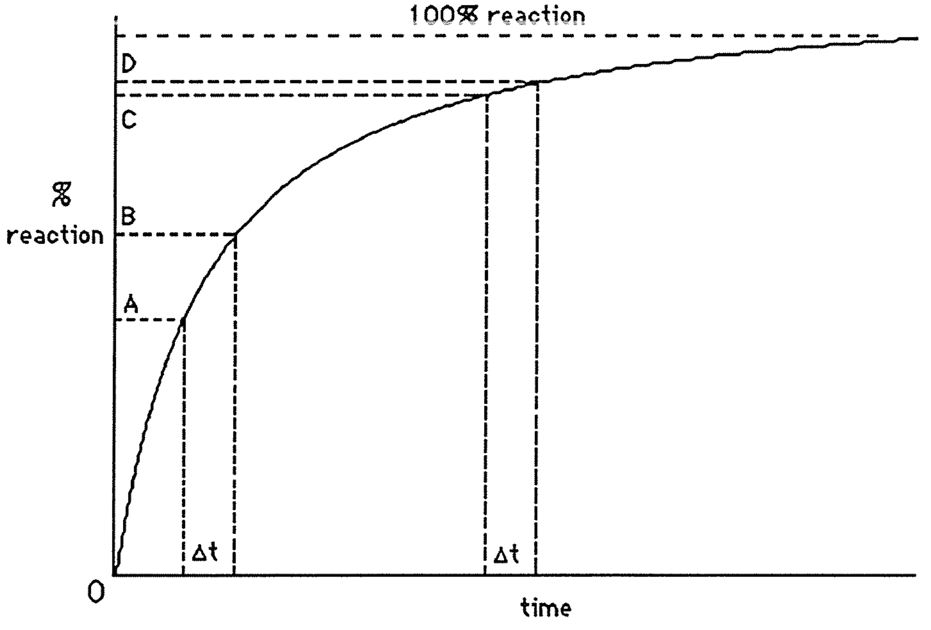

figure 1-4 Variation of reaction rate with time

1.2.3 Rate law

A rate law or rate expression or rate expression is an equation which relates the rate of reaction to the concentration of reactants . It is determined by experiment. In simple reactions the rate law takes one of the forms shown in table 1-1 where x again represents concentration of product at time t.

Order	Rate law (differential form)	Rate law (integrated form)	half-life ($\propto$ to)
0	$dx/dt = k$	$kt = x$	a^1
1	$dx/dt = k(a-x)$	$kt = \ln(a/(a-x))$	a^0
2	$dx/dt = k(a-x)^2$	$kt = x/(a(a-x))$	a^{-1}
3	$dx/dt = k(a-x)^3$	$kt = 1/(2(a-x)^2) - 1/(2a^2)$	a^{-2}
2	$dx/dt = k(a-x)(b-x)$	$kt = 1/(a-b) \ln(b(a-x)/a(b-x))$	—

table 1-1 Simple rate laws

In complex reactions the rate law often takes a more elaborate form and fractional powers occur.

1.1.4 The Order of a reaction

The instantaneous rate of any isothermal process in dilute systems is found to be proportional to the product of the concentrations, n_A, n_B,..... .Thus if n_P denotes the concentration , at any time , of the products in the reaction $\nu_A A + \nu_B B + \ldots\ldots\ldots\ldots \rightarrow P$, the instantaneous rate of reaction is given by the equation

$$\frac{dn_P}{dt} = k_v \, n_A^{\nu_A} \, . \, n_B^{\nu_B} \, \ldots\ldots \qquad \textbf{(1-5)}$$

where k_v is the velocity or rate constant.

The power to which the concentration of a reactant must be raised in order to reproduce the experimental rate of reaction is known as the order of the reaction with respect to that reactant . The net, or over-all , order of reaction ,ν, is the sum of the orders with respect to all the reactants :

$\nu = \nu_A + \nu_B + \ldots\ldots\ldots\ldots$

Experiments show that ν is usually 1 or 2 for reactions in solution. It should also be noted that if a chemical reaction proceeds in a series of sequential stages , then the rate determining or rate contralling stage is the slowest stage.

1.2.5 Half Life

In some cases it is convenient to define the rate of a chemical reaction by stating the time taken for 50% reaction to occur. This time is called the half-life (symbol $t_{1/2}$). The half-life depends on the initial concentrations as well as upon the rate constant. We find this important in Michaelis-Menten reaction kinetics.

1.2.6 Steady State

Chemical reactions approach completion gradually and so there is no instant of time at which the reaction finishes . Because it is often necessary to know what the final concentrations of the reactants are to be, we often define steady state to be the infinite time at which the reaction is complete for practical purposes. Of course for chemistry purposes this is not when we have reached a state of equilibrium (we have a state of equilibrium throughout, at least a local equilibrium) but experimentally one can tell that 'infinite' time has been reached by the constancy of the reaction mixture when we have reached a state of global equilibria.

1.2.7 Determination of the Order of a Reaction

The two most convenient methods of determining the order of a reaction from the experimental results are the method of empirical fit and the half-life method.

1.2.7.1 The method of empirical fit

Experimental data is found of values of x at different times, t. These data are all submitted into each of the rate laws in turn until a law is found that gives constant values of k, or that gives a straight line plot when the appropriate function of x is plotted against time. Thus , if it is suspected that a reaction is first order , a graph of log(a-x) against time is plotted.

1.1.7.2 The half-life method

By combining the results in table 1-1 it is seen that if n equals the order of reaction, then the half-life of a particular order of reaction is given by

$t_{1/2} \propto a^{1-n}$ or

$$t_{1/2} = Ca^{1-n} \qquad \textbf{(1-6)}$$

where C is a proportionality constant .
Taking logs of 1-6 we get

$$\log t_{1/2} = \log C + (1-n) \log a \qquad \textbf{(1-7)}$$

Thus if a graph of the logartihm of the half-life is plotted against the logarithm of the initial concentaration , a straight line will be obtained with a slope of 1,0,-1,or -2 for a zero , first second or third -order reaction respectively.

If a straight line is not obtained in the plot, the kinetics are governed by more complicated equations than those in table 1-1 (e.g. fractional orders or consecutive reactions.

An example of this is the Michaelis-Menten reaction in enzyme catalysis .We can, by a similar process determine the approximate order of this reaction by the half-life method.

1.2.8 Enzyme Catalysis (The Michaelis-Menten reaction)

In biochemical systems, a small amount of enzyme (E) catalyses conversion of a substrate (S) to product (P). In many cases, the rate law is observed to be of the form

$$\frac{d[P]}{dt} = \frac{kE_0[S]}{K_m + [S]} \qquad \textbf{(1-8)}$$

where E_0 is the total enzyme concentration . Other interesting experimentally observed effects are that the rate of reaction is usually proportional to the enzyme concentration. If the substrate concentration is high, the rate of reaction is independent of the substrate concentration (i.e. the reaction is zero order with respect to the substrate) . On lowering the substrate concentration, the order increases until in dilute solution , the rate becomes proportional to the substrate concentration.
The Michaelis-Menten mechanism (1913) is the simplest model consistent with the above observed form.

Here k_1 is the rate constant for the forward reaction and k_1^{-1} is the rate constant for the reverse reaction.

These are not multiplicative inverses of each other.

$$E + S \underset{k_1^{-1}}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_2} E + P \qquad \textbf{(1-9)}$$

Assuming thtat ES is in steady state we find

$$[ES] = \frac{k_1[E][S]}{k_1^{-1} + k_2} \qquad \textbf{(1-10)}$$

and the rate of product formation is

$$\frac{d[P]}{dt} = \frac{k_2[E][S]}{K_m} \qquad \textbf{(1-11)}$$

where

$$K_m = \frac{k_2 + k_1^{-1}}{k_1} \qquad \textbf{(1-12)}$$

K_m is known as the Michaelis-Menten constant or sometimes simply as the Michaelis constant . In general , it is not an equilibrium constant but a 'steady state ' constant.

Since the uncomplexed enzyme concentration is generally not experimentally accessible, equation(1-11) is more useful when expressed in terms of the total enzyme concentration $[E]_0$.

Since
$[E]_0 = [E] + [ES]$, we find that

$$[E] = \frac{Km[E]_0}{(Km + [S])} \qquad \textbf{(1-13)}$$

and hence the reaction rate or reaction velocity

$$v = \frac{d[P]}{dt} = \frac{k_2[E]_0[S]}{Km + [S]} \qquad \textbf{(1-14)}$$

which is precisely the form observed experimentally in (1-8)

By varying the substrate concentration , both k_2 , known as the turnover number and the Michaelis constant can be determined.

Only with reactions for which k_2 is much less than k_1^{-1} is Km numerically equal to the dissociation constant of the equilibrium

$$ES \rightleftharpoons E + S$$

Equation 1-14 shows that the rate of reaction is directly proportional to enzyme concentration ; it also gives the dependency of rate on substrate. Provided the total enzyme concentration is unchanged, a plot of the initial reaction rate against the initial substrate concentration has the characteristic shape illustrated in figure 1-5

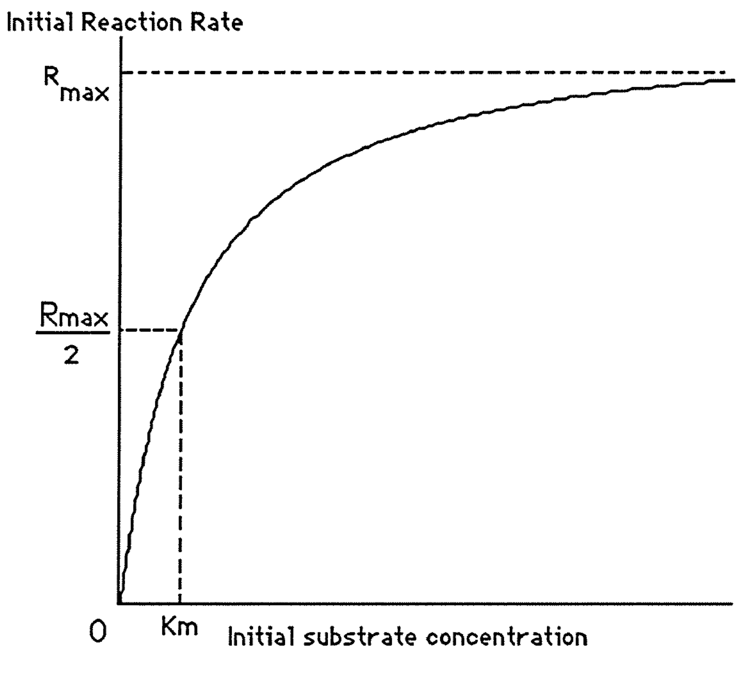

figure 1-5 Initial rate of an enzyme-catalysed reaction obeying equation (1-8) with $[E]_0$ = constant

At very low substrate concentration , [S] is much less than K_m and the plot obeys

$$\text{reaction rate} = v = \frac{k_2\,[E]_0[S]}{K_m} \qquad \textbf{(1-15)}$$

which shows first-order dependency in S.

Under more typical conditions , when [S] is much greater than K_m

$$\text{reaction rate} = k_2[E]_0$$

When this condition applies a maximum or limiting rate of reaction (R_{max}) is attained with effectively all of the enzyme in the form of enzyme-substrate complex , i.e. the enzyme is saturated and there is no free enzyme.
Thus $R_{max} = k_2[E]_0$ and the reaction shows zero-order kinetics with respect to the substrate S.

The equation (1.14) becomes exceptionally simple. The rate of product formation is a constant , $V = R_{max} = k_2[E]_0$. The Michaelis constant can then be determined from the integrated form of 1-14

$$-K_m \ln\left\{\frac{[S]}{[S]_0}\right\} = [S] - [S]_0 + Vt \qquad \textbf{(1-16)}$$

by plotting ln[S] vs. [S] + Vt; the slope is $-K_m$.

We note that

$$\frac{dP}{dt} = -\frac{dS}{dt}$$

Alternatively the reaction velocity v = d[P]/dt can be plotted as a function of substrate concentration in a variety of ways. The most common are

$v^{-1} = 1/V + (K_m/V)[S]^{-1}$ (Lineweaver-Burk)
$v = V - K_m(v/[S])$ (Eadie)
$[S]/v = K_m/V + [S]/V$ (Hanes)

Substituting equation 1-16 into equation 1-14 gives

$$\text{reaction rate} = v = \frac{d[P]}{dt} = \frac{R_{max}[S]}{K_m + [S]}$$

The Michaelis constant has the dimension of concentration and is equal to the concentration of substrate which gives an initial rate of $R_{max}/2$. The ratio of $R_{max}/[E]_0$ is the turnover number. It has the dimension of recriprocal time and indicates the number of substrate molecules converted to products per active site in unit time.

1.3 Biofilm model

We develop diffusion and reaction in any general system which is a solid material with pores through which the reactants and products diffuse. The system is often known as a heterogeneous system. The biofilm which consists of layer of microorganisms held in place by extracellular material around a support material, are analogous to porous catalyst particles employed in conventional heterogeneous reactor systems. We recognise this analogy and attempt an analysis of the biofilm processes . We shall as an assumption model the system as a simple diffusion using an effective diffusion coefficient. A mass balance on a volume of the porous medium gives

$$\frac{\partial S}{\partial t} = \left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right) - R(S) \qquad \textbf{(1-21)}$$

where R(S) is the rate of reaction per unit volume as defined in chap 1.2
(It is positive since the substrate concentration is increasing with time).

Since we are dealing with growth of bacteria as our solid porous media, we must assume that this volume must be solid plus void volume. J is the flux of material (in units of concentration per time per unit area - including again both solid and void area) J_x is the x component of the vector J. We then obtain from Fick's first law

$$\omega = DA\frac{\partial S}{\partial x} \qquad \textbf{(1-22)}$$

where	ω is mass flow and has units	$kg\ s^{-1}$
	D is difusivity constant	$m^2\ s^{-1}$
	A is area	m^2
	S is substrate concentration	kgm^{-3}
	x is distance	m

an equation that expresses the flux J.

$$J = \frac{\omega}{A} = D\,\nabla S \qquad \textbf{(1-23)}$$

units (conc. per unit time per unit area) or

$$J_x = D\frac{\partial S}{\partial x}$$

$$J_y = D\frac{\partial S}{\partial y}$$

$$J_z = D\frac{\partial S}{\partial z}$$

and D is the effective diffusivity constant.

The equation (1-23) assumes equimolar diffusion (exactly the same amount of reactant diffuses in as diffuses out) and all the microscopic details of the porous media are lumped into the diffusion coefficient. Obviously to model a specific physical situation the diffusion coefficient must either be measured or deduced from similar systems. This has been done and this thesis shall use the measured values of the diffusion coefficient and other constants involved. A list of these are given in Chapter 3.6

With this approximation, the equation becomes

$$\frac{\partial S}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial S}{\partial x}\right) + \frac{\partial}{\partial y}\left(D \frac{\partial S}{\partial y}\right) + \frac{\partial}{\partial z}\left(D \frac{\partial S}{\partial z}\right) - R(S) \qquad \textbf{(1-26)}$$

or

$$\frac{\partial S}{\partial t} = \nabla \cdot D \quad \nabla S \quad - R(S)$$

$$= D \nabla^2 S - R(S)$$

since D is constant and where ∇^2 is defined to be the Laplacian operator .

1.3.1 Diffusion in a slab

We assume first that our bioslab is porous and is infinite in extent in two directions giving a large plane sheet with diffusion through the thickness of the sheet

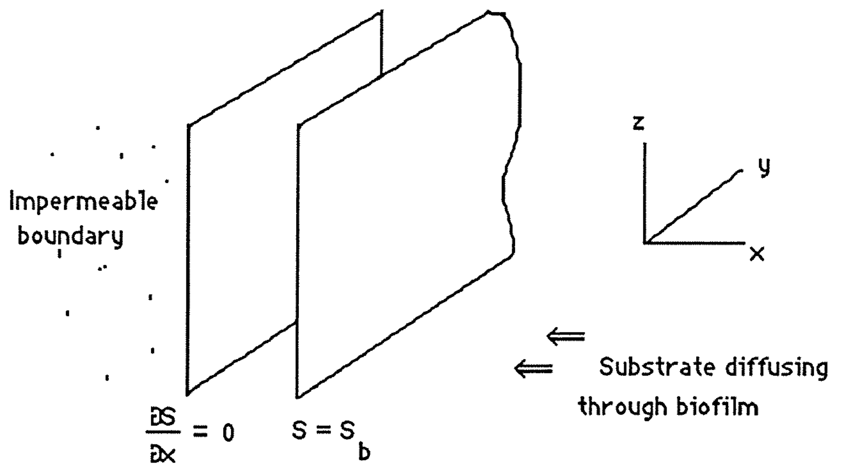

figure 1-6 Substrate diffusing through a slab

We may assume that there is negligible variation of the concentration of the substrates in the z-directions and thus equation simplifies to one dimension.

We then get the partial differential equation

$$\frac{\partial S}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial S}{\partial x}\right) - R(S) \qquad \mathbf{(1\text{-}27)}$$

We notice that equation 1-27 is parabolic (evolutionary in nature)
We require an initial value of the concentration of substrate at each position.
$S(x,0) = S_0(x)$

The concentration S depends on two independent variables. At steady state the time derivative is zero and the above equation reduces to the ordinary differential equation below where the concentration of substrate, S depends on only one independent variable.

$$\frac{d}{dx}\left(D \frac{dS}{dx}\right) - R(S) = 0 \qquad \mathbf{(1\text{-}28)}$$

or

$$D\frac{d^2S}{dx^2} - R(S) = 0 \qquad \mathbf{(1\text{-}29)}$$

since D is a constant

Equations 1-28 and 1-29 are second order and the theory of second order ordinary differential equations says that we must specify two constants in the general solution.

We do that by stating two boundary conditions, one at each side of the slab.

Here we are assuming that one side of the slab is impermeable which means that there is absolutely no flux and the concentration in the bulk liquid of substrate in the bulk liquid is held fixed at the other end.

The boundary conditions are therefore

$$x = L_m \qquad -D \frac{dS}{dx} = 0$$

$$x = L_{bs} \qquad S = S_b$$

where

L_m is the thickness of the support media measured from the centre of the slab

and

L_{bs} is the thickness of the support media with biofilm (bioslab) measured from the centre of the slab.

1.3.2. Diffusion through a cylinder

By solving equation 1-26 in two or three space dimensions, we also have a parabolic partial differential equation with the t variable being evolutionary and the x,y,and z variables being of boundary-value type.

In two dimensions, we have

$$\frac{\partial S}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial S}{\partial x}) + \frac{\partial}{\partial y}(D\frac{\partial S}{\partial y}) - R(S)$$

$$= D(\frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2}) - R(S) \qquad \textbf{(1-30)}$$

for D a constant

At steady-state situations the equation reduces to

$$\frac{\partial}{\partial x}(D\frac{\partial S}{\partial x}) + \frac{\partial}{\partial y}(D\frac{\partial S}{\partial y}) - R(S) = 0 \qquad \textbf{(1-31)}$$

or

$$D(\frac{\partial^2 S}{\partial x^2} + \frac{\partial^2 S}{\partial y^2}) - R(S) = 0$$

for D a constant.

The above equation 1-31 is elliptic in nature.

By assuming that the object we are modelling is an infinite cylinder we may substitute cylindrical coordinates

$x = r \cos \varphi$

$y = r \sin \varphi$

into equation 1-31 to reduce it to only one independent variable - radius.

A Laplacian in cylindrical coordinates is defined to be

$$\nabla^2 S = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial S}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 S}{\partial \varphi^2} + \frac{\partial^2 S}{\partial z^2} \qquad \textbf{(1-32)}$$

By assuming that there is no significant rate of change of substrate concentration with angle and negligible rate of change of substrate in the z direction equation 1-26 reduces to

$$\frac{\partial S}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial S}{\partial r}\right) - R(S) \qquad \textbf{(1-33)}$$

This equation models reaction and diffusion through a cylinder that is very long in the z direction, so that the z variations are negligible. For our purposes we shall take our cylinder to be covered by a layer of biofilm. We model the reaction and diffusion through this biofilm.

We shall also assume that diffusion is isotropic.

The boundary conditions are

at r_{bc} $\quad S = S_b$

at r_{sm} $\quad D\frac{\partial S}{\partial r} = 0$

where

r_{bc} is the total radius of the biocylinder and
r_{sm} is the inner radius or radius of the cylinder support media.

A schematic of our biocylinder is given below

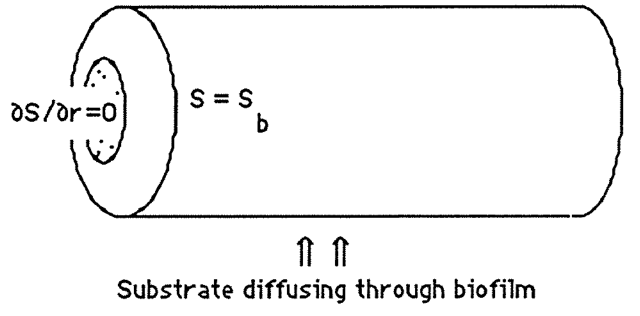

figure 1-7 Substrate diffusing through a biocylinder

3. Diffusion in a sphere

We have equation 1-26 in three dimensions . Since we are modelling reaction and diffusion within a sphere it would be most convenient to substitute spherical coordinates

$x = r \cos \varphi \sin \theta$
$y = r \sin \varphi \sin \theta$
$z = r \cos \theta$

into equation1-26 to reduce the number of independent variables by 2.

A Laplacian in spherical polar coordinates is defined to be

$$\nabla^2 S = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial S}{\partial r}\right) + \frac{1}{r^2 \sin \theta}\frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial S}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 S}{\partial \varphi^2}$$

By assuming that there is no rate of change of concentration with the angles, i.e. is spherically symmetrical, this equation reduces to

$$\frac{\partial S}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial S}{\partial r}\right) - R\,(S) \qquad \textbf{(1-34)}$$

assuming that D is a constant.

As with the biocylinder, we shall also assume that diffusion is isotropic.

A schematic diagram of the bioparticle model is as follows

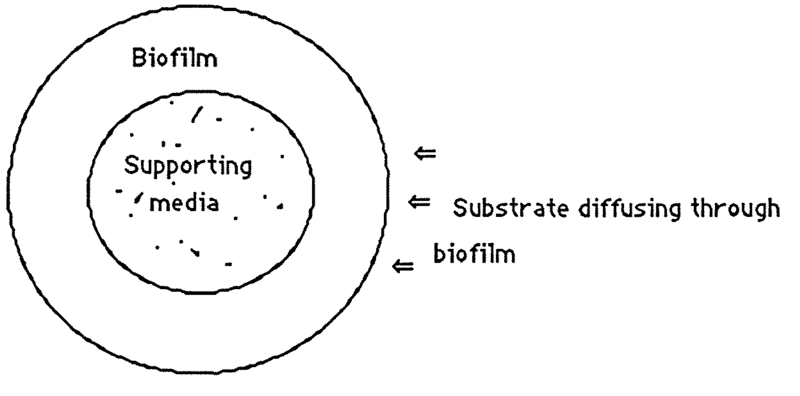

figure 1-8 Substrate diffusing through a bioparticle

Comment

Steady State diffusion problems are generally elliptic in nature and if the problem is unsteady-state or evolutionary the added accumulation term makes them parabolic.

We deduce this classification from the following general linear second-order equation

$$A\frac{\partial^2 S}{\partial x^2} + B\frac{\partial^2 S}{\partial x\,\partial y} + C\frac{\partial^2 S}{\partial y^2} = 0$$

The type of equation is deduced from the discriminant
$\Delta = B^2 - 4AC$

$\Delta < 0$ elliptic
$\Delta = 0$ parabolic
$\Delta > 0$ hyperbolic

This thesis shall be divided into two parts,

i) the first part dealing with the steady state elliptic equations associated with equations 1-27,1-33 and1-34. This is done in Chapter 2.

ii) the second part dealing with the unsteady state , time dependent parabolic equations associated with these equations.This is done in Chapter 3.

1.4 The problem

1.4.1 (The Unsteady State Problem-Non dimensionless coordinates)

We reduce the 3 equations (1-27,1-33 and 1-34) of the previous section to a single equation by specifying a parameter for each type.
The equations are therefore represented by

$$\frac{\partial S}{\partial t} = \frac{D}{r^{a-1}} \frac{\partial}{\partial r} \left(r^{a-1} \frac{\partial S}{\partial r}\right) - R(S) \qquad \textbf{(1-35)} \quad \textbf{(P)}$$

where

D is as before, the Diffusivity constant,
R(S) is the rate of reaction per unit volume,
r is the radius in spherical and cylindrical geometries and thickness measured from the centre of the slab in slab geometries
and

a = 1 represents slab geometry
a = 2 " cylindrical geometry
a = 3 " spherical geometry

Initial conditions

As an initial condition, we specify $S(x,0) = S_0(x) = 0$ to the above problem.

Boundary conditions for total penetration

at inner support media radius radius $r = r_m$, $\partial S/\partial r = 0$
at outer bioparticle radius $r = r_{bp}$, $S = S_b$

Boundary conditions for partial penetration

We shall see that with reaction rates of zero-order kinetics, substrate is able to diffuse only partially into the biofilm if the Thiele modulus ϕ^2 is of a large enough order.

The overall reaction rate will be diffusion or mass transport limited.

We would have to redefine our inner boundary condition to be at some new value of r (call it r_i for new inactive radius) and the appropriate boundary condition for the steady state problem now becomes

at radius of partial penetration $r = r_i$ $\partial S/\partial r = S = 0$
at outer radius $r = r_{bp}$ $S = S_b$

1.4.2 Reaction kinetics we are interested in

The various rates of reactions that we shall be interested in, in this thesis are mainly of simple nth order reactions and Michaelis-Menten reaction kinetics.These have the following form

1. nth order kinetics

has the form

$R_n(S) = \rho_{bf} k_n S^n$

where ρ_{bf} is the biofilm density (kg m^{-3})
k_n is the nth order rate constant
S^n is the substrate concentration (kg m^{-3}) raised to the power of n

2.Michaelis-Menten kinetics

has the form

$$R_{mm}(S) = \frac{\rho_{bf}\mu_m S}{Y_{x/s}(K_s + S)}$$

where

ρ_{bf} is the biofilm density as before
$Y_{x/s}$ is the growth yield of bacteria (kg kg^{-1})
μ_m is a rate constant particular to Michaelis Menten reaction kinetics defined in Chapter 1.1.7

1.4.3 The Unsteady State Problem - dimensionless coordinates

The Problem (P) with reaction rate R(S) may be converted to the dimensionless form

$$\frac{\partial y}{\partial t} = \frac{1}{x^{a-1}}\frac{\partial}{\partial x}\left(x^{a-1}\frac{\partial y}{\partial x}\right) - \phi^2 F(y) \qquad \textbf{(1-36)}$$

by the substitution

$$y = \frac{S}{S_b} \quad \text{and} \quad x = \frac{r}{r_{bp}}$$

1.4.3.1 Dimensionless Parameters

ϕ^2, known as the Thiele modulus is a dimensionless group which in nth order kinetics is the ratio of characteristic time for diffusion r_{bp}^2/D to characteristic time for reaction $1/k_n S_b^{n-1}$.

The Thiele modulus squared is thus the ratio of two characteristic times, diffusion to reaction. If the reaction is very fast its characteristic time is small and the Thiele modulus is large. Likewise, if the diffusion is very fast its characteristic time is small and the Thiele modulus is small.

Therefore

1 In nth order reactions

$$\phi^2 = \frac{k_n r_{bp}^2 S_b^{n-1}}{D}$$

2. In Michaelis-Menten reaction kinetics

$$\phi^2 = \frac{r_{bp}^2 \rho_{bf} \mu_m}{D Y_{x/s} K_s}$$

and we also define another dimensionless constant

$$\beta = \frac{S_b}{K_s}$$

Our problem (P) may then be expressed as

$$\frac{\partial y}{\partial t} = \frac{1}{x^{a-1}} \frac{\partial}{\partial x} (x^{a-1} \frac{\partial y}{\partial x}) - \phi^2 F(y) \qquad \textbf{(1-37)} \qquad \textbf{(P-US)}$$

where

$F(y) = F_n(y) = y^n$ for nth order kinetics and

$F(y) = F_{mm}(y) = \frac{y}{1+\beta y}$ for Michaelis-Menten kinetics

The Unsteady-State problem (P-US) has the boundary conditions

$t > 0 \quad y(1,t)=1$

$t > 0 \quad$ at $x_m = \frac{r_m}{r_{bp}} = \alpha$, $\frac{\partial y}{\partial x}(\alpha,t) = 0$

and the initial condition

$t = 0 \quad \alpha < x < 1, \; y = 0$

1.4.4 The Steady State problem - Dimensionless coordinates

The Steady State problem follows from the Unsteady State problem (P-US) by removing time dependency.

The steady state problem is therefore is therefore

$$\frac{1}{x^{a-1}}\frac{d}{dx}\left(x^{a-1}\frac{dy}{dx}\right) = \phi^2 F(y) \qquad \textbf{(1-38)} \qquad \textbf{(P-SS)}$$

with boundary conditions

$y'(\alpha) = 0$ and $y(1) = 1$

note 1:

It may be noticed that α may be incorporated as a third parameter into the Steady State problem (P-SS) by the substitution

$$z = \frac{x - \alpha}{1 - \alpha}$$

e.g. in Michaelis-Menten kinetics our equation would become

$$\frac{d^2y}{dz^2} + \frac{z(a-1)(1-\alpha)}{(1-\alpha)z + \alpha}\frac{dy}{dz} = \frac{(1-\alpha)^2\phi^2 y}{1+\beta y} \qquad \textbf{(1-39)}$$

with boundary conditions

$y'(0) = 0$ and $y(1) = 1$

and nth order reaction kinetics would be

$$\frac{d^2y}{dz^2} + \frac{z(a-1)(1-\alpha)}{(1-\alpha)z + \alpha}\frac{dy}{dz} = \phi^2 y^n \qquad \textbf{(1-40)}$$

with boundary conditions $y'(0) = 0$ and $y(1) = 1$

However, we shall find it easier to work with the Laplacian form i.e. equation(1-38)

note 2:

It may also be noticed that with Michaelis-Menten Kinetics, all parameters may be incorporated into the boundary conditions by the scalar group transformation.

$y = \bar{y}/\beta$ and

$x = \bar{x}/\phi$

to obtain

$$\bar{y}'' + \frac{(a-1)\bar{y}'}{\bar{x}} = \frac{\bar{y}}{1 + \bar{y}} \qquad \textbf{(1-41)}$$

with boundary conditions

$\bar{y}'(\alpha\phi) = 0$ and $\bar{y}(\phi) = \beta$

note 3:
Likewise, we may reduce the boundary value problem

$$\frac{d^2y}{dx^2} + \frac{(a-1)}{x}\frac{dy}{dx} = \phi^2 y^n$$

with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$
into the form

$$\frac{d^2\bar{y}}{dx^2} + \frac{(a-1)}{x}\frac{d\bar{y}}{dx} = \bar{y}^n \qquad (1\text{-}42)$$

with boundary conditions

$$\bar{y}'(\alpha) = 0 \quad \text{and} \quad \bar{y}(1) = \frac{1}{\phi^{2(\frac{-1}{n-1})}}$$

by the stretching group transfomation

$$y = \phi^{2(\frac{-1}{n-1})}\,\bar{y}\,, \qquad n \neq 1$$

and

$$x = \bar{x}\,/\phi$$

if $n = 1$.

1.4.5 The Effectiveness Factor

The effectiveness factor is, by definition the average reaction rate with diffusion divided by the average reaction rate is evaluated at the boundary conditions(defn. Aris[2],pp59). If the rate of diffusion is very rapid the rate of reaction evaluated at the boundary equals the average reaction rate and the effectiveness factor equals unity.

The effectiveness factor in the domain α to 1 is therefore

$$\eta = \frac{\phi^2 \int_\alpha^1 F(y(x))\, x^{a-1} dx}{\phi^2 \int_\alpha^1 F(y(1))\, x^{a-1}\, dx}$$

Example 1

Effectiveness factors of nth order reactions

Since $y(1) = 1$, $F(y(1)) = 1^n = 1$

Substituting

$$F(y) = \frac{1}{\phi^2} \frac{1}{x^{a-1}} \frac{d}{dx} \left(x^{a-1} \frac{dy}{dx} \right)$$

into the above definition of effective factors we obtain by integrating in the domain α to 1

$$\eta = \frac{\int_\alpha^1 \frac{1}{\phi^2} \frac{1}{\cancel{x^{a-1}}} \frac{d}{dx} \left(x^{a-1} \frac{dy}{dx} \right) \cancel{x^{a-1}} dx}{\int_\alpha^1 x^{a-1} dx}$$

which upon cancelling factors and integrating becomes

$$\eta = \frac{\left. \frac{1}{\phi^2} x^{a-1} \frac{dy}{dx} \right|_\alpha^1}{(1 - \alpha^a) / a}$$

$$= \frac{\left. \frac{1}{\phi^2} \frac{dy}{dx} \right|_1 - \left. \frac{\alpha^{a-1}}{\phi^2} \frac{dy}{dx} \right|_\alpha}{(1 - \alpha^a) / a}$$

$$= \frac{\frac{a}{\phi^2} \left.\frac{dy}{dx}\right|_1}{(1 - \alpha^a)} \quad \text{since } y'(\alpha) = 0$$

Example 2

Effectiveness factor of Michaelis-Menten reaction kinetics

Repeating the procedure for nth order reaction kinetics, and noticing that

$$F_{mm}(y(1)) = \frac{1}{1 + \beta},$$

we obtain

$$\eta = \frac{\frac{1}{\phi^2} x^{a-1} \left.\frac{dy}{dx}\right|_\alpha^1}{\int_\alpha^1 \frac{1}{1+\beta} x^{a-1} \, dx}$$

or

$$\eta = \frac{a(1 + \beta) \left.\frac{dy}{dx}\right|_1}{\phi^2(1 - \alpha^a)}$$

for Michaelis-Menten reaction kinetics with a = 1,2,3 being slab, cylindrical and spherical geometries respectively.

1.5 Definitions and Theorems

An important implement in the investigation of second order elliptic and parabolic problems is the maximum principle. We quote many relevant theorems, some by myself, but most from standard texts on maximum principles and we shall be using these principles in developing proofs for existence and uniqueness theorems . They may also be applied to finding upper and lower bounds to our solutions and are also used in monotonicity properties of differential equations. All the definitions and theorems given below appear to be standard on elliptic and parabolic partial differential equations and they are only included for easy reference. For more thorough and rigourous uses of the maximum principle , the reader of this thesis is advised to consult Sattinger[1] and Protter and Weinberger[16]

1.5.1 One-dimensional Maximum Principle

Definition 1.1 (Linear differential Operator, L[u])

We use the letter L followed by brackets to denote a linear operator acting on functions , i.e. L assigns to each function u of a certain class, a function L[u] of another class. We say that L is linear if, whenever $L[u_1]$ and $L[u_2]$ are defined, the quantities $L[\alpha u_1+\beta u_2]$ and $\alpha L[u_1] + \beta L[u_2]$ are also defined for all constants α and β, and the equation

$L[\alpha u_1+\beta u_2] = \alpha L[u_1]+\beta L[u_2]$ holds.

We define the more general linear differential operator to be

$(L+h)[u] \equiv u'' + g(x)u' + h(x)u$ in 1-dim.

A function that is continuous on the closed interval [a,b] takes on its maximum at a point on this interval. If u(x) has a continuous second derivative, and if u has a relative maximum at some point c between a and b then

$u'(c) = 0$ and $u'' \leq 0$. (i)

Suppose that in an open interval (a,b) , u is known to satisfy a differential inequality of the form

$L[u] \equiv u'' + g(x)u' > 0$ (ii)

where g(x) is any bounded function

It is clear that relations (i) cannot be satisfied at any point c in (a,b). Consequently, whenever (ii) holds, the maximum of u in the interval cannot be attained anywhere except at the endpoints a or b.

Theorem 1.1 (One-dimensional maximum principle)

Suppose $u = u(x)$ satisfies the differential inequality

$L[u] \equiv u'' + g(x)\, u' \geq 0$ for $a < x < b$ with g(x) a bounded function.

If $u(x) \leq M$ in (a,b) and if the maximum M of u is obtained at an interior point c of (a,b) then $u \equiv M$.

Proof:

(1) Suppose $u(c) = M$ and there is a point $d \in (a,b)$ such that $u(d) < M$.
This leads to a contradiction

(2) Without loss of generality, let $d > c$

(3) Define the auxiliary function

$$z(x) = e^{\alpha(x-c)} - 1$$

with α a positive constant that has to be determined.
This function has the properties
$z(x) < 0$ for $a < x < c$
$z(x) > 0$ for $c < x < b$ and
$z(c) = 0$

(4) Compute $L[z]$
$z(x) = e^{\alpha(x-c)} - 1$
$z'(x) = \alpha e^{\alpha(x-c)}$
$z''(x) = \alpha^2 e^{\alpha(x-c)}$
and therefore
$L[z] = z'' + g(x)z' = \alpha[\alpha + g(x)]e^{\alpha(x-c)}$

(5) As mentioned in (3), we choose a positive constant α so that it satisfies the inequality
$\alpha > -g(x)$ for all $x \in (a,b)$
This is always possible since $g(x)$ is bounded.

(6) Define $w(x) = u(x) + \varepsilon z(x)$ where ε is a positive constant chosen so that it satisfies the inequality

$$\varepsilon < \frac{M - u(d)}{z(d)}$$

This is always possible since we assumed in (1) that $u(d) < M$ and $z(d) > 0$

(7) $w(x) < M$ for $a < x < c$
(since z is negative for $a < x < c$)

(8) $w(d) = u(d) + \varepsilon\, z(d) < u(d) + M - u(d) = M$ (by definition of ε)

(9) At the point c
$w(c) = u(c) + \varepsilon\, z(c) = M$

(10) We have shown in (9) that w has a maximum greater than or equal to M which is attained at an interior point of the interval (a,b). But $L[w] = L[u] + \varepsilon\, L[z] > 0$ so that by (0) concerning the strict inequality (ii), we thereby reach a contradiction

(11) Therefore if $u(x) \leq M$ in (a,b) and if the maximum M of u is obtained at an interior point c of (a,b) then $u \equiv M$. ⊠.

Corollary 1.1(One-dimensional minimum principle)

By applying the above theorem to (-u) we have the minimum principle which asserts that a nonconstant function , the differential inequality
$L[u] \leq 0$ cannot attain its minimum at an interior point.

Theorem 1.2

Suppose u is a nonconstant function which satisfies the inequality
$L[u] \equiv u'' + g(x)u' \geq 0$ in (a,b) and has one-sided derivatives at a and b, and suppose g is bounded on every closed subinterval of (a,b) .
If the maximum of u occurs at x=a and g is bounded below at x=a, then $u'(a) < 0$
If the maximum occurs at x=b and g is bounded above at x=b, then $u'(b) > 0$.

Proof:

(1) Suppose that $u(a) = M$, $u(x) \leq M$ for $a \leq x \leq b$ and that for some point $d \in (a,b)$ we have $u(d) < M$
Define as before an auxiliary function
$z(x) = e^{\alpha(x-a)} - 1$ with $\alpha > 0$.

(2) Select $\alpha > -g(x)$ for $a \leq x \leq d$ so that $L[z] > 0$

(3) Form the function $w(x) = u(x) + \varepsilon z(x)$ with ε chosen so that

$$0 < \varepsilon < \frac{M - u(d)}{z(d)}$$

(4) Because $L[w] > 0$, the maximum of w in the interval [a,d] must occur at one of the ends. We have
$w(a) = M > w(d)$
so the maximum occurs at a.

(5) The one-sided derivative cannot therefore be positive at a :
$w'(a) = u'(a) + \varepsilon z'(a) \leq 0$

(6) However $z'(a) = \alpha > 0$ and therefore

(7) $u'(a) < 0$ is the desired result.

(8)If the maximum occurs at x = b, the argument is similar.

⊠.

Theorem 1.3

If u(x) satisfies the linear differential inequality
$(L+h)[u] \equiv u''+g(x)u'+h(x)u \geq 0$ in an interval (a,b) with $h(x) \leq 0$.
If g and h are bounded on every closed subinterval and if u assumes a nonnegative maximum value M at an interior point c, then $u(x) \equiv M$.

Proof:

The proof of theorem 1.3 is an extension of Theorems 1.1 and 1.2. It is easy to see that if the strict inequality $(L+h)[u] > 0$ with $h \leq 0$, holds in an open interval (a,b), then u cannot have a nonnegative maximum in the interior of (a,b). In fact, at any such maximum, we have $u' = 0$, $u'' \leq 0$, $hu \leq 0$ contradicting the above strict inequality. We therefore extend theorems 1.1 and 1.2 by choosing α so large that $(L+h)[u] > 0$. There is no other change in the argument.

(1) The constant α in the function $e^{\alpha(x-c)}-1$ (assuming again that d < c) must only satisfy
$\alpha^2 + \alpha g(x) + h(x)[1 - e^{-\alpha(x-c)}] > 0$

(2) Since $h(x) \leq 0$, it is sufficient to select α so that
$\alpha^2 - \alpha|g(x)| + h(x) > 0$.
This can certainly be done if g(x) and h(x) are bounded.

(3) The rest of the proof follows from the outline of the proof to theorems 1.1 and 1.2 ⊠.

Theorem 1.4

Suppose that u is a nonconstant solution of the differential inequality
$(L+h)[u] \equiv u'' + g(x)u'+h(x)u \geq 0$ (i)
having one-sided derivatives at a and b, that is $h(x) \leq 0$ and that g and h are bounded on every closed subinterval of (a,b) .
If u has a non-negative maximum at a and of the function $g(x) + (x-a)h(x)$ is bounded from below at x=a , then $u'(x) < 0$.
If u has a nonnegative maximum at b and if $g(x)-(b-x)h(x)$ is bounded from above at x = b , then $u'(b) > 0$.

Proof: In extending the proof of theorem 1.2 to theorem 1.4, we need only observe that
$(L+h)[e^{\alpha(x-a)}-1] = e^{\alpha(x-a)}[\alpha^2 + \alpha g + h(1-e^{-\alpha(x-a)})]$

Corollary 1.5.1.4

If u satisfies (i) in (a,b) with $h(x) \leq 0$, if u is continuous on [a,b] and if $u(a) \leq 0$, $u(b) \leq 0$ then $u(x) < 0$ in (a,b) unless $u \equiv 0$.

Theorem 1.5 (Generalised One-dimensional Maximum Principle)

Suppose the operator (L+h)[u] given in (i) with h(x) bounded and with g(x) bounded from below. We note that unlike theorem 1.3,in this theorem, h(x) does not have the condition that it has to be non-positive but that it be bounded.

For any sufficiently short interval [a,b] , a function w can be found which satisfies

$w > 0$ on [a,b],

$(L+h)[w] \leq 0$ in (a,b)

Then if u is any function satisfying (L+h)[u] in (a,b) the function u/w in (a,b) satisfies the maximum principles as given in theorems 1.3 and 1.4

Proof:

(1) We investigate the differential equation

$$(L+h)[u] \equiv u'' + g(x)u' + h(x)u \geq 0, \quad a<x<b \qquad \text{(i)}$$

without the requirement that h(x) be nonpositive.

(2) Suppose we can find a function, w which has a continuous second derivative on [a,b] and which satisfies the inequalities

$$w>0 \text{ on } [a,b] \qquad \text{(ii)}$$

$$(L+h)[w] \leq 0 \text{ in } (a,b) \qquad \text{(iii)}$$

We define the new independent variable

$$v = \frac{u}{w}$$

(3) A simple computation yields

$$(L+h)[u] = (L + h)[vw] = wv''+(2w' + gw)v' + (L+h)[w]\, v \geq 0$$

(4) Dividing through by the positive quantity w, we see that v satisfies the differential inequaltiy

$$v'' + \left(\frac{2w'}{w} + g\right)v' + \frac{1}{w}(L + h)[w]\, v \geq 0 \qquad \text{(iv)}$$

Inequality (iv) when taken in conjunction with (ii) and (iii) shows that v =u/w satisfies theorems 1.3 and 1.4

(6) The argument above depends on the existence of a function w which satisfies (ii) and (iii). It can be shown that a function w that satisfies inequalities (ii) and (iii) is given by

$w = 1 - \beta(x-a)^2$

where the constant β is determined suitably.

⊠.

1.6 Boundary Value Problems

The maximum principle may be used to answer questions about the uniqueness of boundary value problems. The simplest boundary value problems concerns the determination of a solution of the equation

$(L+h)[u] \equiv u'' + g(x)u' + h(x)u = f(x)$ (i)

in an interval (a,b) subject to the boundary conditions

$u(a) = \gamma_1$ (ii)

$u(b) = \gamma_2$

We state a theorem that gives a uniqueness result for boundary value problems

<u>**Theorem 1.6**</u> (Uniqueness theorem for boundary value problems with the simplest kind of boundary conditions)

Suppose that $u_1(x)$ and $u_2(x)$ are solutions of (i) which satisfy the boundary condition (ii). If $h(x) \le 0$ in (a,b) then $u_1 \equiv u_2$.

Proof:

(1) Let $u(x) = u_1(x) - u_2(x)$. Then u satisfies the equation $u'' + g(x)u' + hu = 0$ and the boundary condition $u(a) = u(b) = 0$.

(2) According to theorem 1.3, we know that $u(x) \le 0$ in (a,b). Since the function $-u(x)$ satisfies the same equation with the same boundary conditions, we may apply theorem 1.3 to $-u(x)$ to conclude that $-u(x) \le 0$ in (a,b).

(3) Therefore $u \equiv 0$ in (a,b) and $u_1 \equiv u_2$. ⊠.

<u>**Theorem 1.7**</u> (Uniqueness theorems for boundary value problems with general boundary conditions)

Suppose $u_1(x)$ and $u_2(x)$ are solutions of $u'' + g(x)u' + h(x)u = f(x)$ which satisfy the boundary conditions

$-u'(a)\cos\vartheta + u(a)\sin\vartheta = \gamma_1$

$u'(b)\cos\psi + u(b)\sin\psi = \gamma_2$

where

$\gamma_1, \gamma_2, \vartheta$ and ψ are prescribed constants with $0 \le \vartheta \le \pi/2$, $0 \le \psi \le \pi/2$.

If $h(x) \le 0$ in (a,b) then $u_1 \equiv u_2$ unless $h \equiv 0$, $\vartheta = \psi = 0$, in which case u_1 and u_2 may differ by a constant.

Proof:

(1) As with theorem 1.6, define $u = u_1 - u_2$

(2) Then u satisfies equation $u'' + g(x)\, u' + hu = 0$ and the boundary conditions
$-u'(a)\cos \vartheta + u(a)\sin \vartheta = 0$
$u'(b)\cos \psi + u(b)\sin \psi = 0$

(3) The function $u \equiv M$, a nonzero constant satisfies theses conditions iff $h \equiv 0$ $\vartheta = 0$ and $\psi = 0$.

(4) Suppose u is a nonconstant solution which is positive at some point.

(5) u attains its positive maximum at a or b (theorem 1.3)

(6) Suppose the maximum occurs at a.

(7) We can apply theorem 1.4, which asserts that
$u'(a) < 0$.

(8) Since $0 \leq \vartheta \leq \pi/2$ (and therefore $\cos \vartheta, \sin \vartheta > 0$) and $u(a) > 0$, the first condition of the boundary condition
$-u'(a)\cos \vartheta + u(a)\sin \vartheta = 0$
is violated.

(9) Similarly, if the maximum occurs at b, the second condition of the boundary condition is violated.

(10) This shows a contradiction with (4) and we conclude that any nonconstant solution can never be positive.

(11) We may apply the same reasoning to -u which shows that u can never be negative.

(12) Thus $u \equiv 0$ on [a,b] or $u_1 \equiv u_2$.

⊠.

Example

Consider the two differential equations

1. $\frac{d^2y}{dx^2} + \frac{(a-1)}{x}\frac{dy}{dx} = \phi^2$

and

2. $\frac{d^2y}{dx^2} + \frac{(a-1)}{x}\frac{dy}{dx} = \phi^2 y$

with boundary conditions
$y'(\alpha) = 0$ and $y(1) = 1$

We may choose $\vartheta = 0$ and $\psi = \pi/2$ to satisfy the above more general boundary condition with $a = \alpha$, $b=1$ and $h(x)=0$

Since $0 \le \vartheta \le \pi/2$, $0 \le \psi \le \pi/2$ and $h(x)=0 \le 0$ this clearly show uniqueness of the solutions to the the above two differential equations by the theorem 1.7

1.8 Approximation in Boundary Value Problems

In most cases, it is impossible to find a solution to a boundary value problem explicitly. It is frequently desirable to approximate a solution in such a way that an explicit bound for the error is known. Such an approximation is equivalent to the determination of both upper and lower bounds for the values of the solution. The maximum principles in theorems 1.1 to 1.4 may be used to obtain a bound for a solution u without any actual knowledge of u itself.

1.5.1.8 (Linear Operators)

Theorem 1.8

Suppose that $u(x)$ is a solution of $(L+h)[u] \equiv u'' + g(x)u' + h(x)u= f(x)$ for $a < x < b$,satisfying the boundary condition

$-u'(a)\cos \vartheta + u(a)\sin \vartheta = \gamma_1$

$u'(b)\cos \psi + u(b)\sin \psi= \gamma_2$

where ϑ and ψ are preassigned constants and we assume that $0 \le \vartheta \le \pi/2$ and $0 \le \psi \le \pi/2$, with $h(x) \le 0$.

Suppose also that not all the equalities $\vartheta = 0$, $\psi = 0$, $h \equiv 0$ hold.

If $z_1(x)$satisfies the conditions

$(L+h)[z_1] \le f(x)$ for $a < x < b$

$-z_1'(a)\cos \vartheta + z_1(a)\sin \vartheta = \gamma_1$

$z_1'(b)\cos \psi + z_1(b)\sin \psi= \gamma_2$

and if $z_2(x)$ satisfies the conditions

$(L+h)[z_2] \ge f(x)$

$-z_2'(a)\cos \vartheta + z_2(a)\sin \vartheta = \gamma_1$

$z_2'(b)\cos \psi + z_2(b)\sin \psi= \gamma_2$

then

$z_2(x) \le u(x) \le z_1(x)$

Proof:

(1) We seek a function $z_1(x)$ with the properties :

$(L+h)\ [z_1] \le f(x)$ for $a < x < b$

$-z_1'(a)\cos \vartheta + z_1(a)\sin \vartheta = \gamma_1$

$z_1'(b)\cos \psi + z_1(b)\sin \psi= \gamma_2$

(2) The function $v_1 + u - z_1$ then satisfies
$(L+h)\ [v_1] \geq 0$
$-v_1'(a)\cos\vartheta + v_1(a)\sin\vartheta \leq 0$
$v_1'(b)\cos\psi + v_1(b)\sin\psi \leq 0$

(3) If v_1 is ever positive theorem 1.3 states that its positive maximum occurs at a or at b.
If it occurs at a, we have $v_1(a) > 0,\ \ v_1'(a) \leq 0$.

(4) Since
$-v_1'(a)\cos\vartheta + v_1(a)\sin\vartheta \leq 0$, this can only occur if $\vartheta = 0$ and $v_1'(a) = 0$. Theorem 1.4 then states that $v_1(x)$ is a positive constant thus implying that $h \equiv 0$.

(5) Similarly, v_1 cannot have a positive maximum at b unless $\psi = 0$ and $h \equiv 0$, since-
$v_1'(b)\cos\vartheta + v_1(b)\sin\vartheta \leq 0$

(6) We conclude that unless both ψ and ϑ are zero and $h + 0$, $v_1(x) \leq 0$. That is, $u(x) \leq z_1(x)$

(7) Similarly, if z_2 satisfies the inequalities
$(L + h)[z_2] \geq f(x)$
$-z_1'(a)\cos\vartheta + z_1(a)\sin\vartheta \leq \gamma_1$
$z_1'(b)\cos\psi + z_1(b)\sin\psi \leq \gamma_2$
and if either h is not identically zero or ϑ and ψ are not both zero, then $u(x) \geq z_2(x)$

(8) The result on approximation in boundary value problems then follows

$$z_2(x) \leq u(x) \leq z_1(x)$$

⊠.

Specific functions z_1, z_2 fulfilling the conditions of Theorem 1.8 are easily found in the form of polynomials, exponentials and so forth. We shall use this theorem to develop results that obtain bounds to non-linear boundary value problems that are specific to this thesis.

1.5.1.9 (Non-Linear Operators)

We can extend our results for the linear differential operators to non-linear operators and thereby obtain the theorem

Theorem 1.9

Suppose that

$w'' + H(x,w,w') \geq u'' + H(x,u,u')$

for $a < x < b$ where

$$H, \quad \frac{\partial H}{\partial y} \text{ and } \frac{\partial H}{\partial z} \text{ are continuous and } \frac{\partial H}{\partial y} \leq 0.$$

If $w(x) - u(x)$ attains a nonnegative maximum M in (a,b) then $w(x) - u(x) \equiv M$.

Proof:

(1) Let u(x) be a solution of the non-linear equation

$u'' + H(x,u,u') = 0$ (i)

on an interval $a \leq x \leq b$.

(2) The functions

$$H(x,y,z) \quad , \quad \frac{\partial H(x,y,z)}{\partial y} \quad , \quad \frac{\partial H(x,y,z)}{\partial z}$$

are all assumed to be continuous functions of x,y and z throughout their domains of definition.

(3) We also, in addition , suppose that for each x and z.

$H(x,y_1,z) \leq H(x,y_2,z)$ for all $y_1 \geq y_2$ (ii)

or , this is equivalent to saying that

$$\frac{\partial H}{\partial y} \leq 0.$$

(4) Suppose w(x) satisfies the differential inequality

$w'' + H(x,w,w') \geq 0$ in (a,b) (iii)

(5) We consider the function $v = w - u$ and subtract (i) from (iii) getting

$v'' + H(x,w,w') - H(x,u,u') \geq 0$

(6) After applying the mean value theorem to H above , we find

$$v'' + \frac{\partial H}{\partial z} v' + \frac{\partial H}{\partial y} v \geq 0.$$

We shall assume the quantities

$$\frac{\partial H}{\partial y} \text{ and } \frac{\partial H}{\partial z}$$

are at a value (x, u+λ(w-u), u'+λ(w'-u')) with $0 < \lambda < 1$.

(7) The function v satisfies a linear equation and the maximum principle as given in theorem 1.3 applies.

☒.

We may, in a similar way generalise theorem 1.8 to get the theorem below

Theorem 1.10
Let u(x) be a solution of the boundary value problem

$u'' + H(x,u,u') = 0$ for $a < x < b$ with (i)
$-u'(a)\cos\vartheta + u(a)\sin\vartheta = \gamma_1$
$u'(b)\cos\psi + u(b)\sin\psi = \gamma_2$ (ii)

where $0 \leq \vartheta \leq \pi/2$, $0 \leq \psi \leq \pi/2$ and ϑ and ψ are not both zero.

Suppose that H, $\frac{\partial H}{\partial y}$ and $\frac{\partial H}{\partial z}$ are continuous and $\frac{\partial H}{\partial y} \leq 0$.

If $z_1(x)$ satisfies

$z_1'' + H(x,z_1,z_1') \leq 0$
$-z_1'(a)\cos\vartheta + z_1(a)\sin\vartheta \geq \gamma_1$
$z_1'(b)\cos\psi + z_1(b)\sin\psi \geq \gamma_2$

and if $z_2(x)$ satisfies the conditions

$z_2'' + H(x,z_2,z_2') \geq 0$
$-z_2'(a)\cos\vartheta + z_2(a)\sin\vartheta \leq \gamma_1$
$z_2'(b)\cos\psi + z_2(b)\sin\psi \leq \gamma_2$

then the upper and lower bounds
$z_2(x) \leq u(x) \leq z_1(x)$ are valid.

This theorem implies that a solution of (5) which satisfies boundary conditions (6) must be unique . For if u and û are solutions, we can let $z_1 = z_2 = u$ to find $u \equiv \hat{u}$.

Example 1
nth order reaction kinetics

Consider the differential equation

$$\frac{d^2y}{dx^2} + \frac{(a-1)}{x}\frac{dy}{dx} = \phi^2 y^n$$

with boundary conditions

$y'(\alpha) = 0$ and $y(1) = 1$

Taking boundary conditions
$a = \alpha$
$b = 1$
$\psi = \pi/2$ and $\vartheta = 0$ (which are both not zero) to satisfy the general boundary condition (i), in theorem 1.10

We show that H, $\partial H/\partial y$ and $\partial H/\partial z$ are continuous and $\partial H/\partial y \leq 0$, where

$$H(x,u,u') = (a-1)\frac{y'}{x} - \phi^2 y^n$$

and therefore

$H(x,y,z) = (a-1)\dfrac{z}{x} - \phi^2 y^n$ is continuous in the region $x \in (\alpha,1)$, $y \geq 0$, $z \in \mathbb{R}$

Differentiating with respect to y, we obtain

$\dfrac{\partial H}{\partial y} = -\phi^2 n\, y^{n-1} \leq 0$ for all $n > 0$ since $y \in (0,1)$ for $n > 0$, $n \in \mathbb{R}$

$n = 0,1$ was shown as an example to thm.1.7.

$\dfrac{\partial H}{\partial z} = \dfrac{a-1}{x}$ is continuous in the interval $(\alpha,1)$ where $\alpha \in (0,1)$

It follows from theorem 1.10 that the above differential equation with given boundary conditions must be unique.

Example 2

Michaelis-Menten reaction kinetics

Consider the differential equation

$$y'' + \frac{(a-1)y'}{x} = \frac{\phi^2 y}{1 + \beta y}$$

with boundary conditions

$y'(\alpha) = 0$ and $y(1) = 1$

Taking boundary conditions

$a = \alpha$

$b = 1$

$\psi = \pi/2$ and $\vartheta = 0$ (which are both not zero) to satisfy the general boundary condition (i), as in example 1.

We show that H, $\partial H/\partial y$ and $\partial H/\partial z$ are continuous and $\partial H/\partial y \leq 0$, where

$$H(x,y,y') = (a-1)\frac{y'}{x} - \frac{\phi^2 y}{1 + \beta y}$$

and therefore

$$H(x,y,z) = (a-1)\frac{z}{x} - \frac{\phi^2 y}{1 + \beta y}$$ is continuous in the region $x \in (\alpha,1), y \geq 0, z \in \mathbb{R}$

Differentiating with respect to y, we obtain

$$\frac{\partial H}{\partial y} = -\frac{\phi^2}{(1+\beta y)^2} \leq 0$$ for all $y \in \mathbb{R}$

$$\frac{\partial H}{\partial z} = \frac{a-1}{x}$$ is continuous in the interval $(\alpha,1)$ where $\alpha \in (0,1)$.

It follows that the solution to the above differential equation which satisfies the given boundary conditions must be unique.

For if y and $\hat{y}$

are solutions, we can let $z_1 = z_2 = y$ to find $y \equiv \hat{y}$

1.5.1.11 Approximation to boundary value problems by finding upper and lower bounds

As an example to approximating the boundary value problem

$y'' + H(x,y,y') = 0$ for $\alpha < x < 1$

and where

$$H(x,y,y') = \frac{(a-1)y'}{x} - \frac{\phi^2 y}{1 + \beta y}$$

with boundary conditions

$y'(\alpha) = 0$ and $y(1) = 1$,

we choose z_2 as a lower bound and z_1 as an upper bound such that

$z_1 + H(x,z_1,z_1') \leq 0 \leq z_2 + H(x,z_2,z_2')$ and all boundary conditions are equivalent.

Upper Bounds to y

An appropriate upper bound to y is z_1 where z_1 is such that

$$z_1 + H(x,z_1,z_1') = \frac{(a-1)z_1'}{x} - \frac{\phi^2 z_1}{1 + \beta z_1} \leq 0$$

since

$$\frac{\phi^2 z_1}{1 + \beta z_1} \geq \frac{\phi^2 z_1}{1 + \beta}$$

in the region $z_1 \in (0,1)$

The above inequality assumes that $z_1 > 0$. This will be shown to be true in later chapters.

Lower bounds to y

An appropriate upper bound to y is z_2 where z_2 is such that

$$z_2 + H(x,z_2,z_2') = \frac{(a-1)z_2'}{x} - \phi^2 z_2 \geq 0$$

since

$$\frac{\phi^2 z_2}{1 + \beta z_2} \leq \phi^2 z_1$$

in the region $z_1 \in (0,1)$

As before the, above inequality assumes that $z_1 > 0$.

This will be shown to be true in later chapters.

1.5.2 Elliptic Operators

1.5.2 (The Laplace Operator)

Definition 2.1 (The Laplace Operator)

Let $u(x_1, x_2, \ldots\ldots x_n)$ be twice differentiable function defined in a domain Ω in n-dimensional space.
The Laplace Operator or Laplacian $\Delta \equiv \nabla^2$ is defined as

$$\nabla^2 \equiv \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \ldots\ldots + \frac{\partial^2}{\partial x_n^2}$$

Suppose that u has a local maximum at an interior point of Ω . Then at this point

$$\frac{\partial u}{\partial x_1} = 0 , \quad \frac{\partial u}{\partial x_2} = 0 , \ldots\ldots , \quad \frac{\partial u}{\partial x_n} = 0 .$$

and

$$\frac{\partial^2 u}{\partial x_1^2} \leq 0 , \quad \frac{\partial^2 u}{\partial x_2^2} \leq 0 , \ldots\ldots , \quad \frac{\partial^2 u}{\partial x_n^2} \leq 0.$$

Therefore, at a local maximum, the inequality $\Delta u \equiv \nabla^2 u \leq 0$ must hold.
i.e. If a function satisfies the strict inequality

$$\nabla^2 u > 0 \qquad \text{(i)}$$

at each point of a domain Ω, then u cannot attain its maximum at any interior point of Ω.

Suppose $b_1(x_1, x_2, \ldots\ldots x_n)$, $b_2(x_1, x_2, \ldots\ldots x_n), \ldots\ldots\ldots\ldots b_n(x_1, x_2, \ldots\ldots x_n)$ are any bounded functions defined in Ω .
Without any change in the argument above, we conclude that if u satisfies the strict inequality

$$\Delta u + b_1 \frac{\partial u}{\partial x_1} + b_2 \frac{\partial u}{\partial x_2} + \ldots\ldots + b_n \frac{\partial u}{\partial x} > 0$$

in Ω, then u cannot attain its maximum point at an interior point.

Theorem 2.2 (maximum Principle for the Laplace Operator)
Let $\nabla^2 u \geq 0$ in Ω
If u attains its maximum M at any point of Ω then $u \equiv M$ in Ω

As a consequence of the above theorem, the following result may be obtained. This follows along the lines of theorem 1.10.

Definition 2.2
We have the steady state problem

$$-\Delta u = f(u) \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

Call v a *lower solution* if

$$-\Delta v \leq f(v) \quad \text{in } \Omega$$
$$v \leq 0 \quad \text{on } \partial\Omega$$

and an *upper solution* if the inequalities are reversed

Theorem 2.3
If lower solution v ≤ upper solution w in Ω , then there exists a solution between v and w.

Proof
Based on the maximum principle:
(1) If $-\Delta u \geq 0$ in Ω, then the maximum of u is on $\partial\Omega$.

(2) Suppose first that f is increasing but f' is bounded in Ω.

(3) Let $u_0 = v$ and define u_n inductively as the solution u of the linear equation

$$-\Delta u = f(u_{n-1}) \text{ in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

(4) Maximum principle $\Rightarrow u_{n-1} \leq u_n \leq w$ in Ω.

(5) Therefore u_n converges pointwise to some u between v and w. This u is the required solution.

(6) If f is not increasing, rewrite the pde in the form

$$-\Delta u + cu = f(u) + cu \text{ in } \Omega$$

and choose $c > 0$ so large that $f(u) + cu$ is increasing for
$\min v \leq u \leq \max w$

⊠.

1.5.2.4 Definition (elliptic operators)

$$\mathcal{L} \equiv \sum_{i,j=1}^{n} a_{ij}(x_1, x_2, \ldots\, x_n) \frac{\partial^2}{\partial x_i \partial x_j} \quad , \; a_{ij} = a_{ji} \; , \; i,j = 1,2,..n \tag{i}$$

is called elliptic at each point $\mathbf{x} = (x_1, x_2, \ldots\ldots x_n)$ iff there is a positive quantity $\mu(\mathbf{x})$ such that

$$\sum_{i,j}^{n} a_{ij}(\mathbf{x})\, \xi_i \xi_j \geq \mu(\mathbf{x}) \sum_{i=1}^{n} \xi_i^2 \tag{ii}$$

for all n-tuples of real numbers $(\xi_1, \xi_2, \ldots\ldots \xi_n)$

The operator $\mathcal{L}$ is said to be elliptic in a domain Ω if it is elliptic at each point of Ω. It is uniformly elliptic in Ω if (ii) holds for each point of Ω and if there is a positive constant μ_0 such that $\mu(x) \geq \mu_0$ for all x in Ω.

The operator

$$(L+h) \equiv \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i \frac{\partial}{\partial x_i} + h$$

is said to be elliptic at $\mathbf{x}$ iff

$$\mathcal{L} \equiv \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2}{\partial x_i \partial x_j}$$

is elliptic there.

2.5 Definition (uniformly elliptic)

(L+h) is uniformly elliptic in Ω if $\mathcal{L}$ (the principal part of (L + h)) is uniformly elliptic in Ω,

2.6 The Maximum Principle of E. Hopf

Consider the strict differential inequality

$$L[u] \equiv \sum_{i,j=1}^{n} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i \frac{\partial u}{\partial x_i} > 0$$

in a domain Ω and assume that L is elliptic in Ω. If u has a relative maximum at a point

$\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, \ldots\ldots \bar{x}_n)$

we know from the calculus of several variables that at $\bar{x}$

$$\frac{\partial u}{\partial z_k} = 0 \text{ and } \frac{\partial^2 u}{\partial z_k^2} \leq 0 \text{ , } k = 1,2,.. \text{ n}$$

for any coordinates z_1, z_2, ... z_n

Theorem 2.7
Let $u(x_1,x_2,....x_n)$ satisfy the differential inequality

$$L[u] \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x}) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x}) \frac{\partial u}{\partial x_i} \geq 0$$

in a domain Ω where L is uniformly elliptic. Suppose the coefficients a_{ij} and bi are uniformly bounded. If u attains a maximum M at a point of Ω, then u+M in Ω.

Theorem 2.8
Let u satisfy the differential inequality
$(L+h)[u] \geq 0$
with $h \leq 0$, with L uniformly elliptic in Ω, and with the coefficients of L and h bounded. If u attains a nonnegative maximum M at an interior point of Ω, then $u \equiv M$.

Theorem 2.9
Let u satisfy the inequality

$$L[u] \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x}) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x}) \frac{\partial u}{\partial x_i} \geq 0$$

in a domain Ω in which L is uniformly elliptic. Suppose that $u \leq M$ in Ω and that u = M at a boundary point P.
Assume that P lies on the boundary of a ball K_1 in Ω.
If u is continuous in $\Omega \cup P$ and an outward directional derivative $\partial u/\partial \nu$ exists at P, then

$$\frac{\partial u}{\partial \nu} > 0 \quad \text{at P} \qquad \text{unless } u \equiv M.$$

Theorem 2.10
Let u satisfy the inequality
$(L+h)[u] \geq 0$,
where L is the operator defined in the previous theorem, and $h(\mathbf{x}) \leq 0$ in Ω. Suppose that $u \leq M$ in Ω, that u = M at a boundary point P, and that $M \geq 0$. Assume that P lies on the boundary of a ball in Ω. If u is continuous in $\Omega \cup P$, any outward directional derivative of u at P is positive unless $u \equiv M$ in Ω.

Theorem 2.11
Suppose v_1 and v_2 satisfies the equation

$$(L + h)[v] \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x}) \frac{\partial^2 v}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x}) \frac{\partial v}{\partial x_i} + h(\mathbf{x})v = f$$

subject to boundary conditions

$$\begin{cases} \dfrac{\partial v}{\partial \nu} + \gamma(\mathbf{x})v = g_1 \text{ on } \Gamma_1 \\ v = g_2 \text{ on } \Gamma_2 \end{cases}$$

in a bounded domain Ω. Assume that each point of Γ_1 lies on the boundary of a ball in Ω. If L is uniformly elliptic , $h(\mathbf{x}) \leq 0$ is bounded, and $\gamma(\mathbf{x}) \geq 0$, then $v_1 + v_2$, except when $h \equiv g \equiv 0$ and Γ_2 is vacuous in which case $v_1 - v_2$ must be constant.

Theorem 2.12 (Generalised Maximum Principle for the Elliptic Operator)
Let $u(\mathbf{x})$ satisfy the differential inequality

$$(L + h)[u] \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x}) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x}) \frac{\partial u}{\partial x_i} + h(\mathbf{x}) \geq 0$$

in a domain Ω where L is uniformly elliptic. If there exists a function $w(\mathbf{x})$ such that
$w(\mathbf{x}) > 0$ on $\Omega \cup \partial\Omega$
$(L+h)[w] \leq 0$ in Ω
then $u(\mathbf{x}) / w(\mathbf{x})$ cannot attain a nonnegative maximum at a point P on $\partial\Omega$ which lies on the boundary of a ball in Ω and if u/w is not a constant, then

$\frac{\partial}{\partial \nu}\left(\frac{u}{w}\right) > 0$ at P, where

$\partial/\partial\nu$ is any outward normal vector.

Theorem 2.13
If there exists a function $w(\mathbf{x}) > 0$ on $\Omega \cup \partial\Omega$ such that
$(L+h)[w] \leq 0$ in Ω and Ω is bounded then the problem
$(L+h)[w] = f(\mathbf{x})$ in Ω
$u = g(\mathbf{x})$ on $\partial\Omega$
has at most one solution

Theorem 2.14

Suppose there exists a function $w(x) > 0$ on $\Omega \cup \partial\Omega$ such that

$(L+h)[w] \leq 0$ in Ω

and

$$\frac{\partial w}{\partial \nu} + \gamma(\mathbf{x})w \geq 0 \text{ on } \Gamma_1$$

where

$\partial\Omega$ is composed of two parts Γ_1 and Γ_2.

Suppose that each point of Γ_1 lies on the boundary of a ball in Ω and that Ω is bounded. Then there is at most one solution $u(\mathbf{x})$ of the problem

$(L + h)[u] = f(\mathbf{x})$ in Ω,

$$\frac{\partial u}{\partial \nu} + \gamma(\mathbf{x})\, u = g_1(\mathbf{x}) \text{ on } \Gamma_1$$

$u = g_2(\mathbf{x})$ on Γ_2

unless

(i) $(L+h)[w] \equiv 0$

(ii) $(\partial w/\partial \nu) + g(\mathbf{x})w \equiv 0$

(iii) Γ_2 is vacuous, in which case u is determined to within a constant multiple of w.

1.5.2.15 Approximations in Elliptic Boundary Value Problems

Theorem 2.15

Suppose there exists a function $w > 0$ on $\Omega \cup \partial\Omega$ such that

$(L + h)[w] \leq 0$ in Ω

$$\frac{\partial w}{\partial \nu} + \gamma(\mathbf{x})w \geq 0 \text{ on } \Gamma_1$$

where L is uniformly elliptic and $(\partial u/\partial \nu)$ is an outward directional derivative. We assume that the three conditions below do not all hold.

(i) $(\partial w/\partial \nu) + g(\mathbf{x})w \equiv 0$ on Γ_1

(ii) $(L+h)[w] \equiv 0$ in Ω

(iii) Γ_2 is vacuous,

If $z_1(\mathbf{x})$ satisfies

$(L+h)[z_1] \leq f(\mathbf{x})$ in Ω (i)

with boundary conditions

$$\frac{\partial z_1}{\partial \nu} + \gamma(\mathbf{x})\, z_1 \geq g_1(\mathbf{x}) \text{ on } \Gamma_1 \text{ ,} \tag{ii}$$

$z_1 \geq g(\mathbf{x})$ on Γ_2

and if $z_2(\mathbf{x})$ satisfies

$(L+h)[z_2] \geq f(\mathbf{x})$ in Ω (iii)

with boundary conditions

$$\frac{\partial z_2}{\partial \nu} + \gamma(\mathbf{x})\, z_2 \leq g_1(\mathbf{x}) \text{ on } \Gamma_1 \text{ ,} \tag{iv}$$

$z_2 \leq g_2(\mathbf{x})$ on Γ_2

Then if u is a solution of the problem

$(L + h)[u] = f(\mathbf{x})$ in Ω (v)

which satisfies the boundary conditions

$$\frac{\partial u}{\partial \nu} + \gamma(\mathbf{x})\, u = g_1(\mathbf{x}) \text{ on } \Gamma_1 \text{ ,} \tag{vi}$$

$u = g_2(\mathbf{x})$ on Γ_2

then u satisfies the inequalites

$z_2(\mathbf{x}) \leq u(\mathbf{x}) \leq z_1(\mathbf{x})$ in Ω.

Theorem 2.16
Let z_1 and z_2 satisfiy the conditions (i), (ii), (iii) and (iv) in the previous theorem in such a way that identity does not hold in all of them.

If the above problem (v) with boundary conditions (vi) has solutions for arbitrary continuous boundary values $g_2(\mathbf{x})$, and if u is the solution of the particular problem (v) and (vi) then the bounds

$z_2 \leq u \leq z_1$

are valid iff $z_2 \leq z_1$

1.5.2.17 Non-Linear Elliptic Operators

Theorem 2.17

Let $u(x,y)$ be a solution of

$F(x,y,u,u_x,u_y,u_{xx},u_{xy},u_{yy}) = f(x,y)$ in Ω,

$u = g$ on $\partial\Omega$

Let z and Z satisfy the inequalitues

$F(x,y,Z,Z_x,Z_y,Z_{xx},Z_{xy},Z_{yy}) \le f(x,y) \le F(x,y,z,z_x,z_y,z_{xx},z_{xy},z_{yy})$

in Ω and

$z(x,y) \le g(x,y) \le Z(x,y)$ on $\partial\Omega$

We assume that for each constant ϑ such that $0 \le \vartheta \le 1$, the function F is elliptic with respect to $u + \vartheta(z-u)$ and $u + \vartheta(Z-u)$ in Ω, and that $\partial F/\partial u \le 0$ in Ω. Then we have

$z(x,y) \le u(x,y) \le Z(x,y)$ in Ω.

Proof:

(1) Suppose $u(x,y)$ is a solution of

$F(x,y,u,p,q,r,s,t) = f(x,y)$ in a domain Ω where

$$u = u(x,y) \quad p = \frac{\partial u(x,y)}{\partial x} \quad q = \frac{\partial u(x,y)}{\partial y} \quad r = \frac{\partial^2 u(x,y)}{\partial x^2} \quad s = \frac{\partial^2 u(x,y)}{\partial x \partial y} \quad t = \frac{\partial^2 u(x,y)}{\partial y^2}$$

(2) Suppose that $w(x,y)$ satisfies the differential inequality

$$F(x,y,w,\frac{\partial w}{\partial x}, \frac{\partial w}{\partial y}, \frac{\partial w}{\partial x^2}, \frac{\partial^2 w}{\partial x \partial y}, \frac{\partial^2 w}{\partial y^2}) \le f(x,y)$$

We form the function

$v(x,y) = u(x,y) - w(x,y)$ and consider the inequality

$F(x,y,u,u_x,u_y,u_{xx},u_{xy,}u_{yy}) - F(x,y,w,w_x,w_y,w_{xx},w_{xy,}w_{yy}) \ge 0$

(3) Applying the mean-value theorem of multidimensional calculus to $F(x,y,u,u_x,u_y,u_{xx},u_{xy,}u_{yy})$ we obtain

$$(\frac{\partial F}{\partial r})_0 \frac{\partial^2 v}{\partial x^2} + (\frac{\partial F}{\partial s})_0 \frac{\partial^2 v}{\partial x \partial y} + (\frac{\partial F}{\partial t})_0 \frac{\partial^2 y}{\partial y^2} + (\frac{\partial F}{\partial p})_0 \frac{\partial v}{\partial x} + (\frac{\partial F}{\partial q})_0 \frac{\partial v}{\partial y} + (\frac{\partial F}{\partial u})_0 v \ge 0$$

where subscript zero indicates that the derivatives are evaluated at $(x,y,u_0,p_0,q_{0,}r_0,s_0,t_0)$

with

$u_0 = w + \vartheta(u-w)$

$p_0 = w_x + \vartheta(u_x-w_x)$

$q_0 = w_y + \vartheta(u_y - w_y)$

$r_0 = w_{xx} + \vartheta(u_{xx} - w_{xx})$

$s_0 = w_{xy} + \vartheta(u_{xy} - w_{xy})$

$t_0 = w_{yy} + \vartheta(u_{yy} - w_{yy})$

(4) For each point (x,y) in Ω we assume that F is elliptic for all functions of the form
$\vartheta w + (1 - \vartheta)u$ with $0 \le \vartheta \le 1$.
Then the differential inequality in (3) is elliptic for the function v.

(5) We may apply theorem 2.8 to conclude that if v is not constant and

$$\left(\frac{\partial F}{\partial u}\right)_0 \le 0$$

then v cannot have a nonnegative maximum at any point in Ω.

(6) The theorem then follows trivially.

⊠

1.5.3 Parabolic Operators

1.5.3.1 One-Dimensional Parabolic Operator

3.1 Definition

The differential operator

$$L[u] = a(x,t)\frac{\partial^2 u}{\partial x^2} + b(x,t)\frac{\partial u}{\partial x} - \frac{\partial u}{\partial t}$$

is said to be parabolic at a point (x,t) if a(x,t) > 0.

3.2 Definition

The operator L is uniformly parabolic in a domain Ω of the x,t plane if there is a positive constant μ such that

$a(x,t) \geq \mu$ for all (x,t) in Ω

Theorem 3.1

Suppose that in a domain Λ of the x,t plane, the inequality

$$L[u] = a(x,t)\frac{\partial^2 u}{\partial x^2} + b(x,t)\frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} \geq 0$$

holds, that a and b are bounded and that L is uniformly parabolic in Λ. If the maximum M of u is attained at any interior point (x_1,t_1) of Λ, then $u \equiv M$ on each line segment $t = t_0$ which lies in Λ and contains the point (x_1,t_0) and has the property that the vertical segment $x = x_1$, $t_0 \leq t \leq t_1$ lies in Λ.

Theorem 3.2

Let Λ be a region in the x,t-plane in which u is a solution of the uniformly parabolic inequality

$$L[u] = a(x,t)\frac{\partial^2 u}{\partial x^2} + b(x,t)\frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} \geq 0$$

where a(x,t) and b(x,t) are bounded. Suppose that P is a point on the boundary $\partial\Lambda$ where the maximum of u occurs and that the normal to $\partial\Lambda$ at P is not parallel to the t-axis. Furthermore, suppose that at P a circle tangent to $\partial\Lambda$ can be constructed whose interior lies entirely in Λ and such that u < M in this interior. If $\partial/\partial\nu$ denotes any derivative in an outward direction from L, then

$$\frac{\partial u}{\partial \nu} > 0 \text{ at P.}$$

Theorem 3.3

Suppose that in a domain Λ of the x,t plane the inequality

$$L[u] = a(x,t)\frac{\partial^2 u}{\partial x^2} + b(x,t)\frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} + h(x,t) \geq 0$$

holds, that a and b are bounded, that L is uniformly parabolic in Λ and that $h \leq 0$ in Λ.

If the maximum, M of u is attained at an interior point (x,t) and if $M \geq 0$, then $u \equiv M$ on all line segments t = constant of Λ which lie directly below the horizontal segment of L containing (x_1,t_1). If a nonnegative maximum M occurs at a boundary point P then the conclusion of the previous theorem holds.

1.5.3.4 The General Parabolic Operator

Definition 3.4 (The general parabolic operator)
The operator

$$L \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x},t) \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x},t) \frac{\partial}{\partial x_i} - \frac{\partial}{\partial t}$$

is said to be parabolic at $(\mathbf{x},t) \equiv (x_1,x_2,....x_n,t)$ if for fixed t the operator consisting of the first sum, i.e.

$$L \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x},t) \frac{\partial^2}{\partial x_i \partial x_j}$$

is elliptic at $(\mathbf{x},t)$.
That is, L is parabolic if there is a number $\mu > 0$ such that

$$\sum_{i,j=1}^{n} a_{ij}(\mathbf{x},t)\, \xi_i \xi_j \geq \mu \sum_{i=1}^{n} \xi_i^2 \qquad \text{(i)}$$

for all n-tuples of real numbers $(\xi_1,\xi_2,...\xi_n)$

Definition 3.5 (uniformly parabolic)
The operator L is uniformly parabolic in a domain Λ in $(\mathbf{x},t)$ space if (i) holds with the same number $\mu > 0$ for all $(\mathbf{x},t)$ in Λ.

Theorem 3.4
Let u satisfy the uniformly parabolic differential inequality

$$L \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x},t) \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x},t) \frac{\partial}{\partial x_i} - \frac{\partial}{\partial t} \geq 0.$$

in a domain Λ in (n+1) dimensional space $(x_1,x_2,.....x_n,t)$ and suppose the coefficients of L are bounded. Suppose that the maximum of u in Λ is M and that it is attained at some interior point $P(\mathbf{x},t)$.

Let us denote by $\Lambda(\bar{t})$ the connected component of the intersection of the hyperplane $t = \bar{t}$ with which contains P. Then $u \equiv M$ in $\Lambda(\bar{t})$.
Furthermore, if Q is a point of Λ which can be connected by P by a path in Λ consisting only of horizontal segments and upward vertical segments, then $u = M$ at Q.

Theorem 3.5
Let u satisfy the uniformly parabolic inequality

$$L[u] \equiv \sum_{i,j=1}^{n} a_{ij}(\mathbf{x},t)\frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x},t)\frac{\partial u}{\partial x_i} - \frac{\partial u}{\partial t} \geq 0$$

with bounded coefficients in a domain Λ and suppose that the maximum M of u is attained at a point P on the boundary $\partial\Lambda$. Assume that a sphere through P can be contructed whose interior lies entirely in Λ and in which $u < M$. Also suppose that the radial direction from the centre of the sphere to P is not parallel to the t-axis. Then if $\partial/\partial\nu$ denotes any directional derivative in an outward direction, we have

$$\frac{\partial u}{\partial \nu} > 0$$

at P.

Theorem 3.6
The conclusions of theorems 3.5 and 3.6 remains valid if u is a solution of $(L+h)[u] \geq 0$ provided $h \leq 0$ and $M \geq 0$.

1.5. Uniqueness Theorems for Boundary-Value Problems

Theorem 3.7

Let u be a solution of the uniformly parabolic equation

$$(L + h)\,[u] \equiv \sum_{i,j=1}^{n} a_{ij}\,(\mathbf{x},t)\,\frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i\,(\mathbf{x},t)\frac{\partial u}{\partial x_i} + h(\mathbf{x},t)u - \frac{\partial u}{\partial t} = f(\mathbf{x},t) \qquad \text{(i)}$$

in Λ and let the coefficients of L be bounded.

Suppose $u(\mathbf{x},t) \equiv u(x_1,x_2,....x_n,t)$ satisfies the boundary conditions

$$u(\mathbf{x},0) = g_1(\mathbf{x}) \text{ in } \Lambda \text{ and} \qquad \text{(ii)}$$

$$\gamma_1(\mathbf{x},t)u(\mathbf{x},t) + \gamma_2(\mathbf{x},\, t)\,\frac{\partial u}{\partial \nu} = g_2(\mathbf{x},t) \qquad \text{(iii)}$$

for all $(\mathbf{x},t)$ on Γ, where $\partial/\partial\nu$ is any directional derivative in a direction outward from Γ. and where

Γ is the portion of the boundary of L consisting of $\partial\Omega \times (0,T)$

Assume that $\gamma_1,\gamma_2 \geq 0$ on Γ, that $\gamma_1{}^2 + \gamma_2{}^2 > 0$ at each point and that h(x,t) is bounded above.

If v is another solution of (i) satisfying boundary conditions (ii) and (iii), then $v \equiv u$ in Λ.

Proof:

The result follows form the maximum principle

(1) Define w = u - v

(2) Then w satisfies

$(L+h)[w] = 0$

and the boundary conditions

$w(\mathbf{x},0) = 0$ in Ω and

$$\gamma_1 w + \gamma_2 \frac{\partial w}{\partial \nu} = 0 \quad \text{on} \quad \Gamma$$

(3) We may assume, without loss of generality that $h(\mathbf{x},t) \leq 0$.

(4) According to Theorem 3.6 , the maximum of u must occur either at t = 0 or on Γ.

(5) If then maximum of w is positive, then it must occur on Γ.

(6) Theorem 3.6 , however states that at such a maximum point $\partial w/\partial\nu > 0$

(7) Since γ_1 and γ_2 cannot vanish simultaneously, the condition

$$\gamma_1 w + \gamma_2 \frac{\partial w}{\partial \nu} = 0$$

is violated at a positive maximum. Thus $w \leq 0$ throughout L.

(8) Applying the same reasoning to -w, we find $w \geq 0$.
Therefore $w = u - v \equiv 0$ in Λ.

⊠.

Example
Consider the boundary value problem

$$(L + h)[u] = \frac{\partial^2 u}{\partial x^2} + \frac{2}{x}\frac{\partial u}{\partial x} + \phi^2 u - \frac{\partial u}{\partial t} = 0$$

with boundary conditions
$u(\mathbf{x},0) = g_1(\mathbf{x}) = 0$ in Λ and

$$\gamma_1(\mathbf{x},t)u(\mathbf{x},t) + \gamma_2(\mathbf{x}, t)\frac{\partial u}{\partial \nu} = g_2(\mathbf{x},t)$$

for all $(\mathbf{x},t)$ on Γ where
$\gamma_1(\mathbf{x},t) = 1$, $\gamma_2(\mathbf{x},t) = 0$, $g_2(\mathbf{x},t) = 1$ and
$\gamma_1(\mathbf{x},t) = 0$, $\gamma_2(\mathbf{x},t) = 1$, $g_2(\mathbf{x},t) = 0$
It can be seen that $\gamma_1,\gamma_2 \geq 0$ on Γ, that $\gamma_1{}^2 + \gamma_2{}^2 > 0$ at each point and that $h(x,t) = \phi^2$ is bounded above.
It follows from theorem 3.7 that if v is another solution of the above boundary value problem that satisfies the same boundary conditions, then $v \equiv u$ in Λ.

1.5.3.8 Non-Linear Parabolic Operators

We may use the same methods as chapters 1.5.1 and 1.5.2. to obtain results for nonlinear parabolic equations

We consider the vectors
$\mathbf{x} = (x_1, x_2, \ldots\ldots, x_n)$ and
$\mathbf{p} = (p_1, p_2, \ldots\ldots, p_n)$ and the matrix
$\mathbf{R} = (r_{ij})$, $i = 1,2,\ldots,n$

Let $F(\mathbf{x},t,u,\mathbf{p},\mathbf{R})$ be a continuously differentiable function of its n^2+2n+2 variables.
$F(\mathbf{x},t,u,p_i,r_{ij})$ denotes the above function with p_i and r_{ij} denoting the generic arguments of F.

Definition 3.8
We say that F is elliptic with respect to a function u(x,t) at a given point (x,t) if, for all real vectors
$\xi = (\xi_1, \xi_2, \ldots\ldots \xi_n)$, we have

$$\sum_{i,j=1}^{n} \frac{\partial F}{\partial r_{ij}} \xi_i \xi_j > 0 \quad \text{for } \xi \neq 0 \tag{i}$$

when the values

$$p_i = \frac{\partial u}{\partial x_i}$$

and

$$r_{ij} = \frac{\partial^2 u}{\partial x_i \partial x_j}$$

are substituted in the arguments of the partial derivatives of F appearing in (i), above.
The function F is said to be elliptic in a domain Λ in (x,t)-space if it is elliptic at each point of Λ.
The nonlinear operator

$$L[u] \equiv F(\mathbf{x}, t, u, \frac{\partial u}{\partial x_i}, \frac{\partial^2 u}{\partial x_i \partial x_j}) - \frac{\partial u}{\partial t}$$

is said to be parabolic whenever F is elliptic.

We have the following theorem

Theorem 3.9
Let Ω be a bounded domain in n-dimensional space and let $\Lambda = \Omega \times (0,T]$, as before
Suppose that u is a solution of $L[u] = f(\mathbf{x},t)$ in Λ with L given by

$$L[u] \equiv F(\mathbf{x}, t, u, \frac{\partial u}{\partial x_i}, \frac{\partial^2 u}{\partial x_i \partial x_j}) - \frac{\partial u}{\partial t} \qquad \text{(i)}$$

and that u satisfies the initial and boundary conditions
$u(\mathbf{x},0) = g_1(\mathbf{x})$ in Ω
$u(\mathbf{x},t) = g_2(\mathbf{x},t)$ on $\partial\Omega \times (0,T)$ (ii)

We shall assume that z and Z satisfy the inequalities
$L[Z] \leq f(\mathbf{x},t) \leq L[z]$ in Λ,
and that L is parabolic with respect to the functions
$\vartheta u + (1-\vartheta)z$ and $\vartheta u + (1-\vartheta)Z$ for $0 \leq \vartheta \leq 1$
If $z(\mathbf{x},0) \leq g_1(\mathbf{x}) \leq Z(\mathbf{x},0)$ in Ω,
$z \leq g_2 \leq Z$ on $\partial\Omega \times (0,T)$
then
$z(\mathbf{x},t) \leq u(\mathbf{x},t) \leq Z(\mathbf{x},t)$ in Λ

Proof:
We use the maximum principle, as given in Theorem 3.6 to compare solutions of non-linear parabolic equations

(1) Let u be a solution of
$L[u] = f(\mathbf{x},t)$ where L is given by

$$L[u] \equiv F(\mathbf{x}, t, u, \frac{\partial u}{\partial x_i}, \frac{\partial^2 u}{\partial x_i \partial x_j}) - \frac{\partial u}{\partial t}$$

in a domain Λ in $(\mathbf{x},t)$- space and suppose that $w = w(\mathbf{x},t)$ satisfies
$L[w] \leq f$ in Λ

(2) We form the function
$v(\mathbf{x},t) = u(\mathbf{x},t) - w(\mathbf{x},t)$ and consider the inequality

$$F(\mathbf{x},t,u,u_{x_i}, u_{x_i x_j}) - F(\mathbf{x}, t,w,w_{x_i}, w_{x_i x_j}) - \frac{\partial v}{\partial t} \geq 0$$

(3) We apply the mean value theorem of multidimensional calculus

Letting ϑ be such that $0 \leq \vartheta \leq 1$ and evaluating the derivatives of F at the arguments

$\vartheta u + (1 - \vartheta) w$
$\vartheta u_{x_i} + (1 - \vartheta) w_{x_i}$
$\vartheta u_{x_i x_j} + (1 - \vartheta) w_{x_i x_j}$, we find

$$\sum_{i,j=1}^{n} \left(\frac{\partial F}{\partial r_{ij}}\right) \frac{\partial^2 v}{\partial x_i \partial x_j} + \sum_{i=1}^{n} \left(\frac{\partial F}{\partial p_i}\right) \frac{\partial v}{\partial x_i} + \left(\frac{\partial F}{\partial u}\right) v - \frac{\partial v}{\partial t} \geq 0 \qquad \text{(iii)}$$

(4) We assume that F is elliptic in Λ for all functions of the form
$\vartheta u + (1-\vartheta)w$, for
$0 \leq \vartheta \leq 1$.
Under this assumption, the left hand side of (iii) is a linear parabolic operator for the function v. We may apply the maximum principle of parabolic equations (Theorem 3.6) to conclude that if v is non positive initially and on the boundary, then v is nonpositive in Λ

(5) The approximation result
$z(\mathbf{x},t) \leq u(\mathbf{x},t) \leq Z(\mathbf{x},t)$ in L follows

(6) This theorem implies that a solution of (i) which satisfies boundary conditions (ii) must exist and be unique for if u and $\hat{u}$ are solutions we let

$z_1 = z_2 = u$ to find that $u \equiv \hat{u}$

⊠.

Example

Consider the Boundary Value Problem $(L , \Lambda , \partial\Lambda)$ with

a) $L : L[u] = \nabla^2 u - \dfrac{\partial u}{\partial t} - \dfrac{\phi^2 u}{1 + \beta u.} = 0$

b) region $\Lambda = \Omega \times (0,T]$ where $\Omega = \{ x : \alpha < || \underset{\sim}{x} || < 1 \}$

c) boundary $\partial\Lambda = \partial\Omega \times (0,T)$ where

$$\partial\Omega = \{ x : || \underset{\sim}{x} || = \alpha \text{ or } || \underset{\sim}{x} || = 1 \}$$

$$= \partial\Omega_1 \cup \partial\Omega_2$$

and where $\partial\Omega_1 = \{x : || \underset{\sim}{x} ||=\alpha\}$

and $\partial\Omega_2 = \{x : || \underset{\sim}{x} || = 1\}$

d) The 2 point boundary condition is

i/ $u(|| \underset{\sim}{x} ||=1) = 1$

ii/ $\dfrac{\partial u}{\partial v}(||\underset{\sim}{x} || = \alpha) = 0$

This may be rewritten in the more general form

$$\gamma_1(x) \frac{\partial u}{\partial v} + \gamma_2(x)\, u = g_2(x,t) \quad \text{on} \quad \partial\Omega \times (0,T)$$

where

i/ $|| \underset{\sim}{x} || = \alpha$, i.e. $x \in \partial\Omega_1 \Rightarrow \gamma_1(x) = 1, \gamma_2(x) = 0$ and $g_2(x,t) = 0$

ii/ $|| \underset{\sim}{x} || = 1$, i.e. $x \in \partial\Omega_1 \Rightarrow \gamma_1(x) = 0, \gamma_2(x) = 1$ and $g_2(x,t) = 1$.

e) Initial Condition

$u(x,0) = g_1(x) = 0$ in Ω

Solution

We assume that z and Z satisfy the inequalities
$L[Z] \leq 0 \leq L[z]$ in Λ
and that Λ is parabolic with respect to the functions
$\vartheta u + (1 - \vartheta)z$ and $\vartheta u + (1-\vartheta)Z$ for $0 \leq \vartheta \leq 1$
We therefore have to show that

$$F(x,t,u,p_i, r_{ij}) = \nabla^2 u - \frac{\phi^2 u}{1 + \beta u}$$

is elliptic.

F is elliptic with respect to functions $\vartheta u + (1-\vartheta)z$ and $\vartheta u + (1 - \vartheta)Z$ at a given point (x,t) if , for all real vectors
$\xi = (\xi_1,\xi_2,.....,\xi_n)$, we have

$$\sum_{i,j=1}^{n} \frac{\partial F}{\partial r_{ij}} \xi_i \xi_j > 0 \quad \text{for } \xi \neq 0 \qquad \left(\text{i.e.} \left(\frac{\partial F}{\partial r_{ij}}\right) \text{ is positive definite}\right)$$

For n =1

$$r_{11} = \frac{\partial^2 u}{\partial x_1^2} \quad \text{and} \quad \frac{\partial F}{\partial r_{11}} = 1 > 0 \qquad \text{and } \xi_1^2 > 0$$

For n = 2

$$r_{11} = \frac{\partial^2 u}{\partial x_1^2}, \quad r_{12} = \frac{\partial^2 u}{\partial x_1 \partial x_2} = r_{21} \quad r_{22} = \frac{\partial^2 u}{\partial x_2^2} \quad \text{and} \quad \left(\frac{\partial F}{\partial r_{ij}}\right) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$ which is

positive definite and therefore

$$\sum_{i,j=1}^{n} \frac{\partial F}{\partial r_{ij}} \xi_i \xi_j = \xi_1^2 + \xi_2^2 > 0.$$

For n = 3

$$\left(\frac{\partial F}{\partial r_{ij}}\right) = I_3$$ which is positive definite and

For <u>n-dimensions</u>

$\left(\frac{\partial F}{\partial r_{ij}} \right) = I_n$ which is positive definite and in all cases

$$\sum_{i,j=1}^{n} \frac{\partial F}{\partial r_{ij}} \xi_i \xi_j = \sum_{i=1}^{n} 1 \cdot \xi^2 > 0$$

We have shown that F is elliptic with respect to all functions
$\vartheta u + (1-\vartheta)z$ and $\vartheta u + (1-\vartheta)Z$ at a given point (x,t)

If $z(x,0) \leq g_1(x) \leq Z(z,0)$ in Ω
$z \leq g_2 \leq Z$ on $\partial\Omega \times (0,T)$
then $z(x,t) \leq u(x,t) \leq Z(x,t)$

The existence and uniqueness of the above boundary value problem follows trivially from theorem 3.9 since all conditions and assumptions are satisfied.

1.5.3.9 Approximation to boundary value problems by finding upper and lower bounds.

As an example to approximating u where

$$L[u] = \nabla^2 u - \frac{\partial u}{\partial t} - \frac{\phi^2 u}{1 + \beta u.} = 0$$

and boundary conditions are as in the previous boundary value problem, we choose z as a lower bound and Z as an upper bound such that
$L[Z] \le 0 \le L[z]$

Upper Bounds to u

e.g. An appropriate upper bound to u is Z where Z is such that

$$L[Z] = \nabla^2 Z - \frac{\partial Z}{\partial t} - \frac{\phi^2 Z}{1 + \beta} \le 0$$

since

$$\frac{\phi^2 Z}{1 + \beta Z} \ge \frac{\phi^2 Z}{1 + \beta}$$

in the region $Z \in (0,1)$
The above inequality assumes that $Z > 0$. This will be shown to be true in later chapters.

Lower bounds to u

An appropriate lower bound to u is z where z is such that

$$L[z] = \nabla^2 z - \frac{\partial z}{\partial t} - \phi^2 z \ge 0$$

since

$$\frac{\phi^2 z}{1 + \beta z} \le \phi^2 z$$

in the region $z \in (0,1)$
As before, the above inequality assumes that $z > 0$. This will be shown to be true in later chapters.

Boundary conditions

We take all boundary conditions in L[z], L[Z] and L[u] to be equivalent.

It follows from theorem 3.9 that Z(x,t) and z(x,t) is an upper and lower bound for u for all time.
Z(x,t) and z(x,t) are solutions of linear partial differential equations that provide good analytical bounds and approximations to example. 3.9 for all time.

We may conclude that for any solution u, the maximum and minimum values must occur either at the initial time or at the boundary. The only time that u (which corresponds here to concentration) can be zero is at $t = 0$.
It may be shown that the lower bound z for all time ($\neq 0$) is strictly positive. This is done in the time dependent section of this thesis .

note:
All the above results may be used to prove uniqueness and existence to the boundary value problem

$$L[u] = \nabla^2 u - \frac{\partial u}{\partial t} - \phi^2 u^n$$

$$= F(x,t,u,p_i,r_{ij}) - \frac{\partial u}{\partial t}$$

for all geometries slab, cylinder and sphere and for all kinetic orders, n
As before, F is elliptic and boundary conditions are precisely the same.

Chapter 2 - The Steady State Problem

Chapter 2 The Steady State Problem

2.1 Introduction and some Preliminary results

In this chapter we shall deal with the steady state problem (P-SS).
In our numerical techniques, we shall need some preliminary results

Theorem 2.1.1

Let the function $f(x;\mathbf{u})$ be continuous on the infinite strip
$R: a \le x \le b, \quad |\mathbf{u}| < \infty$
and satisfy there a Lipshitz condition in $\mathbf{u}$ with constant K, uniformly in x; that is,
$|f(x;\mathbf{u}) - f(x;\mathbf{v})| \le K\,|\mathbf{u} - \mathbf{v}|$ for all $(x;\mathbf{u})$ and $(x;\mathbf{v}) \in \mathbb{R}$.
Then the initial-value problem
$\mathbf{u}' = f(x;\mathbf{u}), \quad \mathbf{u}(a) = \alpha$
has a unique solution $\mathbf{u} = \mathbf{u}(x;\alpha)$ defined on the interval [a,b]

2.2 Numerical techniques

One approach to solving boundary-value problems is to convert them to parabolic partial differential equations that are integrated to steady state. We shall use this approach in the time dependency section of this thesis and shall be using an explicit finite difference method technique.
An outline of the method used is as follows

Consider Eq.(1-38). We write this equation with a time derivative on the left-hand side

$$\frac{\partial y}{\partial t} = \frac{1}{x^{a-1}}\frac{\partial}{\partial x}\left(x^{a-1}\frac{\partial y}{\partial x}\right) - \phi^2\, F(y)$$

where a = 0,1,2 represents slab, cylindrical and spherical geometry respectively as before.
We begin the calculation with an initial guess of the solution
$y(x,0) = y_0(x)$
and integrate the above equation until steady state is reached

A boundary-value problem for an ordinary differential equation is obtained by requiring that the dependent variable satisfy conditions at two or more distinct points. We have the theorem (2.1.1) that a unique solution of an nth-order equation is determined by specifying n conditions at one point (that is, for initial-value problems). However, with a total of n boundary conditions imposed at more than one point it is possible that a very smooth nth-order equation has many solutions or even no solution. Thus, as we might very well expect, the existence and uniqueness theorems are considerably more complicated and less thoroughly developed than that for initial-value problems.

As with integrating a parabolic partial differential equation to steady state, there is, however an alternative method of applying initial-value techniques to solve boundary-value problems. We note that we cannot apply initial-value techniques to integrate in x since there may be two or more boundary conditions applied at different positions. If we knew all the conditions at one position x we could integrate with x as a time-like variable. We therefore try to find the conditions of using these initial-value techniques to make the numerical technique easier.

As an example, we suppose the two boundary conditions are that the function takes specified values at $x = \alpha$, for some constant initial value α and $x = 1$. We do not know a priori the value of the function at $x = \alpha$, although once we have the exact solution that value is known. Let us guess the value of $y(\alpha)$ and use the known value of $y'(\alpha)$. Then we have two conditions at the same point, and these are sufficient to solve a second-order equation by integrating forward from $x = \alpha$. We integrate until $x = 1$ and check the value of $y(1)$. If it is correct we make a good guess of $y(\alpha)$; if not we must make another guess and try again. We use this method for linear problems as well as for non-linear problems

2.2.1 Initial Value methods for Linear Boundary-Value Problems

For linear problems we proceed as follows

Suppose the problem is

$$L[y] = g(x)$$

$$y(\alpha) = a \qquad y(1) = b \tag{i}$$

where L[y] is an arbitrary second-order linear differential operator and α is an arbitrary constant initial value. The forcing function g(x) and the boundary values a and b are specified. Consider the three problems:

problem I - solution $y_1(x)$

$$L[y] = g(x) \qquad y(\alpha) = a \qquad y'(\alpha) = 0$$

problem II - solution $y_2(x)$

$$L[y] = 0 \qquad y(\alpha) = 0 \qquad y'(\alpha) = 1$$

problem III- solution $y_3(x)$

$$L[y] = 0 \qquad y(\alpha) = 1 \qquad y'(\alpha) = 0$$

Each of these problems is an initial-value one, and we can and we can solve them numerically by using standard algorithms for solving of differential equations.
We then construct the full solution as

$$y(x) = y_1(x) + c_1y_2(x) + c_2y_3(x)$$

This function satisfies the differential equation for all choices of c_1 and c_2. It satisfies the boundary conditions if we require

$$a = a + c_1y_2(\alpha) + c_2y_3(\alpha)$$

$$b = y_1(1) + c_1y_2(1) + c_2y_3(1)$$

or

$$c_2 = 0 \qquad \& \qquad c_1 = \frac{b - y_1(1)}{y_2(1)}$$

As another example, suppose the problem now is

$$L[y] = g(x) \tag{ii}$$

with boundary conditions
$y'(\alpha) = 0$ for some constant initial value α and $y(1) = 1$.

We would then get
$0 = y_1'(\alpha) + c_1 y_2'(\alpha) + c_2 y_3'(\alpha)$
$1 = y_1(1) + c_1 y_2(1) + c_2 y_3(1)$

$$\therefore \qquad c_1 = 0 \quad \& \quad c_2 = \frac{1 - y_1(1)}{y_3(1)}$$

Thus the solution to the two-point boundary-value problem (ii,above) is to solve two initial-value problems (three in the general case) to find $y_1(x)$ and $y_2(x)$ in the first example and y_1 and y_3 in the second example.

example
Consider the zero order kinetic boundary value problem in slab geometry
$L[y] = y'' = \phi^2$
with boundary conditions
$y'(\alpha) = 0,\ y(1) = 1$

Problem I
$y_1'' = \phi^2, \quad y_1(\alpha) = 0,\ y_1'(\alpha) = 0$
Differentiating, we obtain

$$y_1 = \frac{\phi^2 x^2}{2} + k_1 x + k_2$$

and solving for c_1 and c_2

$$y'(\alpha) = \phi^2\alpha + k_1 = 0$$

$$\Rightarrow k_1 = -\phi^2\alpha$$

$$y(\alpha) = \frac{\phi^2\alpha^2}{2} + k_1\alpha + k_2 = 0$$

$$\Rightarrow k_2 = -\frac{\phi^2\alpha^2}{2}$$

$\therefore$

$$y_1(x) = \frac{\phi^2 x^2}{2} - \phi^2\alpha x - \frac{\phi^2\alpha^2}{2}$$

from which we get

$$y_1(1) = \frac{\phi^2}{2} - \phi^2\alpha - \frac{\phi^2\alpha^2}{2}$$

Problem III

$y_3'' = 0$

$y_3(\alpha) = 1,\ y_3'(\alpha) = 0$

Solving for y_3

$$y_3 = k_1 x + k_2$$

$$y'(\alpha) \Rightarrow k_1 = 0$$
$$y(\alpha) \Rightarrow k_1 x + k_2 = 1$$
$$\Rightarrow k_2 = 1$$

$\therefore$

$$y_3(x) = 1$$
$$y_3(1) = 1$$

We also find

$$c_2 = \frac{1 - y_1(1)}{y_3(1)}$$

$$= 1 - \left(\frac{\phi^2}{2} - \phi^2\alpha - \frac{\phi^2\alpha^2}{2}\right)$$

and therefore

$$y(x) = y_1(x) + c_2 y_3(x)$$

or

$$y(x) = \frac{\phi^2 x^2}{2} - \phi^2\alpha x + 1 - \frac{\phi^2}{2} + \phi^2\alpha$$

A similar initial value technique may be used for non-linear problems in an iterative process. We shall summarise the theory form Keller[12] who uses a system of non-linear equations and applies an iterative method to convert a boundary value problem into an initial value one. The theory and implementation is produced in subsequent chapters of this thesis.

2.2.2 Initial Value methods of Non-Linear Boundary-Value Problems

2.2.2.1 Non-General Two Point Boundary conditions

Let us consider first an important class of boundary-value problems in which the solution, $y(x)$, of a second-order equation

$$y'' = f(x,y,y') \tag{i}$$

is required to satisfy at two distinct points relations of the form

$$\begin{aligned} a_0y(a) - a_1y'(a) &= \gamma_1, \qquad |a_0| + |a_1| \neq 0; \\ b_0y(b) - b_1y'(b) &= \gamma_2, \qquad |b_0| + |b_1| \neq 0. \end{aligned} \tag{ii}$$

defined on the interval [a,b]

A formal approach to the exact solution of this problem is obtained by considering a related initial- value problem, say

$$\begin{aligned} u'' &= f(x,u,u'), \\ a_0u(a) - a_1u'(a) &= \gamma_1, \\ c_0u(a) - c_1u'(a) &= s. \end{aligned} \tag{iii}$$

The second initial condition is to be independent of the first.
This is assured if $a_1c_0 - a_0c_1 \neq 0$.

Without loss of generality we require that c_0 and c_1 be chosen such that $a_1c_0-a_0c_1 = 1$.

With c_0 and c_1 fixed in this manner, we denote the solution of (iii) by
$u = u(x;s)$
to focus attention on its dependence on s.

Evaluating the solution at $x = b$, we seek a value of s for which

$$\Gamma(s) \equiv b_0u(b;s) + b_1u'(b;s) - \gamma_2 = 0 \tag{iv}$$

With b_0 and b_1 fixed, Eq.(iv) is, in general, a transcendental equation in s.
If $s = s^*$ is a root of this equation, we then expect the function $y(x) \equiv u(x;s^*)$ to be a solution of the boundary-value problem (iii) . This is true in many cases, and in fact all solutions of (iii) can frequently be determined in this way .
We shall quote a few theorems from Keller[12],(pp.39-57) that shall be relevant in the numerical approach.

Theorem 1.1

Let the function $f(x,u_1,u_2)$ be continuous on R: $a \leq x \leq b$, $u_1^2 + u_2^2 < \infty$. and satisfy there a uniform Lipshitz condition in u_1 and u_2.
Then the boundary-value problem (iii) has as many solutions as there are distinct roots, $s = s^{(\nu)}$, of equation (iv).

The solutions of (i) are

$$y(x) = y^{(\nu)}(x) \equiv u(x;s^{(\nu)});$$

that is the solutions of the initial-value problem (iii) with initial data $s = s^{(\nu)}$

By means of this theorem the problem of solving a boundary-value problem is 'reduced' to that of finding the root, or roots, of an (in general, transcendental) equation. A very effective class of numerical methods which is widely known as the *initial-value* or *shooting methods* is based on this equivalence. In fact, more general boundary-value problems than (i) can be reduced in this way to solve systems of (transcendental) equations. An important theorem is then developed for a special class of functions to show uniqueness of solutions to boundary-value problems. The proof of the follwing theorem follows from showing that there is a unique solution to the corresponding transcendental equation (iv)

Theorem 1.2

Let the function $f(x,u_1,u_2)$ in (i) satisfy the hypothesis of Theorem 1.1 and have continuous derivatives on R which satisfy, for some positive constant M,

$$\frac{\partial f}{\partial u_1} > 0, \quad \text{and}$$

$$\left|\frac{\partial f}{\partial u_2}\right| \leq M.$$

Let the coefficients in (ii) satisfy
$a_0 a_1 \geq 0$, $b_0 b_1 \geq 0$, $|a_0| + |b_0| \neq 0$.
Then the boundary-value problem (i) has a unique solution.

Example 1

Consider the boundary value problem

$$y'' + \frac{(a-1)y'}{x} = \phi^2 y^n$$

with boundary condtions

$y'(\alpha) = 0$

$y(1) = 1$

This would satisfy the boundary conditions in (ii) if we allow

$a_0=0, a_1=1$

$b_0=1, b_1=0$

and

$\gamma_1=0, \gamma_2=1$

Therefore

$$f(x,y,y') = \phi^2 y^n - \frac{(a-1)y'}{x}$$

$$f(x,u_1,u_2) = \phi^2 u_1^n - \frac{2u_2}{x}$$

$$\frac{\partial f}{\partial u_1} = n\,\phi^2 u_1^{n-1} > 0 \quad \text{for } n > 0$$

and

$$\left|\frac{\partial f}{\partial u_1}\right| = \left|\frac{(a-1)}{x}\right| \leq M \qquad \text{for all } x \in (\alpha, 1)$$

Showing that the allowed coefficients in (ii) satisfy

$a_0 a_1 = 0 \geq 0$

$b_0 b_1 = 0 \geq 0$

$|a_0| + |b_0| = 0 + 1 = 1 \neq 0$

we conclude that a unique solution of the above boundary value problem therefore exists by theorem 1.1

note: We may have difficulties with this theorem if $\alpha = 0$.

Example 2

Consider the boundary value problem

$$y'' + \frac{(a-1)y'}{x} = \frac{\phi^2 y}{1+\beta y}$$

with boundary condtions

$y'(\alpha) = 0$

$y(1) = 1$

This would satisfy the boundary conditions in (ii) if we allow

$a_0=0, a_1=1$

$b_0=1, b_1=0$

and

$\gamma_1=0, \gamma_2=1$

Therefore

$$f(x,y,y') = \frac{\phi^2 y}{1+\beta y} - \frac{(a-1)y'}{x}$$

$$f(x,u_1,u_2) = \frac{\phi^2 u_1}{1+\beta u_1} - \frac{2u_2}{x}$$

$$\frac{\partial f}{\partial u_1} = \frac{\phi^2}{(1+\beta u_1)^2} > 0$$

and

$$\left|\frac{\partial f}{\partial u_1}\right| = \left|\frac{(a-1)}{x}\right| \leq M \quad \text{for all } x \in (\alpha, 1)$$

Showing that the allowed coefficients in (ii) satisfy

$a_0 a_1 = 0 \geq 0$

$b_0 b_1 = 0 \geq 0$

$|a_0| + |b_0| = 0 + 1 = 1 \neq 0$

we conclude that a unique solution of the above boundary value problem... therefore exists by theorem 1.1

note:We may have difficulties with this theorem if $\alpha = 0$.

2.2.2.2 General two-point boundary Value Problems

We now consider second-order equations, which may be nonlinear, of the form

$y'' = f(x,y,y') \quad a \leq x \leq b,$ **(2-1)**

subject to the general two-point boundary conditions of the form

$a_0 y(a) - a_1 y'(a) = \gamma_1, \qquad a_i \geq 0,$
$b_0 y(b) - b_1 y'(b) = \gamma_2, \qquad b_i \geq 0; \qquad a_0 + b_0 > 0.$

The function f(x,y,z) in equation (2-1) will be assumed to satisfy the hypothesis of Theorem 1.2. This assures us that the boundary-value problem (2.1) has a solution which is unique.

As before, the related problem that we consider is

$u'' = f(x,u,u'), \qquad a \leq x \leq b,$ **(2-2)**

$u(a) = a_1 s - c_1 a$
$u'(a) = a_0 s - c_0 a,$

where c_0 and c_1 are constants such that
$a_1 c_0 - a_0 c_1 = 1.$
The solution of this problem, which we denote by $u = u(x;s)$, will be a solution of the boundary-value problem (2-2) if and only if s is a root of

$\Gamma(s) \equiv b_0 u(b;s) + b_1 u'(b;s) - \gamma_2 = 0.$ **(2-3)**

Under the previous-stated conditions on Γ, it can be shown the function $\Gamma(s)$ has a positive derivative which is bounded away from zero for all s, and so Equation (2-3) has a unique root for any value of γ_2.

2.2.3 The Shooting method

The initial-value or shooting methods consists of iterative schemes for approximating the root of Equation (2-3). These iterations all require evaluations of the function $\Gamma(s)$ for a sequence of values of s. This is done by means of numerical solutions of a sequence of initial-value problems of the form 2-2. We note that if f(x,y,z) is linear in y and z, then $\Gamma(s)$ is linear is s and the root of $\Gamma(s) = 0$ could be done in only 2 evaluations of $\Gamma(s)$.

2.2.3.1 Linear second-order equations

We consider first the single linear second-order equation

$$L[y] \equiv -y'' + p(x)y' + q(x) = r(x), \quad a \le x \le b, \qquad \textbf{(2-4)}$$

subject to the general two-point boundary conditions

$$a_0 y(a) - a_1 y'(a) = \gamma_1$$
$$b_0 y(b) + b_1 y'(b) = \gamma_2,$$

such that

$$|a_0| + |b_0| \neq 0.$$

We assume the functions p(x), q(x) and r(x) to be continuous on [a,b] and require the homogeneous problem

$$L[z] = 0;$$
$$a_0 z(a) - a_1 z'(a) = 0,$$
$$b_0 z(b) + b_1 z'(b) = 0$$
have only the trivial solution, $z(x) \equiv 0$.

Then by (Chap.2 theorem 1.2), the solution has a unique solution.

We shall describe and analyze the initial-value or shooting method for computing accurate approximations to the solution of the linear boundary-value problem (2.4)

We shall generalise the method of Chap. 2.2.1. to arbitrary boundary conditions..

Two functions $y^{(1)}(x)$ and $y^{(2)}(x)$ are uniquely defined on [a,b] as solutions of the respective initial-value problems

$L[y^{(1)}] = r(x); \quad y^{(1)}(a) = -\gamma_1 c_1 , \quad y^{(1)'}(a) = -\gamma_1 c_0 ;$
and
$L[y^{(2)}] = 0 ; \quad y^{(2)}(a) = a_1, \quad y^{(2)'}(a) = a_0.$

Here c_0 and c_1 are as before, i.e. constants such that

$a_1c_0 - a_0c_1 = 1.$

Note that these problems have unique solutions on [a,b] (from thm.1.2)

The function y(x) defined by

$y(x) = y(x;s) \equiv y^{(1)}(x) + sy^{(2)}, \quad a \le x \le b,$

satisfies

$a_0y(a) - a_1y'(a) = \gamma_1(a_1c_0 - a_0c_1) = \gamma_1$

and so will be a solution of problem (2-4) if s is chosen such that

$\Gamma(s) \equiv b_0y(b;s) + b_1y'(b;s) - \gamma_2 = 0.$

This equation is linear in s and has the single root

$$s = \frac{\gamma_2 - [b_0y^{(1)}(b) + b_1y^{(1)'}(b)]}{[b_0y^{(2)}(b) + b_1y^{(2)'}(b)]} \qquad \textbf{(2-6)}$$

provided that $[b_0y^{(2)}(b) + b_1y^{(2)'}(b)] \neq 0$.

However, if this quantity does vanish, then $z(x) \equiv y^{(2)}(x)$ would be a nontrivial solution of the homogeneous problem (2-5).

Since this has been excluded, we see that the above construction of a solution of (2-4) is valid.

2.2.3.2 Non-linear second-order equations

As we shall see in this chapter, a non-linear second order equation may require many iterations to determine the root(s) of the subsidiary equation $\Gamma(s)$ .Obviously we should try to employ very rapidly converging iteration schemes as this would reduce the number of initial-value problems that must be solved . We shall discuss the use of several different schemes, one of which is Newton's method and is particularly well-suited for the current class of problems. First we must consider some effects of using numerical approximations to u(b;s) and u'(b;s) in attempting to evaluate $\Gamma(s)$.

Once again, consider the second-order problem

$$y'' = f(x,y,y') \qquad \textbf{(2-7)}$$

where we choose our initial value to be at x = a and integrate in the interval [a,b]

$$a_0y(a) - a_1y'(a) = \gamma_1 \quad \text{for } a_i \geq 0$$
$$b_0y(b) - b_1y'(b) = \gamma_2 \quad \text{for } b_i \geq 0$$

We convert this to

$$u'' = f(x,u,u')$$
$$u(a) = a_1s - c_1\gamma_1$$
$$u'(a) = a_0s - c_0\gamma_2 \qquad \textbf{(2-8)}$$

where we choose the c_0 and c_1 such that

$$a_1c_0 - a_0c_1 = 1 \text{ as before}$$

We next convert the second-order initial-value problem of Eq.(2-8) to two first-order problems

$$u' = v$$
$$v' = f(x,u,v)$$

with boundary conditions

$$u(a) = a_1s - c_1\gamma_1$$
$$v(b) = a_0s - c_0\gamma_2$$

Define the quantity

$$\Gamma(s) = b_0u(1,s) + b_1u'(1,s)-\gamma_2=b_0u(1,s) + b_1v(1,s) - \gamma_2 \quad \textbf{(2-9)}$$

that we would like to make zero.

That is, we would like to find s such that $\Gamma(s) = 0$

We then employ both a successive substitution and a Newton method to do this.
In the successive substitution iteration we replace eqnuation(2-9) by

$$s = s - m\Gamma(s) \quad m \neq 0.$$

Keller[3] showed that if

$$\partial f/\partial y \leq N$$

for some N and $0 < m < 2/\Upsilon$, where Υ increases as N increases, then the iteration scheme

$$s^{k+1} = s^k - m\Gamma(s^k)$$

converges as $k \to \infty$.

The procedure is then to choose an s, solve the initial-value problems of equation (2-8), check the function given by equation (2-9), and iterate with equation (2-10).

For Newton's method of iteration we replace equation (2-10) by the Newton-Raphson formula

$$s^{k+1} = s^k - \frac{\Gamma(s^k)}{\frac{d\Gamma(s^k)}{ds}} \quad \textbf{(2-11)}$$

[3]The convergence of the N-R mathod can be proved under certain conditions. See Isaacson, E. & H.B.Keller "*Analysis of Numerical Methods* " pp.115-116, John Wiley & Sons,Inc, New York,1966

The $d\Gamma/ds$ in the Newton-Raphson formula is determined as the solution to a subsidiary problem.

We let

$$\xi \equiv \frac{\partial u(x,s)}{\partial s} \qquad \eta \equiv \frac{\partial v(x,s)}{\partial s} \qquad \text{(2-12)}$$

$$\xi' = \eta$$

$$\eta' = \frac{\partial f}{\partial v}\eta + \frac{\partial f}{\partial u}\xi$$

with initial-conditions

$$\xi(a) = a_1 \qquad \eta(a) = a_0$$

$$\frac{d\Gamma}{ds} = b_0\xi\,(1,s) + b_1\eta\,(1,s)$$

It must be noted that with shooting methods we can "shoot" in either direction (shooting from $x = b$ to $x = a$ is known as "reverse shooting") and we can use any of the conventional methods for solving initial-value problems such as Predictor-Corrector and Runge-Kutta Methods.

Example

As an example which we shall be using later on, we change the problem

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy}{dx}\right) = \phi^2 R(y)$$

with boundary conditions

$$\frac{dy(\alpha)}{dx} = 0 \qquad y(1) = 1$$

into an initial-value one

$$\frac{1}{z^2}\frac{d}{dz}\left(z^2\frac{dy}{dz}\right) = d^2 R(y)$$

by the choice $x = bz$ and $d = b\phi$.

For any d we choose an arbitrary $y(\alpha)$ and integrate this last problem until the concentration reaches one.

Suppose this happens at $z = z_1$.

Now let

$$b = \frac{1}{z_1}, \quad \phi = \frac{d}{b} = dz_1$$

and we have the exact solution without iteration to eqn.(2-11) for the case $\phi = dz_1$.

For illustration, we apply the shooting method to equation (2-13). The o.d.e. are

$$u' = v$$

$$v' = \phi^2 R(u) - \frac{2v}{x}$$

$$\xi' = \eta$$

$$\eta' = \phi^2 \frac{dR}{du} \xi + \frac{2\eta}{x}$$

where u corresponds to concentration, its first derivative with respect to position is v and and ξ and η are defined in equation (2-12).

We must solve these equations with the boundary conditions
$u(\alpha) = s$
$v(\alpha) = 0$
$\xi(\alpha) = 1$
$\eta(\alpha) = 0$

and the functions Γ and $d\Gamma/ds$ are given by

$$\Gamma(s) = u(1,s) - 1$$

$$\frac{d\Gamma}{ds} = \xi(1,s)$$

The shooting method was demonstrated on problems of the type in the above example and was proven to be exceptionally powerful. It could be used when ϕ^2 was large and y (which corresponds to the concentration) was small (say 10^{-20}) .
The integration uses the initial condition $y'(\alpha) = 0$ and guesses the value of $y(\alpha)$.

Example
Consider the equation

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} = \frac{\phi^2 y}{1 + \beta y}$$

an equation modelling Michaelis-Menten reaction kinetics in a sphere
This has the boundary conditions

$y'(\alpha) = 0$ and $y(1) = 1$.

Choose $\alpha = 0.5$

We therefore have the equations

$$u' = v$$

$$v' = \frac{\phi^2 u}{1 + \beta u} - \frac{2v}{x}$$

$$\xi' = \eta$$

$$\eta = \frac{\phi^2 \xi}{(1+\beta u)^2} + \frac{2\eta}{x}$$

We must solve this system of equations with boundary conditions
$u(\alpha) = s$
$v(\alpha) = 0$
$\xi(\alpha) = 1$
$\eta(\alpha) = 0$

To solve for s we have to find the unique root of $\Gamma(s)$ by the Newton Raphson iterative process.

Since we expect s to be between 0 and 1 , it would be quite reasonable to take s^0, our initial approximation to be equal to 0.5

A summary of the computation is given in the following list of iterations. These were obtained by a program written by the author and only takes a few seconds to run.

Iteration 1

$s^0 = 0.5$

x	u	v	ξ	η
0.5	0.50000	0.00000	1.0000	0.0000
0.6	0.50148	0.02811	1.0025	0.0533
0.7	0.50540	0.04958	1.0113	0.1246
0.8	0.51129	0.06762	1.0280	0.2139
0.9	0.51887	0.08379	1.0547	0.3217
1.0	0.52801	0.09891	1.0930	0.4485

$\Gamma(s^0) = -0.47199$

$$\Gamma(s^0) = u(1,s) - 1 = 0.52801 - 1 = -0.47199$$

$$\Gamma'(s^0) = \xi(1,s) = 1.0930$$

$$s^1 = s^0 - \frac{\Gamma(s^0)}{\Gamma'(s^0)} = 0.5 - \frac{(-0.47199)}{1.0930} = 0.93183$$

Iteration 2

$s^1 = 0.93183$

x	u	v	ξ	η
0.5	0.93183	0.00000	1.0000	0.00000
0.6	0.93397	0.04066	1.0015	0.03215
0.7	0.93965	0.07166	1.0068	0.07499
0.8	0.94814	0.09761	1.0169	0.12854
0.9	0.97145	0.12071	1.0329	0.26815
1.0	0.97223	0.14216	1.0558	0.26815

$\Gamma(s^1) = -0.027769$

$$\Gamma(s^1) = u(1,s) - 1 = 0.97223 - 1 = -0.02777$$

$$\Gamma'(s^1) = \xi(1,s) = 1.0558$$

$$s^2 = s^1 - \frac{\Gamma(s^1)}{\Gamma'(s^1)} = 0.93183 - \frac{(0.97223 - 1)}{1.0558} = 0.95813$$

Iteration 3

$s^2 = 095813$

x	u	v	ξ	η
0.5	0.95813	0.00000	1.0000	0.00000
0.6	0.96030	0.04125	1.0015	0.03129
0.7	0.96606	0.07269	1.0066	0.07298
0.8	0.97468	0.09900	1.0164	0.12510
0.9	0.98577	0.12243	1.0320	0.18771
1.0	0.99911	0.14417	1.0543	0.26092

$\Gamma(s^2) = -0.89252\,e-3$

$\Gamma(s^2) = u(1,s) - 1 = 0.99911 - 1 = -0.00089$
$\Gamma'(s^2) = \xi(1,s) = 1.0543$

$$s^3 = s^2 - \frac{\Gamma(s^2)}{\Gamma'(s^2)} = 0.95813 - \frac{(0.99911 - 1)}{1.0543} = 0.95898$$

Solving for s^3 we find that $s^3 = 0.95898$. This value is the value we are looking for, i.e. our boundary condition $y(\alpha) = 0.95898$ which gives on shooting out, an exact value of $y(1) = 1$ and a value of $\Gamma(s^3) = -1e-5$

"Reverse shooting" techniques were also used with equal success.

The iteration scheme of equations(2-7 to 2-12) was also demonstrated with exceptional results. This iteration scheme proved to converge very rapidly and what would normally take uo to 50 iterations by a Newton bisection method to get y(1) correct to 5 decimal places would now only take 2 iterations for a linear d.e. and at most 10 (usually about 4 to 6 iterations, even for the wildest initial approximation) iterations for a non-linear d.e.

It was also concluded that the iteration scheme works well for simple reactions, such as $R = 1, R = y$, $R = y^2$, is robust for large ϕ being at least 50 but is often not very robust for considerably larger values of ϕ.

As an example to demonstrate the Robustness of the method, a sixth and final iteration in produced in the following sixth iteration for $\phi = 50.$ and where

$$R(y) = \frac{\phi^2 y}{1 + \beta y},$$

$\alpha = 0.5$ and $\beta = 1$

Iteration 6

$\Gamma(s^6) = 1e\text{-}7$

$s \approx 7.19045e\text{-}11$

x	u	v	ξ	η
0.5	0.7190e-10	0.0000	1.0000	0.0000
0.6	0.4638e-08	0.2241e-6	86.350	4466.0
0.7	0.5917e-06	0.2874e-4	15071	7.7757e5
0.8	0.7756e-04	0.3756e-2	2.573e6	1.3196e8
0.9	0.1016e-01	0.49497	4.292e8	2.1803e10
1.0	1.0000	38.1070	4.080e10	1.1339e12

table 2-1 Robustness of the shooting method for large ϕ

The above function is graphed in figure 2-1

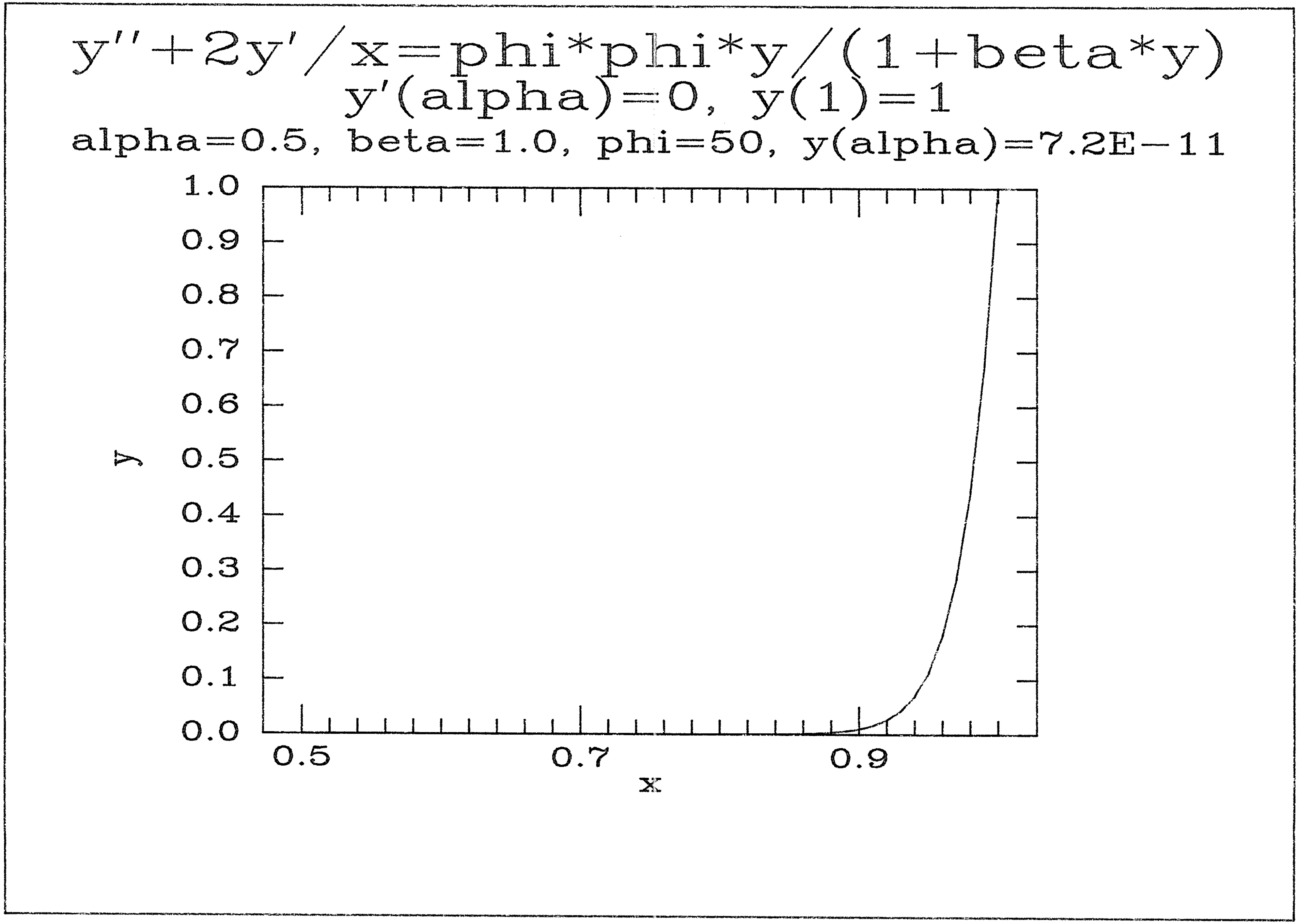

figure 2-1 Robustness of the Shooting Method for large phi

More powerful methods for solving the root of $\Gamma(s)$.

This did not make a considerable difference to the rate of convergence. In particular, a generalised N-R formula was used expecting to give a faster rate of convergence
This is given below

$$s^{k+1} = s^k - \frac{\Gamma(s^k) \pm \sqrt{(\Gamma'(s^k))^2 - 2\,\Gamma(s^k)\Gamma''(s^k)}}{\Gamma''(s^k)}$$

and was obtained by taking the first 3 terms of the Taylor's series expansion of $\Gamma(s^k)$ about 0 and considering only the positive square root.

As seen in figure 2-2 for various functions of $\Gamma(s)$ against s, it is not unexpected that the generalised N-R did not make a considerable difference to convergence compared with the ordinary N-R .
This is obvious noting the approximate linearity behaviour of $\Gamma(s)$.

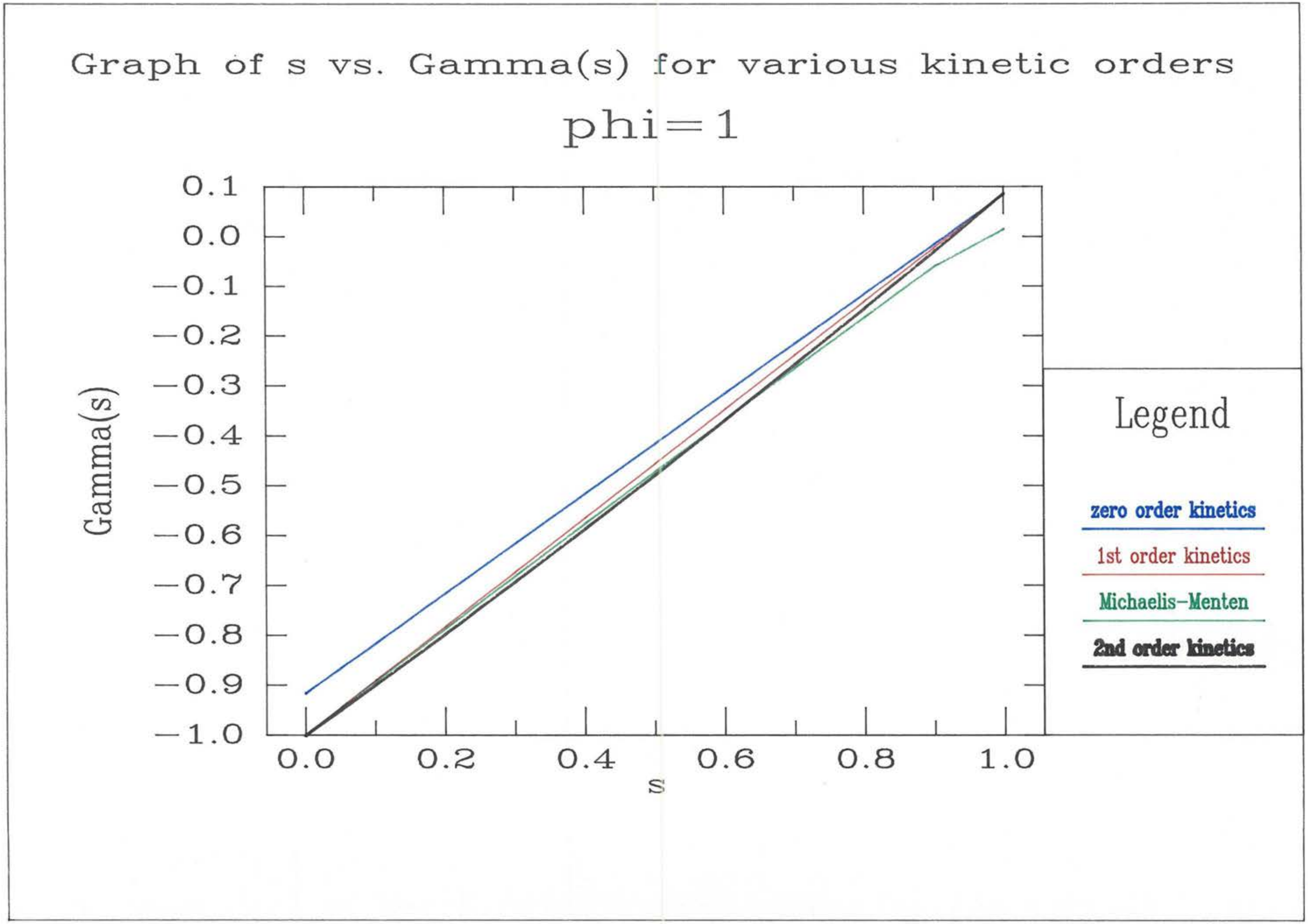

figure 2-2 s vs. Gamma(s)

2.2.3.4 Method of Numerical solutions

The algorithm used in the Initial Value method of Non-Linear boundary value problems was a 5th order Sarafyan algorithm with x interval steps of 1e-4 and printed in steps of 0.1 .

A 4th order Runge Kutta subroutine was also used to generate data but there was no considerable difference between this and the first algorithm at all.

The programs are not included in this thesis.

Absolute and relative errors were taken to be 1e-5 and 1e-4 respectively.

This was plotted and the monotonicity of ϕ^2 and β were studied.

In each case, only one degree of freedom was used, fixing either one of α, β and ϕ and varying the other two variables.

The asymptotic behaviour of problem (P) was studied in the proximity of 0+ and the behaviour of y as α tends to 0+.In particular when $\alpha = 0$ was chosen, a very small positive number (say 1e-7) was taken as an initial starting point instead of $\alpha = 0$. This would make the numerical integration much easier.

In the region of $\alpha = 0$, the approximation

$L[y] = ay''$ was used instead of
$L[y] = y'' + (a-1)y'/x$

The above follows directly from L'Hospital's rule.
where a = 1,2,3 representing a slab, cylinder and sphere respectively.

All results for various kinetic orders and geometries are given in subsequent chapters.

2.3 Zero Order Kinetics

2.3.1 Introduction

For zero order kinetics we solve the equation

$$\frac{D}{r^{a-1}}\frac{d}{dr}\left(r^{a-1}\frac{dS}{dr}\right) = \rho k_0 \qquad \textbf{(2-13)}$$

for a=1,2 and 3 being slab, cylindrical, and spherical geometries respectively.

The external boundary condition is

$S = S_b$ at $r = r_{bp}$

and the internal boundary condition is of two kinds depending on whether substrate is able to fully or partially penetrate the biofilm.

1. Total Penetration

When substrate is able to fully penetrate the biofilm, the following internal boundary condition applies

$$\frac{dS}{dr} = 0 \quad \text{at } r = r_m$$

2. Partial Penetration

When substrate is able to partially penetrate the biofilm, the following internal boundary condition applies

$$\frac{dS}{dr} = S = 0 \quad \text{at } r = r_i$$

where r_i is now the new inactive radius.

The above equation (2-23) has dimensionless form

$$\frac{1}{x^{a-1}}\frac{d}{dx}\left(x^{a-1}\frac{dy}{dx}\right) = \phi^2 \qquad \textbf{(2-14)}$$

with boundary conditions

$y'(\alpha) = 0$, $y(1) = 1$ for total penetration or

$y'(\alpha_i) = y(\alpha_i) = 0$, $y(1) = 1$ for partial penetration

and where

$$y = \frac{S}{S_b}, \quad x = \frac{r}{r_{bp}}, \quad \text{and } \phi^2 = \frac{r_{bp}^2\rho k_0}{S_b D}$$

$\alpha = r_m/r_{bp}$ is as in total penetration and $\alpha_i = r_i/r_{bp}$ is our new α in partial penetration.

A schematic diagram of partial penetration is given below in spherical geometries.

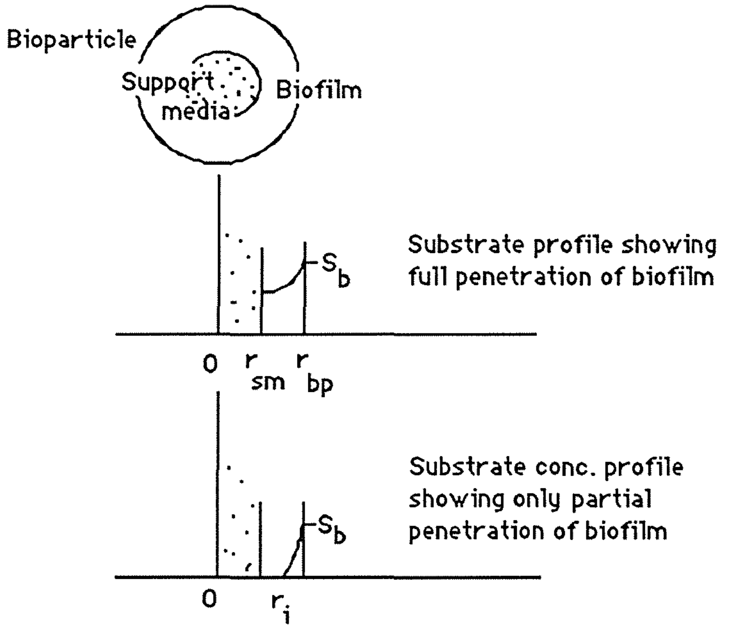

figure 2-3 A schematic diagram of partial penetration of biofilm

2.3.2 Zero Order Kinetics in Slab Geometry

For slab geometry a = 1 in the equation (2-14)

We have as our boundary conditions, $y'(\alpha) = 0$ and $y(1) = 1$.

Solving equation (2-14) with a = 1 we obtain

$$\frac{d^2y}{dx^2} = \phi^2 \tag{2-15}$$

Integrating equation (2-15)with respect to x twice, we obtain

$$\frac{dy}{dx} = \phi^2 x + c_1$$

or the general solution

$$y = \frac{\phi^2 x^2}{2} + c_1 x + c_2$$

Solving for constants c_1 and c_2 in the above equation

$$y'(\alpha) = 0 \Rightarrow c_1 = -\phi^2\alpha$$

$$y(1) = 1 \Rightarrow c_2 = 1 - \frac{\phi^2}{2} - c_1$$

$$= 1 - \frac{\phi^2}{2} + \phi^2\alpha$$

∴

Solution of equation (2-15) is therefore

$$y(x) = \frac{\phi^2 x^2}{2} - \phi^2\alpha x + (1 - \frac{\phi^2}{2} + \phi^2\alpha) \tag{2-16}$$

Evaluating this function at α, we obtain

$$y(\alpha) = -\frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2}{2} + \phi^2\alpha \tag{2-17}$$

Notice that $y(0) = 0$ when $\phi^2 = 2$, i.e this graph can get to zero for certain values of ϕ^2 and α and if $y(\alpha) < 0$ then $\phi^2 > 2$, for all α.

A graph of equation (2-16) is produced in figure 2-4 and figure 2-5 for fixed $\alpha = 0$ and $\alpha = 0.5$. and varying ϕ^2.

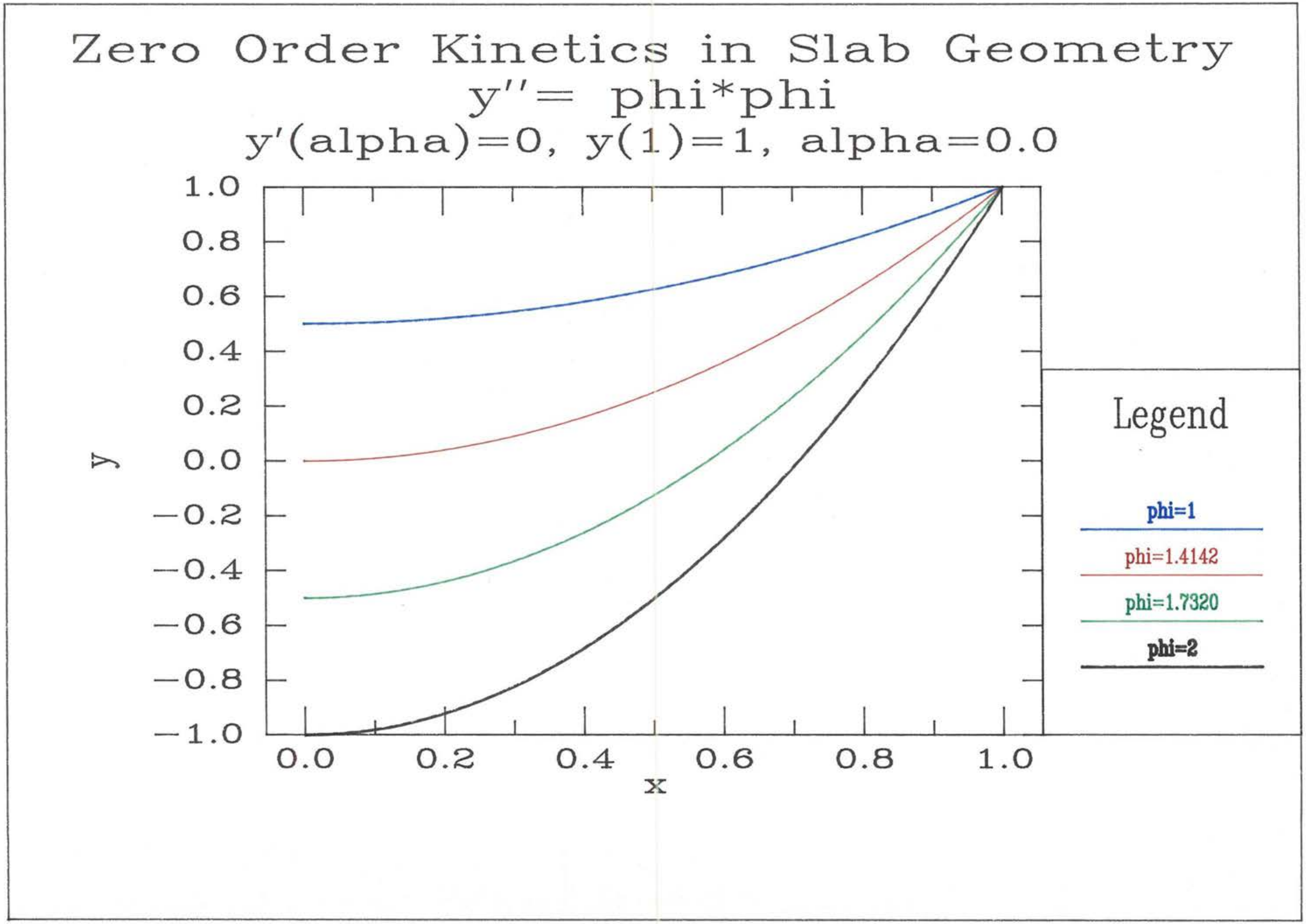

figure 2-4 Zero Order Kinetics in Slab Geometry alpha = 0

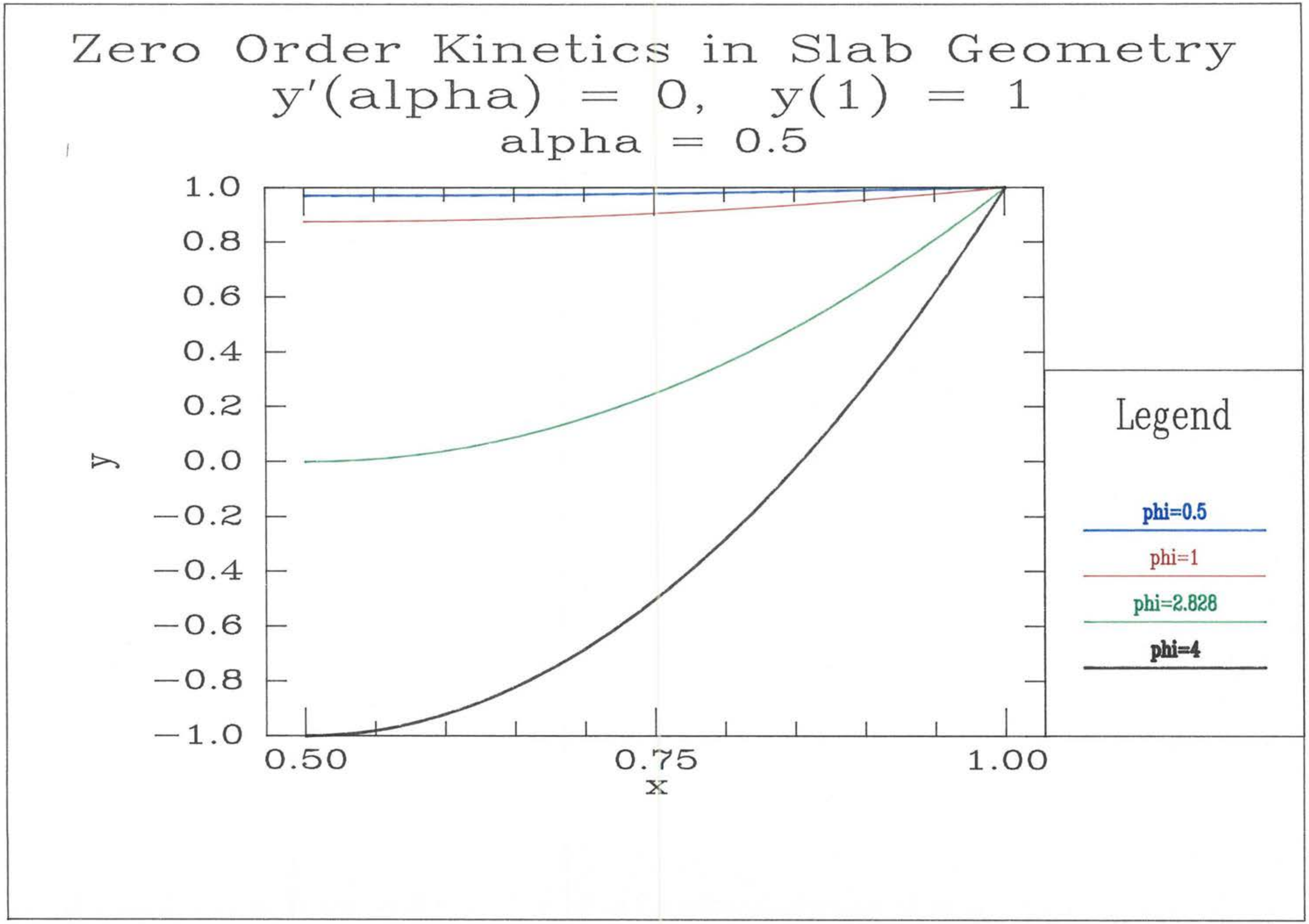

figure 2-5 Zero Order Kinetics in Slab Geometry alpha=0.5

Theorem 2.3.1

Assume $y(\alpha) : y(\alpha) = -\frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2}{2} + \phi^2\alpha$

We then have the following sufficient condition for $y(\alpha)$

$y(\alpha) < 0 \Rightarrow \phi^2 > 2$

Proof:

$$y(\alpha) < 0 \Rightarrow -\frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2}{2} + \phi^2\alpha < 0$$

$$\Rightarrow \quad \frac{\phi^2(\alpha-1)^2}{2} > 1$$

$$\Rightarrow \quad \phi^2 > \frac{2}{(\alpha-1)^2} > 2$$

for all $\alpha \in (0,1)$

⊠.

note: The converse, however, is not true in general.

e.g. take $\phi^2 = 4$, $\alpha = 0.8$ and it follows that $y(\alpha) = 0.92 > 0$.

The above theorem implies that if partial penetration occured in a slab, the Thiele modulus, ϕ^2 would have to be of an order of at least 2.

The necessary condition is demonstrated in the following theorem

Theorem 2.3.2

Assume $y(\alpha) : y(\alpha) = -\frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2}{2} + \phi^2\alpha$

$$\phi^2 > \frac{2}{(1-\alpha)^2} \Rightarrow y(\alpha) < 0$$

Proof:

$$\phi^2 > \frac{2}{(\alpha-1)^2} \Rightarrow \frac{\phi^2(\alpha-1)^2}{2} > 1$$

$$\Rightarrow \quad -\frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2}{2} + \phi^2\alpha < 0$$

$$\Rightarrow \quad y(\alpha) < 0$$

⊠.

2.3.3 Zero Order Kinetics in cylindrical geometry

Letting a = 2 in the equation(2-14) we obtain

$$\frac{1}{x}\left(\frac{d}{dx}\left(x\frac{dy}{dx}\right)\right) = \phi^2 \qquad (2\text{-}18)$$

with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$

Multiplying equation (2-18) through by x , we obtain

$$\frac{d}{dx}\left(x\frac{dy}{dx}\right) = \phi^2 x$$

Integrating twice with respect to x

$$x\frac{dy}{dx} = \frac{\phi^2 x^2}{2} + c_1$$

$$\frac{dy}{dx} = \frac{\phi^2 x}{2} + \frac{c_1}{x}$$

and we finally obtain the general solution with two constants

$$y = \frac{\phi^2 x^2}{4} + c_1 \ln|x| + c_2 \qquad (2\text{-}19)$$

Solving for constants c_1 and c_2

$$y'(\alpha) = 0 \Rightarrow \frac{\phi^2 \alpha}{2} + \frac{c_1}{\alpha} = 0$$

$$\Rightarrow c_1 = -\frac{\phi^2 \alpha^2}{2}$$

$$y(1) = 1 \Rightarrow c_2 = 1 - \frac{\phi^2}{4}$$

$\therefore$

Solution of equation (2-18). is

$$y(x) = \frac{\phi^2 x^2}{4} - \frac{\phi^2 \alpha^2}{2}\ln|x| + 1 - \frac{\phi^2}{4} \qquad (2\text{-}20)$$

Equating this function y(x) at its minimum, α

$$y(\alpha) = \frac{\phi^2\alpha^2}{4} - \frac{\phi^2\alpha^2}{2}\ln|\alpha| + 1 - \frac{\phi^2}{4} \qquad \textbf{(2-21)}$$

It is clear that $y(0) = 0$ at $\phi^2 = 4$ i.e this function gets to zero concentration for some values of ϕ and α and it can be shown in theorem 2.3.4 that if $y(\alpha)<0$ then $\phi^2 > 4$

It is also clear from previous theorems that $y(\alpha)$ is a minimum point

A graph of this is given in figure 2-6 for fixed $\alpha = 0.5$ and varying ϕ^2

Theorem 2.3.3
Assume

$$y(\alpha) : y(\alpha) = \frac{\phi^2\alpha^2}{4} - \frac{\phi^2\alpha^2}{2}\ln|\alpha| + 1 - \frac{\phi^2}{4}$$

We then have the following sufficient condition

$$y(\alpha) < 0 \Rightarrow \phi^2 > 4$$

Proof:

$$y(\alpha) < 0 \Rightarrow y(\alpha) = \frac{\phi^2\alpha^2}{4} - \frac{\phi^2\alpha^2}{2}\ln|\alpha| + 1 - \frac{\phi^2}{4} < 0$$

$$\Rightarrow \quad \phi^2 > \frac{4}{1+2\alpha^2\ln|\alpha| - \alpha^2} > 4$$

for all $\alpha \in (0,1)$

⊠.

The converse, however is not true in general.

The above theorem implies that if partial penetration occured in a cylinder, the Thiele modulus would have to be of an order of at least 4.

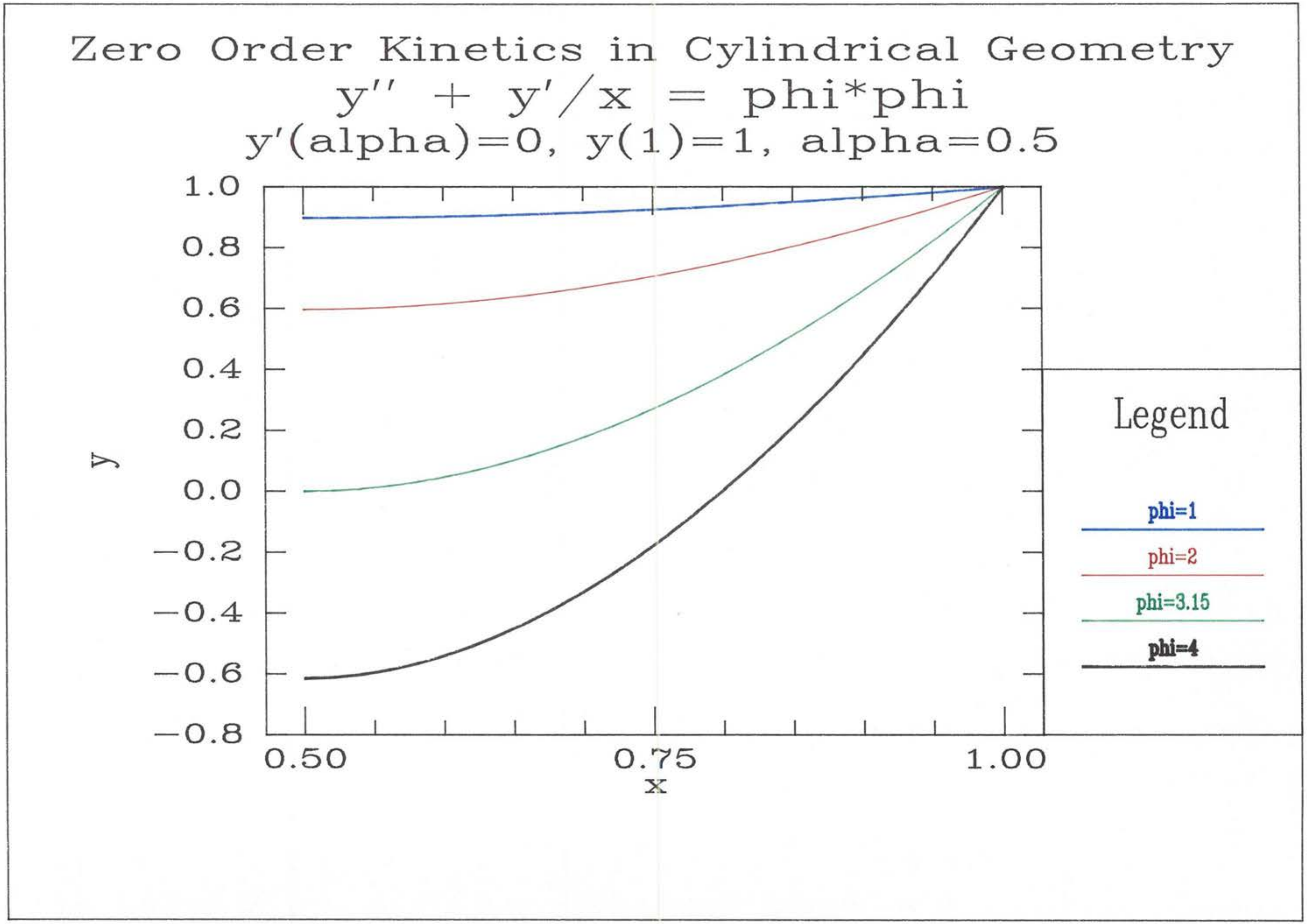

figure 2-6 Zero Order Kinetics in Cylindrical Geometry alpha=0.5

The necessary condition is demonstrated in theorem 2.3.4
We have no way apart from numerical procedures for determining the roots of $y(\alpha)$ that would lead us to ultimately determine conditions on ϕ^2 that would result in $y(\alpha) < 0$.
We however, notice the result

$$\phi^2 > \frac{4}{1+2\alpha^2\ln|\alpha| - \alpha^2} > 4$$

from theorem 2.3.4 and attempt to use this to determine a condition on ϕ^2.
This leads to the following theorem

Theorem 2.3.4

Assume

$$y(a) : y(\alpha) = \frac{\phi^2\alpha^2}{4} - \frac{\phi^2\alpha^2}{2} \ln|\alpha| + 1 - \frac{\phi^2}{4}$$

$$\phi^2 > \frac{4}{1+2\alpha^2\ln|\alpha| - \alpha^2} \Rightarrow y(\alpha) > 0$$

Proof:
Assume

$$\phi^2 > \frac{4}{1+2\alpha^2\ln|\alpha| - \alpha^2}$$

(The denominator always positive in the interval $\alpha \in (0,1)$)

It follows from this assumption that

$$\phi^2(1+2\alpha^2\ln|\alpha|-\alpha^2)-4 > 0$$

$$\Rightarrow \quad \frac{\phi^2}{4}(1+2\alpha^2\ln|\alpha| - \alpha^2) - 1 > 0$$

$$\Rightarrow \quad \frac{\phi^2}{4}(\alpha^2 - 2\alpha^2\ln|\alpha| - 1) + 1 < 0$$

$\Rightarrow$ $y(\alpha) < 0$ in the interval $\alpha \in (0,1)$ ⊠.

2.3.4 Zero Order Kinetics in Spherical Geometry

Letting a = 3 in equation (1-14) we get

$$\frac{d}{dx}\left(x^2 \frac{dy}{dx} \right) = \phi^2 x^2 \qquad \text{(2-22)}$$

with $y'(\alpha) = 0$ & $y(1) = 1$ for total penetration and $y(\alpha) = y'(\alpha) = 0$ & $y(1) = 1$ for partial penetration.

2.3.4.1.Total penetration of substrate through the biofilm

Integrating eqn.(2-22) twice with respect to x while multiplying through by x

$$x^2 \frac{dy}{dx} = \frac{\phi^2 x^3}{3} + c_1$$

$$\frac{dy}{dx} = \frac{\phi^2 x}{3} + \frac{c_1}{x^2}$$

and we finally obtain the general solution

$$y = \frac{\phi^2 x^2}{6} - \frac{c_1}{x} + c_2 \qquad \text{(2-23)}$$

Solving for c_1 and c_2 by substituting the boundary conditions

$$y'(\alpha) = 0 \Rightarrow \frac{\phi^2 \alpha}{3} + \frac{c_1}{\alpha^2} = 0 \quad \Rightarrow c_1 = \frac{-\phi^2 \alpha^2}{3}$$

$$y(1) = 1 \Rightarrow c_2 = 1 + c_1 - \frac{\phi^2}{6} \Rightarrow c_2 = 1 - \frac{\phi^2 \alpha^3}{3} - \frac{\phi^2}{6}$$

$\therefore$

Solution of equation (2-22) is

$$y(x) = \frac{\phi^2 x^2}{6} + \frac{\phi^2 \alpha^3}{3x} + \left(1 - \frac{\phi^2 \alpha^3}{3} - \frac{\phi^2}{6}\right) \qquad \text{(2-24)}$$

We also note with interest that if $\alpha = 0$, we get

$$y(x) = \frac{\phi^2 x^2}{6} + 1 - \frac{\phi^2}{6} \quad , \qquad \text{(2-25)}$$

a parabola

From theorem 1.1 (the one-dimensional maximum principle) we have that the maximum of the unique solution to equation(2-22) and the minimum are found on the boundaries of $(\alpha,1)$ .The maximum of $y(x)$ is at $x = 1$ and the minimum is at $x = \alpha$.
i.e.

$$y(\alpha) \leq y(x) \leq y(1) = 1$$

with $y(\alpha)$ the minimum of $y(x)$ being

$$y(\alpha) = \frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2\alpha^3}{3} - \frac{\phi^2}{6} = \phi^2\left(\frac{\alpha^2}{2} - \frac{\alpha^3}{3} - \frac{1}{6}\right) + 1 \qquad \textbf{(2-26)}$$

We have the following theorem that determines under what conditions, partial penetration will occur.

Theorem 2.3.5
Assume

$$y(\alpha) : y(\alpha) = \frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2\alpha^3}{3} - \frac{\phi^2}{6} = \phi^2\left(\frac{\alpha^2}{2} - \frac{\alpha^3}{3} - \frac{1}{6}\right) + 1$$

$$y(\alpha) < 0 \Rightarrow \phi^2 > 6$$

Proof:

$$y(\alpha) < 0 \Rightarrow y(\alpha) = \frac{\phi^2\alpha^2}{2} + 1 - \frac{\phi^2\alpha^3}{3} - \frac{\phi^2}{6} = \phi^2\left(\frac{\alpha^2}{2} - \frac{\alpha^3}{3} - \frac{1}{6}\right) + 1 \quad < 0$$

$$\Rightarrow \quad \phi^2 > \frac{6}{2\alpha^3 - 3\alpha^2 + 1} > 6$$

for all $\alpha \in (0,1)$

This follows by observing that $2\alpha^3-3\alpha^2+1$ is a decreasing function in the domain $[0,1]$, is minimum at $\alpha = 0$ and is positive.

⊠

The theorem above implies that if partial penetration occured in a sphere, the Thiele modulus would have to be of an order of at least 6. The converse however, is not true in general (except at $\alpha = 0$).

Theorem 2.3.6
Assume

$$y(\alpha) : y(\alpha) = \phi^2 \left(\frac{\alpha^2}{2} - \frac{\alpha^3}{3} - \frac{1}{6} \right) + 1$$

$$\phi^2 > \frac{6}{2\alpha^3 - 3\alpha^2 + 1} \Rightarrow y(\alpha) < 0$$

Proof:

$$\phi^2 > \frac{6}{2\alpha^3 - 3\alpha^2 + 1} \Rightarrow \phi^2 (2\alpha^3 - 3\alpha^2 + 1) > 6$$

$$\Rightarrow \phi^2 \left(\frac{\alpha^2}{2} - \frac{\alpha^3}{3} - \frac{1}{6} \right) + 1 < 0$$

$$\Rightarrow y(\alpha) < 0$$

⊠.

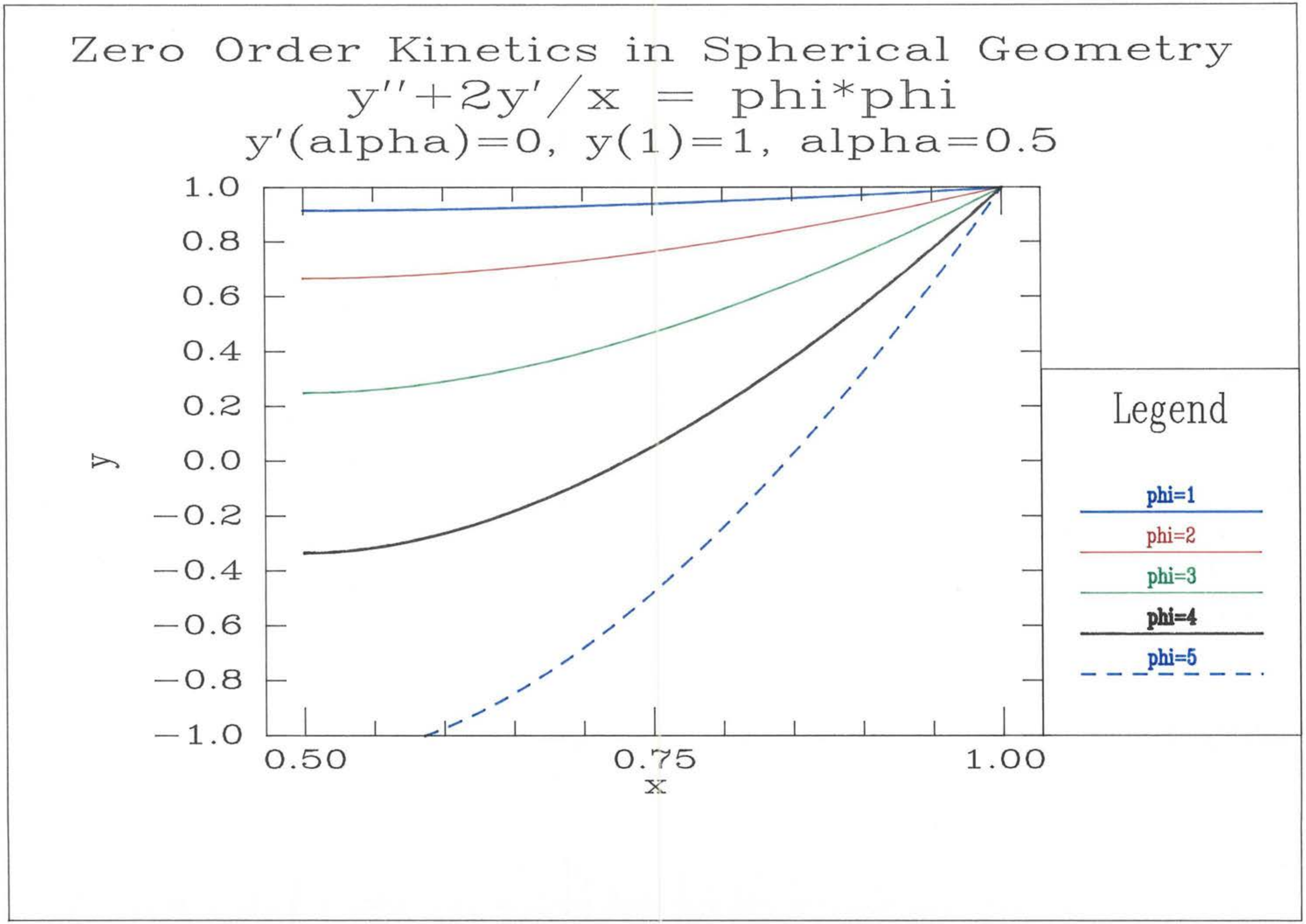

figure 2-7 Zero Order kinetics in Spherical Geometry alpha=0.5

2.3.4.2. Partial Penetration of Substrate through the biofilm

a) concept 1

It can be shown that for certain values of ϕ^2 and α the equation (2-26) can get below zero. This has also been shown with slab and cylindrical geometry where we found that for some α , the Thiele modulus, ϕ^2 has to be greater than 2 and 4 respectively if this happened.

We have just shown, that if $y(\alpha)$ to get below zero in spherical geometry for all α, the Theile modulus ϕ^2 has to be greater than 6.

Having the above function get below zero is not a physical reality for this would imply a negative concentration .

A graph of y(x) vs. x is given in figure 2-7 allowing ϕ^2 to be large enough to make $y(\alpha) < 0$

By increasing ϕ^2 monotonically, and varying α, we find that y(x) first gets to zero when $y(\alpha) = 0$ or equivalently when $\phi^2 = 6$ for all α.

This first occurs at $\alpha=0$.

Assuming that we obtain zero concentration whenever the equation (2-24) gets below zero, we obtain the equation

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} = \phi^2 H(y) = \begin{cases} \phi^2 , & \text{for } y \geq 0 \\ 0 , & \text{for } y \leq 0 \end{cases} \qquad \textbf{(2-27)}$$

for zero order kinetics in a sphere.

note:

If y(x) is continuous, this would imply that dy/dx is continuous.

Since the solution to equation (2-27) is discontinuous when y = 0, the discontinuity must therefore lie in the second and subsequent derivatives.

We shall call this point of discontinuity α_i. Taking a left limit of α_i we see that these derivatives are zero. Our function y must therefore be flat (zero gradient) once it hits zero concentration. Physically this would mean that a discontinuity of flux -DdS/dx (in dimensional coordinates) cannot happen once concentration gets to zero concentration.

In summary, we find that the equation (2-24) can however get to zero before it gets to α , the ratio of the radius of the support media to the radius of the bioparticle. This gives us in zero order kinetics, the concept of partial penetration or sustrate diffusing in the biofilm and reaching zero concentration before it gets to the boundary of the support media.

We can therefore redefine α to be the ratio of the distance to that point in the biofilm where concentration gets to zero to the total radius of the biofilm.

This new α, we shall call α_i.
Mathematically, this is equivalent to imposing a third boundary condition $y(\alpha) = 0$ and determining α in terms of our Thiele Modulus ϕ^2.
This would then preserve our continuity of flux across the boundary α_i .

b)concept 2

We can also get the concept of partial penetration by assuming that for an ideal system there is to be zero concentration of substrate at the boundary.

This would make the system the most efficient , as we do not like there to be still some substrate at the boundary of the support media which could have been broken down by a more efficient system.

We therefore impose the additional boundary condition $S = 0$ at r_m. This is equivalent in dimensionless coordinates to imposing the condition $y = 0$ at $x = \alpha$.

We may then get an expression that links the Thiele modulus ϕ^2 to a giving us an idea of what ϕ^2 to choose.

We shall show that the phenomenon of partial penetration is not true in general for all kinetic orders .

The solution of equation (2-22) is equation (2-23)
Our general solution is then

$$y(x) = \frac{\phi^2 x^2}{6} - \frac{c_1}{x} + c_2$$

with its derivative

$$y'(x) = \frac{\phi^2 x}{3} + \frac{c_1}{x^2}$$

Solving for c_1 and c_2 with boundary conditions $y'(\alpha)=y(\alpha)=0$ and $y(1) = 1$ & where new α_i has to be determined

$$y(\alpha) = 0 \Rightarrow \frac{\phi^2 \alpha^2}{6} - \frac{c_1}{\alpha} + c_2 = 0 \quad \text{(i)}$$

$$y'(\alpha) = 0 \Rightarrow \frac{\phi^2 \alpha}{3} + \frac{c_1}{\alpha^2} = 0 \Rightarrow c_1 = \frac{-\phi^2 \alpha^3}{3} \quad \text{(ii)}$$

$$y(1) = 1 \Rightarrow \frac{\phi^2}{6} - c_1 + c_2 = 1 \quad \text{(iii)}$$

We then solve these three equations for c_1 and c_2 to get

$$c_2 = \frac{-\phi^2\alpha^2}{6} + \frac{c_1}{\alpha} = \frac{-\phi^2\alpha^2}{6} \quad \frac{\phi^2\alpha^2}{3} = - \frac{\phi^2\alpha^2}{2}$$

by substituting c_1 and c_2 into (iii), we obtain

$$\frac{\phi^2}{6} + \frac{\phi^2\alpha^2}{3} - \frac{\phi^2\alpha^2}{2} = 1$$

or simplifying

$$\phi^2(\,1+2\alpha^3 - 3\alpha^2) = 6$$

On further simplification we obtain the equation

$$\phi^2 = \frac{6}{2\alpha^3 - 3\alpha^2 + 1} = \frac{6}{(\alpha-1)^2(2\alpha+1)} \qquad \textbf{(2-28)}$$

a relationship between our new α and Thiele modulus ϕ^2.
The equation (2-28) has asymptotes at $\alpha = 1$ and $\alpha = -0.5$

Of course $\alpha = -0.5$ (which is the ratio of r_i to r_{bp} can never be physically possible) and $\alpha = 1$ means that $r_i = r_{bp}$,
i.e. there is physically no penetration and so the Thiele modulus ϕ^2 will be very large

A graph of ϕ^2 against α is given in figure 2-8

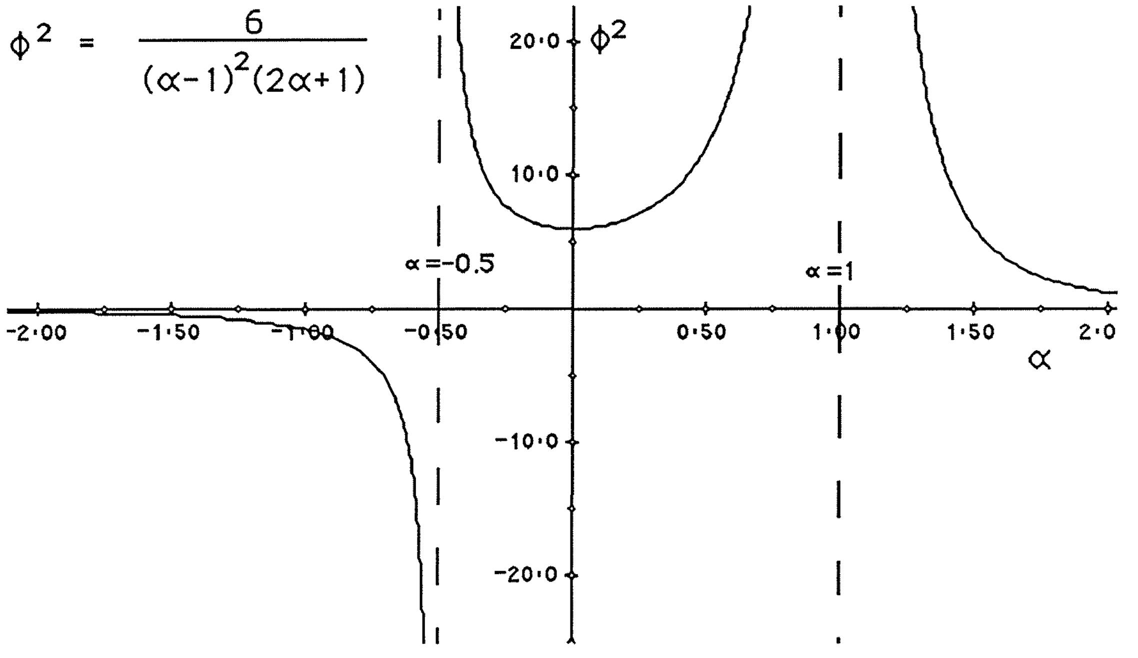

figure 2-8 graph of α vs. φ 2

We write equation (2-28) as

$$2\alpha^3 - 3\alpha^2 + (1 - \frac{6}{\phi^2}) = 0 \quad (2\text{-}29)$$

and call the left hand side F(α,φ) or F(α) for fixed φ.
comment: notice that F(α) = -y(α)

Solving for F(α)=0 for fixed φ

Solve F(α)=0 for α by Cardano's method

1. By Writing F(α) in the normal form of a cubic ($\alpha^3 + a\alpha^2 + b\alpha + c$) we get

$$\alpha^3 - \frac{3}{2}\alpha^2 + \frac{\phi^2 - 6}{2\phi^2} = 0 \quad (2\text{-}30)$$

2. Substituting α = y - a/3 where a = -3/2 into equation (2-29), . we can get the reduced form

$$y^3 - \frac{3}{4}y + \frac{\phi^2 - 12}{4\phi^2} = 0 \quad (2\text{-}31)$$

3. The discriminant of a cubic, Δ is defined to be $q^2 + p^3$ where $y^3 + 3py + 2q = 0$ is the reduced form of a cubic.

We therefore solve for p and q in the above equation and obtain

$$p = -\frac{1}{4} \quad \text{and} \quad q = \frac{\phi^2 - 12}{8\phi^2} \tag{2-32}$$

The discriminant $\Delta = q^2 + p^3$ is therefore

$$\Delta = q^2 + p^3 = \frac{-24\phi^2 + 144}{64\phi^2} = \frac{3(6-\phi^2)}{8\phi^2} \tag{2-33}$$

4. A cubic equation possesses

a) one real root and 2 conjugate complex solutions of the discriminant $\Delta > 0$,
$\Delta > 0 \iff \phi^2 < 6$

b) 3 real solutions, of which at least 2 are equal if $\Delta = 0$,
$\Delta = 0 \iff \phi^2 = 6$

c) 3 real and different solutions if $\Delta < 0$
$\Delta < 0 \iff \phi > 6$ in our case

5. If $\Delta \geq 0$ i.e. $\phi^2 \leq 6$ the 3 roots of eqn.(2.31) are defined to be

$$y_1 = u + v$$
$$y_2 = \frac{u+v}{2} + \frac{i}{2}\sqrt{3}\,(u - v)$$
$$y_3 = \frac{u+v}{2} - \frac{i}{2}\sqrt{3}\,(u - v)$$

where

$$u = \sqrt[3]{-q + \sqrt{q^2 + p^3}} = \sqrt[3]{-q + \sqrt{\Delta}} = \sqrt[3]{\frac{12 - \phi^2}{8\phi^2} + \sqrt{\frac{-24\phi^2 + 144}{64\phi^2}}}$$

$$v = \sqrt[3]{-q - \sqrt{q^2 + p^3}} = \sqrt[3]{-q - \sqrt{\Delta}} = \sqrt[3]{\frac{12 - \phi^2}{8\phi^2} - \sqrt{\frac{-24\phi^2 + 144}{64\phi^2}}}$$

and
therefore the 3 roots of $F(\alpha)$ are

$$\alpha_j = y_j - \frac{a}{3} \quad \text{where } a = -\frac{3}{2}$$

or

$$\alpha_j = y_j + \frac{1}{2} \quad \text{where } j = 1,2,3 \qquad \textbf{(2-34)}$$

6. If $\Delta < 0$ i.e. $\phi^2 > 6$
we evaluate the angle θ

$$\theta = \cos^{-1} \frac{-q}{\sqrt{-p^3}}$$

and solutions are expressed as

$$y_1 = 2\sqrt{-p}\,\cos\left(\frac{\theta}{3}\right)$$

$$y_2 = -2\sqrt{-p}\,\cos\frac{1}{3}(\theta + \pi)$$

and

$$y_3 = -2\sqrt{-p}\,\cos\frac{1}{3}(\theta + \pi)$$

The 3 real roots of $F(\alpha)$ when $\phi^2 > 6$ are therefore

$$\alpha_j = y_j + \frac{1}{2} \quad \text{where } j = 1,2,3 \qquad \textbf{(2-35)}$$

7. If $\Delta = 0$ i.e. $\phi^2 = 6$ then $F(\alpha)$ becomes
$F(\alpha) = 2\alpha^3 - 3\alpha^2 = 0$
$\Rightarrow \alpha^2(2\alpha - 3) = 0$
and the solutions of $F(\alpha)$ where at least two are equal are therefore
$\alpha = 0$ and $\alpha = 3/2$

A table of ϕ^2 vs. the roots (to 4 decimal places) of $F(\alpha)$ is given in table 2-1.

ϕ^2	Real roots α_1	α_2	α_3
0	undefined		
0.5	2.88		
1	2.0786		
2	1.8064		
3	1.6776		
4	1.5980		
5	1.5421		
6	0	0	1.5
7	-0.2047	0.2379	1.4668
8	-0.2660	0.3264	1.4397
9	-0.3039	0.3870	1.4170
10	-0.3305	0.4329	1.3976
∞	-0.5	1	1

table 2-2 ϕ^2 vs. roots of $F(\alpha)$

$F(\alpha)$ is graphed against α in figure 2-9 to illustrate the behaviour of $F(\alpha)$ in the interval $0 < \alpha < 1$.

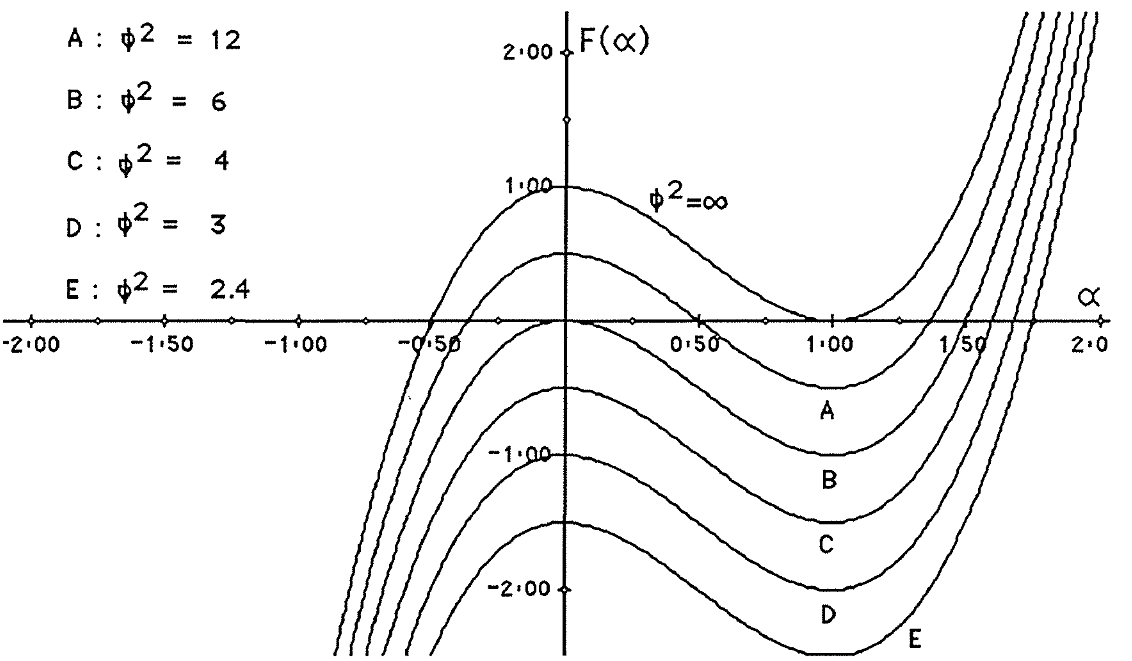

figure 2-9 graph of . α. vs.$F(\alpha)$

Lemma 1
$F(\alpha,\phi)$ is monotonically increasing with ϕ in the interval (0,1)

Proof:

$$\frac{\partial F(\alpha,\phi)}{\partial \phi} = \frac{12}{\phi^3} > 0$$

and it follows that $F(\alpha,\phi)$ is monotonically increasing with ϕ in the interval $\alpha \in (0,1)$.

⊠.

Lemma 2
$F(\alpha,\phi)$ is monotonically decreasing with α in the interval (0,1)

Proof:

$$\frac{\partial F(\alpha,\phi)}{\partial \phi} = 6\alpha^2 - 6\alpha = 6\alpha(\alpha-1) < 0$$

since $\alpha(\alpha-1)$ does not change sign in the interval (0,1) i.e. $\alpha(\alpha-1)$ is always negative
It therefore follows that $F(\alpha,\phi)$ is monotonically decreasing with α in the interval (0,1).

⊠.

It can be shown by Lemma 2 that $\alpha = 0$ and $\alpha = 1$ are critical points
Moreover, performing a 2-dim. second derivative test to see whether these points are local maxima or minima, we obtain the discriminant

$$\Delta(\alpha,\phi) = F_{\alpha\alpha}(\alpha,\phi)\, F_{\phi\phi}(\alpha,\phi) - [\, F_{\alpha\phi}(\alpha,\phi)\,]^2$$

$$= 6(2\alpha - 1)\,\frac{(-36)}{\phi^4} - 0^2$$

$$= \frac{-216}{\phi^4}(2\alpha - 1)$$

from which we obtain that $\alpha = 0$ is a local maximum and $\alpha = 1$ is a saddle point.

Fixing ϕ^2 and performing a one dimensional first and second derivative test, we obtain

$$\frac{dF(\alpha)}{d\alpha} = \alpha(\alpha-1) < 0$$

i.e.
$F(\alpha)$ is monotonically decreasing with α, with critical points $\alpha = 0$ and $\alpha = 1$.
and

$$\frac{d^2F(\alpha)}{d\alpha^2} = 2\alpha - 1$$

It therefore follows that

$\alpha = 0.5$ is a point of inflection of $F(\alpha)$
$\alpha = 1$ is a minimum point of $F(\alpha)$
$\alpha = 0$ is a maximum point of $F(\alpha)$

This is observed in figure 2-9.

We have the following theorem

Theorem 2.3.7

There exists a unique (real) root of the cubic $F(\alpha)$ in the interval (0,1) iff $\phi^2 > 6$. for fixed ϕ^2

Proof

($\Rightarrow$)

This follows directly from the discriminant q^2+p^3 of the reduced form of the cubic $F(\alpha)$ i.e. equation (2-31).

If the condition must hold for the reduced form of the equation $F(\alpha)$, it must hold for $F(\alpha)$ since they are both isomorphic.

From earlier work

$$\Delta = \frac{-24\phi^2 + 144}{64\phi^2} = \frac{3(6-\phi^2)}{8\phi^2}$$

and

$$p = \frac{1}{4} \qquad q = \frac{\phi^2 - 12}{8\phi^2}$$

It may be noticed that

1. $\Delta = q^2 + p^3 \geq 0 \Leftrightarrow \phi^2 \leq 6$

2. $\Delta = q^2 + p^3 \leq 0 \Leftrightarrow \phi^2 \geq 6$

3. $q = 0 \Leftrightarrow \phi^2 > 12$

4. Decrease $\phi^2 \Rightarrow$ decrease q

5. $F(\alpha,\phi^2) = F(\alpha,6)$ has roots $\alpha_1=0$, $\alpha_2=0$, $\alpha_3=1.5$
   decrease $\phi^2 \Rightarrow y_1 = u+v$ increases $\Rightarrow y_1 > 1 \Rightarrow \alpha_1 > 1.5$

This is only real root. (from soln. of roots of $F(\alpha)$ eqn.4)

6. We need thus, only look at the case when $\Delta = q^2 + p^3 \leq 0$
i.e. when $\phi^2 \geq 6$

7. Assume $\phi^2 \geq 6$

8. The uniqueness of the root α of $F(\alpha)$ in the interval (0,1) follows from the Intermediate Value Theorem which when applied to $F(\alpha)$ states that if $F(\alpha)$ is continuous on (0,1), (which it is in our case) and is strictly increasing or decreasing (which we have shown from our two lemmas).

Then if $F(\alpha) = 0$ is between $F(0)$ and $F(1)$ which are of opposite sign then there is a unique α in (0,1) such that $F(\alpha) = 0$.

We have yet to show that $F(0)$ and $F(1)$ are of opposite signs

9. Assuming $\phi^2 > 6$

$$\phi^2 > 6 \quad \Rightarrow \quad F(0) = 1 - \frac{6}{\phi^2} > 0$$

$$\phi^2 > 6 \quad \Rightarrow \quad F(1) = -\frac{6}{\phi^2} < 0$$

Thus if $\phi^2 > 6$ then $F(\alpha)$ has a unique root in the interval (0,1)

($\Leftarrow$)

1. Suppose there exists a (unique) root of $F(\alpha)$ in the interval (0,1)

2. Call this root α

3. Substitute into $F(\alpha)$: $F(\alpha) = 2\alpha^3 - 3\alpha^2 + \left(1 - \frac{6}{\phi^2}\right) = 0$

4. Since $2\alpha^3 < 3\alpha^2$ in the interval (0,1) it follows that

$$1 - \frac{6}{\phi^2} > 0$$

and therefore

5. $\phi^2 > 6$

⊠.

Corollary 2.3.7

There exists a unique (real) root α of the cubic $y(\alpha)$ $(=-F(\alpha))$ where

$$\alpha = \frac{1}{2} - 2\sqrt{-p}\,\cos\frac{1}{3}(\theta + \pi)$$

$$p = -\frac{1}{4}$$

$$\theta = \cos^{-1}\frac{-q}{\sqrt{-p^{3}}}$$

and

$$q = \frac{12 - \phi^2}{\phi^2}$$

in the interval (0,1) ,

iff $\phi^2 > 6$

Interesting Observation

1. It may be noticed that by imposing the condition $y(\alpha) = 0$ in the total penetration problem which has solution

$$y(x) = \frac{\phi^2 x^2}{6} - \frac{c_1}{x} + c_2$$

with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$
we get a quadratic equation when $\alpha = 0$

$$y = \frac{\phi^2 x^2}{6} \qquad \textbf{(2-36)}$$

2. It has also been observed that for partial penetration in a slab , cylinder and sphere the Thiele modulus has to be of an order $\phi^2 > 2,4$ and 6 respectively for some $\alpha \in [0,1]$

3. A graph of Partial Penetration of Substrate in Spherical Geometries with Zero Order kinetics is given in figure 2-10.

4. A comparison of the graphs of substrate concentrations in slab, cylindrical and spherical geometries with Zero Order kinetics is given in figure 2-11. Here α and ϕ is chosen so that partial penetration does not occur.

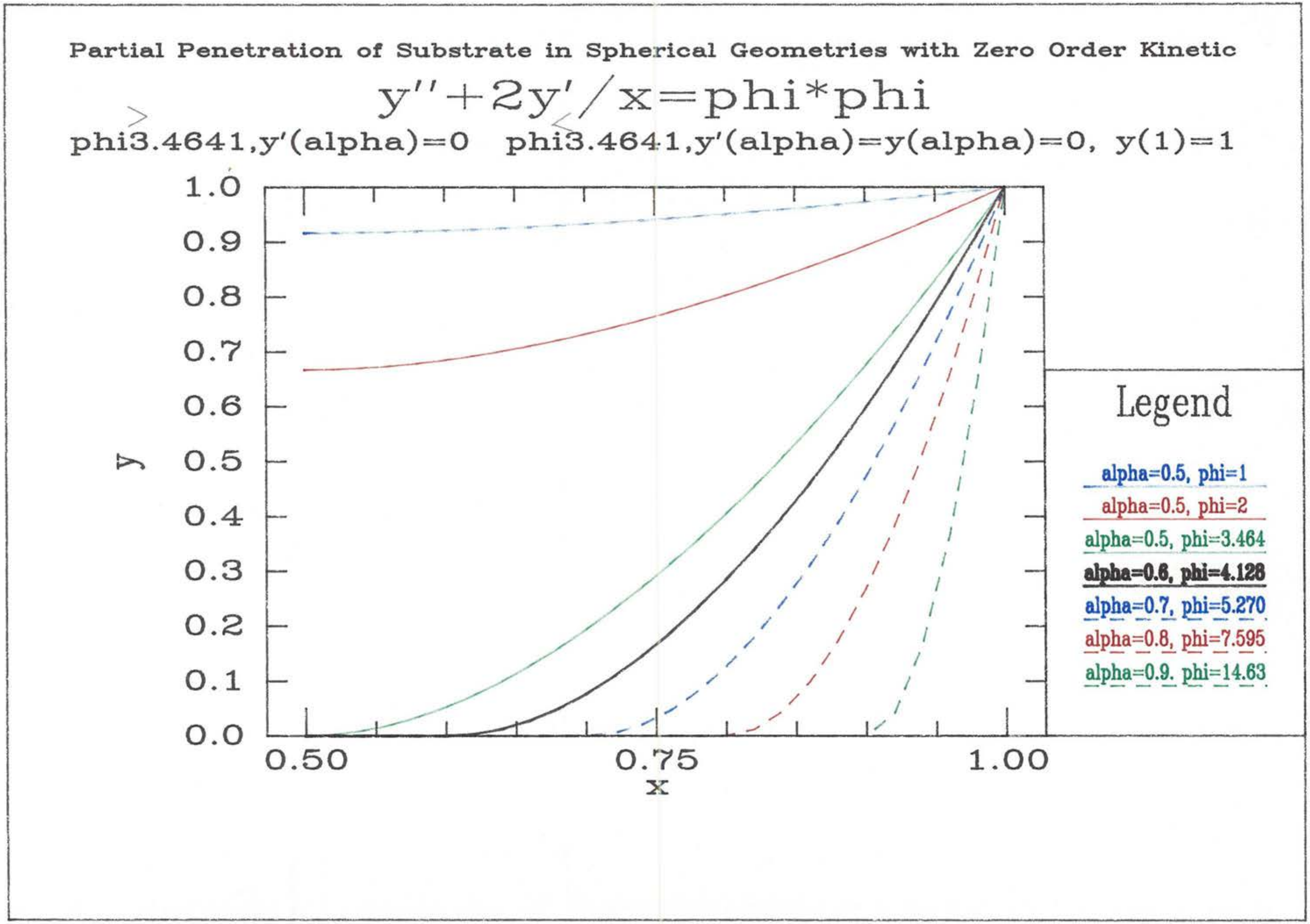

figure 2-10 Partial Penetration

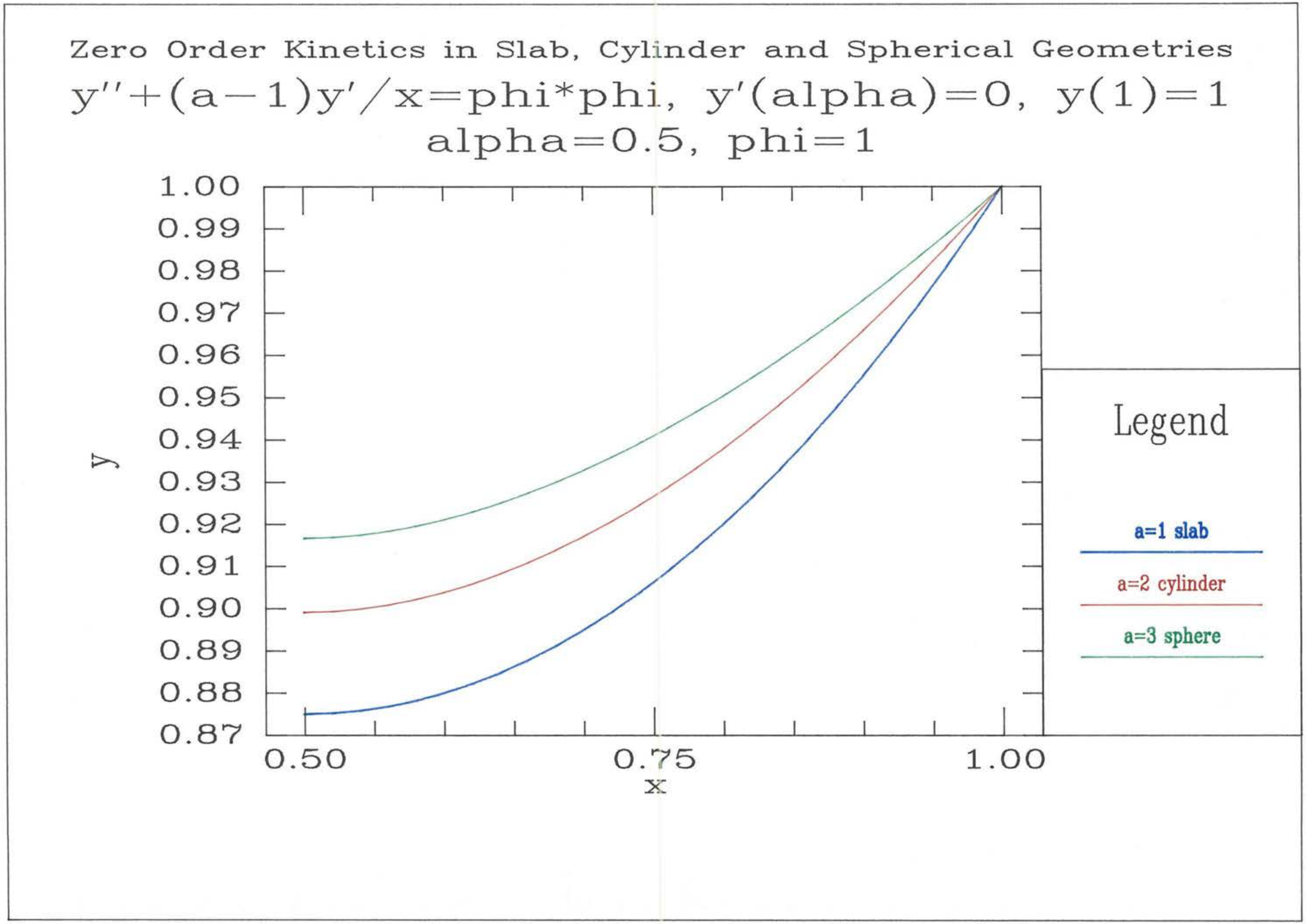

figure 2-11 Zero Order kinetics in Slab,Cylindrical and Spherical Geometries

2.4 First Order Kinetics

2.4.1 Introduction

For first order kinetics, we solve the equation

$$\frac{D}{r^{a-1}}\frac{d}{dr}\left(r^{a-1}\frac{dS}{dr}\right) = \rho k_1 S \qquad \textbf{(2-38)}$$

for a = 1,2 and 3 being slab, cylindrical and spherical geometries respectively.

The external boundary condition is
$S = S_b$ at $r = r_{bp}$
and the internal boundary condition is

$$\frac{dS}{dr} = S \quad \text{at } r = r_m$$

This has dimensionless form

$$\frac{1}{x^{a-1}}\frac{d}{dx}\left(x^{a-1}\frac{dy}{dx.}\right) = \phi^2 y \qquad \textbf{(2-39)}$$

or equivalently

$$\frac{d^2y}{dx^2} + \frac{(a-1)}{x}\frac{dy}{dx} = \phi^2 y \qquad \textbf{(2-40)}$$

where $y = S/Sb$
$x = r/r_{bp}$ and

$$\phi^2 = \frac{k_1 r_{bp}^2}{D}$$

with external boundary conditions now becoming y = 1 at x = 1 and internal boundary condition y' = 0 at $x = \alpha$.

It may be noticed that the equation (2-39) is a special case of Michaelis-Menten kinetics with parameter $\beta = 0$. It is of interest to study first order kinetics because it provides upper and lower bounds to solutions of equations with Michaelis-Menten kinetics.

2.4.2 The concept of partial penetration in first and other order kinetics

To examine the concept of having partial penetration in first order kinetics we include a third boundary condition $y(\alpha) = 0$ and hope to write α_i as a function of ϕ^2 . This was done in chapter 2.3 with zero order kinetics.

Taking 2 out of our 3 boundary conditions , $y(\alpha) = 0$ and $y'(\alpha) = 0$ and substituting them into equation (2-39) would imply that $y''(\alpha) = 0$.

This would obviously mean that all derivatives are zero and by expanding y(x) in a Taylor's series expansion, we conclude that the solution to eqn. (2-39) with these two boundary conditions would clearly be $y \equiv 0$.

We have also shown from Example 1 in Chapter 1.7 that any solution to the above differential equation must be unique.

This shows that our conditions are mutually exclusive;

y cannot be zero throughout but be 1 at the third boundary condition $y(1) = 1$

There is therefore no concept of partial penetration in first order kinetics.

In a similar manner, the above outline of a proof can be generalised to all F(y) with $F(0)=0$ and $F(y) > 0$..

(We must note that we may get equations such as $F(y)= -1/y$ where it is possible to get $y(x) < 0$.)

2.4.3 First Order Kinetics in Slab Geometry

We have to solve equation 2-39 for a = 1.

We then obtain the equation 2-41

$$\frac{d^2y}{dx^2} = \phi^2 y \tag{2-41}$$

or

$$\frac{d^2y}{dx^2} - \phi^2 y = 0$$

This has gereral solution

$$y = c_1 e^{\phi x} + c_2 e^{-\phi x} \tag{2-42}$$

or

$$y = A'\cosh(\phi x) + B'\sinh(\phi x) \tag{2-43}$$

for some constants A' and B'

To make it more convenient to satisfy the boundary conditions
$y(1) = 1$ and
$y'(\alpha) = 0$,
we rewrite equation 2-43 as

$$y = A \cosh \phi(1-x) + B \sinh \phi(1-x) \tag{2-44}$$

Solving for constants A and B

$$y(1) = 1 \Rightarrow A + 0 = 1$$
$$\Rightarrow A = 1$$
$$y'(\alpha) = 0 \Rightarrow -\phi \sinh \phi(1-\alpha) - B\phi \cosh \phi(1-\alpha) = 0$$
$$\Rightarrow B = -\frac{\phi \sinh \phi(1-\alpha)}{\phi \cosh \phi(1-\alpha)}$$
$$= -\tanh \phi(1-\alpha)$$

and

$\therefore$

$$y(x) = \cosh \phi(1-x) - \tanh \phi(1-\alpha) \sinh \phi(1-x) \tag{2-45}$$

with a graph of equation 2-45 given in figure 2-12 for $\alpha = 0.5$

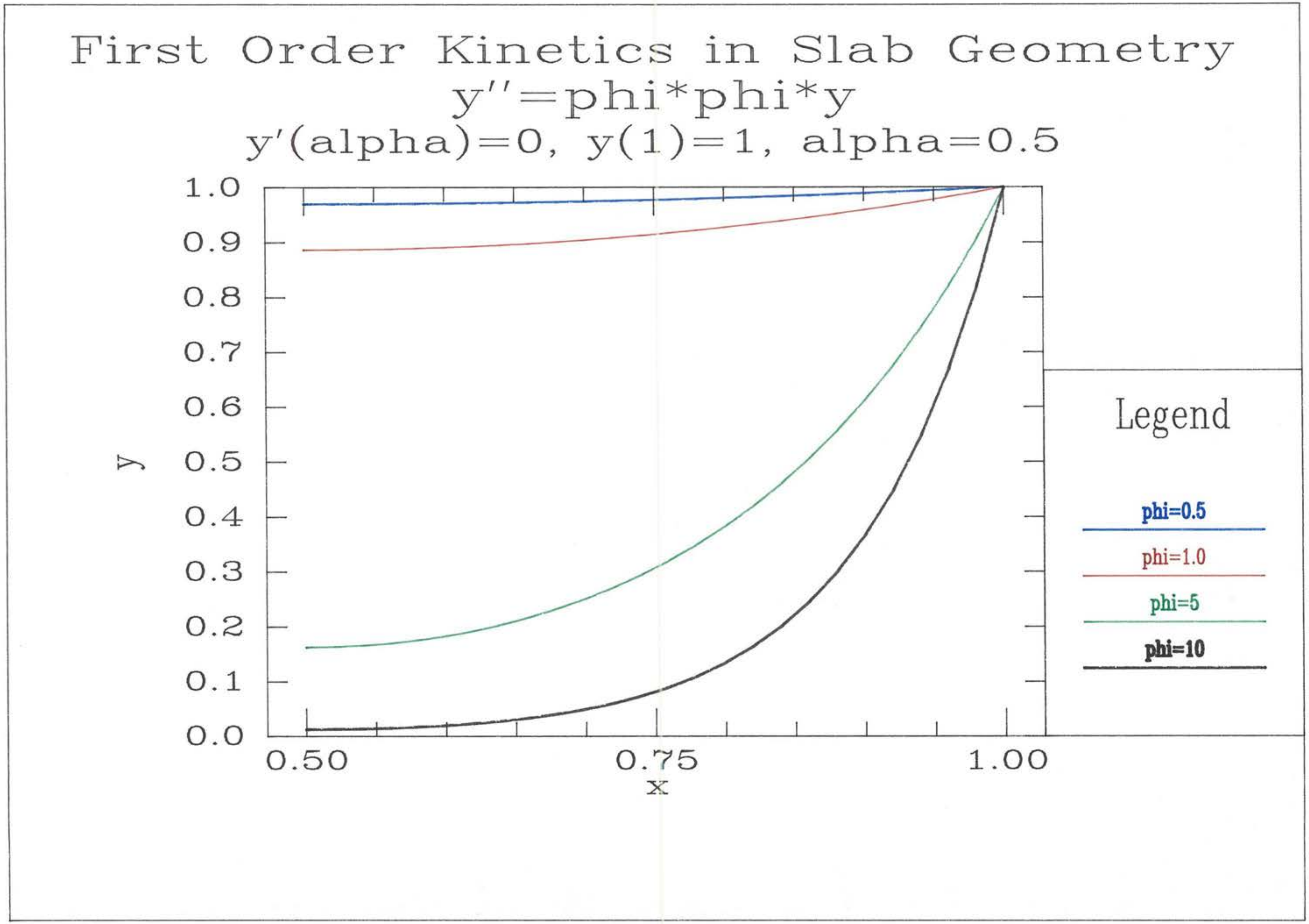

figure 2-12 First Order kinetics in a Slab alpha=0.5

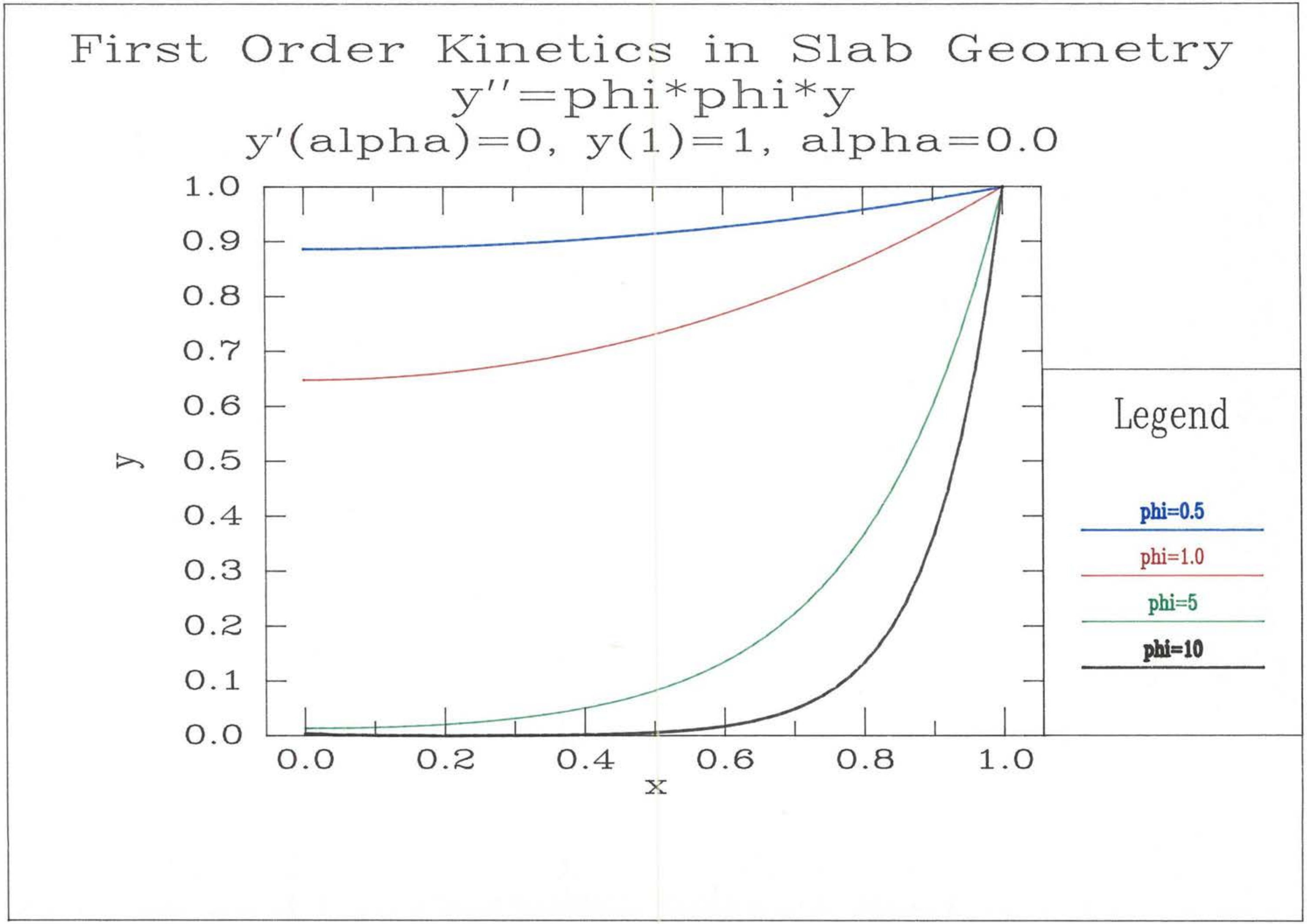

figure 2-13 First Order kinetics in a Slab alpha=0.0

Theile modulus vs. effectiveness factor in a Slab with first order kinetics

eta = 1/phi*tanh phi

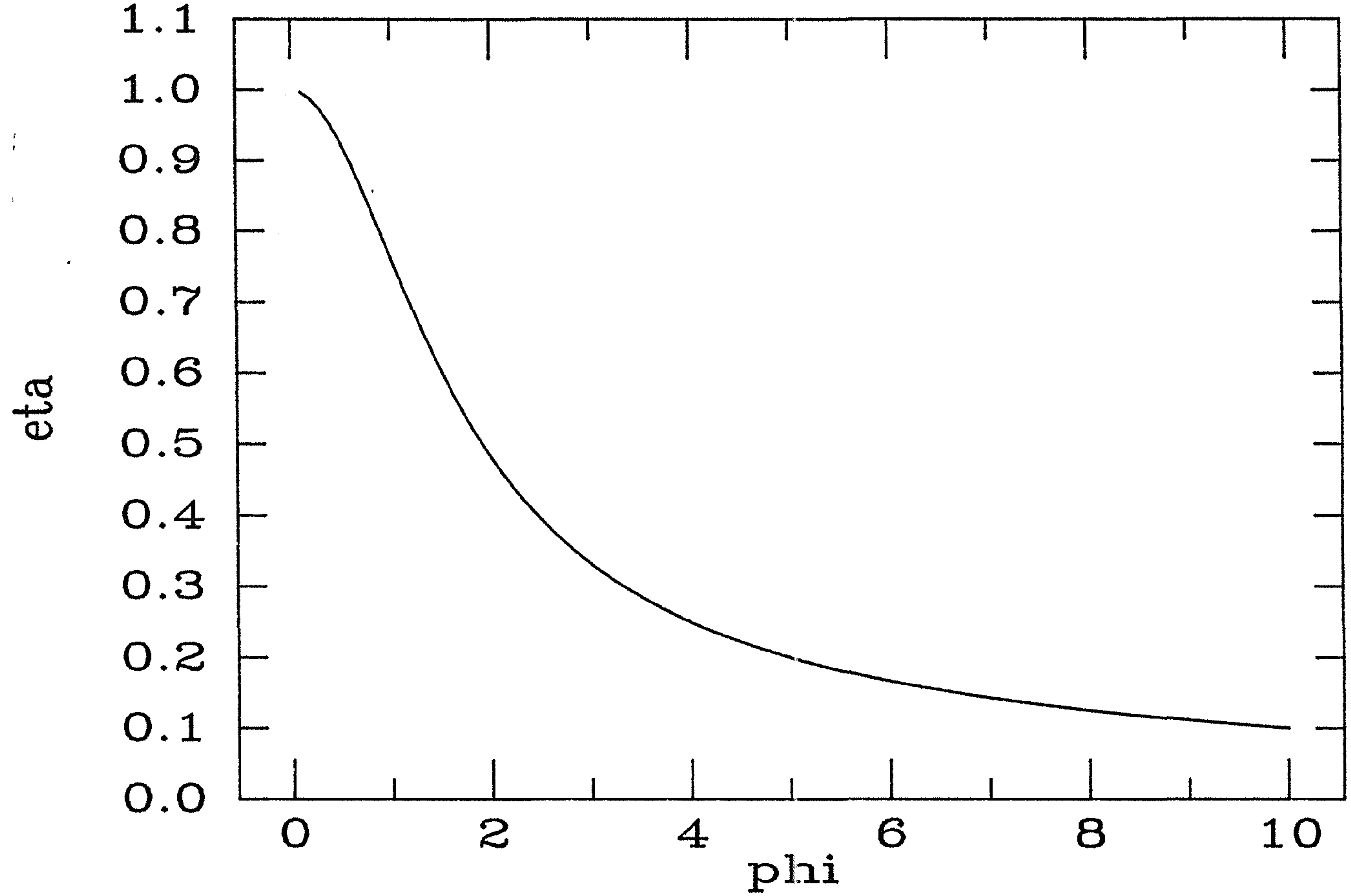

figure 2-14

Equating this function y(x) at its minimum, α,we obtain the equation

$$y(\alpha) = \cosh \phi(1-\alpha) - \tanh \phi(1-\alpha) \sinh \phi(1-\alpha) > 0 \qquad \textbf{(2-46)}$$

As an example that is not particular to biofilms, is common in many other slabs where diffusion may occur, and is used for illustration, we take $\alpha = 0$ in slab geometry. This would in physical terms be a very thin slab with a lot of biological growth.

Repeating the above procedure for $y'(0) = 0$ and $y(1) = 1$

From equation 2-43

$y(x) = A' \cosh(\phi x) + B' \sinh(\phi x)$
$y'(x) = A'\phi \sinh(\phi x) + B'\phi \cosh(\phi x)$
$y'(0) = 0 \Rightarrow B' = 0$
$y(1) = 1 \Rightarrow \quad A \sinh \phi = 1 \Rightarrow A = 1/ \sinh \phi$
$\therefore$

$$y(x) = \frac{\cosh \phi x}{\cosh \phi} \qquad \textbf{(2-47)}$$

The graph of equation 2-47 is given in figure 2-13

We note with interest that
$y(0) = 1/\cosh \phi \geq 0$

Effectiveness factor for $\alpha = 0$
Solving for y'(1) , we obtain

$y'(1) = \phi \tanh \phi$
and therefore

$$\eta = \frac{1}{\phi^2} y'(1) = \frac{1}{\phi} \tanh \phi \qquad \textbf{(2-48)}$$

The effectiveness factor is plotted as a function of Thiele modulus in figure 2-14.
At small ϕ, the effective factor is 1, i.e. this means that the rate of reaction is relatively uninfluenced by diffusion.
For large ϕ the effectiveness factor is smaller than one, meaning that the average rate is reduced below what it would be without diffusion limitations.

2.4.3.1 Perturbation solutions

We attempt to obtain perturbation solutions for diffusion and reaction in a slab

We apply the perturbation method for small ϕ.

The series

$y(x,\phi) = \phi^0 y_0(x) + \phi^2 y_1(x) + \phi^4 y_2(x) + \ldots\ldots$

is substituted into equation 2-41 to obtain

ϕ^0 : $y_0'' = 0$ $\quad y_0'(0) = 0 \quad y_0(1) = 1$

ϕ^2 : $y_1'' = y_0$ $\quad y_i'(0) = 0 \quad y_i(1) = 0 \quad i \geq 1$

ϕ^4 : $y_2'' = y_2$

These equations are solved to obtain

$$y_0(x) = 1$$

$$y_1(x) = -\frac{(1+x)}{2}$$

$$y_2(x) = \frac{5 - 6x^2 + x^4}{24}$$

which are finally substituted into

$$y(x) = y_0(x) + \phi^2 y_2(x) + \phi^4 y_2(x) \qquad \textbf{(2-49)}$$

to give an approximate analytic solution.

We also get the effectiveness factor

$$\eta = 1 - \tfrac{1}{3}\phi^2 + 2/15\phi^4 \qquad \textbf{(2-50)}$$

which agrees with. equation (2-48). for small ϕ.

We realise that this perturbation solution is only valid for small ϕ, i.e. we need ϕ tending to zero

If the 2nd. term is 10% of the first approximation this leads to the solution being good for $\phi < 0.5$. This may be used as a criterion of how good an approximation η is.

2.4.4 First Order Kinetics in cylindrical Geometry

We have to solve equation 2-39 for a = 2
We then get

$$\frac{1}{x}\frac{d}{dx}\left(x\frac{dy}{dx}\right) = \phi^2 y \qquad (2\text{-}51)$$

or

$$\frac{d^2y}{dx^2} + \frac{1}{x}\frac{dy}{dx} = \phi^2 y \qquad (2\text{-}52)$$

By making the scalar group transformation

$$\bar{x} = \frac{x}{\phi^2}$$

we may reduce the above problem to the form

$$\frac{d^2y}{d\bar{x}^2} + \frac{1}{\bar{x}}\frac{dy}{d\bar{x}} = y \qquad (2\text{-}53)$$

with boundary conditions

$$\frac{dy}{d\bar{x}}(\phi\alpha) = 0 \quad , \quad y(\alpha) = 1$$

It may be noticed that equation (2-53) is a Bessel's modified Differential equation of order zero.

A Bessel's modified Differential equation of order n is of the form

$$x^2y'' + xy' - (x^2 + n^2)y = 0 \quad \text{where } n \geq 0. \qquad (2\text{-}54)$$

The General solution of the Bessel's modified equation is of the form where

$$y = AI_n(x) + BK_n(x) \quad \text{for all n.} \qquad (2\text{-}55)$$

$I_n(x)$ is defined to be the Modified Bessel function of the first kind of order n and
$K_n(x)$ is the Modified Bessel function of the second kind of order n .
These are defined below

$$I_n(x) = i^{-n} J_n(ix) = e^{-n\pi i/2} J_n(ix)$$

$$= \frac{x^n}{2^n\,\Gamma(n+1)}\left\{1 + \frac{x^2}{2(2n+2)} + \frac{x^4}{2\cdot 4(2n+2)(2n+4)} + \ldots\ldots\right\}$$

$$= \sum_{k=o}^{\infty} \frac{(x/2)^{n+2k}}{k!\,\Gamma(n+k+1)}$$

$$I_{-n}(x) = iJ_{-n}(ix) = e^{n\pi i/2} J_{-n}(ix)$$

$$= \frac{x^{-n}}{2^{-n}\Gamma(1-n)} \{1 + \frac{x^2}{2(2-2n)} + \frac{x^4}{2 \cdot 4(2-2n)(4-2n)} + ...\}$$

$$= \sum_{k=0}^{\infty} \frac{(x/2)^{2k-n}}{k!\,\Gamma(k+1-n)}$$

$I_{-n}(x) = I_n(x) \quad n = 0,1,2,....$

If $n \neq 0,1,2,...$, then $I_n(x)$ and $I_{-n}(x)$ are linearly independent.

J_n and and J_{-n} are Bessel functions of the first kind of order n. It may be noticed that Modified Bessel Differential equations may be obtained from Bessel's equation by substituting ix for x.

$$K_n(x) = \begin{cases} \dfrac{\pi}{2 \sin n\pi} \{ I_{-n}(x) - I_n(x) \} & n \neq 0,1,2,3,.. \\ \lim\limits_{p \to n} \dfrac{\pi}{2 \sin p\pi} \{ I_{-p}(x) - I_p(x)\} & n = 0,1,2,.. \end{cases}$$

For n = 0,1,2,... , L'Hopital's rule yields

$$K_n(x) = (-1)^{n+1}\{\ln(x/2)+\gamma\}\, I_n(x) + \frac{1}{2}\sum_{k=0}^{n-1} (-1)^k(n-k-1)!(x/2)^{2k-n}$$
$$+ \frac{(-1)^n}{2}\sum_{k=0}^{\infty}\frac{(x/2)^{n+2k}}{k!(n+k)!} \{ \phi(k) + \phi(n+k)\}$$

where
$\gamma = 0.5772156...$ is Euler's constant and
$\phi(p) = 1 + 1/2 + 1/3 + ...+ 1/p$
$\phi(0) = 0$

A general solution of equation (2-53) is therefore

$$y = A\, I_0(x) + B\, K_0(x) \qquad \textbf{(2-56)}$$

where

$$I_0(x) = 1 + \frac{x^2}{2^2} + \frac{x^4}{2^2 \cdot 4^2} + \frac{x^6}{2^2 \cdot 4^2 \cdot 6^2} + \ldots..$$

$$= 1 + \frac{x^2}{2^2(1!)^2} + \frac{x^4}{2^4(2!)^2} + \frac{x^6}{2^6(3!)^2} + \ldots...$$

and

$$K_0(x) = -\{\ln(x/2) + \gamma\}\, I_0(x) + \frac{x^2}{2^2} + \frac{x^4}{2^2 \cdot 4^2}(1+1/2) + \frac{x^6}{2^2 \cdot 4^2 \cdot 6^2}(1+1/2+1/3) + \ldots...$$

$$= -(\gamma + \ln\,(x/2))I_0(x) + \sum_{r=1}^{\infty} \frac{(x/2)^{2r}}{r!\; r!}(1 + 1/2 + 1/3 + \ldots.. + 1/r)$$

For small values of x these series show that

$I_0(x) \approx 1$

$K_0(x) \approx -\gamma - \ln(x/2)$

The General solution of equation (2-52).is therefore

$$y = A\, I_0(\phi x) + BK_0(\phi x) \qquad \textbf{(2-57)}$$

with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$

We consider without loss of generality equation 2-56 with .$\phi^2 = 1$

The general solution is therefore

$$y = A\, I_0(x) + BK_0(x)$$

where A and B have to be determined

Solving for A and B with the given boundary conditions

$y'(\alpha) = 0 \Rightarrow A\, I_0'(\alpha) + BK_0'(\alpha) = 0$
$y(1) = 1 \Rightarrow A\, I_0(1) + BK_0(1) = 1$

To determine constants A and B we note that we have recurrence formulas for modified Bessel functions of the first and second kind of order n. These are as follows

1. $I_n'(x) = 1/2\{I_{n-1}(x) + I_{n+1}(x)\}$
2. $K_n'(x) = -1/2\{K_{n-1}(x) + K_{n+1}(x)\}$

If $n \neq 0,1,2,....$ then $I_n(x)$ and $I_{-n}(x)$ are linearly independent and the general solution of Bessel's modified equation is then
$y = A\, I_n(x) + B\, I_{-n}(x)$

If n=0,1,2,.... then

$I_{-n}(x) = I_n(x)$ and
$K_{-n}(x) = K_n(x)$

We therefore obtain from the recurrence the equalities
$I_n'(x) = I_{n+1}$ and
$K_n'(x) = -K_{n+1}$

$I_0'(x)$ can therefore be defined as a function of $I_1(x)$ and similarly $K_0'(x)$ with $K_1(x)$.

$$I_0'(x) = I_1(x) = \frac{x}{2} + \frac{x^3}{2^2 \cdot 4} + \frac{x^5}{2^2 \cdot 4^2 \cdot 6} + \frac{x^7}{2^2 \cdot 4^2 \cdot 6^2 \cdot 8} + \ldots$$

$$= \frac{x}{2} + \frac{x^3}{2^3 1!2!} + \frac{x^5}{2^5 2!3!} + \ldots.$$

$$\simeq x/2$$

$$K_0'(x) = -K_1(x) = -(\gamma + \ln(\frac{x}{2}))I_1(x) - \frac{1}{x} + \frac{1}{2}\sum_{r=0}^{\infty} \frac{(x/2)^{2r+1}}{r!(r+1)!}\{2(1+\frac{1}{2}+\ldots\ldots+\frac{1}{r}) + \frac{1}{r+1}\}$$

$$\simeq -1/x$$

2.4.4.1 Solving with boundary conditions

We may therefore solve for A and B by solving

$A\,I_1(\alpha) - B\,K_1(\alpha) = 0$
$A\,I_0(1) + B\,K_0(1) = 1$

It may be noted that rather than solving for A and B as an infinite sum involving α , it would be more convenient to consult tables or graphs of Bessel's Modified Functions of the first and second kind of kinetic orders zero and one.
The method demonstrates the conversion of a Laplacian to a Bessel function.

For practical purposes, it illustrates the uses of graphs or tables for calculating concentration gradients in our model. We could linearise non-linear equations, to obtain upper or lower solutions that are obtained by the use of Bessel functions.

A graph of Bessel's modified Functions of the first and second kind are given in figures 2-15 and 2-16 respectively. These were obtained from the first few terms in the infinite sum of $K_n(x)$ and $I_n(x)$ and plotted by a program written by the author.

We are of course only interested in the function when x is greater than zero.

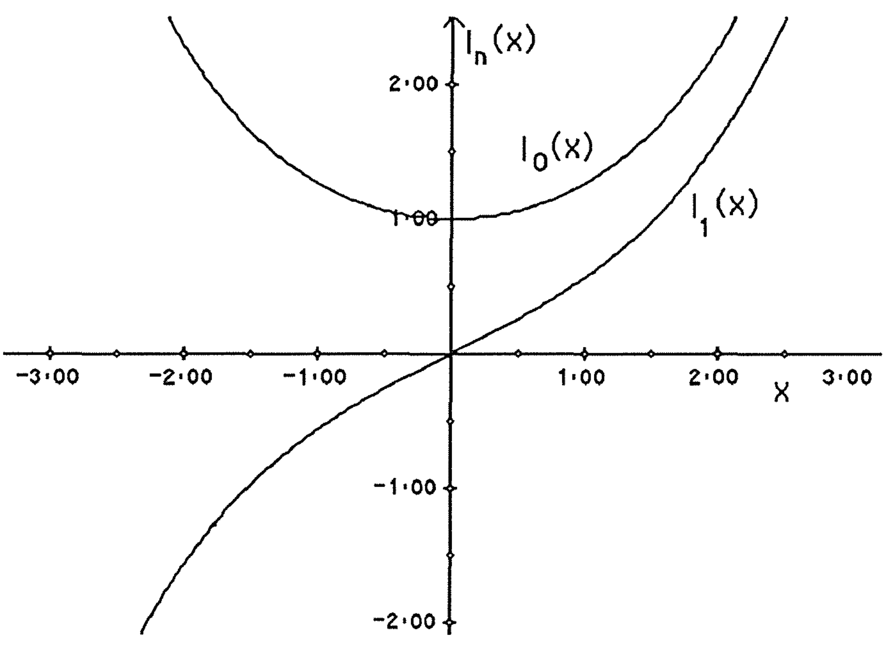

figure 2-15 A graph of the first 3 terms in the infinite sum of $I_0(x)$ and $I_1(x)$.

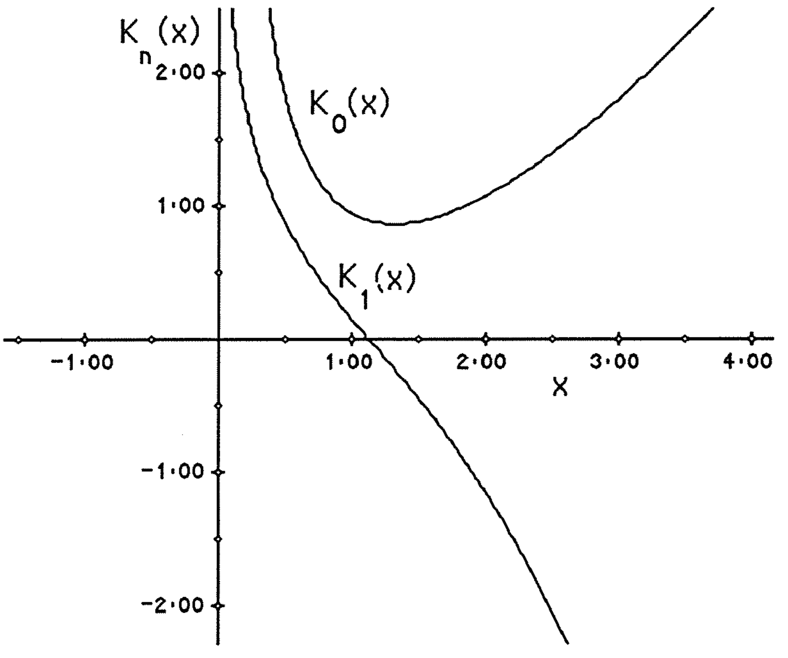

figure 2-16 A graph of the first 3 terms in the infinite sum of $K_0(x)$ and $K_1(x)$.

For large and very small values of ϕ^2, the reader is recommended to consult a book on asymptotic analysis. Most books on asymptotic analysis do contain asymptotic solutions of Bessel functions and the reader is recommended to see Tranter[14] p. 49-53 and Murray[20] pp.65,78,105 keeping in mind the relationships between $J_n(x)$, $I_n(x)$ and $K_n(x)$.

The equation 2-51 was solved numerically for $\phi = 1$ and $\alpha = 0$
For $\alpha = 0$, numerical values were obtained by starting with very small numbers of the order of 1e-7.

Two methods of numerical integration were used to calculate y(0).

1. y(0) = 0.78993 by taking α to be of the order 1e-7

2. y(0) = 0.75 by making the approximation

$$y'' + \frac{y'}{x} \approx 2y'' = \phi^2 y$$

2.4.5 First Order Kinetics in Spherical Geometry

2.4.5.1 Exact solutions

We have to solve equation 2-39. for a = 3
We then obtain

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} = \phi^2 y \tag{2-58}$$

or

$$x\frac{d^2y}{dx^2} + 2\frac{dy}{dx} = \phi^2 xy \tag{2-59}$$

with boundary conditions $y'(\alpha)$ and $y(1) = 1$.

Let $u(x) = xy$ **(2-60)**

$$\frac{du}{dx} = y + x\frac{dy}{dx}$$

$$\frac{d^2y}{dx^2} = \frac{dy}{dx.} + \frac{dy}{dx} + x\frac{d^2y}{dx^2} = x\frac{d^2y}{dx^2} + 2\frac{dy}{dx}$$

and

$$x\frac{d^2y}{dx^2} = \frac{d^2u}{dx^2} - 2\frac{dy}{dx}$$

Substituting the above equalities into equation 2-59, we obtain

$$\frac{d^2u}{dx^2} - 2\frac{dy}{dx} + 2\frac{dy}{dx} = \phi^2 xy$$

$$\frac{d^2u}{dx^2} = \phi^2 u$$

or

$$\frac{d^2u}{dx^2} - \phi^2 u = 0. \tag{2-61}$$

The solution of equation 2-61 is an Airy function.

As with first order Kinetics with cylindrical geometry, it is a special kind of Bessel equation and Airy functions are often expressed in terms of Bessel functions of fractional order.

Solving of equation, 2-61, we obtain

$$
\begin{aligned}
u(x) &= c_1 e^{\phi x} + c_2 e^{-\phi x} \\
&= c_3 \cosh(\phi x) + c_4 \sinh(\phi x) \\
&= A \cosh \phi(1-x) + B \sinh \phi(1-x)
\end{aligned}
$$

and from equation 2-60, it follows that

$$
y = \frac{A \cosh \phi(1-x)}{x} + \frac{B \sinh \phi(1-x)}{x} \qquad \textbf{(2-62)}
$$

for constants A and B.

To solve for A and B we have to differentiate equation

$$
\begin{aligned}
\frac{dy}{dx} = y' &= \frac{A(-\phi)x \sinh \phi(1-x) - A \cosh \phi(1-x)}{x^2} + \\
&\quad \frac{B(-\phi)x \cosh \phi(1-x) - B \sinh \phi(1-x)}{x^2} \\
&= A\{ \frac{\phi \sinh \phi(1-x)}{x} \quad \frac{\cosh \phi(1-x)}{x^2}\} + \\
&\quad B\{ -\frac{\sinh \phi(1-x)}{x^2} - \frac{\phi \cosh \phi(1-x)}{x}\}
\end{aligned}
$$

$$
\begin{aligned}
y(1) = 1 &\Rightarrow A \cosh(0) + B \sinh(0) = 1 \\
&\Rightarrow A = 1
\end{aligned}
$$

$y'(\alpha) = 0 \Rightarrow$

$$
-\frac{\phi \sinh \phi(1-\alpha)}{\alpha} - \frac{\cosh \phi(1-\alpha)}{\alpha^2} - B\{\frac{\sinh \phi\ (1-\alpha)}{\alpha^2} + \frac{\phi \cosh \phi(1-\alpha)}{\alpha}\} = 0.
$$

$$
\Rightarrow \quad B = -\frac{\alpha\phi \sinh \phi(1-\alpha) + \cosh \phi(1-\alpha)}{\sinh \phi(1-\alpha) + \phi \cosh \phi(1-\alpha)}
$$

Therefore the solution of equation 2-58 is

$$y(x) = \frac{\cosh\phi(1-x)}{x} - \frac{\sinh\phi(1-x)}{x}\left\{\frac{\alpha\phi\sinh\phi(1-\alpha)+\cosh\phi(1-\alpha)}{\phi\alpha\cosh\phi(1-\alpha)+\sinh\phi(1-\alpha)}\right\}$$

which is simplified to

$$y(x) = \frac{\alpha\phi\cosh(x-\alpha)+\sinh(x-\alpha)}{x(\alpha\phi\cosh\phi(1-\alpha)+\sinh\phi(1-\alpha))} \qquad \textbf{(2-63)}$$

by using hyperbolic trig. identities

The graph of this function is observed in Michaelis-Menten kinetics where the parameter β is taken to be zero.

Theorem

$$y(x) : \ y(x) = \frac{\alpha\phi\cosh(x-\alpha)+\sinh(x-\alpha)}{x(\alpha\phi\cosh\phi(1-\alpha)+\sinh\phi(1-\alpha))} > 0$$

Proof:

It is sufficient to show that y(x) > 0 at its minimum, α

Evaluating the function at it's minimum i.e. at α we obtain

$$y(\alpha) = \frac{\alpha\phi\cosh(0)+\sinh(0)}{\alpha(\alpha\phi\cosh\phi(1-\alpha)+\sinh\phi(1-\alpha))}$$

$$= \frac{\alpha\phi}{\alpha(\alpha\phi\cosh\phi(1-\alpha)+\sinh\phi(1-\alpha))}$$

$$= \frac{\phi}{\alpha\phi\cosh\phi(1-\alpha)+\sinh\phi(1-\alpha)}$$

$$> 0 \quad \text{for all } \alpha \in [0,1]$$

We also note with interest that

$$y(0) = \frac{\phi}{\sinh\phi}$$

2.4.5.2 Particular solutions in the form of Bessel functions

It may be noted that solutions to equation 2-58 may also be obtained in form of Bessel functions

e.g.

$$y(x) = x^{-1/2} I_{1/2}(x)$$

is a particular solution of equation where $I_{1/2}$ is a Modified Bessel function of the first kind of order 1/2.

Solution

$$y'(x) = -1/2\ x^{-3/2} I_{1/2}(x) + x\text{-}1/2I'_{1/2}(x)$$

$$y''(x) = 3/4x^{-5/2}I_{1/2}(x) - x^{-3/2}I''_{1/2}(x) + x^{1/2}I''_{1/2}(x)$$

and therefore

$$xy'' = 3/4x^{-3/2}I_{1/2}(x) - x^{-1/2}I'_{1/2}(x) + x^{1/2}I''_{1/2}(x)$$

$$2y' = -x^{-3/2}I_{1/2}(x) + 2x^{-1/2}I'_{1/2}(x)$$

$$xy = x^{1/2}I_{1/2}(x)$$

Substituting into equation 2-59

$$xy'' + 2y' + xy = x^{-3/2}\left[I_{1/2}\left(\frac{1}{4} + x^2\right) + I'_{1/2}x + I''_{1/2}x^2 \right]$$

$$= x^{-3/2} . 0$$

$$= 0.$$

2.4.5.3 Asymptotic cases

Noting the relation of equation 2-61 with Bessel functions we may also obtain two asymptotic cases when $\phi^2 \rightarrow \infty$ and when $\phi^2 \rightarrow 0$

1. $\phi^2 \rightarrow \infty$

Using the method of steepest descents and a generalised transform method of contour integration the following result was obtained

$$u = Ai\,(\phi^2) \sim \frac{1}{2} (\pi\phi)^{-1/2} e^{-2/3\phi^2}$$

$$= xy$$

and y is solved in terms of u/x

$$y \sim \frac{1}{2x} (\pi\phi)^{-1/2} e^{-2/3\phi^2} \qquad \textbf{(2-64)}$$

2. $\phi^2 \rightarrow 0$

We get the linear equation

$y = A + B/x$

which when solved with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$ gives

$y(x) = 1$

2.4.5.4 Perturbation solutions

We have the equation

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} = \phi^2 y$$

with boundary conditions $y'(\alpha) = 0$ and $y(1) = 1$.

Let

$y(x,\phi) = \phi_0 y_0(x) + \phi^2 y_1(x) + \phi^4 y_2(x) + ...$

$y'(x,\phi) = \phi_0 y_0'(x) + \phi^2 y_1'(x) + \phi^4 y_2'(x) + ...$

$y''(x,\phi) = \phi_0 y_0''(x) + \phi^2 y_1''(x) + \phi^4 y_2''(x) + ...$

substituting this into the above equation

(1) $\phi^0 : y_0''+2y_0'/x = 0$ $\quad y_0'(\alpha) = 0 \quad y_0(1) = 1$

(2) $\phi^2 : y_1''+2y_1'/x - y_0 = 0$ $\quad y_i'(\alpha) = 0 \quad y_i(1) = 1$

(3) $\phi^4 : y_2''+ 2y_2'/x - y_1 = 0$

Solving eqn (1)

$y_0(x) = 1$

Solving eqn. (2) with $y_0(x) = 1$, we get

$$y_1(x) = \frac{x^2}{6} + \frac{\alpha^3}{3x} - \frac{1}{6}(2\alpha^3 + 1)$$

Solving eqn.(3) with $y_0(x)$ and $y_1(x)$, we obtain

$$y(x) = \frac{x^4}{120} + \frac{\alpha^3 x}{6} + A\frac{x^2}{6} - \frac{B}{x} + C \qquad (2\text{-}65)$$

where

$$A = -\frac{1}{6}(2\alpha^3 + 1)$$

$$B = -\alpha^3\left(\frac{3}{10}\alpha^2 + \frac{A}{3}\right)$$

and

$$C = 1 - \frac{1}{120} - \frac{\alpha^3}{6} - \frac{A}{6} + B$$

2.5 Michaelis-Menten reaction kinetics

2.5.1 Introduction

For Michaelis-Menten Kinetics, we solve the equation

$$\frac{D}{r^{a-1}}\frac{d}{dr}\left(r^{a-1}\frac{dS}{dr}\right)=\frac{\rho_{bf}\,\mu_m\,S}{Y_{x/s}\,(K_s+S)} \qquad (2\text{-}66)$$

for a=1,2 and 3 being slab,cylindrical and spherical geometries respectively

The external boundary condition is
$S = Sb$ at r_{bp}
and the internal boundary condition is
$dS/dr = S$ at $r = r_m$

This has dimensionless form

$$\frac{1}{x^{a-1}}\frac{d}{dx}\left(x^{a-1}\frac{dy}{dx}\right)=\frac{\phi^2 y}{1+\beta y} \qquad (2\text{-}67)$$

or equivalently

$$\frac{d^2y}{dx^2}+\frac{(a-1)}{x}\frac{dy}{dx}=\frac{\phi^2 y}{1+\beta y}$$

where

$y = S/S_b$
$x = r/r_{bp}$

$$\phi^2=\frac{r_{bp}^2\rho_{bf}\mu_m}{DY_{x/s}K_s}$$

and

$$\beta=\frac{S_b}{K_s}$$

The external boundary condition is $y(1) = 1$ and the internal boundary condition is $y'(\alpha) = 0$

2.5.2 The concept of partial penetration in Michaelis-Menten kinetics

As with first order kinetics, there is no partial penetration in Michaelis-Menten kinetics for the same reasons given in first order kinetics, Chap.2.4.2.

2.5.3 Uniqueness and Existence

Uniqueness and existence of equation 2-67 are given as trivial examples to theorems 2.2.2.1.2 and 1.5.1.10.

2.5.4 Upper and Lower bounds

Upper and Lower bounds are given as trivial examples to theorem 1.5.1.11

2.5.5 Monotonicity with β and ϕ^2

Theorem 5.1

y is monotonically increasing with β

Proof

1. Assume $\beta_1 > \beta_2$
2. Let y_1 be the solution to 2-67 with β_1

$$L[y_1] = \frac{d^2 y_1}{dx^2} + \frac{2}{x}\frac{dy_1}{dx} = \frac{\phi^2 y_2}{1+\beta_2 y_2}$$

with $y_1'(\alpha) = 0$ and $y_1(1) = 1$ and

3. Let y_2 be the solution to 2.67 with β_2

$$L[y_2] = \frac{d^2 y_2}{dx^2} + \frac{2}{x}\frac{dy_2}{dx} = \frac{\phi^2 y_2}{1 + \beta_2 y_2}$$

with $y_2'(\alpha) = 0$ and $y_2(1) = 1$.

4. We look at $y_2 - y_1 = z$

$$L[z] = \frac{\phi^2 y_2}{1 + \beta_2 y_2} - \frac{\phi^2 y_1}{1 + \beta_1 y_1}$$

with

$z'(\alpha) = y_2'(\alpha) - y_1'(\alpha) = 0$ and

$z(1) = y_2(1) - y_1(1) = 0$ i.e.

L[z] has homogeneous boundary conditions

5. Simplifying L[z]

$$L[z] = \phi^2 \left(\frac{y_2}{1+\beta_2 y_2} - \frac{y_1}{1+ \beta_1 y_1} \right)$$

$$= \frac{\phi^2 (y_2+\beta_1 y_1 y_2 - y_1 - \beta_2 y_1 y_2)}{(1+\beta_2 y_2)(1+ \beta_1 y_1)}$$

$$< \frac{\phi^2 (y_2 - y_1)}{(1+\beta_2 y_2)(1+\beta_1 y_1)}$$ since we have assumed that $\beta_1 > \beta_2$

$$< \phi^2 (y_2 - y_1)$$ since we have shown that $y(x) > 0$

$$= \phi^2 z$$

i.e.
We have the problem $L[z] - \phi^2 z < 0$
with homogeneous boundary conditions
$z'(\alpha) = z(1) = 0$

It follows from theorem 1.5.1.9 and 1.5.1.10 that if $L[z] - \phi^2 z < 0$
with boundary conditions above then $z > 0$

$z > 0 \Rightarrow y_1 - y_2 > 0 \Rightarrow y_1 > y_2$

Thus y is increasing with β and by taking successive iterations we may show that it is monotonic.

⊠.

Graphs of the monotonicity behaviour of β is observed in figure 2-17 and figure 2-18 between the intervals (0.5,1) and (0.1,1) respectively.
α is chosen to be 0.5

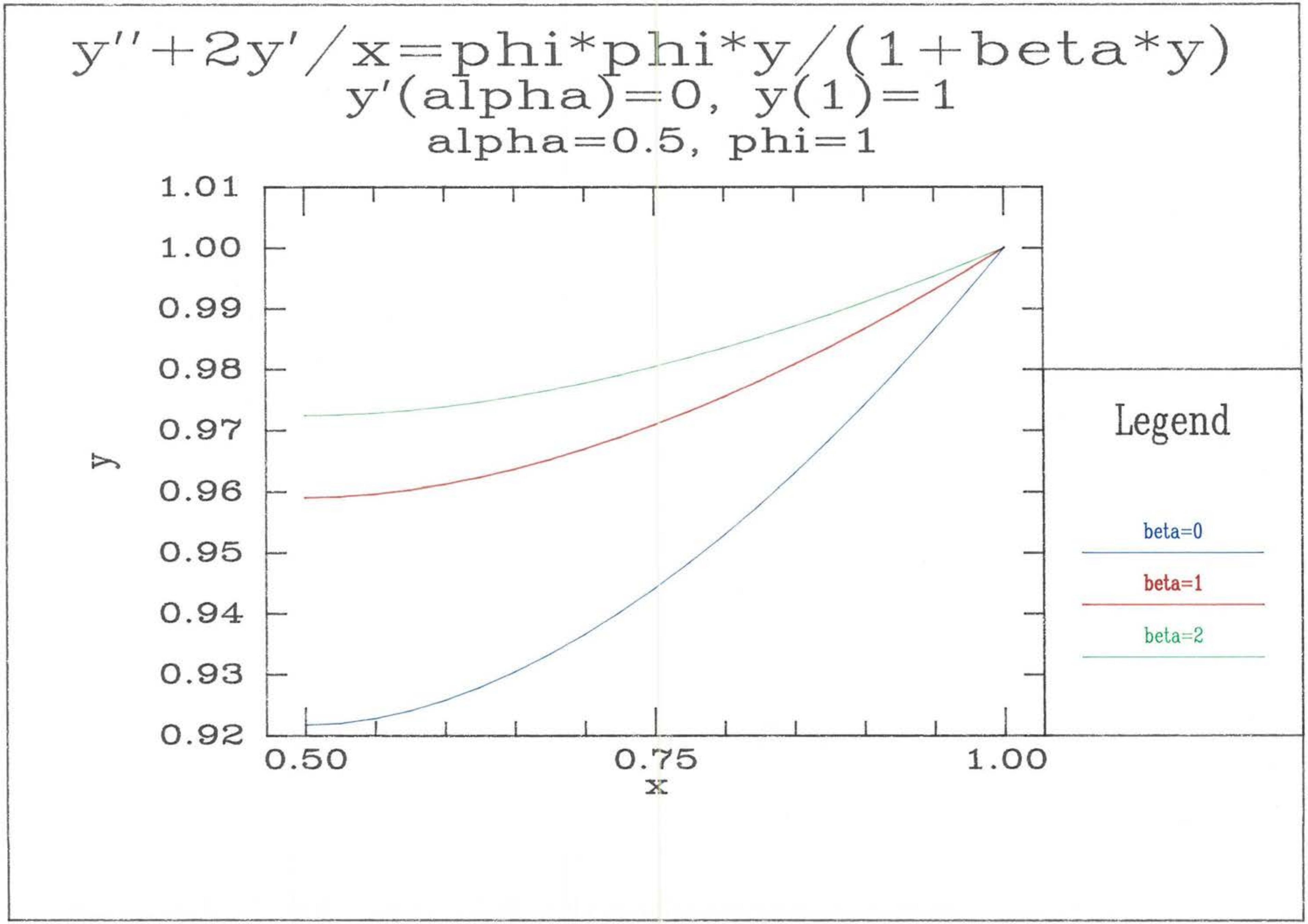

figure 2-17 Monotonicity of beta

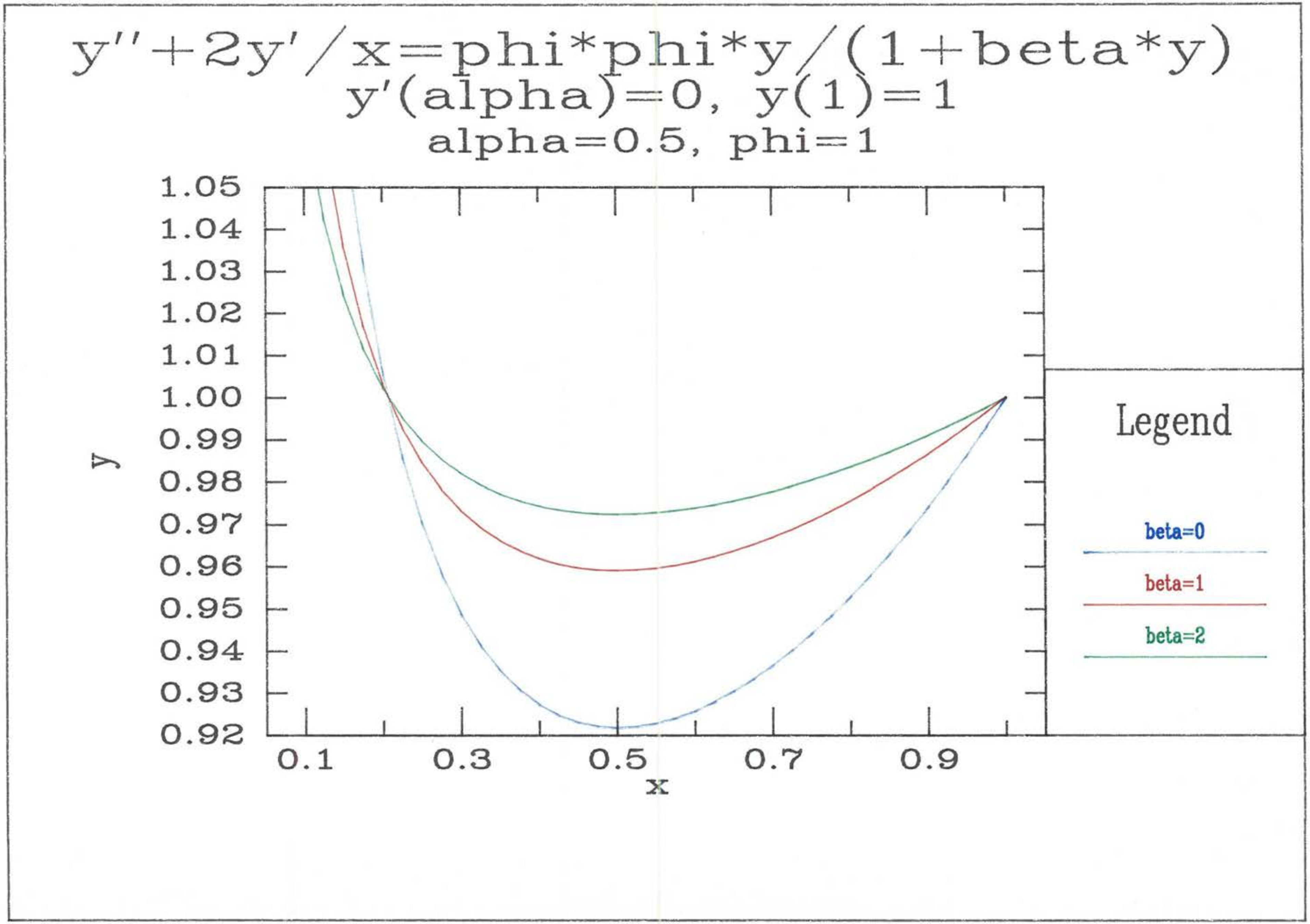

figure 2-18 Monotonicity of beta

Theorem 5.2
y is monotonically decreasing with ϕ

Proof
1. Assume $\phi_1 > \phi_2$

2. Let y_1 be a solution 2-67 with ϕ_1

$$L[y_1] = \frac{d^2y_1}{dx^2} + \frac{2}{x}\frac{dy_1}{dx} = \frac{\phi^2 y_2}{1+\beta_2 y_2} \qquad y_1'(\alpha) = 0,\ y_1(1) = 1$$

3. Let y_2 be a solution of 2-67 with ϕ_2

$$L[y_2] = \frac{d^2y_2}{dx^2} + \frac{2}{x}\frac{dy_2}{dx} = \frac{\phi^2 y_2}{1 + \beta_2 y_2} \qquad y_2'(\alpha) = 0,\ y_2(1) = 1$$

4. Look, as before at $y_2 - y_1 = z$

$$L[z] = \frac{\phi_2^2 y_2}{1 + \beta y_2} - \frac{\phi_1^2 y_1}{1 + \beta y_1}$$

with homogeneous boundary conditions $B(z) = 0$ as before

5. Simplifying

$$L[z] = \frac{\phi_2^2(1 + \beta y_1)y_2 - \phi_1^2(1 + \beta y_2)y_1}{(1 + \beta y_2)(1 + \beta y_1)}$$

$$< \frac{\phi_1^2(1 + \beta y_1)y_2 - \phi_1^2(1 + \beta y_2)y_1}{(1 + \beta y_2)(1 + \beta y_1)}$$

$$< \phi_1^2 y_2 + \phi_1^2 \beta y_1 y_2 - \phi_1^2 y_1 - \phi_1^2 \beta y_1 y_2$$

$$< \phi_1^2(y_2 - y_1)$$

$$< \phi_1^2 z$$

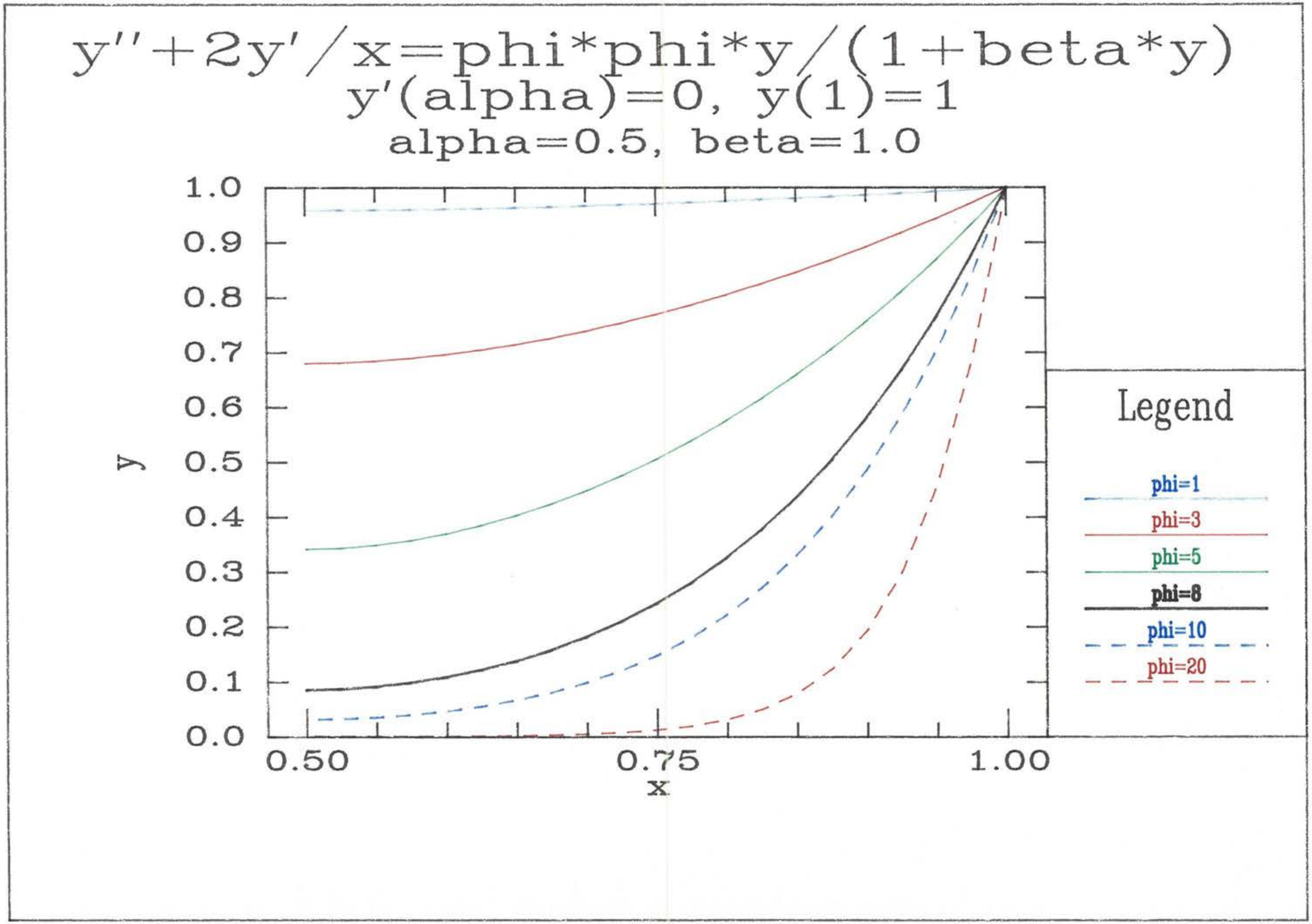

figure 2-19 Monotonicity of phi

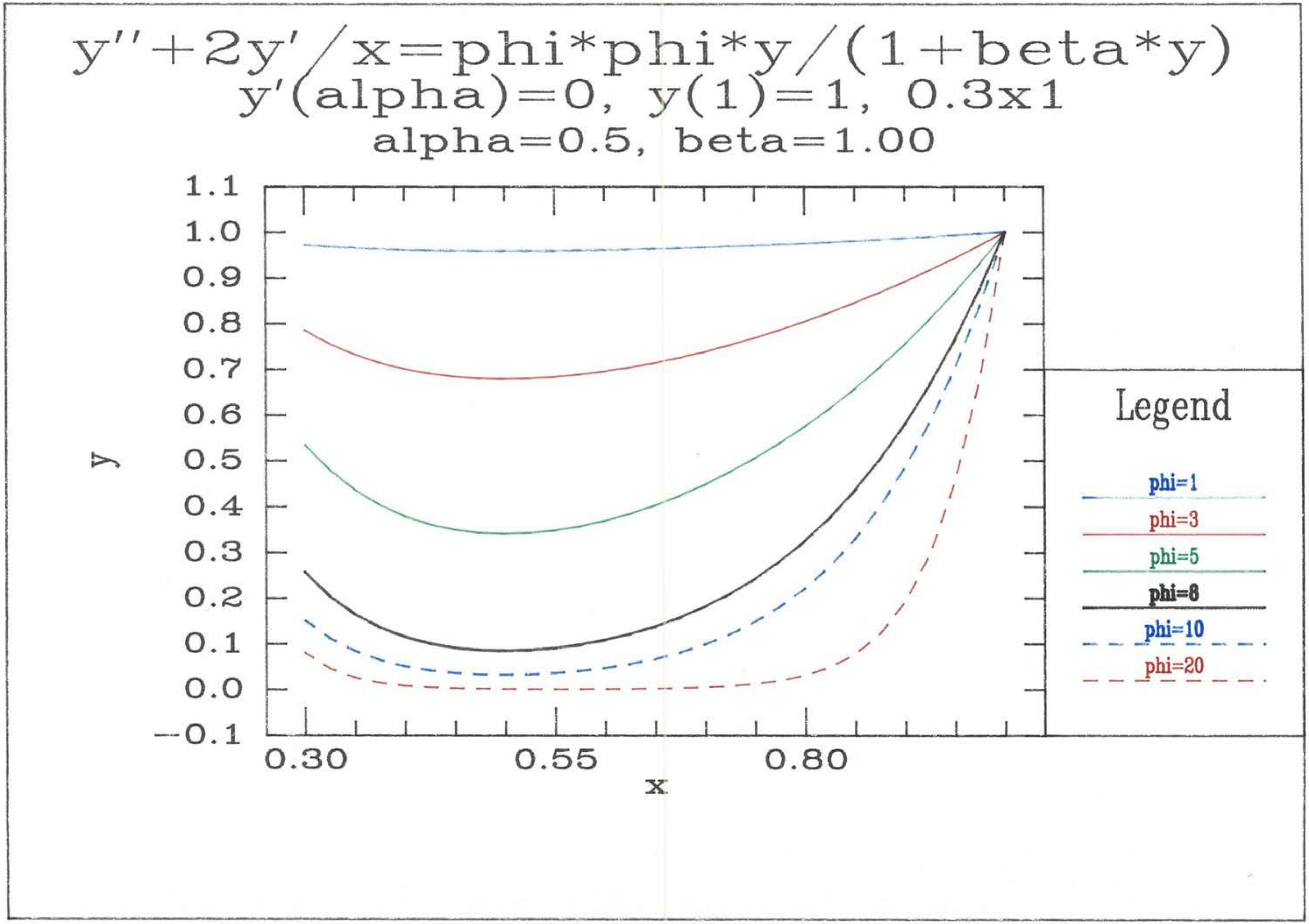

figure 2-20 Monotonicity of phi

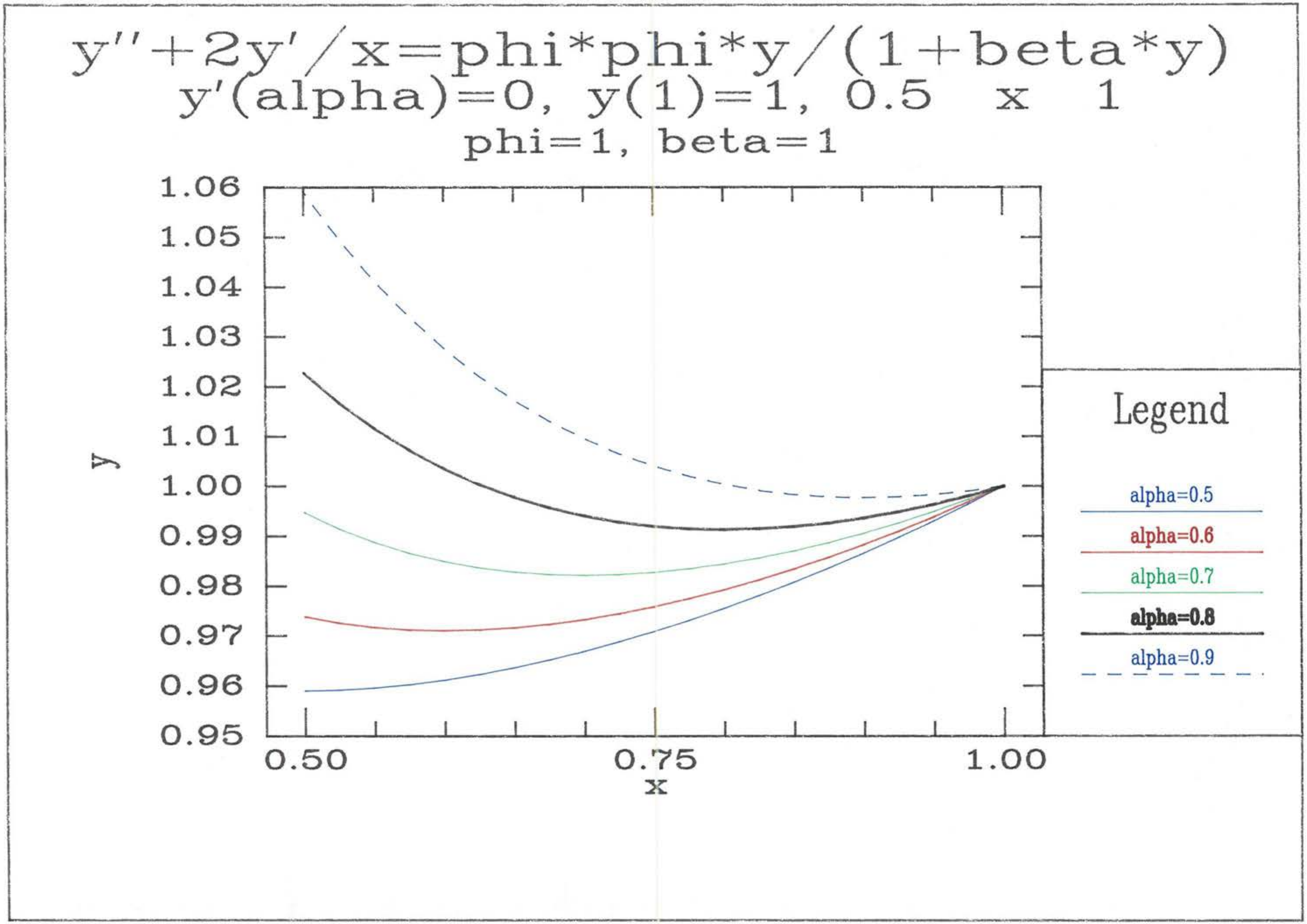
y''+2y'/x=phi*phi*y/(1+beta*y)
y'(alpha)=0, y(1)=1, 0.5 x 1
phi=1, beta=1
1.06
1.05
1.04
1.03
1.02
1.01
1.00
0.99
0.98
0.97
0.96
0.95
y
0.50
0.75
1.00
x
Legend
alpha=0.5
alpha=0.6
alpha=0.7
alpha=0.8
alpha=0.9

figure 2-21

6. Therefore

$L[z] - \phi_1^2 z < 0$

with boundary conditions $B(z) = z'(\alpha) = z(1) = 0$

7. It follows again from theorem 1.5.1.9 and 1.5.1.10 that

$L[z] - \phi_1^2 z < 0 \Rightarrow z > 0$

$\Rightarrow y_1 - y_2 > 0$

$\Rightarrow y_1 > y_2$

thus y is monotonically decreasing with ϕ

⊠.

A graph of the monotonicity behaviour of ϕ is demonstrated in figure 2-19 and figure 2-20 in the interval (0.5,1) and (0.1,1) respectively.
α is taken to be 0.5 and β is taken to be 1.

The monotonicity behaviour of α is illustrated in figure 2-21.

2.5.6 Approximate analytical solutions

2.5.6.1 Perturbation solutions for small ϕ

For small ϕ, we must use the regular perturbation method but we must expand in y(x)

$$y = y_0 + \phi^2 y_1 + \phi^4 y_2 + \ldots\ldots$$

$$F(y) = F(y_0) + \left(\frac{dF}{dy}\right)\Big|_{y_0} \phi^2 y_1 + \ldots$$

or

$$\frac{y}{1+\beta y} = \frac{y_0}{1+\beta y_0} + \frac{1}{(1+\beta y_0)^2}\phi^2 y_1 + \ldots$$

We then get the simpler problems

(1) $\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy_0}{dx}\right) = 0 \qquad y_0'(\alpha) = 0 \quad y_0(1) = 1$

(2) $\frac{1}{x^2}\frac{d}{dx.}\left(x^2\frac{dy_1}{dx}\right) = F(y_0) \qquad y_1'(\alpha) = 0 \quad y_1(1) = 0$

Solving for equation (1) we get the equation

$y_0 = 1$

Substituting $y_0 = 1$ into (2) and solving for y_1 with the given boundary conditions, we obtain the equation

$$y_1(x) = \frac{Kx^2}{6} - \frac{A}{x} + B$$

where

$$K = \frac{1}{1+\beta}, \quad A = -\frac{K\alpha^3}{3} \quad \text{and} \quad B = -\frac{K}{6} - \frac{K\alpha^3}{3}$$

Thus a perturbation solution fo small ϕ^2 is

$$y = y_0 + \phi^2 y_1 \tag{2-68}$$

where $y_0 = 1$ and y_1 is as above.

We don't know how good the solution is, although we know we need $\phi \to 0$. It can also be observed that this perturbation solution is a lower solution. This is done below

Consider the perturbation solution

$y_{ps} = y_0 + \phi^2 y_1$

Differentiating

$$y_{ps} = 1 + \frac{\phi^2 K}{6} x^2 - \frac{A}{x} + B$$

$$y_{ps}' = \frac{K\phi^2}{3} x + \frac{A}{x^2}$$

$$y_{ps}'' = \frac{K\phi^2}{3} - \frac{2A}{x^3}$$

Therefore

$$y_{ps}' + \frac{2y_{ps}'}{x} = \frac{K\phi^2}{3} - \frac{2A}{x^3} + \frac{2}{x}\left(\frac{K\phi^2}{3} x - \frac{A}{x^2}\right)$$

$$= K\phi^2$$

$$= \frac{\phi^2}{1+\beta} \geq \frac{\phi^2 y_{ps}}{1+\beta y_{ps}}$$

(assuming that $y_{ps} \leq 1$)

It follows from theorem 1.5.1.10. that y_{ps} is a lower solution of y.

2.5.6.2 Comparison of the Numerical Solution to the first perturbation solution

Rather than comparing all points between the exact numerical solution and the perturbation solution, we compare only values at $y(\alpha)$.

Since the perturbation solution is a lower solution, the maximum error will occur at $y(\alpha)$.(by the nature of $y(x)$)

A summary of results is given in table 2-3

ϕ	β	$y(\alpha)$ (perturbation solution)	$y(\alpha)$ (numerical solution)	Absolute error
0.1	0.1	0.99924	0.99924	0
0.5	0.5	0.98611	0.98621	1e-4
0.3	0.3	0.99423	0.99425	2e-5
1	1	0.95833	0.95898	6.4e-4
1	5	0.98611	0.98612	1e-5
1	10	0.99242	0.99242	0
1	20	0.99603	0.99603	0
1	50	0.99837	0.99837	0
1	100	0.99917	0.99917	0
2	2	0.88889	0.89217	3.3e-3
2	5	0.94444	0.94485	4.1e-4
5	5	0.65278	0.67194	2e-2
5	10	0.81061	0.81350	3e-3

table 2-3 A comparison of the numerical solution to the first perturbation solution

(Of course ϕ <<1 for this procedure to work most effectively)

Although this method assumes that ϕ is small (of course ϕ <<1 for this procedure to work most effectively), it seems to work remarkably well for all ϕ and β of practical interest.

Maximum relative error for the chosen parameters is of the order of 3%

Notice that this perturbation solution is very good for ϕ very small and β moderate to very large.

2.5.6.3 A Second perturbation solution

Many other perturbation techniques were also implemented, in particular, perturbation solutions were obtained for large β and small ϕ. One of the methods of obtaining this was just done in section 2.5.6.2 . However , a second approximation, y_2 was also obtained after considerable effort and verified computationally.

This is summarised below and numerical results produced in table 2-4

Solving for y_2,
where

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy_2}{dx}\right) = \frac{1}{(1+\beta y_0)^2}\phi^2 y_1$$

and boundary conditions
$y_2'(\alpha) = 0$ and $y_2(1) = 0$
we obtain

$$y_2 = \frac{\phi^2}{(1+\beta)^2}\left(\frac{Kx^4}{120} - \frac{Ax}{2} + \frac{Bx^2}{6}\right) - \frac{C}{x} + D$$

where
K,A and B have been defined and

$$C = \frac{\alpha^2}{(1+\beta)^2}\left(\frac{-K\phi^2\alpha^3}{30} + \frac{A\phi^2}{2} - \frac{B\phi^2\alpha}{3}\right)$$

and

$$D = \frac{\phi^2}{(1+\beta)^2}\left(\frac{-K}{120} + \frac{A}{2} - \frac{B}{6}\right) + C$$

We then obtain our second perturbation solution

$$y(x) = y_0 + \phi^2 y_1 + \phi^4 y_2 \qquad \textbf{(2-69)}$$

As with our first perturbation solution, we compare results with our numerical solution. These results are summarised in table 2-4

ϕ	β	$y(\alpha)$ (perturbation solution)	$y(\alpha)$ (numerical solution)	Absolute error
0.1	0.1	0.99924	0.99924	0
0.5	0.5	0.98618	0.98621	3e-4
0.3	0.3	0.99424	0.99425	1e-5
1	1	0.96022	0.95898	1.2e-3
1	5	0.98618	0.98612	6e-5
1	10	0.99242	0.99242	0
1	20	0.99603	0.99603	0
1	50	0.99837	0.99837	0
1	100	0.99917	0.99917	0
2	2	0.92469	0.89217	3.3e-3
2	5	0.94892	0.94485	4.1e-3
5	5	1.70321	0.67194	1.00
5	7	1.20005	0.74742	0.45
5	10	0.98792	0.81350	1.7e-1

table 2-4A comparison of the numerical solution to the second perturbation solution

It may be seen that the second perturbation solution, is far more sensitive to large ϕ than our first perturbation solution.

It is suspected, from the numerical data that this perturbation solution is an upper solution (except for one value at ϕ=0.3 and β = 0.3 which could be due to numerical error)

For most values of ϕ and β, it seems as if the second perturbation solution gives no better results than our first perturbation solution.

1.4.4 Other Perturbation techniques for various parameters

Perturbation methods were also done with small β and small ϕ.

These perturbation methods provide useful information in limited regions of parameter space.

It is usually easy to find the first approximation but it gets considerably difficult to get the second and sucessive approximations.

It was particularly difficult to obtain a perturbation solution expanded in β

This is not produced in this thesis because of its complexity.

Effectiveness factor for small ϕ

We obtain the effectiveness factor for small ϕ from the equation (2-68). and the definition of effectiveness factor in Michaelis-Menten kinetics

For small ϕ^2

$$y = y_0 + \phi^2 y_1$$

$$= 1 + \frac{\phi^2 K}{6} x^2 - \frac{A}{x} + B$$

where

$$K = \frac{1}{1+\beta}$$

$$A = -\frac{K\alpha^3}{3}$$

and

$$B = \frac{-(K + 2\alpha^3)}{6}$$

Differentiating and equating at x = 1

$$y'(x) = K\phi^2 x/3 + A/x^2$$
$$y'(1) = K\phi^2/3 + A$$

The effectiveness factor

$$\eta = \frac{3(1+\beta)\ y'(1)}{\phi^2(1-\alpha)} \tag{2-70}$$

for Michaelis-Menten kinetics with small ϕ^2 is therefore

$$\eta = \frac{3\ (1+\beta)\ (\frac{\phi^2 K}{3} + A\ )}{\phi^2(1-\alpha)} \tag{2-71}$$

where A, B and K were defined previously.

2 Approximate analytical solutions for arbitrary ϕ and β

As stated in Chapter 1.8, it is frequently impossible to find a solution to boundary value problems explicitly. It is frequently desirable to approximate a solution in such a way that an explicit bound for the error is known. Such an approximation is equivalent to the determination of both upper and lower bounds for the values of the solution. We shall once again, use with the help of the maximum principle, obtain bounds to problem(2-67).
This follows from theorem 1.5.1.10

We state the inequality

$$0 \leq \frac{\phi^2 y}{1+\beta} \leq \frac{\phi^2 y}{1+\beta y} \leq \phi^2 y \leq \phi^2 \qquad \text{(i)}$$

for $0 < y < 1$

It follows from theorem 1.5.1.10 that if
z_1 satisfies

$$z_1'' + \frac{2z_1'}{x} - \frac{\phi^2 z_1}{1+\beta z_1} \leq 0$$

with boundary conditions
$z_1'(\alpha) = 0, \quad z_1(1) = 1$

and if z_2 satisfies

$$z_2'' + \frac{2z_2'}{x} - \frac{\phi^2 z_2}{1+\beta z_2} \geq 0$$

with boundary conditions
$z_2'(\alpha) = 0$ and $z_2(1) = 1$

then the upper and lower bounds
$z_2(x) \leq y(x) \leq z_1(x)$ are valid.

We immediately see from the above inequality (i), that it follows that

$$1 \geq z_1\left(x; \frac{\phi^2}{1+\beta}\right) \geq y(x) \geq z_2(x; \phi^2) \geq 0$$

where

$z_1(x; \frac{\phi^2}{1+\beta})$

is the solution to the linearised problem

$$z_1'' + \frac{2z_1'}{x} - \frac{\phi^2 z_1}{1+\beta} = 0$$

with boundary conditions $z_1'(\alpha) = 0$, $z_1(1) = 1$

and

$z_2(x;\phi^2)$ is the solution to the linearised problem

$$z_2'' + \frac{2z_2'}{x} - \phi^2 z_2 = 0$$

with boundary conditions $z_2(\alpha) = 0$, $z_2(1) = 1$.

A graph of y(x) and its upper and lower bounds is given in figure 2-22 for $\beta=1$ and $\phi=1$.

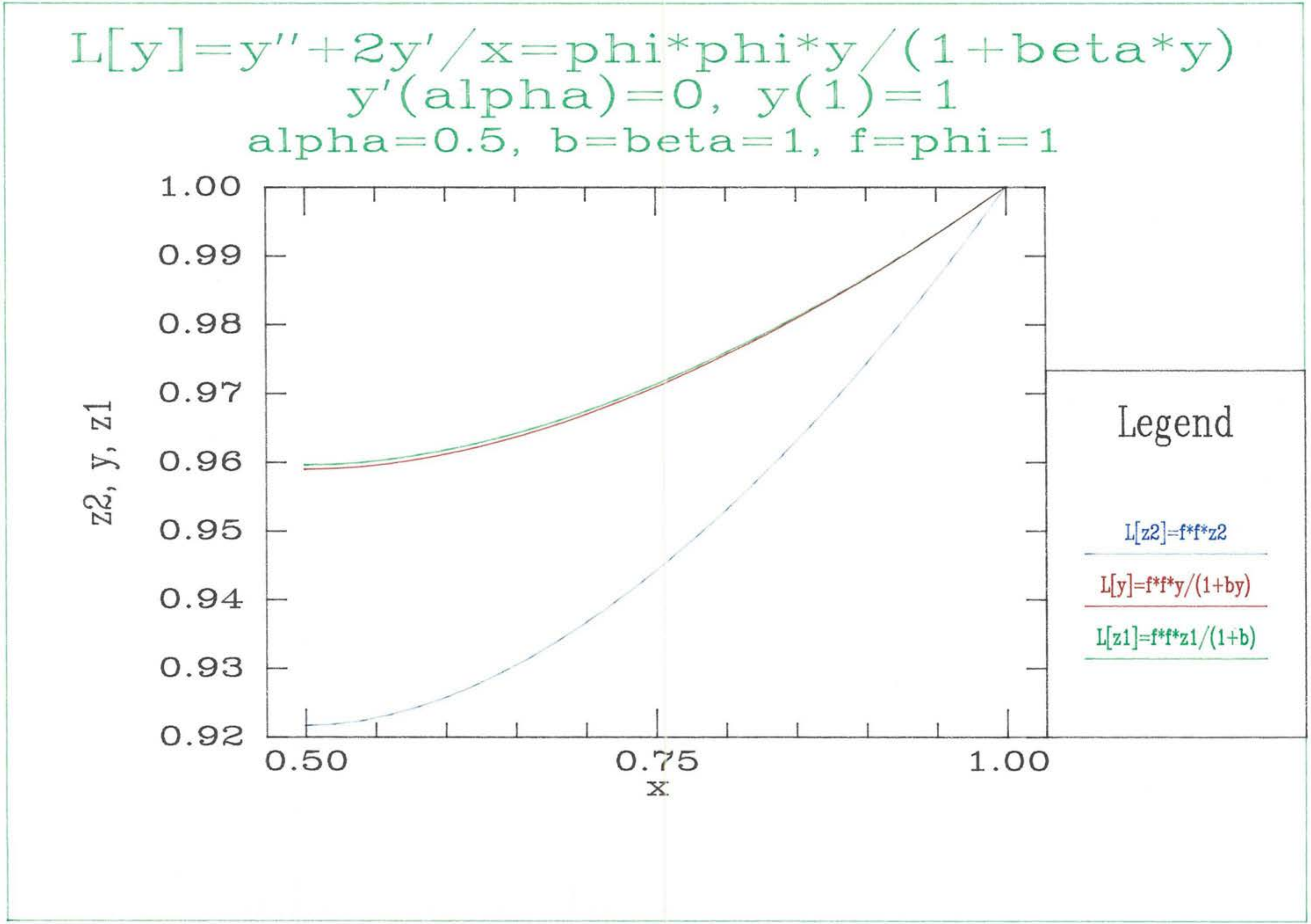

figure 2-22 Upper and Lower Bounds to L[y]

2.5.6.5 Attempts to produce better upper and lower bounds

The following facts may be noticed

1. $F(y) = \frac{\phi^2 y}{1+\beta y}$ is convex and any linearisation of F(y) will be strictly greater than F(y).
Check :

$$F''(y) = \frac{\phi^2}{(1+\beta)^2} > 0$$

2. $F(y) = \frac{\phi^2 y}{1+\beta y} \approx \phi^2 y$ when $\beta \approx 0$.

3. $F(y) = \frac{\phi^2 y}{1+\beta y} \approx \frac{\phi^2 y}{1+\beta}$ when $y \approx 1$ and β very large .
This is also the best linearisation below F(y)

4. $f(y) = \frac{\phi^2 y}{1+\beta y} \approx \frac{\phi^2 y_0}{1+\beta y_0} + \frac{\phi^2}{(1+\beta y_0)^2}(y - y_0) + \dots$

where f(y) is linearised about y_0

Example 1
linearising about $y_0 = 0$, we obtain $F(y) \approx \phi^2 y$

Example 2

Linearising about $y_0 = 1$, we obtain $F(y) \approx \frac{\phi^2}{1+\beta} + \frac{1}{(1+\beta)^2}(y-1)$

A graph of F(y) and its linearisations at y_0=0 and y_0=1 is produced in figure 2-23.

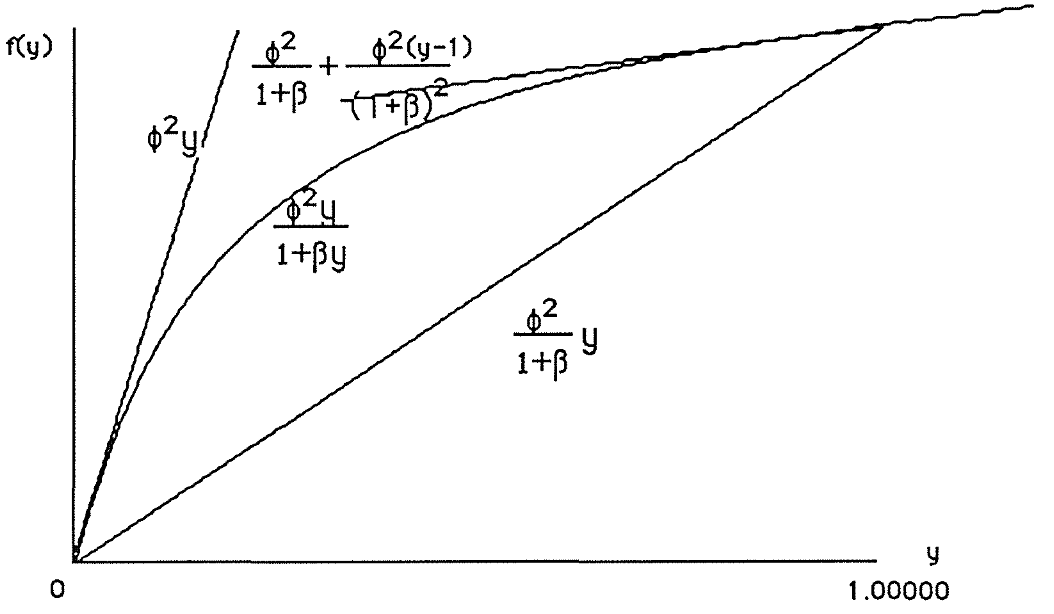

figure 2-23 A graph of F(y) and its linearisations about $y_0=0$ and $y_0=1$.

2.5.6.6 Other linearisations

We take a linearised Taylors series expansion about ε where $0 < \varepsilon < 1$ in the hope of getting a better lower bound for y(x) .

Here we aim to choose the most appropriate ε to linearise about

$$\frac{\phi^2 y}{1+\beta y} \approx \frac{\phi^2 \varepsilon}{1+\beta\varepsilon} + \frac{\phi^2(y-\varepsilon)}{(1+\beta\varepsilon)^2}$$

$$= \frac{\phi^2 \varepsilon}{1+\beta\varepsilon} - \frac{\phi^2 \varepsilon}{(1+\beta\varepsilon)^2} + \frac{\phi^2}{(1+\beta\varepsilon)^2} y$$

$$= \lambda + \psi y$$

where

$$\lambda = \frac{\phi^2 \varepsilon}{1+\beta\varepsilon} - \frac{\phi^2 \varepsilon}{(1+\beta\varepsilon)^2}$$

and

$$\psi = \frac{\phi^2}{(1+\beta\varepsilon)^2}$$

We choose the most appropriate ε to expand about to be at the point

$$\varepsilon = \frac{-1 + \sqrt{1+\beta}}{\beta}$$

where ε is the the value of y that gives a tangent of slope

$$\frac{1}{1+\beta}$$

on the graph

$$F(y) = \frac{\phi^2 y}{1 + \beta y}$$

This tangent occurs at the point (ε,k) where

$$k = \frac{\phi^2 \varepsilon}{1+\beta\varepsilon}$$

We finally obtain the linearised problem

$$y_\varepsilon'' + \frac{2y_\varepsilon'}{x} = \lambda + \psi y_\varepsilon \qquad \textbf{(2-72)}$$

with boundary conditions

$y_\varepsilon'(\alpha) = 0, \quad y_\varepsilon(1) = 1$

and ε, λ, ψ defined previously

An average of the upper and lower bound may then be taken to give an approximate analytical solution for practical purposes.
This is neither an upper nor a lower solution.
There are many ways to choose an average that would minimise the error between our approximate analytical solution and our numerical solution.
Of these would be to find an optimum linearised problem
between lower bound
y_ε
and
upper bound

$$z_1\left(x; \frac{\phi^2}{1+\beta}\right)$$

We simply take an arithmetic mean of the source terms

$$\lambda + \frac{\phi^2}{1+\beta} y$$

and

$$\frac{\phi^2}{1+\beta} y$$

This is seen in figure 2-24

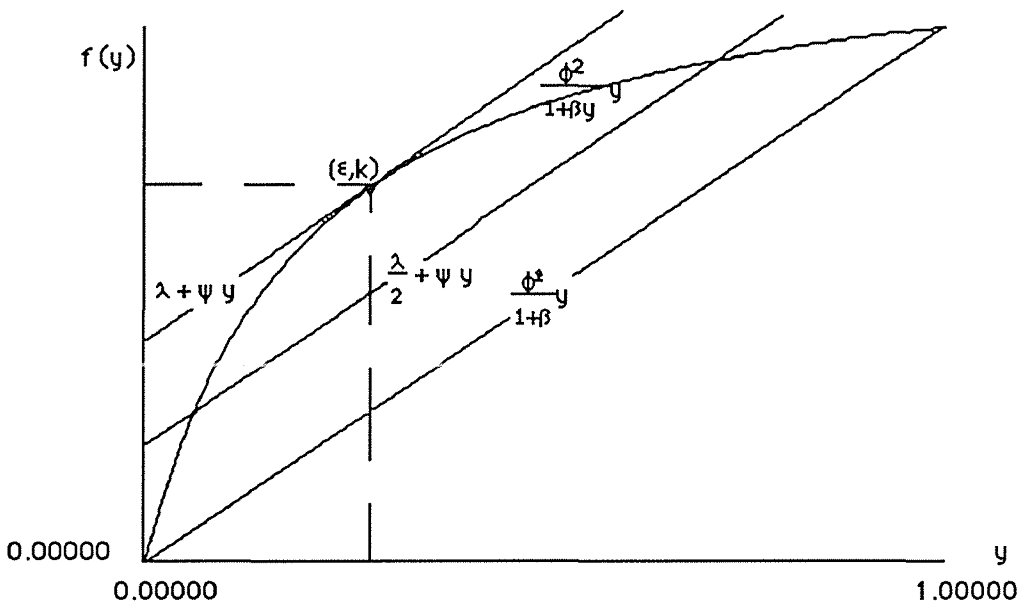

figure 2-24 A graph of linearisations about ε and an average

We then obtain the linearised problem

$$y_{av}'' + \frac{2y_{av}'}{x} = \frac{\lambda}{2} + \frac{\phi^2}{1+\beta} y \qquad \textbf{(2-72)}$$

with boundary condtions $y_{av}'(\alpha) = 0$, $y_{av}(1) = 1$
where
y_{av} is neither an upper nor a lower solution and has the exact solution

$$y_{av}(x) = \frac{A \cosh \sqrt{\psi}(1-x)}{x} + \frac{B \sinh \sqrt{\psi}(1-x)}{x} + \frac{\lambda}{2} \qquad \textbf{(2-73)}$$

where we found in Chap. 2.4.5 that

$$A = 1 - \frac{\lambda}{2}$$

and

$$B = \frac{\alpha\sqrt{\psi}\ \sinh\sqrt{\psi}\ (1-\alpha) + \cosh\sqrt{\psi}\ (1-\alpha)}{\sqrt{\psi}\ \alpha \cosh\sqrt{\psi}\ (1-\alpha) + \sinh\sqrt{\psi}\ (1-\alpha)}$$

2.5.6.7 A comparison of the numerical solution with an approximate analytical solutions

Results for the previous chapter were obtained and tabulated for various values of ϕ and β of practical significance.

These are given in the table below.

ϕ	β	$y(\alpha)$	$z_1(\alpha)$	$z_2(\alpha)$	$y_\varepsilon(\alpha)$	$y_{av}(\alpha)$	relative error between y_{av} and numerical soln
0.1	0.1	0.99924	0.99924	0.99917	0.99924	0.99924	0 %
0.5	0.5	0.98620	0.98626	0.97948	0.985	0.98620	0.02%
1	1	0.95897	0.95964	0.92170	0.958	0.9562	0.3%
1	2	0.97240	0.97280	0.92170	0.965	0.96950	0.3%
1	5	0.98612	0.98625	0.92170	0.985	0.98350	0.3%
2	2	0.89209	0.89775	0.73556	0.87	0.88400	0.9%
2	5	0.94480	0.94672	0.73556	0.93	0.93620	0.9%
2	10	0.96973	0.97036	0.73556	0.96	0.96300	0.7%
3	3	0.81975	0.83623	0.52997	0.79	0.80920	1.3%
4	4	0.74584	0.77947	0.35844	0.70	0.73700	1.2%
5	1	0.34642	0.43250	0.23361	0.33	0.38400	12.5%
5	3	0.54473	0.8818	0.23361	0.51	0.57000	5%
5	5	0.67172	0.72686	0.23361	0.61	0.6700	0.3%
5	10	0.81334	0.83594	0.23361	0.745	0.79100	2.8%
6	6	0.59822	0.67960	0.14898	0.53	0.60600	1.3%

table 2-5 A comparison of the numerical solution with an approximate analytical solution

We notice that for very large values of β, $z_2(x)$ is not a very good lower bound.

We also notice that when ϕ is large and β is small, we do not get a good approximation by this method. i.e. it seems that the method seems to be highly sensitive to ϕ^2/β.

Expanding f(y) about ε gives considerably better solutions for all values of ϕ and β than expanding about 0, i.e. $y_\varepsilon(x)$ is a far better lower bound than $z_2(x)$.

For most values of ϕ and β of practical interest, this approximate analytical solution is very good.

The parameters we shall be interested in are
ϕ of the order of 1 to 5 and
β of the order of 2 to 10.

2.6 nth Order Kinetics

2.6.1 Introduction

For nth Order Kinetics, we solve the equation

$$\frac{D}{r^{a-1}}\frac{d}{dr}\left(r^{a-1}\frac{dS}{dr}\right) = \rho_{bf}\, k_n\, S^n \qquad \textbf{(2-74)}$$

for a = 1,2 and 3 being slab, cylindrical and slab geometries respectively.
The external boundary conditions is S = Sb

S = Sb at $r = r_{bp}$

and the internal boundary condition is

$$\frac{dS}{dr} = 0 \quad \text{at } r = r_m$$

This has dimensionless form

$$\frac{1}{x^{a-1}}\frac{d}{dx}\left(x^{a-1}\frac{dy}{dx}\right) = \phi^2 y^n \qquad \textbf{(2-75)}$$

or equivalently

$$\frac{d^2y}{dx^2} + \frac{(a-1)}{x}\frac{dy}{dx} = \phi^2 y^n \qquad \textbf{(2-76)}$$

where

$$y = \frac{S}{S_b}$$

$$x = \frac{r}{r_{bp}}$$

and $\phi^2 = \dfrac{k_n r_{bp}^2 S_b^{n-1}}{D}$

2.6.2 Uniqueness and existence of solutions

These are done as trivial examples to theorems 1.10 in Chapter 1 and theorem 1.2 in Chap.2

2.6.3 Finding exact solutions

We may reduce the problem (2-76) into the form

$$\frac{d^2\bar{y}}{dx^2} + \frac{(a-1)}{x}\frac{d\bar{y}}{dx} = \bar{y}^{\,n} \qquad \textbf{(2-77)}$$

with boundary conditions

$$\bar{y}'(\alpha) = 0 \quad \text{and} \quad \bar{y}(1) = \frac{1}{\phi^{2(\frac{-1}{n-1})}}$$

by the stretching group transformation defined in eqn.(1-42)

$$y = \phi^{2(\frac{-1}{n-1})}\bar{y}$$

The equation (2-77) can then be transformed to the more simpler form

$$u'' - x^{1-n}u_n = 0 \qquad \textbf{(2-78)}$$

by the transformation

$$u(x) = xy \qquad \textbf{(2-79)}$$

A particular solution of equation (2-78) may be obtained by Lie Group methods and has the form

$$u(x) = [2(1 + \frac{1}{n})(1 + \frac{2}{n})]^{1+\frac{1}{n}}\, x^{-1(1+\frac{2}{n})} \qquad \textbf{(2-80)}$$

The equation (2-77) is a form of the Emden-Fowler equation and has been extensively studied.

Taking the equation 2-76 and looking for a simple stretching group

$x_1 = e^{\varepsilon x}$, $y_1 = e^{a\varepsilon}y$

that leaves the equation 2-76 invariant, we find

$k = \frac{2}{1-n}$, provided $n \neq 1$

Assuming that this is the case, we take

$u = yx^{-k}$ as the new independent variable so that equation 2-76 becomes

$$\{x^2u''+((a+1)+2k)xu'+k((a-1) + k-1)u\} -\phi^2u^n = 0 \quad (2\text{-}81)$$

With the substitutions
t = log x
p = du/dt

equation 2-81 becomes

$$up\frac{dp}{du} + ((a-1)+2k-1)pu + k((a-1)+k-1)u^2 -\phi^2u^{-2/k} = 0 \quad (2\text{-}82)$$

In general, this is an Abel equation of the second kind (Murphy[ ], pg. 25) However special cases give rise to standard equations.

This does not guarantee that our boundary conditions will be solved.

For example, if $n = 3$, the equation is homogeneous while if $a \neq 0$ and $n = (a+2)/(a-2)$, the equation is of the Bernoulli type

Clearly n=0 and n=1 are cases which have been solved in earlier chapters.

2.6.4 Comparison of Michaelis-Menten Kinetics with nth order Kinetics

To compare Michaelis-Menten Kinetics with nth order Kinetics it must be noted that

$$F_{mm}(y) = \frac{y}{1 + y}$$

is a function that goes form 0 to 0.5 for $y \in [0,1]$ and that

$$F_n(y) = y^n$$

is a function that goes from 0 to 1 for $y \in [0,1]$.

It would therefore seem obvious to scale $F_{mm}(y)$ by a factor of 2 and try to find a suitable order, n that best approximates Michaelis-Menten Kinetics.
The method chosen to identify deviances of nth order kinetics with Michaelis-Menten Kinetics is a method of least squares where root mean squared values of the differences was tabulated and compared for different orders,n. Rather than using integration techniques to minimise the area between the two curves this method seems useful in that it can be used to see exactly where the graphs best fit one another.
A result of the comparison of Michaelis-Menten Kinetics with nth order kinetics is given in table 2-6 for n between 0.63 and 0.68. It was found by a Newton bisection method that Michaelis-Menten kinetics best approximates 0.641 order kinetics giving the overall lowest RMS value when over 1e5 points or more were taken in the interval [0,1].
A graph of 0.641 order kinetics with Michaelis-Menten kinetics is given in figure 2-25
Note that we could have used many other techniques for approximating Michaelis-Menten kinetics with nth order kinetics and where n has to be determined.
An obvious integration technique would be to minimise the area between the two curves, over n ,i.e. find

$$\min_{n} \int_0^1 \left| \frac{2y}{1 + y} - y^n \right|$$

for a suitable n that has to be determined.
This was performed numerically by a program written by the author and it was concluded that although brilliant results were not achieved, values of n that minimised the area was of the order 0.625 with a total area of 0.02225 (compare this with the RMS value of 0.026 over the interval (0,1))

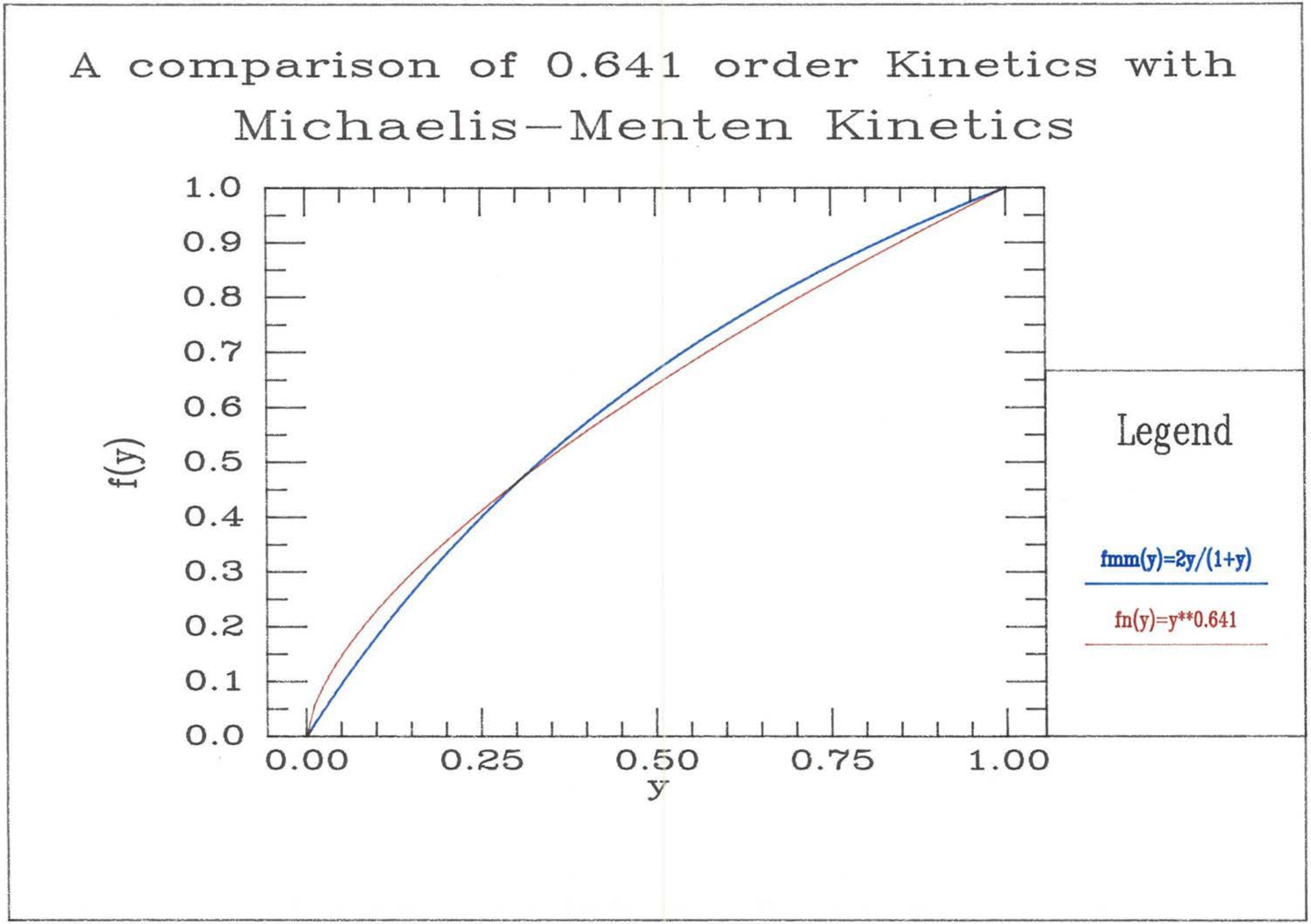
A comparison of 0.641 order Kinetics with Michaelis-Menten Kinetics
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
f(y)
0.00
0.25
0.50
0.75
1.00
y
Legend
fmm(y)=2y/(1+y)
fn(y)=y**0.641

figure 2-25

A graph of the function $F(y) = y^{0.625}$ is given in figure 2-26 with a difference of this function with Michaelis-Menten kinetics given in figure 2-27

y	$\frac{2y}{1+y}$	$y^{0.63}$	$y^{0.64}$	$y^{0.65}$	$y^{0.66}$	$y^{0.67}$	$y^{0.68}$
0.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.10	0.18182	0.23442	0.22909	0.22387	0.21878	0.21380	0.20839
0.20	0.33333	0.36278	0.35699	0.35129	0.34568	0.34017	0.33473
0.30	0.46154	0.46837	0.46276	0.45722	0.45175	0.44635	0.44100
0.40	0.57143	0.56143	0.55631	0.55124	0.54621	0.54123	0.53629
0.50	0.66667	0.64618	0.64171	0.63728	0.63288	0.62851	0.62416
0.60	0.75000	0.72483	0.72114	0.71746	0.71380	0.71017	0.70655
0.70	0.82353	0.79875	0.79591	0.79307	0.79025	0.78744	0.78463
0.80	0.88889	0.86885	0.86692	0.86498	0.86306	0.86113	0.85921
0.90	0.94737	0.93578	0.93479	0.93381	0.93282	0.93184	0.93086
1.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
RMS over							
10 intervals -		0.02579	0.02557	0.02608	0.02726	0.02900	0.03119
100 intervals -		0.02667	0.92619	0.02641	0.02727	0.02868	0.03055
1000 intervals -		0.02665	0.02609	0.02631	0.02716	0.02856	0.03042

table 2-6 A comparison of Michaelis-Menten kinetics with nth order kinetics where n is fractional and is determined by a lowest RMS value

Here

$$RMS = \sqrt{\frac{\sum_{i=1}^{k} (\frac{2y}{1+y} - y^{n})}{k-1}}$$

for all y between 0 and 1 taken in steps of 0.1(above), 0.01 and 0.001.
k = no. of interval steps 10,100,1000.

It may be noticed that Michaelis-Menten Kinetics is initially approximately of 0.67-0.68 order, the overall RMS value in the interval [0,1] is found to be lowest at 0.64 order. A Newton iterative scheme was performed between 0.63 and 0.65 order kinetics and it was found that Michaelis-Menten Kinetics best approximates 0.641 order Kinetics with an overall RMS value of approximately 0.02618 when taking 100 interval steps. It was also shown to converge to 0.641 order kinetics as the number of interval steps between 0 and 1 was increased beyond 10000 intervals and the RMS value was minimised.

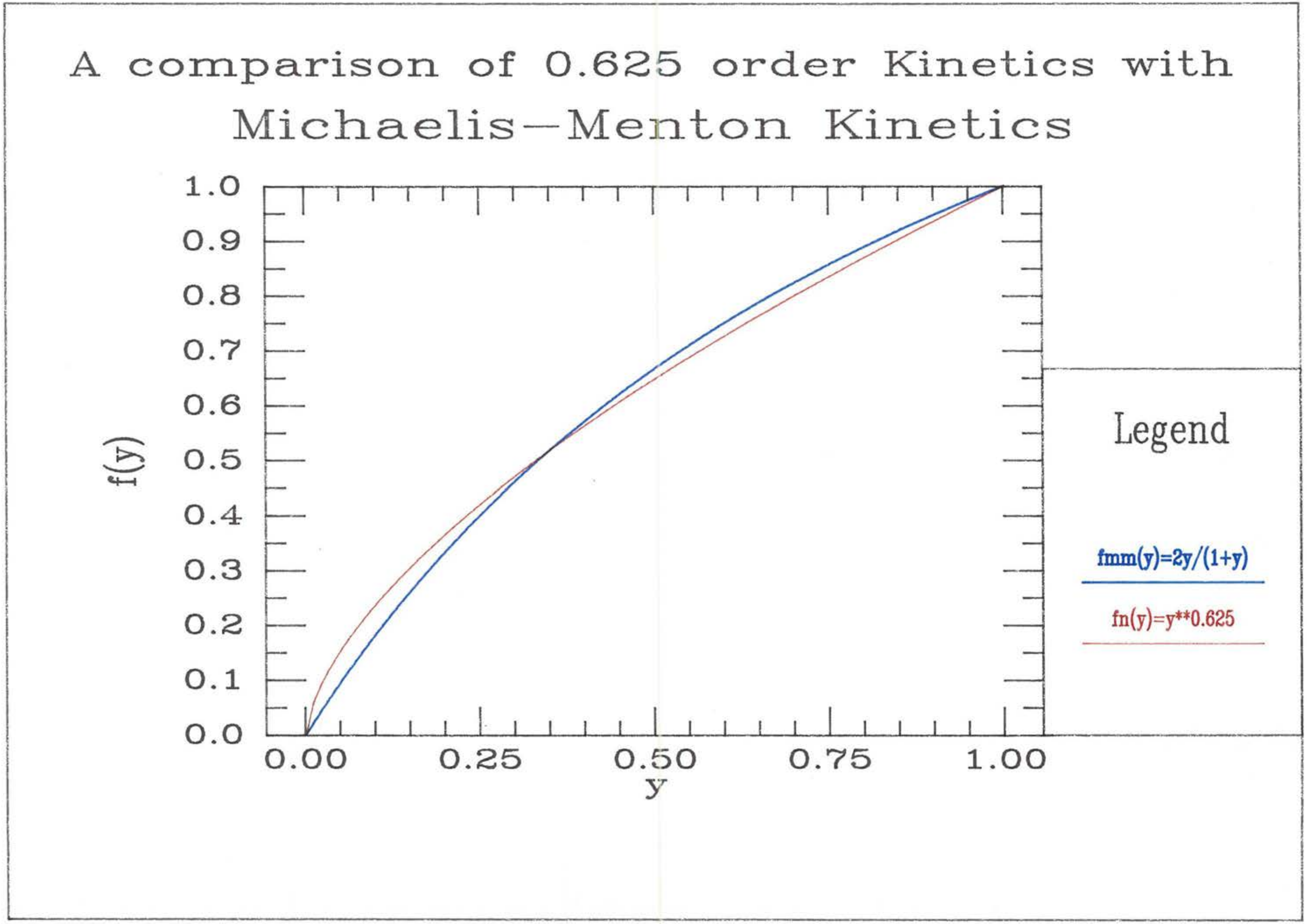
A comparison of 0.625 order Kinetics with Michaelis–Menton Kinetics
f(y)
y
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.00
0.25
0.50
0.75
1.00
Legend
fmm(y)=2y/(1+y)
fn(y)=y**0.625

figure 2-26

A difference of 0.625 order Kinetics with Michaelis–Menten Kinetics

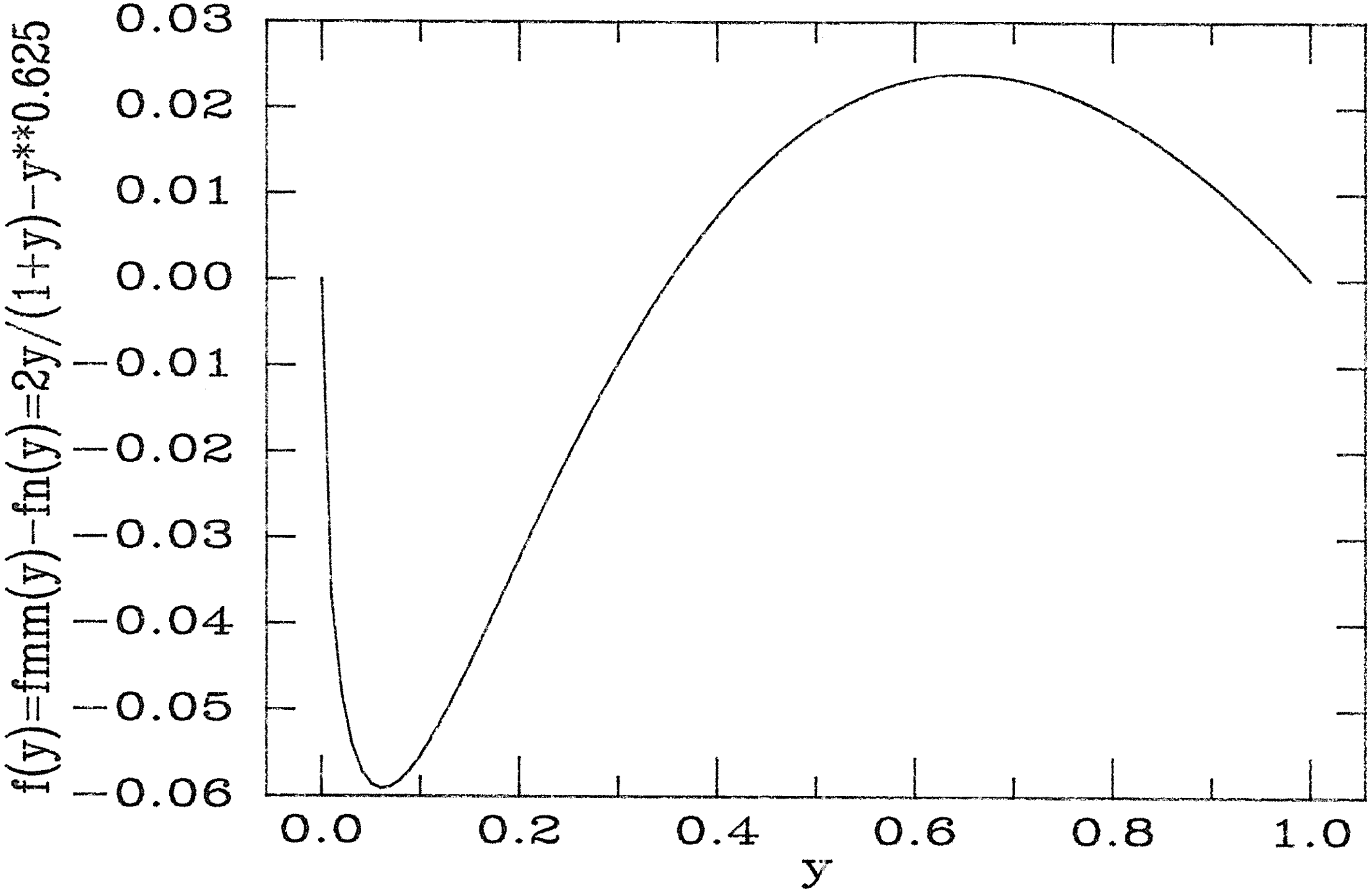

figure 2-27

y	$\frac{2y}{1+y}$	$y^{0.625}$	absolute error
0.00	0.00000	0.00000	0.00000
0.10	0.18182	0.22856	0.04674
0.20	0.33333	0.35642	0.02308
0.30	0.46154	0.46220	0.00666
0.40	0.57143	0.55580	-0.01563
0.50	0.66667	0.64127	-0.02540
0.60	0.75000	0.72077	-0.02923
0.70	0.82353	0.79562	-0.02791
0.80	0.88889	0.86672	-0.02216
0.90	0.94737	0.93469	-0.01267
1.00	1.00000	1.00000	0.00000

table 2-7 Absolute error between 0.625 order kinetics and Michaelis-Menten kinetics.

Chapter 3 Unsteady State

Chapter 3 Unsteady state

3.1 Introduction

This chapter shall deal primarily with Michaelis-Menten reaction kinetics. We shall deal with solving of the equation

$$\frac{\partial y}{\partial t} = \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial y}{\partial x}\right) - \frac{\phi^2 y}{1+\beta y} \qquad \textbf{(3-1)}$$

with boundary conditions

$$\frac{\partial y(\alpha,t)}{\partial x} = 0 \quad \text{and} \quad y(1,t) = 1$$

All results may easily be generalised to a first order reaction by taking parameter $\beta = 0$.

It would be an interesting exercise to examine the movement of boundary α, with time of reactions exibiting zero order kinetics and partial penetration.

3.2 Uniqueness and Existence

These follow as trivial examples to Theorem 3.9 , Chapter 1.5

3.3 Monotonicity with β and ϕ

Monotonicity with parameters ϕ and β may be shown to be the same as for steady state.

We may use the techniques of theorem 2.5.5 and theorem 3.9 of Chapter 1.5. to show that this is indeed true.

3.4 Upper and Lower bounds

Examples of lower and upper bounds are given in Chap. 1.5 section 3.9 as an example to theorem 3.9

These lower and upper bounds are graphed for all time in figures 2-28, and 2-30 respectively with the numerical solution of equation 3-1 given in figure 2-29.

We choose $\phi^2 = 1$, $\alpha = 0.5$ and $\beta = 1$ for mathematical convenience.

Notice that these are upper and lower bounds for all time.(Thm. 3.9)

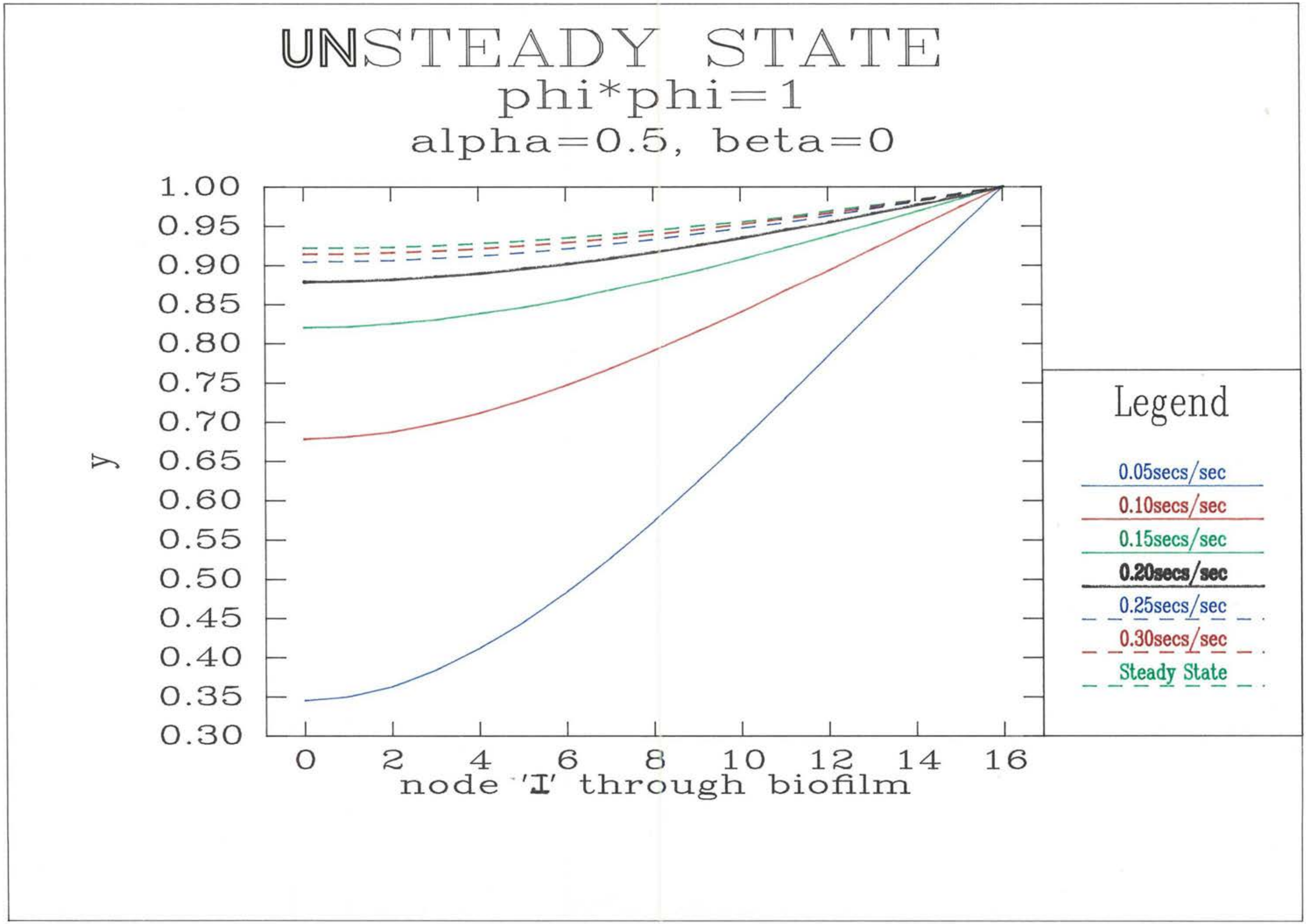
UNSTEADY STATE
phi*phi=1
alpha=0.5, beta=0
y
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0
2
4
6
8
10
12
14
16
node 'I' through biofilm
Legend
0.05secs/sec
0.10secs/sec
0.15secs/sec
0.20secs/sec
0.25secs/sec
0.30secs/sec
Steady State

figure 2-28

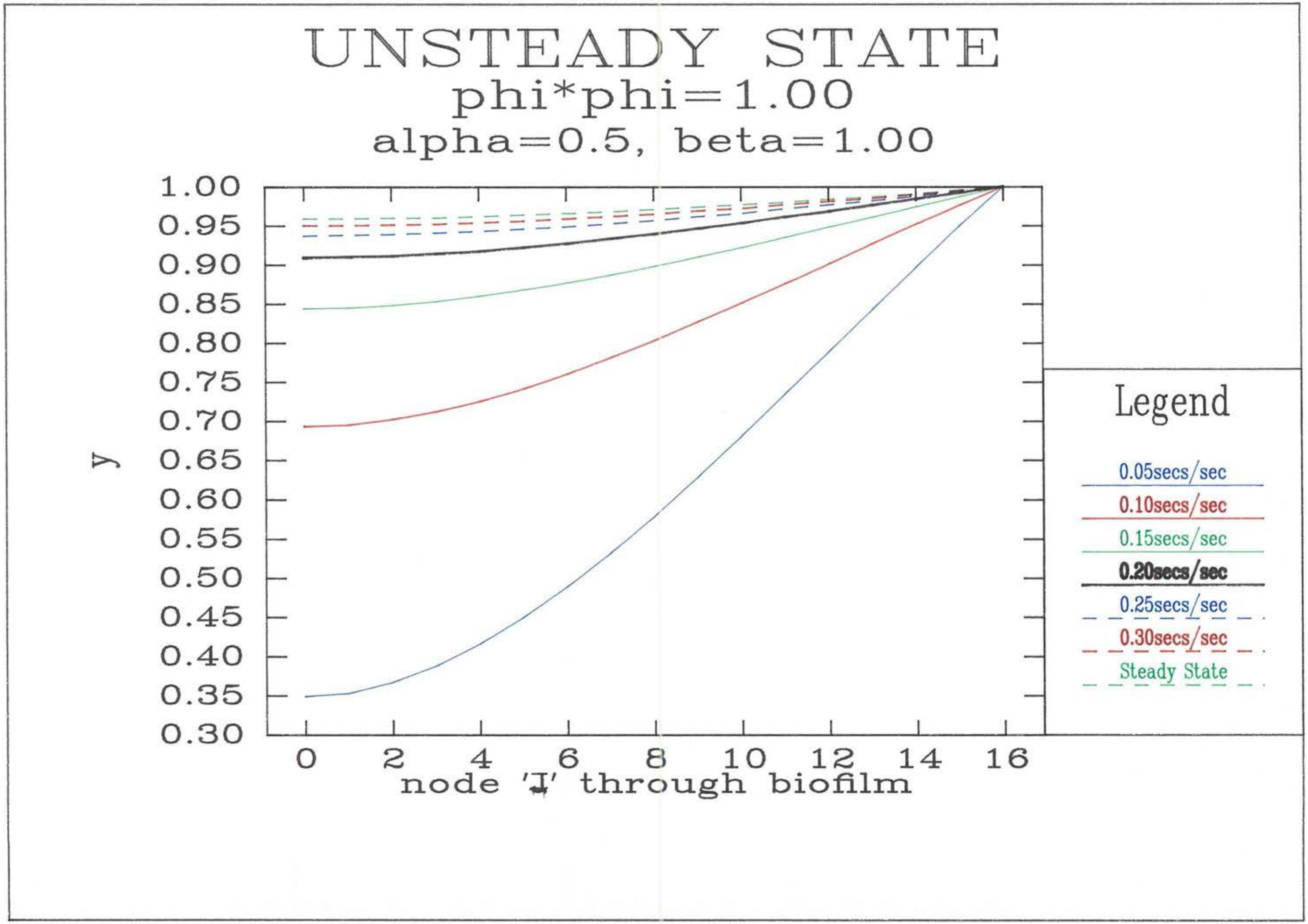
UNSTEADY STATE
phi*phi=1.00
alpha=0.5, beta=1.00
y
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0
2
4
6
8
10
12
14
16
node 'I' through biofilm
Legend
0.05secs/sec
0.10secs/sec
0.15secs/sec
0.20secs/sec
0.25secs/sec
0.30secs/sec
Steady State

figure 2-29

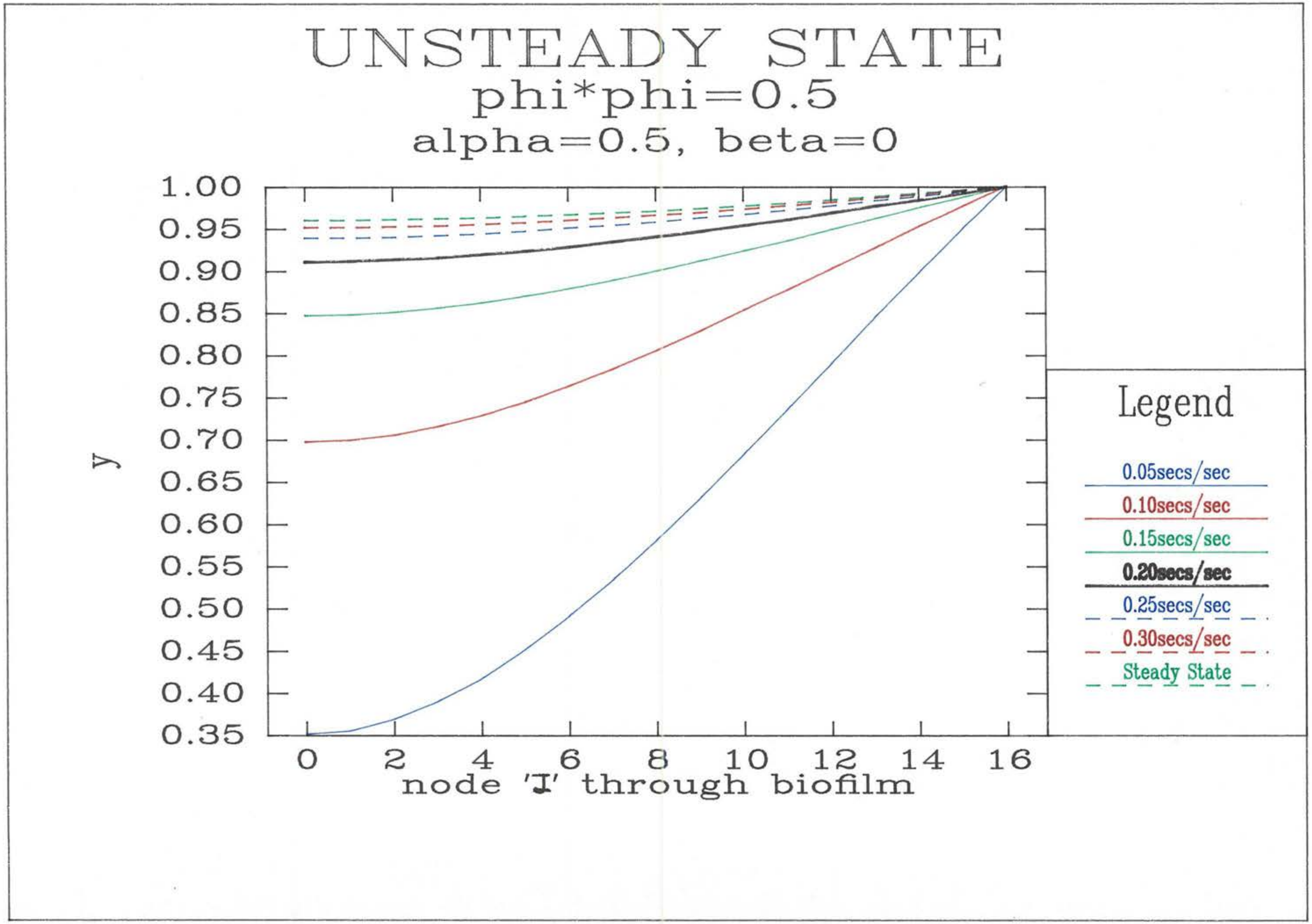
UNSTEADY STATE
phi*phi=0.5
alpha=0.5, beta=0
y
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0
2
4
6
8
10
12
14
16
node 'I' through biofilm
Legend
0.05secs/sec
0.10secs/sec
0.15secs/sec
0.20secs/sec
0.25secs/sec
0.30secs/sec
Steady State

figure 2-30

3.5 Numerical technique

The numerical technique used to solve equation 3-1 was an explicit finite difference algorithm.

This is given as a Pascal program in appendix 1 and is very explanatory.

To implement this program on a computer, we shall take experimental values of our constants and substitute these into the program.

node 'I' is taken from r_m to r_{bp}
distance from one node to another = Δr where

$$\Delta r = \frac{r_{bp} - r_m}{J} = \frac{r_{bp} - r_m}{J}$$

and J is the last node.

The distance to the ith node is therefore

$$r_m + i\left(\frac{r_{bp} - r_m}{J}\right)$$

and the distance to the Jth node from the centre of the bioparticle is r_{bp}.

Writing

$$C_j^{i+1}$$

as

$$C_j^{i+1} = k_1 C_{j-1}^i + k_2 C_{j+1}^i + k_3 C_j^i$$

and noting that for numerical stability to occur

$k_3 > 0$.

This corresponds to time interval steps $\Delta t < 10^{-5}$ for stability to occur given that we use 64 nodes

This is printed every 4th node in the program.

3.6 Model Verification

We take experimental values of constants from literature (Rao[17],1985)and implement these on the computer using our program.

K_s = 0.2 e-4 gcm^{-3}
$Y_{x/s}$ = 0.9223 g g-1
r_m = 0.01375 cm
r_{bp} = 0.02975 cm
D = 2.743202e-6 cm^2sec^{-1}
ρ_{bf} = 0.03267 g cm^{-3}
μ_m = 0.40/3600 sec^{-1}
Sb = 1e-4 g cm^{-3}

These values correspond in dimensionless coordinates to
$\phi^2 = 63.49223$
$\beta = 5$

and dimensionless time

$$\tau = \frac{D\,t}{r_{bp}^2}$$

These values were implemented on the computer and graphed for various times in figure 2-32.

Also graphed in figure 2-31 is its lower bound
$z(x,t;\phi^2;\beta) = z(x,t;\phi^2;0)$
which can be seen to be a lower bound for all time(Thm. 3.9)

and upper bound in figure 2-33
$Z(x,t;\phi^2;\beta) = Z(x,t,\phi^2/(1+\beta);0)$
which is also an upper bound for all time. (Thm.3.9)

This was shown to reach steady state in 0.3 secs/sec

This corresponds in real time to be about one and a half minutes and is physically realistic.

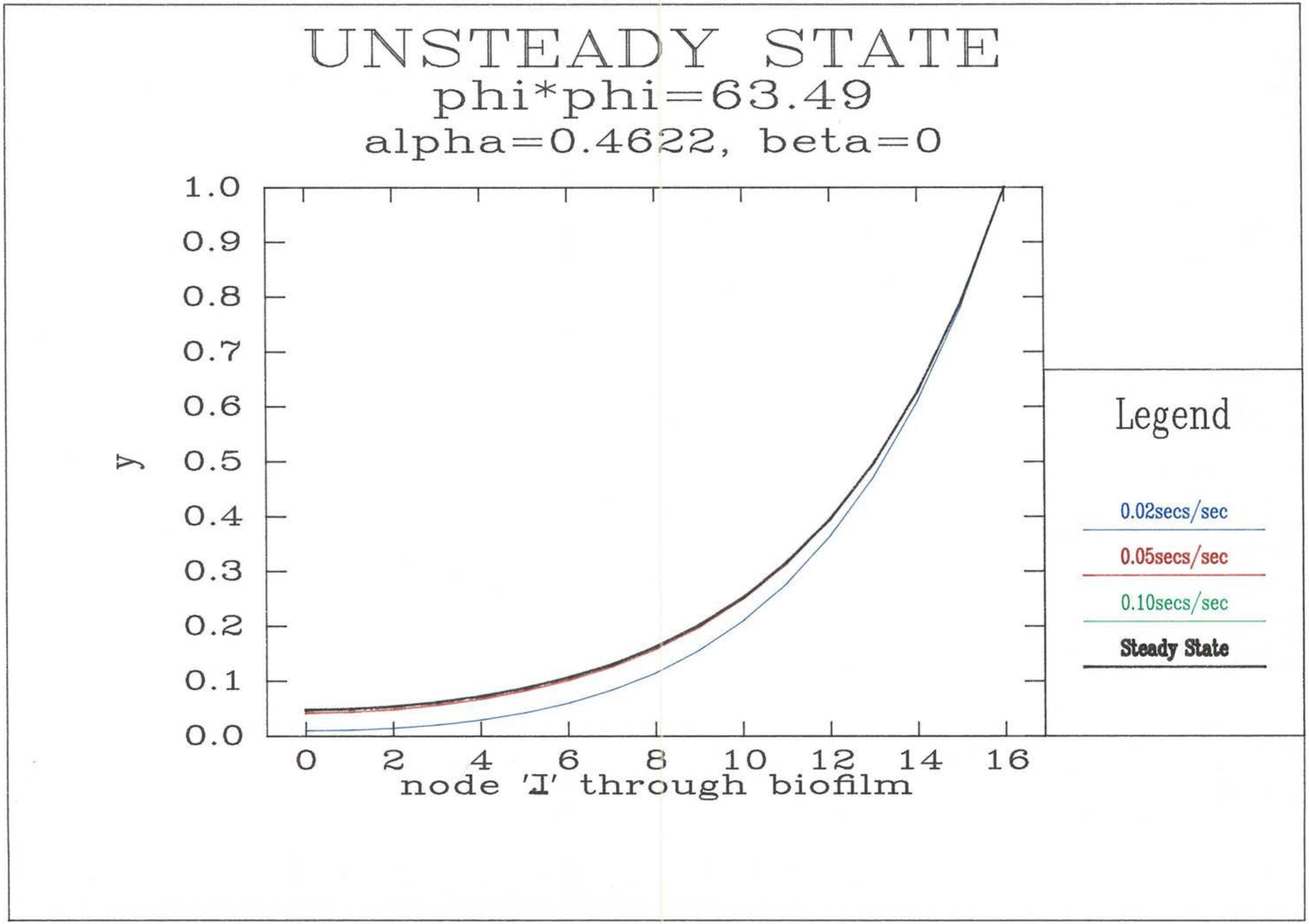

figure 2-31 Model verification :Lower bound

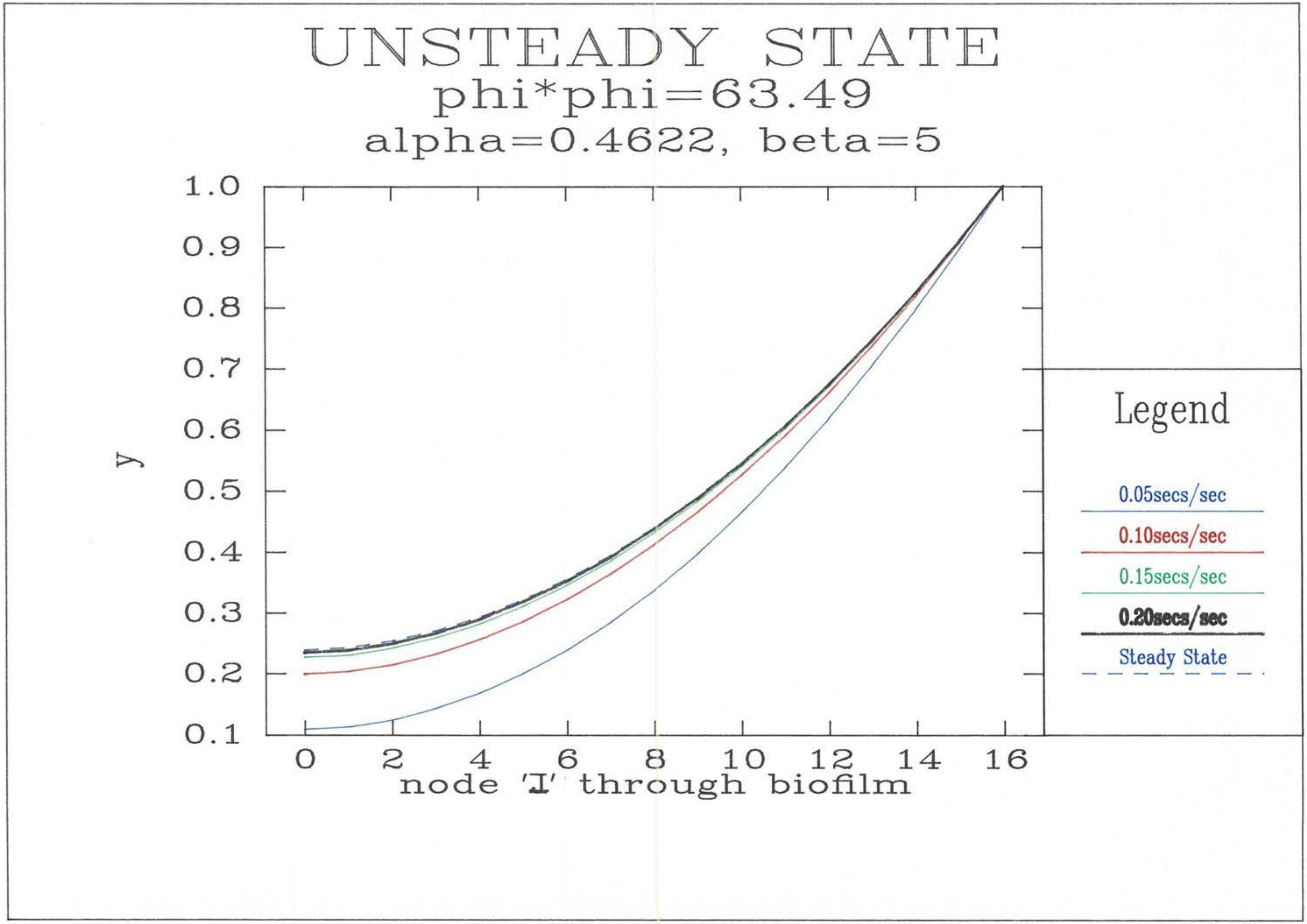

figure 2-32 Model verification

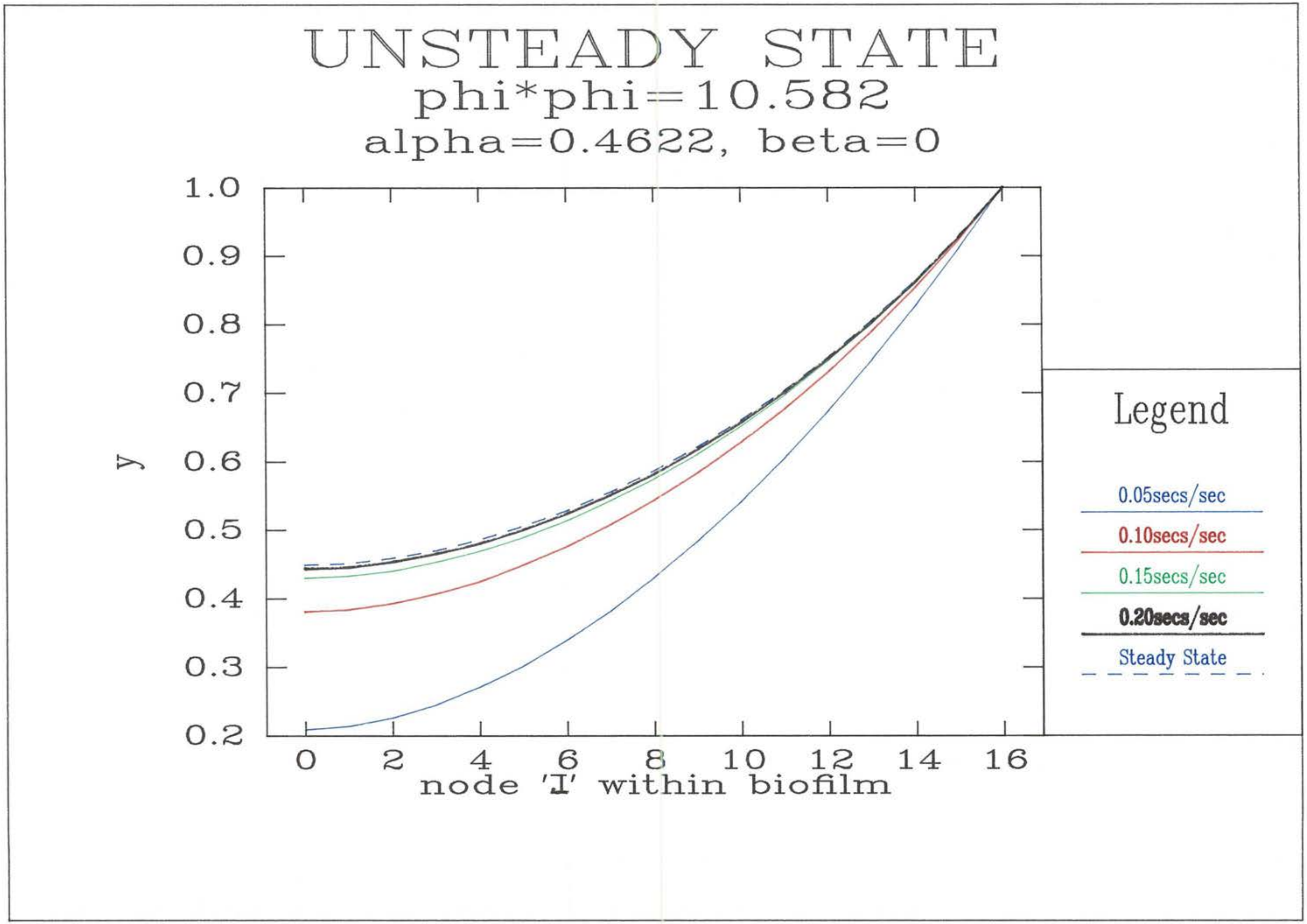

figure 2-33 Model verification : Upper bound

3.7 Applications and Conclusions

Attached growth biological systems have been increasingly considered for bioprocessing in manufacturing and wastewater treatment. The work presented in this thesis analyses the biofilm process characteristics and establishes the theoretical basis for the behaviour of such systems.

Surface supported biofilms incorporating reaction and diffusion concepts have been formulated and methods have been developed for numerical solution of both steady state and unsteady-state problems with zero order, first order and Michaelis-Menten kinetics.

Although, numerical solutions do exist in literature, the question of existence, uniqueness and monotonicity have not been rigorously examined.

The non-linear reaction coupled with diffusion results in a complex system of equations. Although these can be solved numerically using standard algorithms, this approach is however time consuming and expensive. It is , however desirable to simplify the procedure provided the resulting solutions lie within tolerence limits. An approximate analytical solution is presented for Steady-State problems. It would not be too diffucult to generalise the procedure to the Unsteady-State problem. A comparison of approximate and numerically exact solutions over realistic parameter ranges indicates a good agreement.

Unsteady-State problems have been solved to verify the Steady-State solutions and to determine the process time constants.

In addition to the above, the concept of partial substrate penetration has been examined. It has been shown that partial penetration is possible only for the intrinsic zero order case.

The constraint for partial penetration has been discovered to be
$\phi^2 > 2$ for a flat plate
$\phi^2 > 4$ for a cylinder and
$\phi^2 > 6$ for a sphere

The study of the reaction-diffusion equations may not only be applied to biofilm and floc reactors and the general areas mentioned in the introduction. It is also motivated by the study of the microbial processes in technology especially in the field of antibiotics, flocculation processes in fermentation, production of interferon - a protein that inhibits viral replication that may be used in the control of Aids. It may gather much knowledge in microbiology that may be used in the production of cell cultures that follow a 'social' behaviour e.g. mammalian cells which have to be anchored to a support media, etc.

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Appendix

Explicit finite difference program for the Unsteady-State problem

```pascal
program spherical_bioparticle(input,output);
const  pi=3.14159;
       secs=1814400;  {Later on put sec,radius,J in input}
       rc=0.4622;
       beta=0;
       phi2=63.4922287;
       J=64;

var Dt, time,telaps,tprint,dr,
    A0,V0,AJ,VJ,A0half,AJhalf:Real;
    i,K :integer;
    cnow,cnew,Vol,Ajplushalf,Ajminushalf  :Array[0..J] of Real;

BEGIN

{read in data}
{================}
Writeln;Writeln;
{Write('No. of space steps ');Readln(J);}
Write ('Time step (s) ');Readln(Dt);
Write ('Time between printouts (s) ');Readln(Tprint);


{initialisation}
{======================}
Dr:=(1-rc)/J;

writeln('Dt =',Dt:6,'    Tprint=',Tprint:6);


{ set initial conditions}
{========================================}
For i:=0 to J do
    begin
        cnow[i]:=0;

        Vol[i]:=0;
        cnow[J]:=1;
    end;

{complete initialisation}
{========================}
Telaps :=0;
TIME:=0;

{algebraic equations}
{===================}


{calculation loop starts}
{=============================}
While Time +Dt <=secs Do
    BEGIN
      TIME := TIME +Dt;
      Telaps:=Telaps+Dt;
```

```
{internal nodes}
{=====================}
For I:=1 to J-1 DO
    BEGIN

         Cnew[i]:=cnow[i]+Dt/Dr/Dr*(Cnow[i+1]-2*Cnow[i]+Cnow[i-1])+
            2*Dt/(rc+i*Dr)*(Cnow[i+1]-Cnow[i-1])/Dr/2--
              phi2*Dt*Cnow[i]/(1+beta*Cnow[i])

   End;

{inner boundary of spherical bioparticle}
{===========================================================================}
    A0:=4*pi*rc*rc;
    A0half:=4*pi*(rc+0.5*Dr)*(rc+0.5*Dr);
    V0:=4/3*pi*((rc+0.5*Dr)*(rc+0.5*Dr)*(rc+0.5*Dr)-rc*rc*rc);
    Cnew[0]:=(A0half/V0/Dr*(Cnow[1]-Cnow[0])-
    phi2*Cnow[0]/(1+beta*Cnow[0]))*Dt+Cnow[0];


{outer boundary of the spherical bioparticle}
{==============================================}

    Cnew[J]:=1;


{write final output}
{===================}
IF telaps >=Tprint then
    begin
      telaps:=0;
      write(Time:36:6,' secs');

writeln;writeln('Conc.   ');

For i:=0 to trunc(J/4) do


        writeln(i,'    ',Cnew[4*i]);

  end;

{update arrays}
{================}
For i:=0 to J do
begin

Cnow[i]:=Cnew[i];
end;
end;
end.
```