MULTIPLICITY OF SOLUTIONS OF A NONLINEAR BOUNDARY VALUE PROBLEM ARISING IN COMBUSTION THEORY.

by

Patrick Joseph Kelly

A thesis
presented to Massey University of Palmerston North
in fulfilment of the
thesis requirement for the degree of
Master of Science
in
Mathematics.

Palmerston North, New Zealand, 1991
Patrick Joseph Kelly.

Abstract

The problem of self-heating in spherical and spherically annular domains is addressed in this thesis. In particular, the Frank-Kamenetskii model is used to investigate the multiplicity of steady state solutions in these geometries. The differential equations describing this model depend crucially on a parameter, the "Frank-Kamenetskii" parameter; for spherical geometries it is known that: (a) a unique solution exists for sufficiently small parameter values, (b) there is a value of the parameter such that an infinite number of solutions exist. A convergent infinite series solution is developed for the problem in a spherical domain. The multiplicity of solutions when the problem is posed in spherically annular domains is then explored. It is shown, in contrast to (b), that multiple solutions exist for arbitrarily small parameter values and that no value of the parameter produces infinite multiplicity.

ACKNOWLEDGEMENTS.

To my supervisor Professor G.C. Wake....

Thanks Graeme for a wonderful year. Your guidance and patience were invaluable.

To Doctor Bruce van Brunt...

Thanks for your help in proof reading this thesis and for the discussions on series convergence.

To our computer consultant Richard Rayner, who was always available with cheerful efficient advice on matters computing. I have finished now so your weekends are your own and the equipment will work properly.

To my roomates, Daniel and Kim, who were always there with cheerful thoughts and helpful advice. Thanks for putting up with me. A special thanks to Daniel for putting up with my lousy chess playing, those stress relieving games were a godsend.

To Margaret and Graeme Murdoch with whom i boarded for four years while completing my studies. Thanks for everything.

DEDICATION.

I dedicate this thesis to those i love

My parents, Roxy and Brian,

My brothers and sisters,

Chris and Annette,

Jason,

Deborah,

Richard,

Rebecca.

My nephews

Daniel,

David.

Thanks for all the love and support you have given me over the years.

Yes i have finally finished and here it is...

CONTENTS

Chapter 1

Introduction

1.1 The theory of thermal ignition

The theory of thermal ignition addresses the question of what happens to a combustible substance when it is placed in a vessel, the walls of which are maintained at a prescribed temperature T_0 (usually constant). Under certain conditions, one observes a rapid rise in the temperature of the substance to a high value near the theoretical maximum temperature of explosion. Under other conditions, in contrast, only a small rise to a stationary level is observed. This small temperature rise remains constant until a large portion of the material has reacted. The conditions under which the transition occurs from one range to the other, for a small change in the external parameters, are termed the critical conditions of ignition.

When investigating the problem of thermal ignition, we consider the equation of heat conduction with continuously distributed sources of heat,

$$c\rho\frac{\partial T}{\partial t} = \nabla.(\lambda\nabla T)+q, \tag{1.1}$$

where T is the temperature, c the heat capacity, ρ the density of the substance, λ the thermal conductivity, and q the density of the sources of heat, that is, the quantity of heat evolved as a result of chemical reactions in a unit volume per unit time.

Solving this equation under the boundary conditions involving a given temperature T_0 at the surface of the wall gives the temperature distribution in the vessel as a function of time. The nature of this dependence changes sharply at the critical conditions, where there is an abrupt transition from a small constant temperature rise to a large and rapid rise. Owing to the formidable mathematical difficulties involved in integrating the partial differential equation (1.1) one normally resorts to one of two approximations which are well known in the nonstationary and stationary theories of thermal explosion.

In the stationary theory, the spatial temperature is not taken into consideration; instead, a mean temperature is introduced and assumed to be equal at all points of the reaction vessel. This assumption is admittedly not valid in the conduction range where the temperature is by no means localised at the wall. This approach, however, does allow the temperature dependence on time to be examined; consequently, one can also determine the induction period, that is, the time within which an explosion occurs. Although the nonstationary theory is an integral part of the theory of thermal ignition, we will not deal with it any further. Instead, we will examine the stationary theory of thermal ignition in symmetrical regions.

In the stationary theory, only the temperature distribution over the vessel is considered and its change in time is not taken into account. The conditions under which the stationary temperature distribution becomes highly sensitive or even discontinuous due to changes in the external parameters are termed the critical conditions of ignition.

The stationary form of the heat conduction equation (1.1) is

$$\nabla . (\lambda \nabla T) + q = 0 . \tag{1.2}$$

In most cases, however, the temperature dependence of the heat conductivity is neglected and the above equation reduces to

$$\lambda \nabla^2 T + q = 0 . \tag{1.3}$$

If the rate of reaction depends on the temperature in accordance with Arrhenius' Law then it can be represented by

$$Z = ze^{-E/RT} \tag{1.4}$$

where Z is the rate of reaction, T the absolute temperature, R the gas constant, and E and z are parameters characteristic of the given chemical reaction. The quantity E is termed the activation energy and represents the amount of energy required for a mole of the substance to react. The factor z depends on the pressure and composition of the substance, but not on the temperature in a first approximation. In this approximation one also assumes that the rate of reaction is independent of the loss of reactant. The density of the sources of heat can thus be expressed as

$$q = Qze^{-E/RT} ,$$

where Q is the thermal effect of the reaction per unit volume. Equations (1.3) can now be written in the form

$$\nabla^2 T + \frac{Q}{\lambda} ze^{-E/RT} = 0 . \tag{1.5}$$

We can rewrite this equation in terms of a dimensionless temperature and spatial coordinate by taking

$$u = RT/E \tag{1.6}$$

as the dimensionless temperature and

$$\underset{\sim}{y} = \frac{1}{\ell} \underset{\sim}{x}$$

as the dimensionless spatial coordinates, where, $\underset{\sim}{x}$ are the dimensional spatial coordinates and ℓ is a typical length such as the radius or half-width of the vessel such that, on the surface $\|\underset{\sim}{y}\|=1$, the boundary condition is

$$u=u_0=RT_o/E.$$

In this way we have only the one dimensionless parameter

$$\gamma=QzR\ell^2/\lambda E$$

in the differential equation and a second dimensionless parameter

$$u_0=RT_0/E$$

in the boundary condition. The equation now has the form

$$\nabla^2_{\underset{\sim}{y}}u+\gamma e^{-1/u}=0. \qquad (1.7)$$

If u is a solution to this equation and satisfies the boundary condition, then

$$u=f(\underset{\sim}{y},\gamma,u_0), \qquad (1.8)$$

giving the temperature u as a function of $\underset{\sim}{y}$ with the two parameters γ and u_0. This represents the most general solution of the problem of thermal ignition in a purely conductive heat exchange. The condition under which a stationary temperature distribution is parametrically sensitive, that is, when a rapid rise in temperature occurs for a small change in the parameter γ, should be of the form

$$\gamma=g(u_0), \qquad (1.9)$$

as neither the equation nor the boundary condition contain any parameters other than u_0 and γ. However, an empirical fact of great importance is that u_0 is small, i.e.

$$u_0 = RT_0/E << 1,$$

and so it is reasonable to look for the limiting form of (1.9) corresponding to $u_0 \to 0$. Moreover, if we consider $u_0 << 1$, we not only obtain more tractable results, but also specific features proper to combustion stand out more distinctly [13]. In examining this limiting case, we must keep in mind that we are considering a stationary temperature distribution below the explosion limit where the temperature rises are small.

Let $\upsilon = T - T_0$ where it is assumed that $\upsilon << T_0$: this is equivalent to $u_0 << 1$, a fact that will be established later. Now

$$e^{-E/RT} = e^{-E/R\,(\upsilon + T_0)} = e^{-E/RT_0\,(1/(1+\frac{\upsilon}{T_0}))},$$

and since $\upsilon << T_0$, the quantity

$$\frac{1}{1+\frac{\upsilon}{T_0}},$$

can be estimated using a binomial series expansion and neglecting all terms of order $\left(\frac{\upsilon}{T_0}\right)^2$; thus,

$$e^{-E/RT} \approx e^{-E/RT_0\,(1-\frac{\upsilon}{T_0})} = e^{-E/RT_0}\,e^{E\upsilon/RT_0^2}. \quad (1.10)$$

Using the above approximation, equation (1.5) can be written

$$\nabla^2 \upsilon + \frac{Q}{\lambda z} e^{-E/RT_0} e^{E\upsilon/RT_0^2} = 0\,, \tag{1.11}$$

subject to the boundary condition $\upsilon=0$ at the wall of the vessel.

Let
$$\theta = E\upsilon / RT_0^2. \tag{1.12}$$

Transforming (1.11) into the dimensionless variables θ and $\underset{\sim}{y}$ we now have

$$\nabla_{\underset{\sim}{y}}^2 \theta + \frac{QE}{\lambda R T_0^2} z \ell^2 e^{-E/RT_0} e^{\theta} = 0\,, \tag{1.13}$$

and the boundary condition at the surface $\|\underset{\sim}{y}\|=1$ is $\theta = 0$. The differential equation and boundary condition now contain only the one dimensionless parameter

$$\delta = \frac{QE}{R\lambda T_0^2} z \ell^2 e^{-E/RT_0}\,, \tag{1.14}$$

which, in this approximation, characterises the properties of the substance and the vessel shape. The problem of thermal ignition can therefore be represented by the non-linear differential equation

$$\nabla_{\underset{\sim}{y}}^2 \theta + \delta e^{\theta} = 0 \tag{1.15}$$

and the boundary condition at the surface of the vessel $\theta=0$, $\|\underset{\sim}{y}\| = 1$. This approach was first developed by Frank-Kamenetskii [13] and the parameter δ is called the Frank-Kamenetskii parameter.

If θ is a solution to (1.15) representing a stationary distribution then

$$\theta = f(\underset{\sim}{y},\delta). \tag{1.16}$$

The critical condition of ignition depends solely on δ as neither the differential equation nor the boundary condition contain any parameters other than δ. Thus, there exists a

$$\delta = \text{constant} = \delta_{cr} \tag{1.17}$$

such that a stationary temperature distribution becomes impossible. If the conditions of any experiments give a value of δ less than the critical value δ_{cr} a stationary temperature distribution should establish itself; if not, an explosion or thermal runaway will occur (see figure 1.1).

The value of δ_{cr} depends crucially on the shape of the vessel, and the values are well known for simple geometric shapes. For a spherical vessel, δ_{cr}=3.3219; for an infinitely long cylindrical vessel, δ_{cr}=2.00; and for a vessel with two infinitely long parallel planar surfaces (the infinite slab), δ_{cr}=0.878. These values calculated from the theory of thermal ignition are in close agreement with the experimental values obtained from substances whose kinetics are known [8].

From the solution (1.16), we can see that the maximum temperature rise below the explosion limit is given by

$$\upsilon_{max} = (T - T_0)_{max} = \frac{RT_0^2}{E} f(\underset{\sim}{0}, \delta_{cr}), \tag{1.18}$$

where we have assumed that the vessel is symmetric, and consequently the hottest point is at $\underset{\sim}{y} = \underset{\sim}{0}$. Since $\upsilon \propto \frac{RT_0^2}{E}$, below the explosion limit $RT_0 << E$ and therefore $\upsilon << T_0$. Thus the assumption $\upsilon << T_0$ made in the derivation

Bifurcation Diagram.

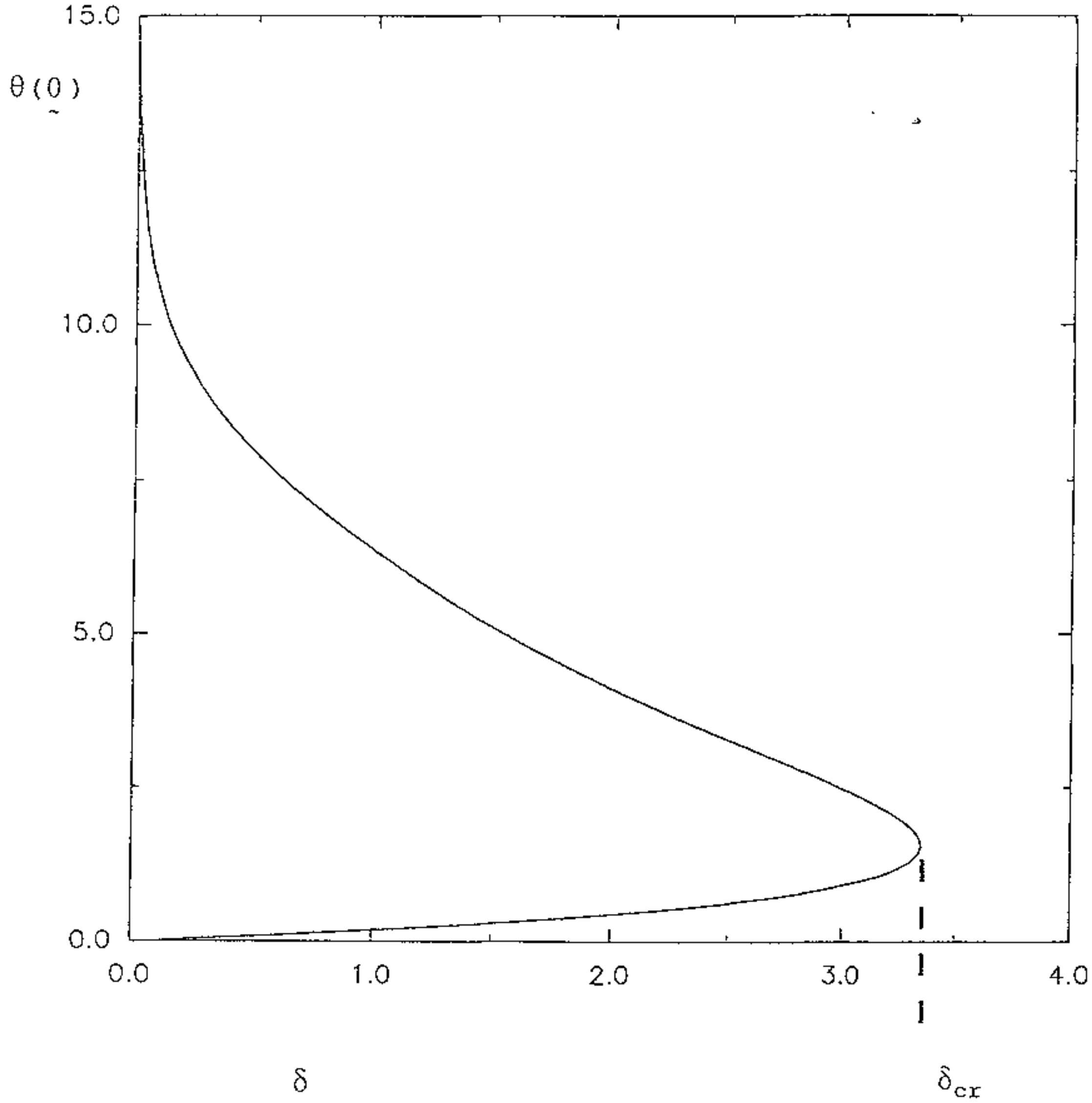


Figure 1.1
The critical value of the parameter δ.

of (1.10) is equivalent to $u_0 << 1$. If, however, RT_0 is not small compared to E then we do not get the characteristic picture of the combustion phenomena; instead, we are dealing with the theory of the nonisothermal course of a chemical reaction, a limiting form of which is considered in the theory of combustion and thermal ignition.

1.2 Formulating The Problem And Boundary Conditions.

Thus far we have considered only vessels whose walls were held at a fixed temperature equal to that of the surrounding medium. We now consider the case when heat released in the reaction warms the vessel walls and the surrounding medium, whose temperature typically changes if the heat exchange between the two mediums is not too rapid. Any steady-state theory of thermal explosion that includes this effect must begin with the complicated manner in which heat is exchanged between the reactive medium and the vessel walls. This problem is not addressed here but has been discussed by Borzykin and Marzhanov [9] and by Thomas [10]. The temperature distribution inside such a wall rapidly becomes quasistationary and the temperature on the inner surface of the wall is given by the Newtonian heat exchange equation [7],

$$\lambda \frac{\partial T}{\partial n} = -\alpha (T - T_0), \qquad (1.19)$$

where the heat flux on the left is calculated for the reacting substance next to the vessel surface ($\underset{\sim}{n}$ is a unit outward normal to the wall) and the heat flux on the right is calculated from the conditions of heat exchange between the wall and the surroundings. Here T_0 is the temperature of the surroundings far from the vessel surface, λ the heat conductivity, α the heat transfer coefficient depending on the nature of the heat transfer between the vessel and the surroundings and ℓ a measure of length. Equation (1.12) can be rearranged as

$$(T - T_0) = \frac{RT_0^2}{E}\theta.$$

Differentiating the above equation yields

$$\lambda\frac{\partial T}{\partial n} = \frac{1}{\ell}\frac{\lambda R T_0^2}{E}\frac{\partial \theta}{\partial n},$$

and substituting this into (1.19) gives

$$\frac{1}{\ell}\frac{\lambda R T_0^2}{E}\frac{\partial \theta}{\partial n} = -\alpha\frac{RT_0^2}{E}\theta,$$

which in turn yields

$$\frac{\partial \theta}{\partial n} + \frac{\alpha\ell}{\lambda}\theta = 0.$$

The Biot number is defined as

$$Bi = \frac{\alpha\ell}{\lambda},$$

giving the so called arbitrary Biot number condition on the boundary

$$\frac{\partial \theta}{\partial n} + Bi\theta = 0. \tag{1.20}$$

When $Bi \to \infty$ equation (1.20) becomes the Frank-Kamenetskii boundary condition $\theta=0$. When $Bi \to 0$ there is no heat exchange and an adiabatic thermal explosion occurs. Our problem can thus be stated

$$\nabla^2_{\underset{\sim}{y}}\theta + \delta e^{\theta} = 0 \qquad \text{in region,}$$

$$\frac{\partial\theta}{\partial n} + Bi\,\theta = 0 \qquad \text{on boundary.} \tag{1.21}$$

<u>The sphere.</u>

In the next chapter we consider a sphere of reactive material with radius R. Neglecting reactant consumption and using the Frank-Kamenetskii truncation along with the dimensionless variables θ and r, the dimensionless form of the radius, the governing system of equations is (1.21) where

$$\delta = \frac{QE}{R\lambda T_0^2} z\ell^2 e^{-E/RT_0}$$

is the Frank-Kamenetskii parameter. The symmetry of the reactive medium implies that there is no heat flux at the centre of the sphere therefore we have the condition

$$\left.\frac{d\theta}{dr}\right|_{r=0} = 0$$

It is known [2], that the non-linear heat conduction equation in a spherical region with sources depending on the temperature, admits only spherically symmetric solutions (provided the boundary conditions are also spherically symmetric). Thus for spherical geometries, system (1.21) is equivalent to

$$\frac{d^2\theta}{dr^2}+\frac{2}{r}\frac{d\theta}{dr}+\delta e^{\theta}=0, \quad 0<r\leq 1,$$

$$\frac{d\theta}{dr}(1)+Bi\theta(1)=0, \qquad (1.22)$$

$$\frac{d\theta}{dr}(0)=0,$$

This is the Frank-Kamenetskii model for steady state thermal regimes in a spherical region, and it is known [1], to have a gross multiplicity of steady state solutions for an arbitrary Biot number. The analytic condition for infinite multiplicity is $\delta_{\infty}=2e^{\frac{-2}{Bi}}$. In chapter two we find an infinite series solution to the system (1.22). We then generalise some results found in [1] to spheres in n dimensions. Finally, we apply the infinite series solution to n-dimensional spheres.

The spherical annulus.

In chapter 3 we consider spherically annular geometries. The problem consists of a sphere of inert material completely enclosed by a spherical annulus of reactive material. We define this problem by considering the inert core to have radius α' and the outer radius of the reactive sphere to be R. Neglecting reactant consumption, using the Frank-Kamenetskii truncation, and by choosing the dimensionless variables θ and r, the governing system of equations is

$$\frac{d^2\theta}{dr^2}+\frac{2}{r}\frac{d\theta}{dr}+\delta e^{\theta}=0, \quad \alpha<r\leq 1,$$

$$\frac{d\theta}{dr}(1) + Bi\theta(1) = 0,$$

where $\alpha = \alpha'/R$ and

$$\delta = \frac{QE}{R\lambda T_0^2} z\ell^2 e^{-E/RT_0}$$

is the Frank-Kamenetskii parameter.

In spherically annular geometries, heat transfer occurs at the inner surface. Dust explosions with laser optics give the linear boundary condition

$$\frac{d\theta}{dr}(\alpha) = A < 0,$$

where A is the heat flux at the inner surface of the reactive medium. Using phase plane analysis we investigate the multiplicity of steady state solutions. In spherical geometries it is known that:

(1) for δ small enough there is only one steady state solution;

(2) when $\delta = \delta_\infty = 2e^{\frac{-2}{Bi}}$ there is an infinite multiplicity of steady state solutions.

We show in chapters three and four the above results are not valid for spherically annular geometries . Specifically, we find, that for small values of δ there are two steady state solutions, and, although arbitrarily large multiplicity is obtainable given suitable values for α and A, we do not get infinite multiplicity.

Chapter 2

An Infinite Series Solution

2.1 A Solution to the Frank-Kamenetskii Equations with Infinite Biot Number.

In chapter one we formulated the problem in which a spherical object of reactive material undergoes an exothermic chemical reaction with the resultant heat production causing the temperature of the object to rise. The governing system of differential equations is

$$\frac{d^2\theta}{dr^2}+\frac{2}{r}\frac{d\theta}{dr}+\delta e^{\theta}=0, \quad 0<r\leq 1$$

$$\frac{d\theta}{dr}(1)+Bi.\theta(1)=0, \qquad (2.0)$$

$$\frac{d\theta}{dr}(0)=0.$$

Following Wake *et al.* [1] we introduce the following transformations similar to those employed by Chandrasekhar in the study of stellar structure [5]:

$$p=\delta r^2 e^{\theta},$$

$$q=r\frac{d\theta}{dr}+2,$$

$$r=e^{-s}, 0\leq r\leq 1. \qquad (2.1)$$

Using these transformations, system (2.0) reduces to the autonomous first order equations

$$\frac{dq}{ds} = p + q - 2, \tag{2.2}$$

$$\frac{dp}{ds} = -pq.$$

The phase plane corresponding to these was examined in [1]. We use a similar analysis to examine multiplicity of steady states in n-dimensional spheres.

The boundary conditions in (2.0) transform under (2.1) to

$$q(0) - 2 + Bi\, \ln\frac{p(0)}{\delta} = 0, \tag{2.3}$$

and

$$q \to 2 \quad \text{as} \quad s \to \infty. \tag{2.4}$$

In terms of the new variables p and q, the Frank-Kamenetskii model is (2.2) together with the boundary conditions (2.3) and (2.4). We consider a solution for p and q of the form

$$p = \sum_{n=1}^{\infty} a_n e^{-2ns}, \tag{2.5}$$

$$q = 2 + \sum_{n=1}^{\infty} b_n e^{-2ns}.$$

This, it is noted, is equivalent to a power series in r. We proceed under the assumptions that the above Dirichlet series can be differentiated term by term and can be multiplied together to give a convergent series. As is shown later these are valid assumptions. Substituting (2.5) into (2.2) yields

$$a_n = -b_n(1+2n) \qquad n \geq 1, \tag{2.6}$$

$$a_n = \frac{1}{2(n-1)} \sum_{k=1}^{n-1} a_{n-k} b_k \qquad n \geq 2, \tag{2.7}$$

and using (2.6), (2.7) can be written as a recursive relation for a_n, viz.

$$a_n = \frac{1}{2(n-1)} \sum_{k=1}^{n-1} \frac{-a_{n-k} a_k}{1+2k} \qquad n \geq 2. \tag{2.8}$$

Letting a_1 be our undetermined constant, we find

$$p = \sum_{n=1}^{\infty} \alpha_n a_1^n e^{-2ns}, \tag{2.9}$$

$$q = 2 + \sum_{n=1}^{\infty} \beta_n a_1^n e^{-2ns} \tag{2.10}$$

where

$$\alpha_n = -\beta_n(1+2n) \qquad n \geq 1, \tag{2.11}$$

$$\alpha_n = \frac{1}{2(n-1)} \sum_{k=1}^{n-1} \frac{-\alpha_{n-k} \alpha_k}{1+2k}, \quad \alpha_1 = 1, \quad n \geq 2 \tag{2.12}$$

Appendix A contains values for α_n and β_n calculated using equations (2.11) and (2.12).

When considering the convergence of the series solutions for p and q it is obvious that, if $\sum_{n=1}^{\infty} \alpha_n$ converges then the series (2.5) converge for sufficiently small values of a_1.

Theorem 2.0

The series

$$\sum_{n=1}^{\infty}\alpha_n,$$

where $\alpha_1 = 1,$

$$\alpha_{n+1} = \frac{1}{2n}\sum_{k=1}^{n}\frac{-\alpha_{n-k+1}\alpha_k}{1+2k},$$

is absolutely convergent.

Proof

Let P_n be the following proposition:

$$P_n : \left|\alpha_m\right| \le \frac{1}{2^{m-1}} \quad 1 \le m \le n.$$

Clearly P_1 is true. Suppose P_n is true. Now

$$\left|\alpha_{n+1}\right| \le \frac{1}{2n}\sum_{k=1}^{n}\frac{\left|-\alpha_{n-k+1}\right|\left|\alpha_k\right|}{1+2k},$$

and since P_n is true,

$$\left|\alpha_{n+1}\right| \le \frac{1}{2n}\sum_{k=1}^{n}\frac{1/2^{n-1}}{1+2k} < \frac{1}{2^n n}\sum_{k=1}^{n}\frac{1}{1+2k}$$

$$< \frac{1}{2^n n}\,\frac{n}{3} < \frac{1}{2^n}.$$

Therefore by the principle of mathematical induction P_n is true for all $n \in Z^+$. The geometric series $\sum_{n=1}^{\infty} \frac{1}{2^n}$ converges; thus (the comparison test implies) $\sum_{n=1}^{\infty} |\alpha_n|$ converges and the theorem follows. □

Thus justifying the assumptions made earlier.

Consider the case when the Biot number is infinite, i.e. the reactive medium is a perfect conductor. Here we have the Frank-Kamenetskii boundary conditions with $\theta=0$ at $r=1$ $(s=0)$. From (2.1) and $\theta=0$ when $s=0$ we get

$$p(0) = \delta,$$

which, using equation (2.9), gives

$$\delta = \sum_{n=1}^{\infty} \alpha_n a_1^n. \tag{2.13}$$

Equations (2.1) and (2.9) imply that

$$p = \sum_{n=1}^{\infty} \alpha_n a_1^n e^{-2ns} = \delta e^{-2s} e^{\theta}.$$

Dividing by e^{-2s} and evaluating the limit as $s \to \infty$ yields

$$a_1 = \delta e^{\theta_0}, \tag{2.14}$$

where θ_0 denotes $\lim_{s\to\infty} \theta(s)$. Substituting (2.14) into (2.13), dividing by δe^{θ_0} gives

$$\sum_{n=1}^{\infty} \alpha_{n+1} (\delta e^{\theta_0})^n = e^{-\theta_0} - 1 \quad (\alpha_1 = 1). \tag{2.15}$$

Before we can proceed any further with (2.15) we must address reversion of a power series. Given a convergent power series

$$y = \sum_{n=1}^{\infty} c_n x^n,$$

where $c_1 \neq 0$ there exist coefficients $\bar{c}_n$ such that, for y sufficiently small, the power series

$$x = \sum_{n=1}^{\infty} \bar{c}_n y^n$$

converges. The $\bar{c}_n$ are functions of $c_1, c_2, \ldots c_n$ and the new series is called the "reverted" series. The series is unique and it represents the inverse of the function defined by the original power series. The $\bar{c}_n$ can be calculated by substituting the original series into the reverted series and comparing coefficients. While it is theoretically possible to obtain any number of these reverted coefficients, it is numerically difficult to do so in our case because the coefficients of the original series become small quickly. Given the finite precision of the computer and subsequent introduced rounding errors our calculated reverted coefficients started to "blow up" after a small number of coefficients (around 50) were calculated.

Now $\alpha_2 = {}^{-1}\!/_{6} \neq 0$, and, assuming series (2.15) is convergent, it can be reverted, i.e.

$$\delta e^{\theta_0} = \sum_{n=1}^{\infty} \bar{\alpha}_{n+1} (e^{\theta_0} - 1)^n. \tag{2.16}$$

2.2 A solution to the Frank-Kamenetskii equations with arbitrary Biot number.

In the previous section we considered the special case when the Biot number was infinite we now turn our attention to the more general problem where Bi can be any positive number. We no longer have the Frank-Kamenetskii boundary conditions and so are reliant on the general boundary condition (2.3). The derivation of (2.14), it is noted is independent of the Biot number and therefore it is valid for any Bi as is (2.9) and (2.10). Equations (2.9) and (2.10) give

$$p(0) = \sum_{n=1}^{\infty} \alpha_n a_1^n,$$

$$q(0) = 2 + \sum_{n=1}^{\infty} \beta_n a_1^n,$$

and using (2.14) this yields

$$p(0) = \sum_{n=1}^{\infty} \alpha_n (\delta e^{\theta_0})^n \quad ,$$

$$q(0) = 2 + \sum_{n=1}^{\infty} \beta_n (\delta e^{\theta_0})^n .$$

Substituting the above expression equation into (2.3) gives

$$\sum_{n=1}^{\infty} \beta_n (\delta e^{\theta_0})^n + Bi \ln \sum_{n=1}^{\infty} \alpha_n \delta^{n-1} e^{n\theta_0} = 0 ,$$

which is equivalent to

$$\sum_{n=1}^{\infty} \alpha_n \delta^{n-1} e^{n\theta_0} = e^{-1/Bi \sum_{n=1}^{\infty} \beta_n (\delta e^{\theta_0})^n} .$$

The above expression implies

$$e^{\theta_0}\left(1+\sum_{n=1}^{\infty}\alpha_{n+1}(\delta e^{\theta_0})^n\right)=e^{-1/Bi\sum_{n=1}^{\infty}\beta_n(\delta e^{\theta_0})^n}\quad(\alpha_1=1),$$

and

$$e^{1/Bi\sum_{n=1}^{\infty}\beta_n(\delta e^{\theta_0})^n}\left(1+\sum_{n=1}^{\infty}\alpha_{n+1}(\delta e^{\theta_0})^n\right)=e^{-\theta_0}. \quad (2.17)$$

The exponential factor in the left hand side of (2.17) is an infinite series in δe^{θ_0}, and the left-hand side of (2.17) can be expanded as a power series,

$$1+\sum_{n=1}^{\infty}\Gamma_n(Bi)(\delta e^{\theta_0})^n;$$

thus,

$$\sum_{n=1}^{\infty}\Gamma_n(Bi)(\delta e^{\theta_0})^n=e^{-\theta_0}-1, \quad (2.18)$$

which, upon inverting gives a "formal" solution to (1.22) with arbitrary Biot number,

$$e^{-\theta_0}\sum_{n=1}^{\infty}\bar{\Gamma}_n(e^{-\theta_0}-1)^n=\delta. \quad (2.19)$$

Solving

$$\left.\frac{d\delta}{d\theta_0}\right|_{\delta=\delta_{cr}}=0,$$

yields

$$\delta_{cr} = -e^{-2\theta_0} \sum_{n=1}^{\infty} n\overline{\Gamma}_{n+1} \left(e^{-\theta_0} - 1 \right)^{n-1}.$$

Depending on the value of Bi, between forty and sixty of the $\overline{\Gamma}_n$ were calculated before numerical rounding errors crept in and the $\overline{\Gamma}_n$ started to "blow up". Appendix A contains values for $\overline{\Gamma}_n$. By using the available $\overline{\Gamma}_n$ the following values of the critical parameter were calculated using (2.19), see table 1.

Table 1

δ_{cr}	Bi	θ_0
0.0011	.001	1.00
0.011	.01	1.00
0.108	.1	1.03
0.9010	1	1.25
2.7390	10	1.59
3.2564	100	1.61
3.3153	1000	1.61

Critical values of the parameter δ for various Biot numbers, calculated using the infinite series solution.

2.3 A Look at Exothermic Chemical Reactions in n-Spherical Domains.

Certain results obtained by Wake *et al.* in their study of exothermic chemical reactions in spherical geometries are easily adapted to spherical geometries of n dimensions. We found in chapter one the governing system of differential equations is

$$\nabla^2_{\underset{\sim}{y}} \theta + \delta e^{\theta} = 0 \quad \text{in region,}$$

$$\frac{\partial \theta}{\partial n} + Bi\theta = 0 \quad \text{on boundary.}$$

In n-spherical domains our system becomes

$$\frac{d^2\theta}{dr^2} + \frac{(n-1)}{r}\frac{d\theta}{dr} + \delta e^{\theta} = 0, \tag{2.20}$$

$$\frac{d\theta}{dr}(1) + Bi.\theta(1) = 0,$$

$$\frac{d\theta}{dr}(0) = 0.$$

Following a line of argument similar to that of Wake *et al.* we show that the system (2.20) has a gross multiplicity for 2<n<10 and arbitrary Biot number with the analytic condition for infinite multiplicity given as

$$\delta_{\infty} = 2(n-2)e^{-2/Bi}.$$

We also show for n≥10

$$\delta_{cr} = 2(n-2)e^{\frac{-2}{Bi}},$$

where δ_{cr} is the critical value of the parameter: a value of the parameter lower than δ_{cr} implies the existence of steady states; whereas, a value higher than δ_{cr} implies no such steady states exist and thermal ignition occurs.

Using transformations (2.1), system (2.20) becomes a pair of autonomous first order equations, viz.

$$\frac{dq}{ds} = (n-2)(q-2)+p, \tag{2.21}$$

$$\frac{dp}{ds} = -pq,$$

The boundary conditions are

$$q(0)-2+Bi\ln\frac{p(0)}{\delta} = 0, \tag{2.22}$$

$$q \to 2 \quad \text{as} \quad s \to \infty. \tag{2.23}$$

System (2.21) can be examined in the p-q phase plane. There are two singular points: S1= (p=2(n-2), q=0) which has eigenvalues

$$\lambda_{\pm} = \frac{n-2 \pm \sqrt{(n-2)(n-10)}}{2},$$

and S2=(p=0,q=2) which has eigenvalues

$$\lambda_{-} = -2, \qquad \lambda_{+} = n-2.$$

It is evident that S1 has complex eigenvalues for 2<n<10; thus, S1 corresponds to a spiral focus (see Figure (2.1).

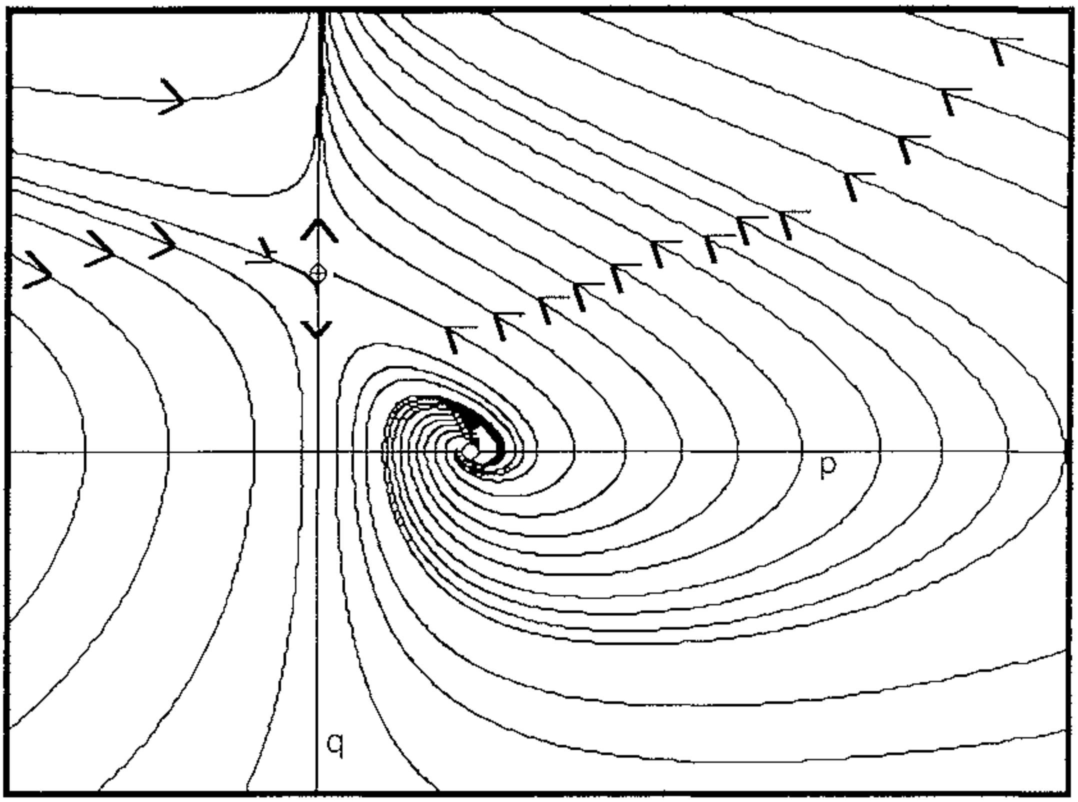


Figure (2.1)
Phase plane for 2<n<10.

The transformations made (equations 2.1) indicate that we need consider only that part of the phase plane in which $p \geq 0$. There are two separatrices in the phase plane: the ordinate axis $p=0$, and a spiral that winds anti-clockwise out of the focus up to the saddle point. The other trajectories also wind anti-clockwise out of the focus. It is not hard to show that the only curve satisfying the boundary conditions is the spiral separatrix. As demonstrated in [1] the number of steady state solutions corresponds to the number of times the initial condition locus (equation 2.22) intersects the spiral separatrix. The outer boundary condition (2.22), indicates that it is possible for this initial condition locus to intersect the spiral separatrix any number of times. Because of the focal nature of the singularity S1 there is an infinite number of intersections when the initial condition locus passes through this point. The value of δ for which the initial condition locus intersects this point is $\delta_\infty(Bi)$. Substituting $q(0)=0$, $p(0)=2(n-2)$ into (2.22) yields the following relation:

$$\delta_\infty = 2\,(n-2)\,e^{-2/Bi}.$$

Criticality can be seen as a tangency condition in the phase plane. Specifically, the critical values of the parameter δ are those for which the initial condition locus is tangent to the separatrix.

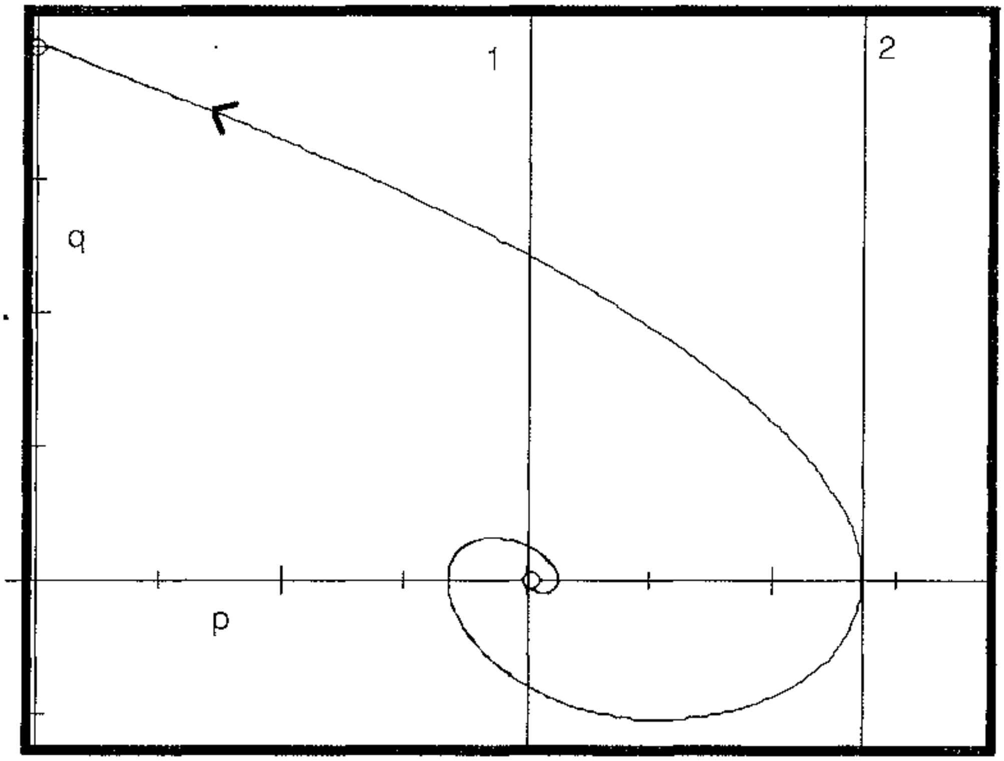


Figure 2.2
The initial condition locus when: 1, $\delta=\delta_\infty$, 2, $\delta=\delta_{cr}$.

If $n\geq10$ the eigenvalues associated with S1 are positive real numbers and the singularity S1 is a nodal point (cf. Figure 2.3). As before, the number of steady states corresponds to the number of times the initial condition locus crosses the separatrix, it is clear that it can intersect the separatrix at most once. It follows that the value of δ which causes the initial condition locus to pass through the focus is δ_{cr}; therefore,

$$\delta_{cr} = 2\,(n-2)\,e^{\frac{-2}{Bi}} \qquad n \geq 10.$$

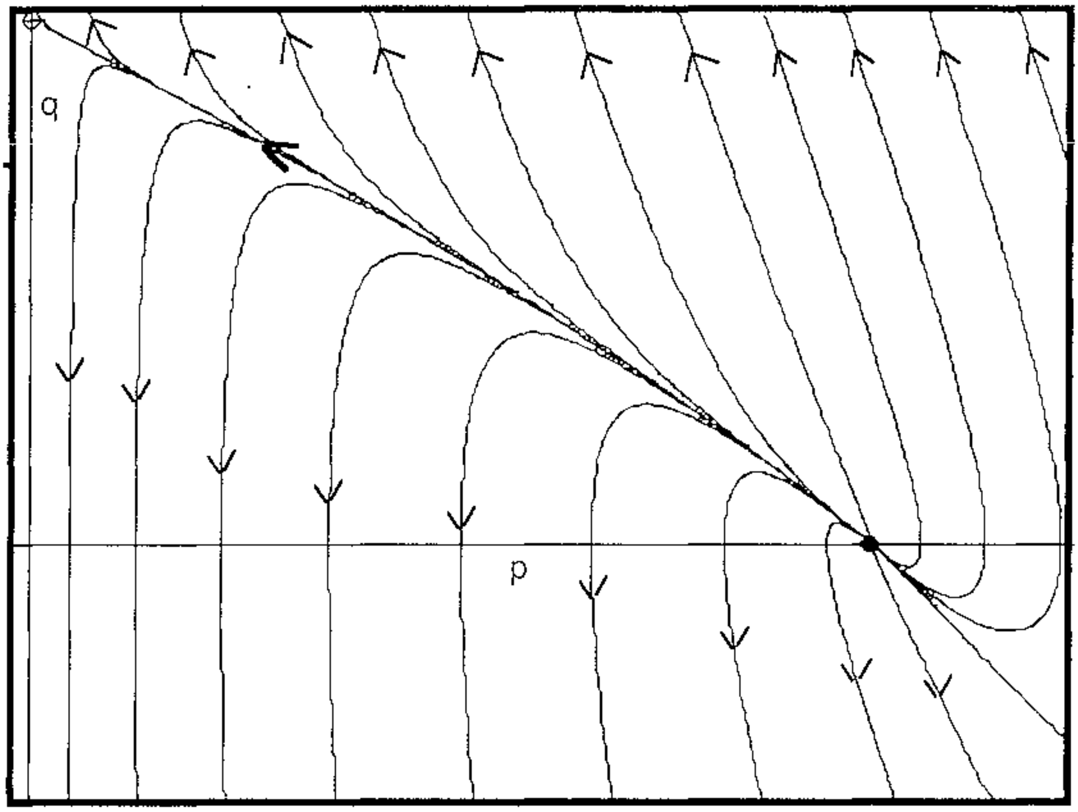


Figure (2.3)
Phase plane for $n \geq 10$.

2.4 An Infinite Series Solution to the Frank-Kamenetskii Equations with Arbitrary Biot Number in n Dimensions.

Following the procedure used for $n=3$, series solutions for p and q can be readily derived, viz.

$$p = \sum_{k=1}^{\infty} \alpha_k a_1^k e^{-2ks},$$

$$q = \sum_{k=1}^{\infty} \beta_k a_1^k e^{-2ks},$$

where

$$\alpha_k = -\beta_k\,(n-2+2k)\ , \qquad k \geq 1$$

$$\alpha_k = \frac{1}{2\,(k-1)} \sum_{j=1}^{k-1} \frac{-\alpha_j \alpha_{k-j}}{(n-2+2j)}\ , \qquad k \geq 2$$

and n is the dimension. Adapting the methods in section (2.1) the solution

$$e^{-\theta_0} \sum_{i=1}^{\infty} \overline{\Gamma}_i\,(e^{-\theta_0}-1)^i = \delta$$

can be derived for the n-dimensional case.

Chapter 3

The Spherical Annulus

In chapter one we formulated the problem in which a spherical annulus of reactive material undergoes an exothermic chemical reaction with the resultant heat production causing the temperature of the reactive medium to rise. After choosing the standard dimensionless form for the parameters, ignoring reactant consumption and applying the Frank-Kamenetskii truncation the governing system of equations is

$$\frac{d^2\theta}{dr^2}+\frac{2}{r}\frac{d\theta}{dr}+\delta e^{\theta},\quad \alpha<r\leq 1,$$

$$\frac{d\theta}{dr}(1)+Bi.\theta(1)=0, \tag{3.1}$$

$$\frac{d\theta}{dr}(\alpha)=A<0,$$

where δ is the Frank-Kamenetskii parameter, A represents the heat flux at the inner surface and α the dimensionless form of the inner radius.

Using the same transformations as in the spherical case, i.e.

$$p=\delta r^2 e^{\theta},$$

$$q=r\frac{d\theta}{dr}+2,$$

$$r=e^{-s},\ 0\leq r\leq 1,$$

equations 3.1 reduce to the autonomous system

$$\frac{dq}{ds}=p+q-2\,,$$
$$\frac{dp}{ds}=-pq\,, \qquad 0\le s\le -\ln(\alpha)\,,$$

along with the boundary conditions

$$q(s=-\ln(\alpha))=\alpha A+2\,,$$

$$q(0)-2+Bi\ln\left(\frac{p(0)}{\delta}\right)=0\,.$$

We examine this system in the p-q phase plane, noting from the transformation that we need only consider p≥0. The phase plane is the same as that given in chapter two (cf. figure 2.1) except the boundary condition is below the singularity (0,2). The question that now arises is, given an initial condition locus, which curves in the phase plane satisfy the boundary condition? We first look at this problem for the case A=0. To investigate this problem we introduce a new function. For a given initial condition locus (this effectively means knowing values for the parameters δ and Bi) we define a new function $T(\delta,Bi,q_0)=T_{\delta,Bi}(q_0)$ as follows: given (p_0,q_0) on the initial condition locus, the function $T_{\delta,Bi}(q_0)$ is the change in the independent variable s along the trajectory that passes through the point (p_0,q_0) in the direction of increasing s, from the point (p_0,q_0) to the boundary condition q=2. We note that the variable s can take any positive value and in this sense acts in a "time-like" manner. It is helpful to think of s as "time", and in this thesis we exploit this and refer to such concepts as the time taken to travel from point B to point C (where C and B are on the same trajectory). We think of $T_{\delta,Bi}(q_0)$ as representing the "time" taken to traverse the trajectory from (p_0,q_0) to the boundary condition q=2, and examine some properties of it. (see figures in appendix C).

Property 1

We note first that any trajectory emanating from the initial condition locus crosses the boundary condition only once; thus, $T_{\delta,Bi}(q_0)$ is single-valued.

Property 2

If $q_0 = 2$, then $T_{\delta,Bi}(q_0) = 0$.

This is a somewhat obvious result, the initial point is on the boundary condition .

Property 3.

If $q_0 < 2$ then $T_{\delta,Bi}(q_0) > 0$.

Given we traverse the trajectories only in the direction of increasing s the above property follows easily .

A not so intuitive result is

Property 4.

$$T_{\delta,Bi}(q_0) \to 0 \quad \text{as}\, q_0 \to -\infty.$$

Although we had no luck in providing a proof of this result, it is reinforced by numerical evidence see table 3.1 .

Property 5.

If the point $(p_0, q_0) \neq (2,0)$ is on the spiral separatrix then $T_{\delta,Bi}(q_0) \to \infty$.

If A=0 the boundary condition is q=2, and that part of the phase plane which contains the solution curves also contains the singularity (0,2), and the whole of the spiral separatrix. As was seen in chapter two the spiral separatrix is the solution curve satisfying the boundary condition $q \to 2$ as $s \to \infty$, and it is evident that the separatrix takes infinite time to reach the boundary condition from any starting point on the separatrix.

<u>Table 3.1</u>

Bi=∞ A = 0

δ / q_c	2	0	-2	-80	-1000	-100000	-1e8
.1	0	2.05	1.37	1.4e-1	1.9e-2	2.1e-3	2.7e-4
2	0	∞	1.12	1.1e-1	1.3e-2	1.9e-3	2.3e-4
4	0	1.01	8.7e-1	1e-1	1.3e-2	1.8e-3	2.3e-4

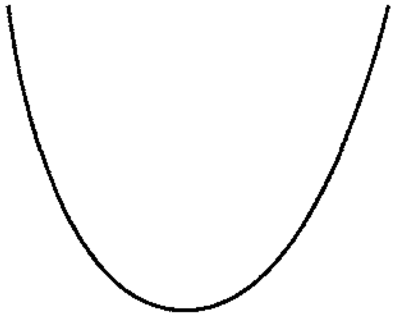
Values for $T_{\delta,Bi}(q_0)$.

Property five has an important implication on the structure of the graph for the function $T_{\delta,Bi}(q_0)$ as it indicates the possible presence of vertical asymptotes. In particular, the graph of $T_{\delta,Bi}(q_0)$ has a vertical asymptote whenever the initial condition locus intersects the separatrix. As seen in chapter two the initial condition locus can intersect the separatrix any number of times, in particular when $\delta = 2e^{\frac{2}{\pi^2}}$ there is an infinite number of intersections, which in turn indicates an infinite number of asymptotes in the graph of the function $T_{\delta,Bi}(q_0)$. Figure C3 shows a typical such graph. The nature of the spiral separatrix indicates that if a large number of asymptotes are present in the graph of $T_{\delta,Bi}(q_0)$, they cluster around the $T_{\delta,Bi}(q_0)$ axis. Specifically, if there is an infinite number of vertical asymptotes present in the $T_{\delta,Bi}(q_0)$ graph then between any asymptote and the origin there are an infinite number of vertical asymptotes. The boundary conditions indicate that a trajectory which takes a time of $-\ln(\alpha)$ to travel from the initial condition locus to the line $q=2$ is a solution curve. Therefore the solution curves are those parts of the trajectories, which emanate from $(\delta e^{\frac{2-q_0}{Bi}}, q_0)$ and end at $(p(-\ln(\alpha)), 2)$ where q_0 is a solution of $T_{\delta,Bi}(q_0) = -\ln(\alpha)$.

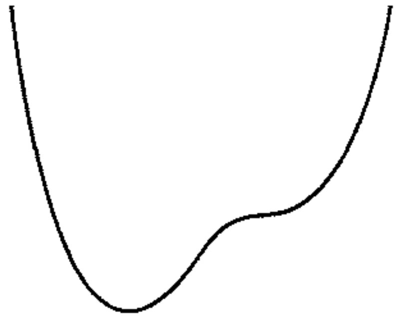
The number of steady state solutions is then given by

$$N_\alpha = \left|\left\{ q_0 \;\middle|\; -\ln(\alpha) = T_{\delta,Bi}(q_0) \right\}\right|.$$

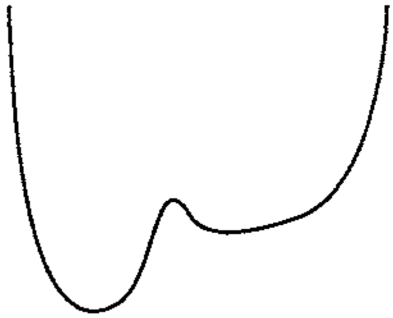
The number N_α, it is noted depends only the inner radius α; this is because we are considering the special case of no heat flux at the inner surface (A=0). To determine multiplicity of steady state solutions a careful examination of the function $T_{\delta,Bi}(q_0)$ is required. The first thing to note is that the value of the Biot number does not affect the qualitative structure of the $T_{\delta,Bi}(q_0)$ graph. Given δ sufficiently close to $2e^{\frac{-2}{Bi}}$ (the value for δ which causes the initial condition locus to pass through the focus), the graph of $T_{\delta,Bi}(q_0)$ contains a number of vertical asymptotes. Between consecutive pairs of these asymptotes is either a curve of type 1, type 2, or type 3 (see figure 3.1). The only place that curves of type 2 or type 3 occur is between the pair of asymptotes that straddle the $T_{\delta,Bi}(q_0)$ axis. Before the first asymptote there is a curve of type 4 or type 5 (see figure 3.1). Beyond the last asymptote there is a curve of type 5 (see figure 3.1). Actual graphs of the function $T_{\delta,Bi}(q_0)$ are contained in appendix C. If δ is sufficiently large the initial condition locus cannot intersect the separatrix; the corresponding $T_{\delta,Bi}(q_0)$ graph thus does not have asymptotes. In this situation the $T_{\delta,Bi}(q_0)$ graph has a maximum at q_0^1. The function is strictly increasing for $q<q_0^1$ and strictly decreasing $q_0^1<q<2$. See figure C7. The following theorems give some insight into the behaviour of the function $T_{\delta,Bi}(q_0)$:



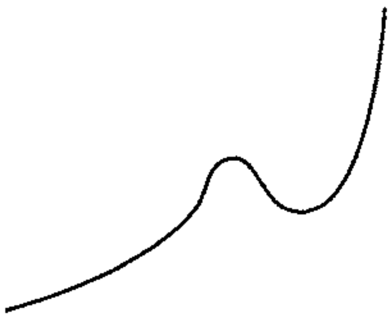
Type 1.



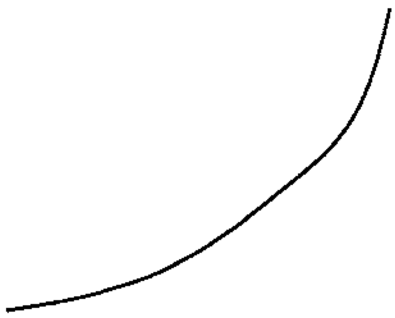
Type 2.



Type 3.



Type 4.



Type 5.

Figure 3.1.

A type 1 curve has, 1 minimum, no maximum and no inflection points; a type 2 curve has, 1 minimum, no maximum and 2 inflection point; a type 3 curve has, 2 minimum points, 1 maximum point and 2 points of inflection; a type 4 curve has, 1 minimum, 1 maximum and 2 inflection points; a type 5 curve has, no minimum, no maximum and no inflection points.

Theorem 3.1.

If $T_{\delta,Bi}(q_0)$ has exactly one local minimum between consecutive pairs of asymptotes, and has minima at q_0^1 and q_0^2 and $0 < q_0^1 < q_0^2$ then $T_{\delta,Bi}(q_0^2) < T_{\delta,Bi}(q_0^1)$

Proof.

The result is easily seen by examining the phase plane. Since q_0^1 and q_0^2 are the q coordinates of distinct minima the corresponding parts of the $T_{\delta,Bi}(q_0)$ graph are between a different set of asymptotes (with perhaps one common asymptote). In terms of the phase plane this means that the q values corresponding to the minima occur between different crossings of the initial condition locus with the separatrix. As $0 < q_0^1 < q_0^2$, the value q_0^1 occurs on the initial condition locus after the locus has crossed the separatrix at least once more after the occurrence of q_0^2. The point on the initial condition locus with q coordinate q_0^1 is inside at least another "loop" of the spiral separatrix compared to the point with q coordinate q_0^2. Given that to travel from this inner "loop" to the boundary condition we must cross the initial condition locus (at a point (p,q)), inside the "loop" corresponding to the minimum at q_0^2. We conclude from this that $T_{\delta,Bi}(q_0^1) > T_{\delta,Bi}(q) \geq T_{\delta,Bi}(q_0^2)$, and it follows that $T_{\delta,Bi}(q_0^2) < T_{\delta,Bi}(q_0^1)$. A similar argument shows that if $q_0^1 < q_0^2 < 0$ then $T_{\delta,Bi}(q_0^1) < T_{\delta,Bi}(q_0^2)$. □

The only time that more than one minimum occurs between consecutive pairs of asymptotes is when that pair straddles the $T_{\delta,Bi}(q_0)$ axis. In this case theorem 3.1 is easily adapted by choosing the smallest minimum between the asymptotes.

So we now have that the $T_{\delta,Bi}(q_0)$ graph (given a value of δ which causes the initial condition locus to intersect the separatrix) contains a number of vertical asymptotes. Contained between these asymptotes are curves of type 1 (or under some conditions curves of type 2 or type 3). Given a value of δ that causes the initial condition locus to intersect the separatrix a sufficient number of times we have shown in theorem 3.1 that the curves between the asymptotes, have local minima whose values are increasing as the q coordinate tends to 0. Therefore when we have an infinite number of vertical asymptotes, we have an infinite number of minima which are clustered around the q=0 axis and have values that are increasing as they approach the q=0 axis. A point to note here is that it takes the separatrix an infinite time to spiral out of the focal point, this coupled with the continuity of integral curves in the phase plane gives the following result: if $\delta = 2e^{\frac{-2}{Bi}}$ and a minimum occurs at q, then $T_{\delta,Bi}(q) \to \infty$ as $q \to 0$. We are now in a position to consider the multiplicity of the steady state solutions. Recall that the number of steady state solutions is

$$N_\alpha = \left|\left\{q_0 \;\middle|\; -\ln(\alpha) = T_{\delta,Bi}(q_0)\right\}\right|.$$

It follows from this that the number of steady states is limited only by the number of vertical asymptotes in the graph of $T_{\delta,Bi}(q_0)$. On the other hand we see that for δ sufficiently large, the initial condition locus does not intersect the separatrix, and, as will be discussed later, there exists a critical value of δ beyond which the system has no steady states. Given a value of δ sufficiently large so that the initial condition locus does not intersect the separatrix we see given appropriate values of α (the inner radius) it is possible to have 0,1 or 2 steady state solutions (see figure C7).

For a given δ and Bi, the corresponding $T_{\delta,Bi}(q_0)$ graph has k asymptotes, and if $1 \le k$ we see that, for appropriate values of α it is possible for N_α to be any integer value between, 2 and 2k if no curve of type 3 or occurs or 2 and 2k+2 if a curve of type 3 or occurs. We can have the initial condition locus intersecting the separatrix an arbitrarily large number of times (and even an infinite number of times) so we investigate the possibility of infinite multiplicity. In spherical domains we know infinite multiplicity exists: we will show that it does not exist for spherically annular domains.

We know that the number of steady states depends on the number of vertical asymptotes in the $T_{\delta,Bi}(q_0)$ graph and the presence of a type 3 curve. Let the initial condition locus cross the separatrix $k \ge 1$ times (k finite). We define $\bar{\alpha}$ as that value of α which $\max\limits_{0<\alpha<1} N_\alpha = N_{\bar{\alpha}}$ and examine the behaviour of $\bar{\alpha}$ as $k \to \infty$. As $k \to \infty$ the $T_{\delta,Bi}(q_0)$ graph has an infinite number of type 1 curves clustered around the q=0 axis. As seen earlier the minimum points of these type 1 curves tend to infinity as q approaches 0; therefore, $\bar{\alpha} \to 0$ as $k \to \infty$. This reverts the problem to the spherical case. Although it is possible to have arbitrarily large multiplicity, infinite multiplicity is not possible in the case of a spherical annulus. Based on numerical evidence, we conjecture that for a given Bi and inner radius α, $\max\limits_{\delta} N_\alpha$ occurs when $\delta = 2e^{\frac{-2}{Bi}}$. Tables B1-B6 in appendix B show values for N_α.

A Look At Criticality.

In the spherical case, criticality is equivalent to the initial condition locus being tangent to the spiral separatrix. The analogous condition for the spherical annulus is that the line $T_{\delta_{cr},Bi}=-\ln(\alpha)$ is tangent to the $T_{\delta_{cr},Bi}(q_0)$ graph (see figure 3.2)

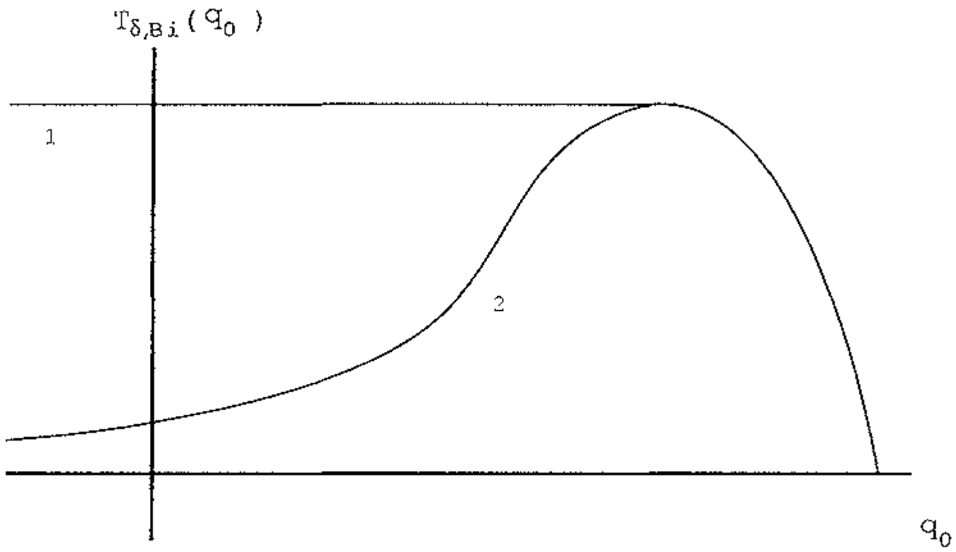


Figure 3.2

The line $T_{\delta_{cr},Bi}=-\ln(\alpha)$ (1) tangent to the $T_{\delta_{cr},Bi}(q_0)$ graph (2).

The following two theorems can be established for the case where there is no heat flux at the inner surface:

Theorem 3.2.

For A=0 and a given Biot number. $\delta_{cr}(\alpha)>\delta_{cr}(0)$ for all $0<\alpha<1$.

Proof.

Suppose $\delta_{cr}(\alpha)<\delta_{cr}(0)$ The initial condition locus

$$q(0)-2+Bi\ln\left(\frac{p(0)}{\delta_{cr}(0)}\right)=0,$$

is by the definition of $\delta_{cr}(0)$ tangent to the separatrix [1], and this implies that the $T_{\delta_{cr}(\alpha),Bi}(q_0)$ graph has at least one vertical asymptote. As seen earlier, this means that $N_\alpha \geq 2$ and this contradicts the assumption that $\delta_{cr}(\alpha) < \delta_{cr}(0)$ consequently

$$\delta_{cr}(\alpha) \geq \delta_{cr}(0).$$

Equality is easily seen not to hold, as criticality in the spherical case was when the initial condition locus was tangent to the separatrix. The result thus follows ❑

<u>Theorem 3.3</u>

Let A=0 and Bi be a given Biot number. If $0<\alpha_1<\alpha_2<1$ then $\delta_{cr}(\alpha_1)<\delta_{cr}(\alpha_2)$.

<u>Proof.</u>

Assume $\delta_{cr}(\alpha_1)>\delta_{cr}(\alpha_2)$, then $-\ln(\alpha_2)<-\ln(\alpha_1)$, and it follows from theorem 3.2 that the graph of $T_{\delta_{cr}(\alpha_1),Bi}(q_0)$ has no asymptotes and therefore is continuous. Now $\delta_{cr}(\alpha_1)$ is the critical value of the parameter for α_1 so that by definition, $N_{\alpha_1} = 1$. The continuity of $T_{\delta_{cr}(\alpha_1),Bi}$ and the above inequality, however, imply $N_{\alpha_2}=2$. This contradicts our assumption and hence

$$\delta_{cr}(\alpha_1) \geq \delta_{cr}(\alpha_1).$$

As $-\ln(\alpha_2) < -\ln(\alpha_1)$ equality can be seen not to hold and hence the result follows ❑

Numerical evidence given in chapter four suggests the above theorem holds for any value of A. We conjecture that $\delta_{cr}(A,\alpha)$ is monotonic increasing in α for any A<0.

We considered the case when there is no heat flux at the inner surface; we now turn our attention to the case when heat is flowing from the reactive medium into the inert core. The boundary condition for this case is

$$\frac{d\theta}{dr}(\alpha) = A < 0,$$

which transforms to

$$q = 2 + \alpha A \quad < 2 \cdot$$

Although the $T_{\delta,Bi}(q_0)$ function was useful for exploring multiplicity for the special case when A=0, we no longer take the approach of introducing a new function. Since the boundary condition locus is below the singularity it is possible for the trajectories emanating from the initial condition locus to cross the boundary condition more than once (see figure 3.3). These multiple crossings cause any function analogous to $T_{\delta,Bi}(q_0)$ to be multivalued. We not only have the problem of multiple crossings of the boundary condition, but we also have to contend with the fact that there exists solution curves which emanate from points on the initial condition locus above the boundary

A Look At Criticality.

An increase in the heat flow from the reactive medium to the inert core causes an increase in temperature at the centre. Therefore we expect on physical grounds that as (A<0) decreases, $\delta_{cr}(A,\alpha)$ decreases. We conjecture that $\delta_{cr}(A,\alpha)$ is monotonic decreasing in A. In chapter four, numerical evidence supports this conjecture.

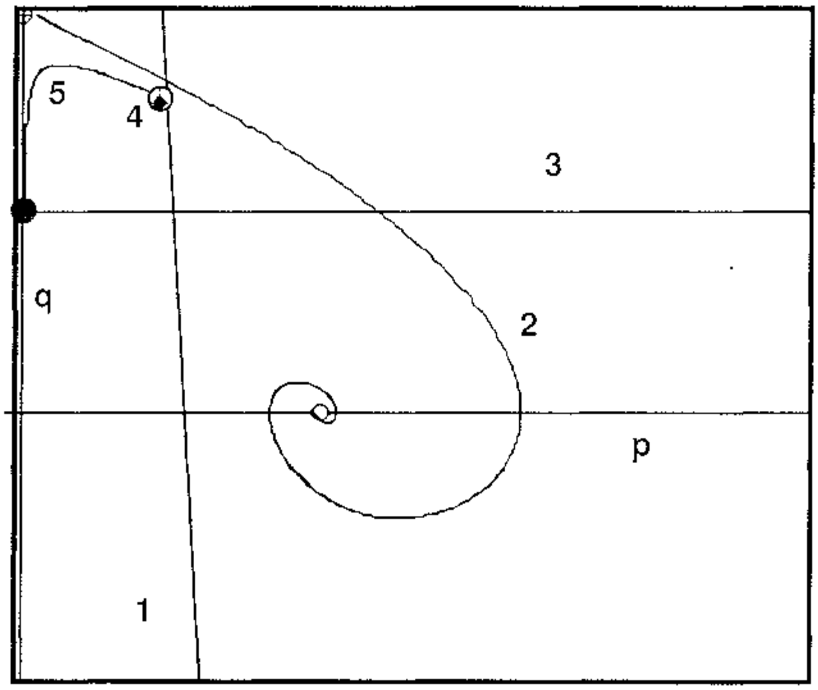


Figure 3.4.
Initial condition locus (1), the spiral separatrix (2), the boundary condition (3), (4) the starting point of the solution curve (5).

Chapter 4

Bifurcation Diagrams

The aim of this chapter is twofold: firstly to derive the bifurcation diagram for the spherical annulus and secondly to investigate how changes in the parameters affect the qualitative structure. The bifurcation diagram is a plot of the parameter δ versus $\|\theta\|$ where we have

$$\|\theta(r)\| = \max_{\alpha \le r \le 1} |\theta(r)| = \max_{\alpha \le r \le 1} \theta(r).$$

The following theorem shows that the maximum value of θ occurs at $r = \alpha$:

Theorem 4.0

Consider a spherical annulus of reactive material enclosing a sphere of inert material with relative radius α, then

$$\forall k \quad \alpha < k < 1, \; \theta(k) < \theta(\alpha),$$

where θ is the dimensionless form of the temperature.

Proof

We have from the boundary condition that

$$\frac{d\theta}{dr}(\alpha) = A < 0.$$

Assume θ has a local minimum at $r = \ell$ where $\alpha<\ell<1$. Evaluating the original differential equation (from system 1.22) at $r=\ell$,

$$\frac{d^2\theta}{dr^2}(\ell)+\frac{2}{\ell}\frac{d\theta}{dr}(\ell)+\delta e^{\theta(\ell)}=0,$$

and since a minimum occurs at $r=\ell$,

$$\frac{d\theta}{dr}(\ell)=0;$$

thus

$$\frac{d^2\theta}{dr^2}(\ell)=-\delta e^{\theta(\ell)}. \tag{4.1}$$

The right hand side of (4.1) is always negative so that

$$\frac{d^2\theta}{dr^2}(\ell)<0.$$

This contradicts the assumption that a minimum occurs at $r = \ell$; therefore, no such minimum can exist. Given that θ is decreasing at the boundary $r=\alpha$ and there are no local minima for $\alpha<r<1$ it follows there are no local maxima for $\alpha<r<1$. Hence, the hottest temperature occurs at the inner boundary $r=\alpha$ ❑

From the transformation equations,

$$p=\delta r^2 e^{\theta},$$

which, at r=α, implies

$$p(\alpha)=\delta\alpha^2 e^{\theta(\alpha)} ,$$

and thus

$$\theta_\alpha=\ln(\frac{p(\alpha)}{\delta\alpha^2}).$$

Before calculating values of θ_α we must first determine p at r=α. This is accomplished using the phase plane. Given A=0 and values for δ, Bi and α we must find points (p_0,q_0) on the initial condition locus such that $T_{\delta,Bi}(q_0)=-\ln(\alpha)$ (if any exist). Remember this means that it takes -ln(α) time for the trajectory passing through the point (p_0,q_0) to travel from the point (p_0,q_0) to the point $(p_\alpha,2)$ on the boundary condition. This quantity determines the value of p_α as the value of the p coordinate at the end of a solution curve in the phase plane. The above definition for p_α is valid for A≠0. Numerically, an efficient approach to take when calculating points on the bifurcation diagram is to choose a point $(p_\alpha,2+\alpha A)$ that satisfies the boundary condition and integrate along the trajectory backwards -ln(α) in time to find the starting point (p_0,q_0). Once this is determined, δ can be calculate, i.e. $\delta=p_0 e^{\frac{2-q_0}{Bi}}$ and thus θ_α, i.e. $\theta_\alpha=\ln(\frac{p(\alpha)}{\delta\alpha^2})$; this determines the point (δ,θ_α) on the bifurcation diagram. By varying $0<p_\alpha<\infty$ the bifurcation diagram can be obtained. Once the bifurcation diagram is obtained the qualitative structure can be investigated when A=0. As seen earlier, the value of the Biot number does not affect the qualitative structure of the $T_{\delta,Bi}(q_0)$ graph. Typically values for the Biot number are large and we consider only the case where the Biot number is infinite. Earlier we saw that for any positive value of the parameter δ less than the critical value $N_\alpha \geq 2$; therefore the bifurcation diagram has at least two branches. We conjectured in chapter three that for a given α, $\max_\delta N_\alpha$ occurs when $\delta = 2e^{\frac{-2}{Bi}}$. The number of relative maxima in the bifurcation diagram is

$$\frac{\max_\delta N_\alpha}{2},$$

and, when $\delta = 2e^{\frac{-2}{Bi}}$,

$$\frac{\max_\delta N_\alpha}{2} = \frac{N_\alpha}{2},. \qquad (4.2)$$

Table (4.1) shows some values of the number of maxima present calculated in this manner.

<u>Table 4.1.</u>

α / Bi	1e-1	1	10	42	1e2	1e3	1e4	infinity
1e-1	2	1	1	1	1	1	1	1
1e-2	2	2	2	2	2	2	2	2
1e-3	3	3	3	3	3	3	3	3
1e-4	4	4	4	4	4	4	4	4
1e-5	5	5	5	5	5	5	5	5
1e-6	6	6	6	6	6	6	6	6

The number of relative maxima present in the bifurcation diagram for various α and Bi calculated using equation 4.2.

Table 4.1 suggests the following two conjectures; (a) if Bi>1 the number of relative maxima in the bifurcation diagram depends only on α. (b)N_α is proportional to $-\ln(\alpha)$. Diagrams D.1.0, D.2.0 and D.3.0 support these conjectures (appendix D).

Having investigated the bifurcation diagrams for A=0, we now explore how the parameter A influences this structure. Consider the system

$$\frac{d^2\theta}{dr^2}+\frac{2}{r}\frac{d\theta}{dr}+\delta e^{\theta}=0,$$

$$\frac{d\theta}{dr}(\alpha)=A,$$

$$\frac{d\theta}{dr}(1)+Bi\,\theta(1)=0.$$

When $\delta=0$,

$$\frac{d^2\theta}{dr^2}+\frac{2}{r}\frac{d\theta}{dr}=0, \tag{4.2}$$

$$\frac{d\theta}{dr}(\alpha)=A, \tag{4.3}$$

$$\frac{d\theta}{dr}(1)+Bi\,\theta(1)=0. \tag{4.4}$$

This system is easily solved analytically giving

$$\theta(r)=\alpha^2A\left(\frac{Bi-1}{Bi}-\frac{1}{r}\right), \tag{4.5}$$

and it follows that

$$\theta(\alpha)=\theta_\alpha=\alpha^2A\left(\frac{Bi-1}{Bi}-\frac{1}{\alpha}\right).$$

As $Bi\rightarrow\infty$,

$$\theta(\alpha)=\theta_\alpha\rightarrow\ \alpha A(\alpha-1),$$

and this implies that the bifurcation diagram no longer passes through the origin but passes through the point $(0,\theta_\alpha)$ with $\theta_\alpha > 0$.

As we let $Bi \to \infty$ the terminal point on the bifurcation diagram is given by $(0,\alpha A(\alpha-1))$, where $\alpha A(\alpha-1) > 0$ for A<0. In terms of the phase plane, this analytic solution of our system when $\delta = 0$ represents a solution curve on the q axis (which as noted earlier, is a separatrix). This solution curve is the line segment joining $(0,2+\alpha^2 A)$ with $(0,2+\alpha A)$.

Numerical calculations produced the bifurcation diagrams contained in appendix D. These diagrams suggest that for any value of α, the bifurcation diagrams with A sufficiently close to 0, are qualitatively the same as those with A=0 i.e. $\delta(A,\alpha)$ is a continuous function of A. It can be seen that as A<0 decreases the number of relative maxima in the bifurcation diagram decreases and the qualitative structure resembles that of a bifurcation diagram for a larger value of α. This indicates that the number of relative maxima in the bifurcation diagram for A<0 is dependent on both A and α. The diagrams provide numerical evidence to support our conjecture that $\delta_{cr}(A,\alpha)$ is monotonic increasing in both A and α.

Conclusions.

The problem of self-heating in spherical domains has been studied extensively in the past and values for $\delta_{cr}(Bi)$ are well documented. It was shown in chapter two that an infinite series solution to the Frank-Kamenetskii equations for exothermic chemical reactions in spherical domains with arbitrary Biot number exists. This solution was shown to converge for θ_0 small enough. An explicit relation for δ_{cr} in terms of θ_0 was obtained by differentiating the series term by term. This relation holds if θ_0 is small enough at criticality. It is well known that an infinite multiplicity of steady state solutions exists for exothermic chemical reactions in spherical domains. Wake *et al.* showed that the analytic condition needed for this to occur is $\delta=\delta_\infty=2e^{\frac{-2}{Bi}}$. This result was generalised for n-dimensional spheres (2<n<10) in chapter two with the analytic condition being $\delta=\delta_\infty=2(n-2)e^{\frac{-2}{Bi}}$. This poses the interesting question (not addressed in this thesis): what makes the tenth dimension so special? For n≥10 we showed $\delta_{cr}=2(n-2)e^{\frac{-2}{Bi}}$. This result is directly related to the previous result and both relations are obtained via simple phase plane analysis.

The major portion of this thesis dealt with the problem in spherically annular domains. In chapters 3 and 4, it was shown that infinite multiplicity of steady state solutions is not possible. This was first obtained for the case A=0 and then generalised for A<0 using a simple continuity argument. In spherical domains, there exists a unique steady state solution. We showed in chapter 3 that in spherically annular domains there exist at least two steady state solutions for any value of $0<\delta<\delta_{cr}$. In chapter 4, we saw that $\delta_{cr}(A, \alpha)$ is monotonically increasing in both A, the heat flux, and α, the inner radius.

In this thesis, several conjectures were made motivated by numerical evidence, e.g. $N_\alpha \propto -\ln(\alpha)$. Analysis may be conclusive to resolving these questions and ultimately to extending the analytical theory underlying self-heating in spherical and spherically annular geometries.

Attention was restricted to the self-heating problem in spherical and spherically annular geometries. There are, however, other simple geometries of interest which remain to be explored analytically, e.g. an infinitely long cylindrical annulus and the infinite slab. Another area for future work would be to investigate the problem in these and other geometries.

References

[1] Wake, G.C., Scott, S.K., and Brindley, J., Multiplicity of steady state solutions for combustion in a solid sphere with arbitrary Biot number, *Physics Letters A*, Volume 153, number 1 February 1991

[2] Gidas, B., Nirenberg, W.M Ni., and Nirenberg, L., Symmetry And Related Properties Via The Maximum Principle. *Commun, Math. Phys.* 68 (1979) 209.

[3] Keller, H.B., and Fier, J.M., Equilibrium Chaos and Related Parameter Sequences, *Analyse Mathematique et Applications*, Gauthier-Villars, Paris, 1988.

[4] Abramowitz, M., and Stegun, I.A., *Handbook of Mathematical Functions*, Dover Publications, 1972

[5] Chandrasekhar, S., *Introduction To The Study Of Stellar Structure,* Dover Publications, 1930, p.160.

[6] Williams, F.A., *Combustion Theory*, The Bejamin/Cummings Publishing Company, Inc 1985.

[7] Zeldovich, Ya.B., Barenblatt, G.I., Librovich, V.B., and Makhviladze, G.N., *The Mathematical Theory of Combustion and Explosions*, Academy of sciences of the U.S.S.R.

[8] Bowes, P.C., *Self-heating: Evaluating and Controlling the Hazards,* Elsevier Science Publishers B.V.

[9] Barzykin, V.V., and Merzhanov, A.G., *Kraevaya zadacha v teorii teplovogo vzaryva (Boundary Value Problems in The Theory of Thermal Explosions)*, Dokl, AN SSSR, 120:1271 (1958).

[10] Thomas, P.L., *On The Thermal Conduction Equation For Self-heating Materials with Surface Cooling,* Trans. Faraday Soc., 54:pt 1, p. 60 (1958).

[11] Keller, J.B., and Antman, S., *Bifurcation Theory and Non-Linear Eigenvalue Problems*, W.A Benjamin Inc, 1969

[12] Boyce, W.E., and DiPrima, R.C., *Elementary Differential Equations and Boundary Value Problems*, John Wiley and Sons Inc.

[13] Frank-Kamenetskii D.A., *Diffusion and Heat Exchange in Chemical Kinetics*, Princeton University Press, 1955.

Appendix A.

Coefficients of the Series Solutions.

Coefficients α_n and β_n.

a 1	=	1.00000000000000E+0000	b 1	=	-3.33333333333333E-0001
a 2	=	-1.66666666666667E-0001	b 2	=	3.33333333333333E-0002
a 3	=	2.22222222222222E-0002	b 3	=	-3.17460317460317E-0003
a 4	=	-2.68959435626102E-0003	b 4	=	2.98843817362336E-0004
a 5	=	3.08152067411327E-0004	b 5	=	-2.80138243101206E-0005
a 6	=	-3.40738365429723E-0005	b 6	=	2.62106434945941E-0006
a 7	=	3.67492372195488E-0006	b 7	=	-2.44994914796992E-0007
a 8	=	-3.89083335972654E-0007	b 8	=	2.28872550572149E-0008
a 9	=	4.06102244741984E-0008	b 9	=	-2.13738023548412E-0009
a 10	=	-4.19076321480907E-0009	b 10	=	1.99560153086146E-0010
a 11	=	4.28478315845212E-0010	b 11	=	-1.86294919932701E-0011
a 12	=	-4.34733214859744E-0011	b 12	=	1.73893285943898E-0012
a 13	=	4.38223507895534E-0012	b 13	=	-1.62305002924272E-0013
a 14	=	-4.39293548631422E-0013	b 14	=	1.51480534010835E-0014
a 15	=	4.38253296955721E-0014	b 15	=	-1.41372031276039E-0015
a 16	=	-4.35381600599748E-0015	b 16	=	1.31933818363560E-0016
a 17	=	4.30929113823459E-0016	b 17	=	-1.23122603949560E-0017
a 18	=	-4.25120916824707E-0017	b 18	=	1.14897545087759E-0018
a 19	=	4.18158880382699E-0018	b 19	=	-1.07220225739154E-0019
a 20	=	-4.10223808739188E-0019	b 20	=	1.00054587497363E-0020
a 21	=	4.01477386442072E-0020	b 21	=	-9.33668340562957E-0022
a 22	=	-3.92063950031317E-0021	b 22	=	8.71253222291817E-0023
a 23	=	3.82112102059436E-0022	b 23	=	-8.13004472466885E-0024
a 24	=	-3.71736182456926E-0023	b 24	=	7.58645270320258E-0025
a 25	=	3.61037610356052E-0024	b 25	=	-7.07916883051082E-0026
a 26	=	-3.50106107981094E-0025	b 26	=	6.60577562228480E-0027
a 27	=	3.39020816980588E-0026	b 27	=	-6.16401485419251E-0028
a 28	=	-3.27851316541133E-0027	b 28	=	5.75177748317777E-0029
a 29	=	3.16658551733576E-0028	b 29	=	-5.36709409717925E-0030
a 30	=	-3.05495679767312E-0029	b 30	=	5.00812589782478E-0031
a 31	=	2.94408841144016E-0030	b 31	=	-4.67315620863518E-0032
a 32	=	-2.83437862091934E-0031	b 32	=	4.36058249372206E-0033
a 33	=	2.72616894113741E-0032	b 33	=	-4.06890886736927E-0034
a 34	=	-2.61974995985981E-0033	b 34	=	3.79673907226059E-0035
a 35	=	2.51536663099019E-0034	b 35	=	-3.54276990280308E-0036
a 36	=	-2.41322308617843E-0035	b 36	=	3.30578504955949E-0037
a 37	=	2.31348700571221E-0036	b 37	=	-3.08464934094962E-0038
a 38	=	-2.21629358635993E-0037	b 38	=	2.87830335890899E-0039
a 39	=	2.12174914071370E-0038	b 39	=	-2.68575840596671E-0040
a 40	=	-2.02993435972325E-0039	b 40	=	2.50609180212746E-0041
a 41	=	1.94090726748987E-0040	b 41	=	-2.33844249095165E-0042
a 42	=	-1.85470589498483E-0041	b 42	=	2.18200693527627E-0043
a 43	=	1.77135069714729E-0042	b 43	=	-2.03603528407734E-0044
a 44	=	-1.69084673578905E-0043	b 44	=	1.89982779302141E-0045
a 45	=	1.61318564886964E-0044	b 45	=	-1.77273148227433E-0046
a 46	=	-1.53834742499318E-0045	b 46	=	1.65413701612170E-0047
a 47	=	1.46630200040541E-0046	b 47	=	-1.54347578990043E-0048
a 48	=	-1.39701069432329E-0047	b 48	=	1.44021721064257E-0049
a 49	=	1.33042749710129E-0048	b 49	=	-1.34386615868817E-0050
a 50	=	-1.26650022451770E-0049	b 50	=	1.25396061833435E-0051
a 51	=	1.20517155034272E-0050	b 51	=	-1.17006946635216E-0052
a 52	=	-1.14637992831960E-0051	b 52	=	1.09179040792343E-0053
a 53	=	1.09006041374364E-0052	b 53	=	-1.01874805022770E-0054
a 54	=	-1.03614539395440E-0053	b 54	=	9.50592104545318E-0056
a 55	=	9.84565236258252E-0055	b 55	=	-8.86995708340768E-0057
a 56	=	-9.35248861065282E-0056	b 56	=	8.27653859349807E-0058

Reverted Coefficients for Bi = 1e-2 calculated using methods discussed in chapter two.

g1	=	-2.98507462686567E-0002	g2	=	1.50142581811371E-0002
g3	=	-1.00394106562267E-0002	g4	=	7.54458069713687E-0003
g5	=	-6.04470640330430E-0003	g6	=	5.04329740530821E-0003
g7	=	-4.32715023573548E-0003	g8	=	3.78950446355507E-0003
g9	=	-3.37097804130389E-0003	g10	=	3.03590632594863E-0003
g11	=	-2.76157428840117E-0003	g12	=	2.53282727499792E-0003
g13	=	-2.33916663986616E-0003	g14	=	2.17308886964259E-0003
g15	=	-2.02908839799547E-0003	g16	=	1.90303399289094E-0003
g17	=	-1.79176502355472E-0003	g18	=	1.69282217121706E-0003
g19	=	-1.60426309393779E-0003	g20	=	1.52453333693338E-0003
g21	=	-1.45237408894281E-0003	g22	=	1.38675507089286E-0003
g23	=	-1.32682491442814E-0003	g24	=	1.27187393344832E-0003
g25	=	-1.22130582157261E-0003	g26	=	1.17461587444851E-0003
g27	=	-1.13137404672316E-0003	g28	=	1.09121163604359E-0003
g29	=	-1.05381071934419E-0003	g30	=	1.01889569976944E-0003
g31	=	-9.86226488044269E-0004	g32	=	9.55592961062080E-0004
g33	=	-9.26810426996683E-0004	g34	=	8.99715889888197E-0004
g35	=	-8.74164953940290E-0004	g36	=	8.50029243236020E-0004
g37	=	-8.27194239421545E-0004	g38	=	8.05557460387133E-0004
g39	=	-7.85026918719255E-0004	g40	=	7.65519810884594E-0004
g41	=	-7.46961397599546E-0004	g42	=	7.29284043281719E-0004
g43	=	-7.12426388382204E-0004	g44	=	6.96332633229139E-0004
g45	=	-6.80951916352832E-0004	g46	=	6.66237775050677E-0004
g47	=	-6.52147682921570E-0004	g48	=	6.38642671480286E-0004
g49	=	-6.25687066490339E-0004	g50	=	6.13248413849199E-0004
g51	=	-6.01297749007256E-0004	g52	=	5.89810495887406E-0004
g53	=	-5.78768479187348E-0004	g54	=	5.68163778341987E-0004

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Reverted Coefficients for Bi = 1e-1 calculated using methods discussed in chapter two.

g1	=	-2.85714285714286E-0001	g2	=	1.50826044703596E-0001
g3	=	-1.03436442928321E-0001	g4	=	7.90843297470071E-0002
g5	=	-6.41988675651577E-0002	g6	=	5.41341532698961E-0002
g7	=	-4.68626874201897E-0002	g8	=	4.13566858255592E-0002
g9	=	-3.70387864034960E-0002	g10	=	3.35593315912890E-0002
g11	=	-3.06940190568024E-0002	g12	=	2.82922549942502E-0002
g13	=	-2.62491233844067E-0002	g14	=	2.44892565857101E-0002
g15	=	-2.29570973961269E-0002	g16	=	2.16107786008851E-0002
g17	=	-2.04181423631337E-0002	g18	=	1.93540739702673E-0002
g19	=	-1.83986695938869E-0002	g20	=	1.75359485121113E-0002
g21	=	-1.67529297734748E-0002	g22	=	1.60389582828951E-0002
g23	=	-1.53852050147236E-0002	g24	=	1.47842909787821E-0002
g25	=	-1.42300005708230E-0002	g26	=	1.37170604387500E-0002
g27	=	-1.32409670178651E-0002	g28	=	1.27978506674911E-0002
g29	=	-1.23843676465866E-0002	g30	=	1.19976134859247E-0002
g31	=	-1.16350529650816E-0002	g32	=	1.12944630918480E-0002
g33	=	-1.09738863487439E-0002	g34	=	1.06715921103348E-0002
g35	=	-1.03860446108371E-0002	g36	=	1.01158761991375E-0002
g37	=	-9.85986488961226E-0003	g38	=	9.61691542456744E-0003
g39	=	-9.38604322388004E-0003	g40	=	9.16636072097385E-0003
g41	=	-8.95706567946868E-0003	g42	=	8.75743115624253E-0003
g43	=	-8.56679682480624E-0003	g44	=	8.38456139208889E-0003
g45	=	-8.21017581460748E-0003	g46	=	8.04313690627011E-0003
g47	=	-7.88298064314162E-0003	g50	=	7.43954374976561E-0003
g51	=	-7.30263227406864E-0003	g52	=	7.17025857448661E-0003
g53	=	-7.04148611837828E-0003	g54	=	6.91465859646943E-0003
g55	=	-6.78658819942612E-0003			

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Reverted Coefficients for Bi = 1 calculated using methods discussed in chapter two.

g1	=	-2.00000000000000E+0000	g2	=	1.33333333333333E-0000
g3	=	-1.05185185185185E+0000	g4	=	8.91005291005291E-0001
g5	=	-7.84953164805017E-0001	g6	=	7.08873219753878E-0001
g7	=	-6.51160856155520E-0001	g8	=	6.05607417906409E-0001
g9	=	-5.68566298104328E-0001	g10	=	5.37743423134466E-0001
g11	=	-5.11617373999053E-0001	g12	=	4.89135991318664E-0001
g13	=	-4.69546416219099E-0001	g14	=	4.52294498783298E-0001
g15	=	-4.36962504182641E-0001	g16	=	4.23229042360168E-0001
g17	=	-4.10842446011966E-0001	g18	=	3.99602583536799E-0001
g19	=	-3.89348129047204E-0001	g20	=	3.79947459778371E-0001
g21	=	-3.71292022946211E-0001	g22	=	3.63291419790631E-0001
g23	=	-3.55869706574749E-0001	g24	=	3.48962572885833E-0001
g25	=	-3.42515162230378E-0001	g26	=	3.36480369522024E-0001
g27	=	-3.30817497227153E-0001	g28	=	3.25491184438200E-0001
g29	=	-3.20470545895038E-0001	g30	=	3.15728474123612E-0001
g31	=	-3.11241069471414E-0001	g32	=	3.06987171263511E-0001
g33	=	-3.02947969512956E-0001	g34	=	2.99106681259042E-0001
g35	=	-2.95448279212480E-0001	g36	=	2.91959263532757E-0001
g37	=	-2.88627471114857E-0001	g38	=	2.85441922321105E-0001
g39	=	-2.82392715798572E-0001	g40	=	2.79471004038416E-0001
g41	=	-2.76669127806542E-0001	g42	=	2.73981081302460E-0001
g43	=	-2.71403676209592E-0001	g44	=	2.68939199961719E-0001
g45	=	-2.66601337322424E-0001	g46	=	2.64428418690486E-0001
g47	=	-2.62513496283609E-0001	g48	=	2.61073367934797E-0001
g49	=	-2.60606765386745E-0001	g50	=	2.62251138015474E-0001
g51	=	-2.68564320886832E-0001	g52	=	2.85170640967523E-0001
g53	=	-3.24062867822842E-0001	g54	=	4.09847911653151E-0001
g55	=	-5.90715561688978E-0001			

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Reverted Coefficients for Bi = 10 calculated using methods discussed in chapter two.

g1	=	-5.00000000000000E+0000	g2	=	3.95833333333333E+0000
g3	=	-3.44659391534392E+0000	g4	=	3.12801408179012E+0000
g5	=	-2.90520631251296E+0000	g6	=	2.73809974129621E+0000
g7	=	-2.60676922837554E+0000	g8	=	2.50003590907758E+0000
g9	=	-2.41107613468118E+0000	g10	=	2.33545618736804E+0000
g11	=	-2.27015284318319E+0000	g12	=	2.21302390899039E+0000
g13	=	-2.16250313702737E+0000	g14	=	2.11741512602269E+0000
g15	=	-2.07685813420260E+0000	g16	=	2.04012718432259E+0000
g17	=	-2.00666204354367E+0000	g18	=	1.97601109178606E+0000
g19	=	-1.94780564224534E+0000	g20	=	1.92174131745465E+0000
g21	=	-1.89756429771845E+0000	g22	=	1.87506100307936E+0000
g23	=	-1.85405023912543E+0000	g24	=	1.83437713989698E+0000
g25	=	-1.81590844109077E+0000	g26	=	1.79852875133247E+0000
g27	=	-1.78213758149060E+0000	g28	=	1.76664695618616E+0000
g29	=	-1.75197947690554E+0000	g30	=	1.73806673819015E+0000
g31	=	-1.72484802060226E+0000	g32	=	1.71226919773190E+0000
g33	=	-1.70028179786783E+0000	g34	=	1.68884214840954E+0000
g35	=	-1.67791049083114E+0000	g36	=	1.66744986780375E+0000
g37	=	-1.65742443669573E+0000	g38	=	1.64779668628992E+0000
g39	=	-1.63852305393125E+0000	g40	=	1.62954855959995E+0000
g41	=	-1.62080635724576E+0000	g42	=	1.61224746702680E+0000
g43	=	-1.60399091019402E+0000	g44	=	1.59689414831766E+0000
g45	=	-1.59450531497301E+0000	g46	=	1.60940312127353E+0000
g47	=	-1.68309798554633E+0000	g48	=	1.94676081190827E+0000
g49	=	-2.80149349017254E+0000	g50	=	5.43842013107610E+0000
g51	=	-1.32957351246095E+0001	g52	=	3.60215684183974E+0001
g53	=	-9.99447711671997E+0001	g54	=	2.74996776173989E+0002
g55	=	-7.42248735876477E+0002			

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Reverted Coefficients for Bi = 100 calculated using methods discussed in chapter two.

g1 =	-5.88235294117647E+0000	g2 =	4.70520388086030E+0000
g3 =	-4.11131759661929E+0000	g4 =	3.73784671301747E+0000
g5 =	-3.47525460873438E+0000	g6 =	3.27765825047220E+0000
g7 =	-3.12201487452431E+0000	g8 =	2.99531420334547E+0000
g9 =	-2.88957949899587E+0000	g10 =	2.79961087463255E+0000
g11 =	-2.72185376070772E+0000	g12 =	2.65378443214823E+0000
g13 =	-2.59355468503643E+0000	g14 =	2.53977564703236E+0000
g15 =	-2.49138058905909E+0000	g16 =	2.44753473158548E+0000
g17 =	-2.40757412752146E+0000	g18 =	2.37096315213701E+0000
g19 =	-2.33726425322409E+0000	g20 =	2.30611598890645E+0000
g21 =	-2.27721679571893E+0000	g22 =	2.25031279917743E+0000
g23 =	-2.22518852798778E+0000	g24 =	2.20165974798734E+0000
g 25 =	-2.17956786644232E+0000	g26 =	2.15877551534124E+0000
g27 =	-2.13916303068470E+0000	g28 =	2.12062562026703E+0000
g29 =	-2.10307106576825E+0000	g30 =	2.08641784298525E+0000
g31 =	-2.07059357097652E+0000	g32 =	2.05553371874376E+0000
g33 =	-2.04118050533037E+0000	g34 =	2.02748191529424E+0000
g35 =	-2.01439067705807E+0000	g36 =	2.00186278715023E+0000
g37 =	-1.98985431406915E+0000	g38 =	1.97831266154679E+0000
g39 =	-1.96715124716632E+0000	g40 =	1.95617730378756E+0000
g41 =	-1.94489408585198E+0000	g42 =	1.93198347033760E+0000
g43 =	-1.91401482887556E+0000	g44 =	1.88237037048341E+0000
g45 =	-1.81625793652136E+0000	g46 =	1.66757748466387E+0000
g47 =	-1.32977858552376E+0000	g48 =	5.77283656712317E-0001
g49 =	1.04521753978389E+0000	g50 =	-4.41269620235019E+0000
g51 =	1.11342958894200E+0001	g52 =	2.41186333415351E+0001
g53 =	4.89428302364219E+0001	g54 =	9.84665096439660E+0001
g55 =	2.10347043102764E+0002		

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Reverted Coefficients for Bi = 1000 calculated using methods discussed in chapter two.

g1	=	-5.98802395209581E+0000	g2	=	4.79041200470442E+0000
g3	=	-4.18590630970364E+0000	g4	=	3.80571446844773E+0000
g5	=	-3.53838344576266E+0000	g6	=	3.33721541841173E+0000
g7	=	-3.17875577315844E+0000	g8	=	3.04976085017862E+0000
g9	=	-2.94211048814731E+0000	g10	=	2.85051115264476E+0000
g11	=	-2.77134418069222E+0000	g12	=	2.70204029886873E+0000
g13	=	-2.64071792203779E+0000	g14	=	2.58596307765684E+0000
g15	=	-2.53668974862604E+0000	g16	=	2.49204805494240E+0000
g17	=	-2.45136203486541E+0000	g18	=	2.41408636802797E+0000
g19	=	-2.37977557963981E+0000	g20	=	2.34806168172513E+0000
g21	=	-2.31863764797718E+0000	g22	=	2.29124500404693E+0000
g23	=	-2.26566437388872E+0000	g24	=	2.24170818412655E+0000
g25	=	-2.21921496717052E+0000	g26	=	2.19804486469985E+0000
g27	=	-2.17807604347422E+0000	g28	=	2.15920181232639E+0000
g29	=	-2.14132828352555E+0000	g30	=	2.12437246061082E+0000
g31	=	-2.10826066326914E+0000	g32	=	2.09292722215584E+0000
g33	=	-2.07831339802437E+0000	g34	=	2.06436650835938E+0000
g35	=	-2.05103929186030E+0000	g36	=	2.03828960836123E+0000
g37	=	-2.02608059755322E+0000	g38	=	2.01438110081985E+0000
g39	=	-2.00316443746140E+0000	g40	=	1.99239744461149E+0000
g41	=	-1.98199294845072E+0000	g42	=	1.97164793635874E+0000
g43	=	-1.96036238345656E+0000	g44	=	1.94513600658498E+0000
g45	=	-1.91768375796877E+0000	g46	=	1.85663671406631E+0000
g47	=	-1.70995013710460E+0000	g48	=	1.35698573820419E+0000
g49	=	-5.30087359068193E-0001	g50	=	-1.34127774682865E+0000
g51	=	5.42630845029775E+0000	g52	=	-1.40137195168585E+0001
g53	=	3.12752767568014E+0001	g54	=	-6.37051233420559E+0001
g55	=	1.16782352280492E+0002			

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Reverted Coefficients for Bi = 10000 calculated using methods discussed in chapter two.

g1	=	-5.99880023995201E+0000	g2	=	4.79904012000479E+0000
g3	=	-4.19344694880114E+0000	g4	=	3.81257074468559E+0000
g5	=	-3.54475838502425E+0000	g6	=	3.34322809389786E+0000
g7	=	-3.18448306596720E+0000	g8	=	3.05525580944013E+0000
g9	=	-2.94741154753355E+0000	g10	=	2.85564721653638E+0000
g11	=	-2.77633763849574E+0000	g12	=	2.70690891390950E+0000
g13	=	-2.64547606953221E+0000	g14	=	2.59062258658067E+0000
g15	=	-2.54126049219333E+0000	g16	=	2.49653837579256E+0000
g17	=	-2.45577905823533E+0000	g18	=	2.41843623700650E+0000
g19	=	-2.38406363497291E+0000	g20	=	2.35229260136145E+0000
g21	=	-2.32281555685684E+0000	g22	=	2.29537356154280E+0000
g23	=	-2.26974684422000E+0000	g24	=	2.24574749361992E+0000
g25	=	-2.22321375121758E+0000	g26	=	2.20200550649892E+0000
g27	=	-2.18200070604015E+0000	g28	=	2.16309246471803E+0000
g29	=	-2.14518672167625E+0000	g30	=	2.12820032233978E+0000
g31	=	-2.11205943538887E+0000	g32	=	2.09669823348475E+0000
g33	=	-2.08205778230184E+0000	g34	=	2.06808510156776E+0000
g35	=	-2.05473240399399E+0000	g36	=	2.04195663202365E+0000
g37	=	-2.02971970364593E+0000	g38	=	2.01799053021145E+0000
g39	=	-2.00675106960089E+0000	g40	=	1.99601015367763E+0000
g41	=	-1.98582810099869E+0000	g42	=	1.97634213517061E+0000
g43	=	-1.96772468041027E+0000	g44	=	1.95980821378841E+0000
g45	=	-1.95050843850498E+0000	g46	=	1.93047075350502E+0000
g47	=	-1.86672565681713E+0000	g48	=	1.65592150296197E+0000
g49	=	-9.96528325001958E-0001	g50	=	-9.47066269789015E-0001
g51	=	6.39326596987562E+0000	g52	=	-2.09902315045323E+0001
g53	=	5.84626886545748E+0001	g54	=	-1.50281910498445E+0002
g55	=	3.63064157953565E+0002			

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

<u>Reverted coefficients for Bi = ∞, calculated using methods discussed in chapter two.</u>

g1 =	-6.00000000000000E+0000	g2 =	4.80000000000000E+0000
g3 =	-4.19428571428571E+0000	g4 =	3.81333333333333E+0000
g5 =	-3.54546740878169E+0000	g6 =	3.34389680922252E+0000
g7 =	-3.18512003013162E+0000	g8 =	3.05586692623569E+0000
g9 =	-2.94800109377431E+0000	g10 =	2.85621840839456E+0000
g11 =	-2.77689296708058E+0000	g12 =	2.70745035552677E+0000
g13 =	-2.64600522347334E+0000	g14 =	2.59114076881710E+0000
g15 =	-2.54176880108852E+0000	g16 =	2.49703773941667E+0000
g17 =	-2.45627026921343E+0000	g18 =	2.41891997869533E+0000
g19 =	-2.38454050146712E+0000	g20 =	2.35276311301966E+0000
g21 =	-2.32328017251645E+0000	g22 =	2.29583268824899E+0000
g23 =	-2.27020084506476E+0000	g24 =	2.24619669413671E+0000
g25 =	-2.22365844469115E+0000	g26 =	2.20244595853662E+0000
g27 =	-2.18243715885085E+0000	g28 =	2.16352514185693E+0000
g29 =	-2.14561583473969E+0000	g30 =	2.12862608259204E+0000
g31 =	-2.11248207606044E+0000	g32 =	2.09711805262372E+0000
g33 =	-2.08247521913246E+0000	g34 =	2.06850084844576E+0000
g35 =	-2.05514748362876E+0000	g36 =	2.04237208377709E+0000
g37 =	-2.03013458355339E+0000	g38 =	2.01839416352757E+0000
g39 =	-2.00709802965982E+0000	g40 =	1.99614795708253E+0000
g41 =	-1.98530629384253E+0000	g42 =	1.97395188422468E+0000
g43 =	-1.96050486911356E+0000	g44 =	1.94123835962808E+0000
g45 =	-1.90831943431656E+0000	g46 =	1.84821452099100E+0000
g47 =	-1.74711715937690E+0000	g48 =	1.62864190724752E+0000
g49 =	-1.70413900124699E+0000	g50 =	2.86605334037847E+0000
g51 =	-8.13756519500374E+0000	g52 =	2.66167789622140E+0001
g53 =	-8.35863647600009E+0001	g54 =	2.45179360545769E+0002
g55 =	-6.76095282054375E+0002		

Where $g_n = \overline{\Gamma}_n$ in formula 2.19.

Appendix B.

Calculated Values For N_{α}.

Table B1.

α | δ	1e-120	1e-100	1e-80	1e-20	1e-14	1e-7
1e-1	2	4	4	2	2	0
1e-2	2	4	?	2	2	0
1e-3	2	6	?	2	2	0
1e-4	2	6	?	2	2	0
1e-5	2	6	?	2	2	0
1e-6	2	6	?	2	2	0

Values for N_α when Bi=.01 A=0.

Table B2

α | δ	1e-11	1e-10	1e-9	1e-8	1e-7	1e-4	1e-3	1e-2	1e-1	1
1e-1	4 *	4	4	2(3)	2	2	2	2	2	0
1e-2	2	6	4	4	4	4	4	4	2	0
1e-3	2	6	6	6	4	4	4	4	2	0
1e-4	2	6	8	6	4	4	4	4	4	0
1e-5	2	6	8	6	4	4	4	4	4	0
1e-6	2	6	8	6	4	4	4	4	4	0

Values for N_α when Bi=.1 A=0

Table B3

α | δ	.1	.2	.27 **	.3	.4	.5	.7	.8	.9	1
1e-1	2	2	2	2	2	2	2	2	2	0
1e-2	2	4	4	4	4	4	2	2	2	0
1e-3	2	6	6	6	4	4	4	4	4	0
1e-4	2	6	8	8	4	4	4	4	4	0
1e-5	2	6	10	8	4	4	4	4	4	0
1e-6	2	6	>10	8	4	4	4	4	4	0

Values for N_α when Bi=1 A=0.

?: Number of solutions undetermined.

** :δ_∞.

>10: At least 10 solutions.

*:Type 3 curve present.

Table B4

α | δ	1	1.5	1.6	* *	1.7	1.8	2	2.7	2.8	3
1e-1	2	2	2	2	2	2	2	2	2	0
1e-2	2	4	4	4	4	4	3(4)	2	0	0
1e-3	2	5	6	6	6	4	4	4	0	0
1e-4	2	6	6	8	6	4	4	4	0	0
1e-5	2	6	6	10	8	4	4	4	0	0
1e-6	2	6	6	>10	8	4	4	4	0	0

Values for N_α when Bi=10 A=0.

Table B5

α | δ	.1	.5	1.7	1.8	1.9	* *	2.2	2.5	3.2	3.5
1e-1	2	2	2	2	2	2	2	2	2	0
1e-2	2	2	4	4	4	4	4	2	2	0
1e-3	2	2	4	4(5)	6	6	4	4	2	0
1e-4	2	2	6	6	6	8	4	4	4	0
1e-5	2	2	6	6	6	10	4	4	4	0
1e-6	2	2	6	6	6	>10	4	4	4	0

Values for N_α when Bi=100 A=0.

Table B6

α | δ	.1	1.6	1.7	1.8	1.9	* *	2.1	2.8	3.2	3.4
1e-1	2	2	2	2	2	2	2	2	2	0
1e-2	2	2	4	4	4	4	4	2	2	0
1e-3	2	2	4	4	6	6	6	4	4	0
1e-4	2	2	6	6	6	8	6	4	4	0
1e-5	2	2	6	6	6	10	8	4	4	0
1e-6	2	2	6	6	6	>10	8	4	4	0

Values for N_α when Bi=10000 A=0.

?: Number of solutions undetermined.

* * : δ_∞.

>10: At least 10 solutions.

*:Type 3 curve present.

Appendix C.

Graphs of the Function $T_{\delta,Bi}(q_0)$.

Graph of the Function $T_{\delta,Bi}$.

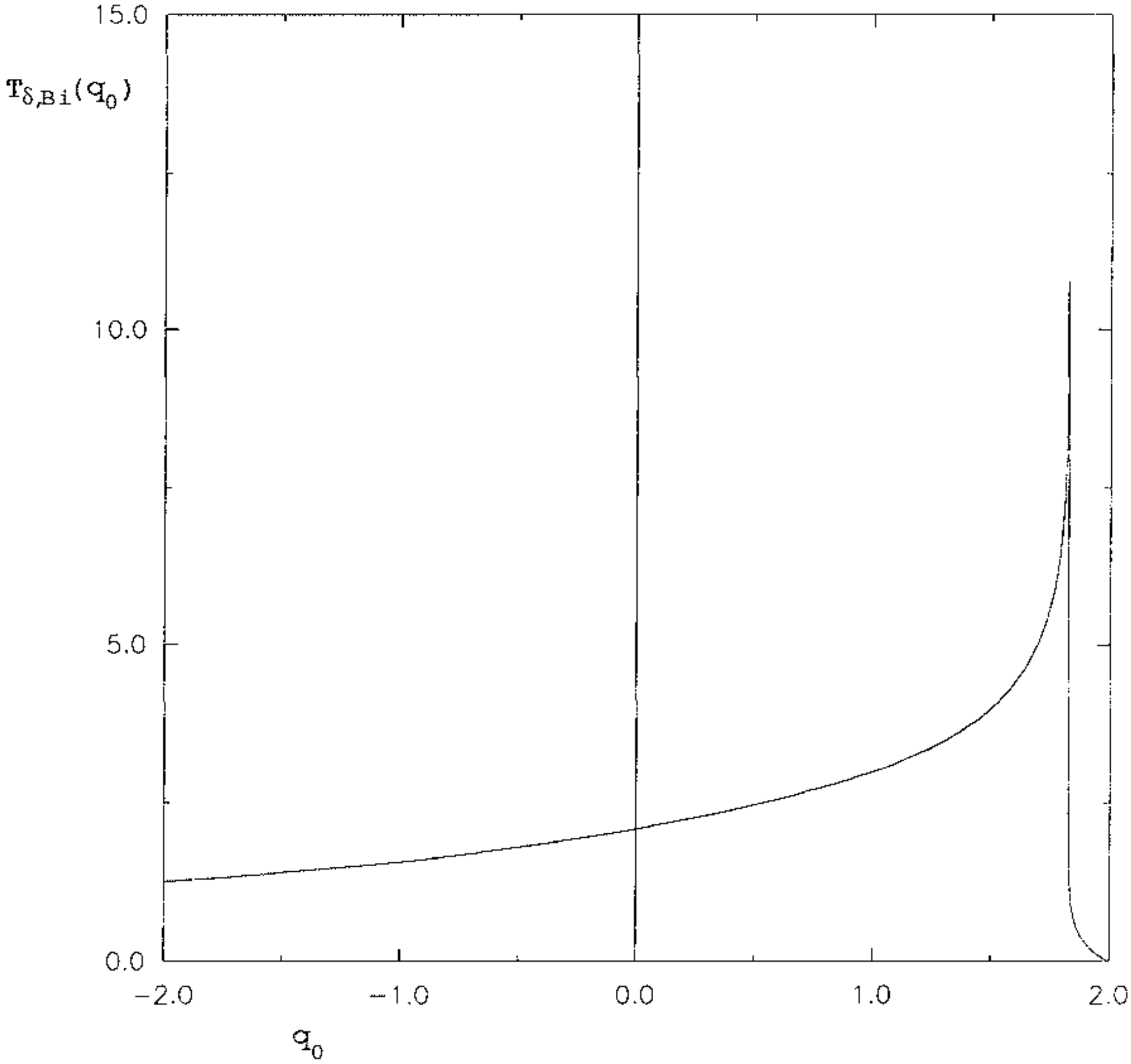


Figure C1.

Bi	= ∞
A	= 0
δ	= .5

Graph of the Function $T_{\delta,Bi}$.

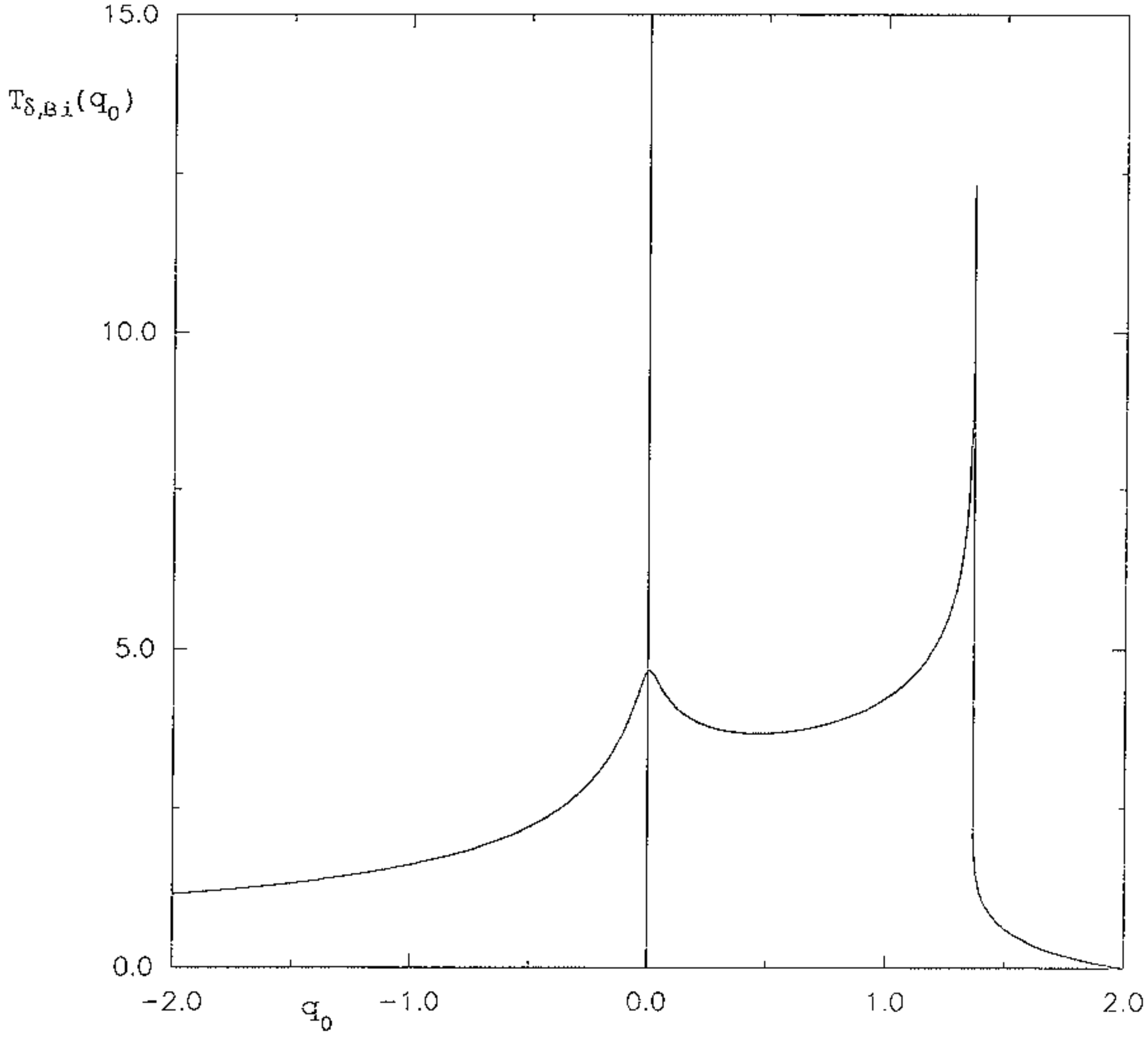


Figure C2

Bi = ∞
A = 0
δ = 1.66

Graph of the Function $T_{\delta,Bi}$

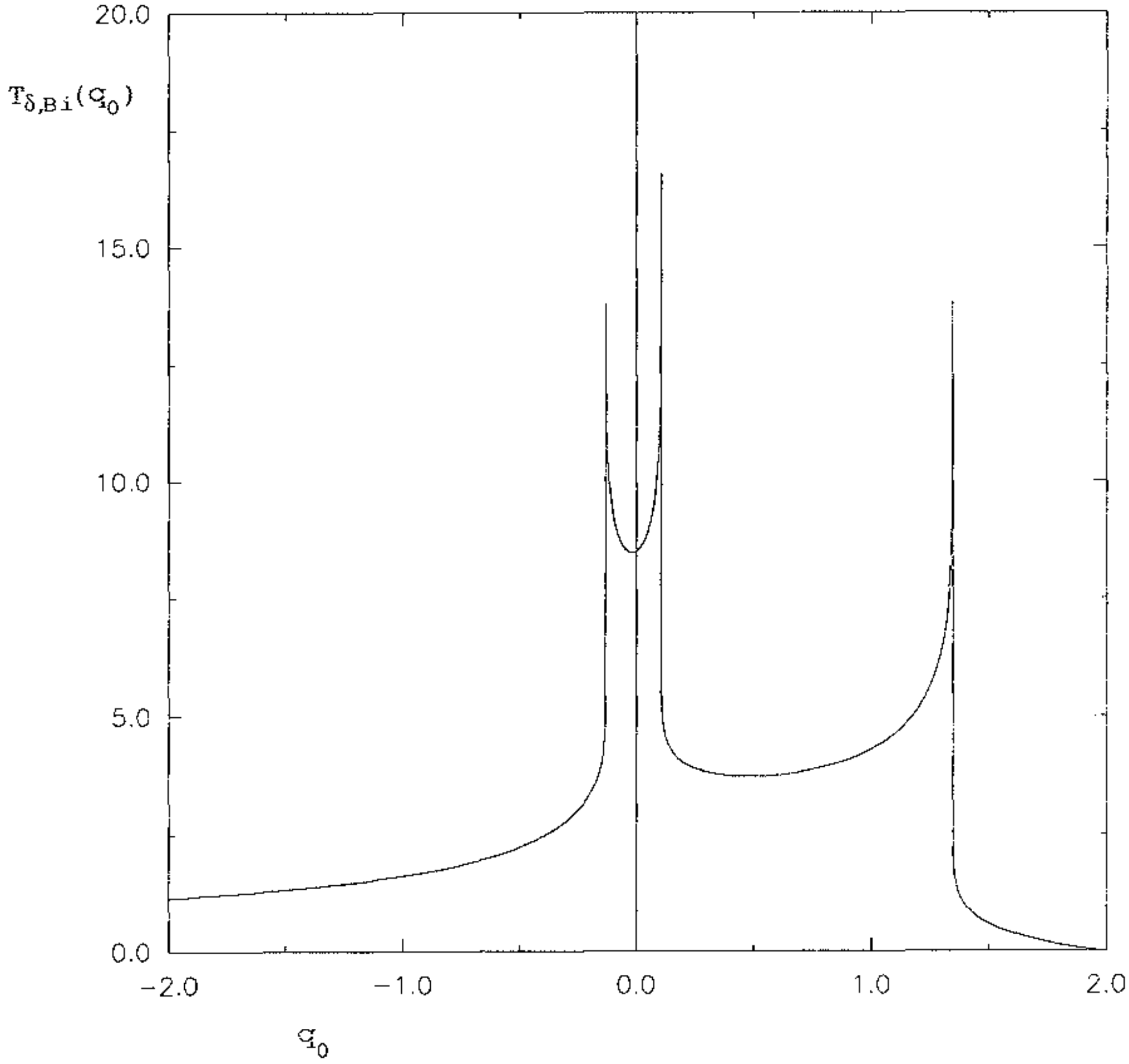


Figure C3.

$Bi = \infty$
$A = 0$
$\delta = 1.7$

Graph of the Function $T_{\delta,Bi}$.

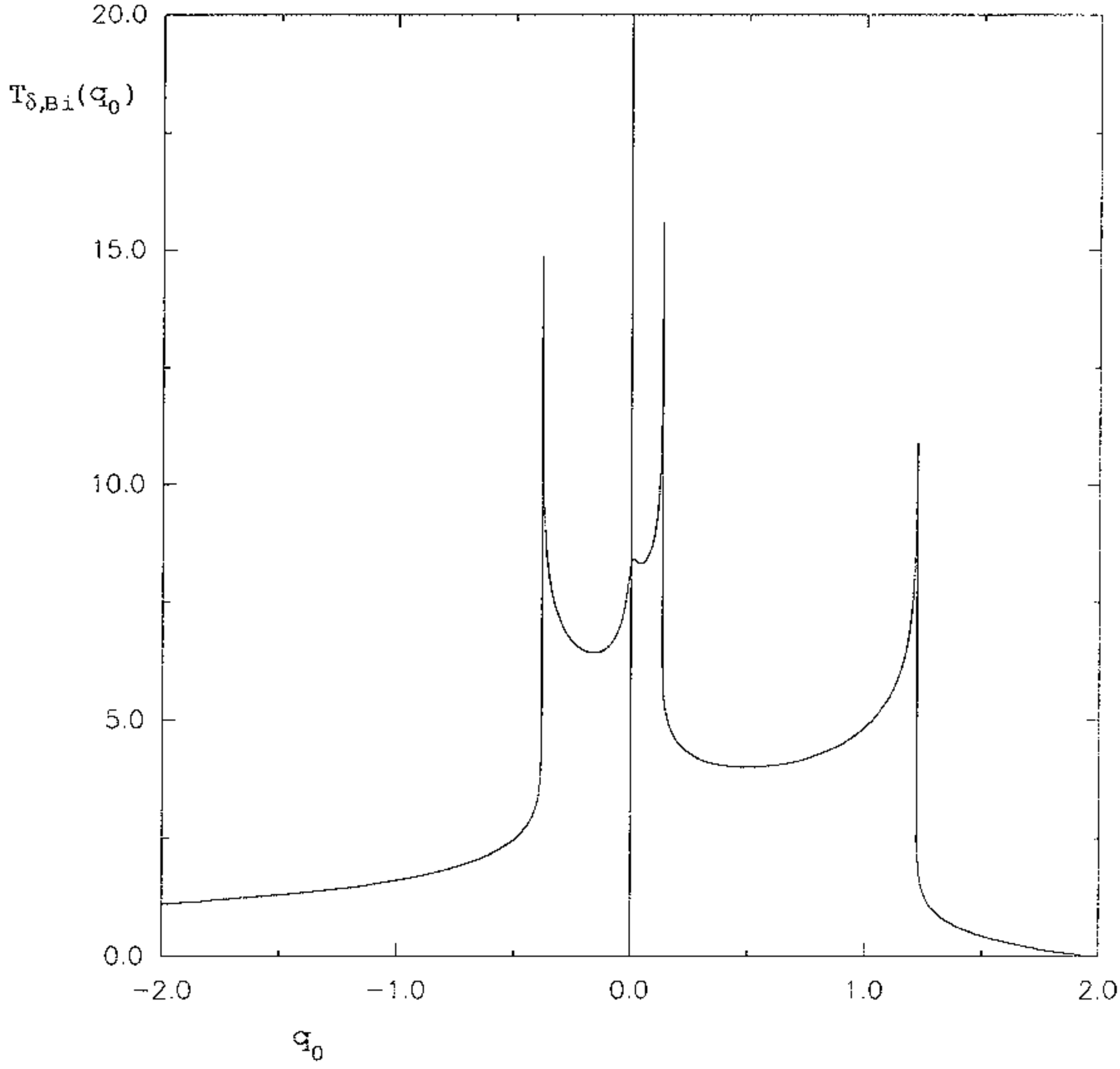


Figure C4.

Bi = ∞
A = 0
δ = 1.96

Graph of the Function $T_{\delta,Bi}$

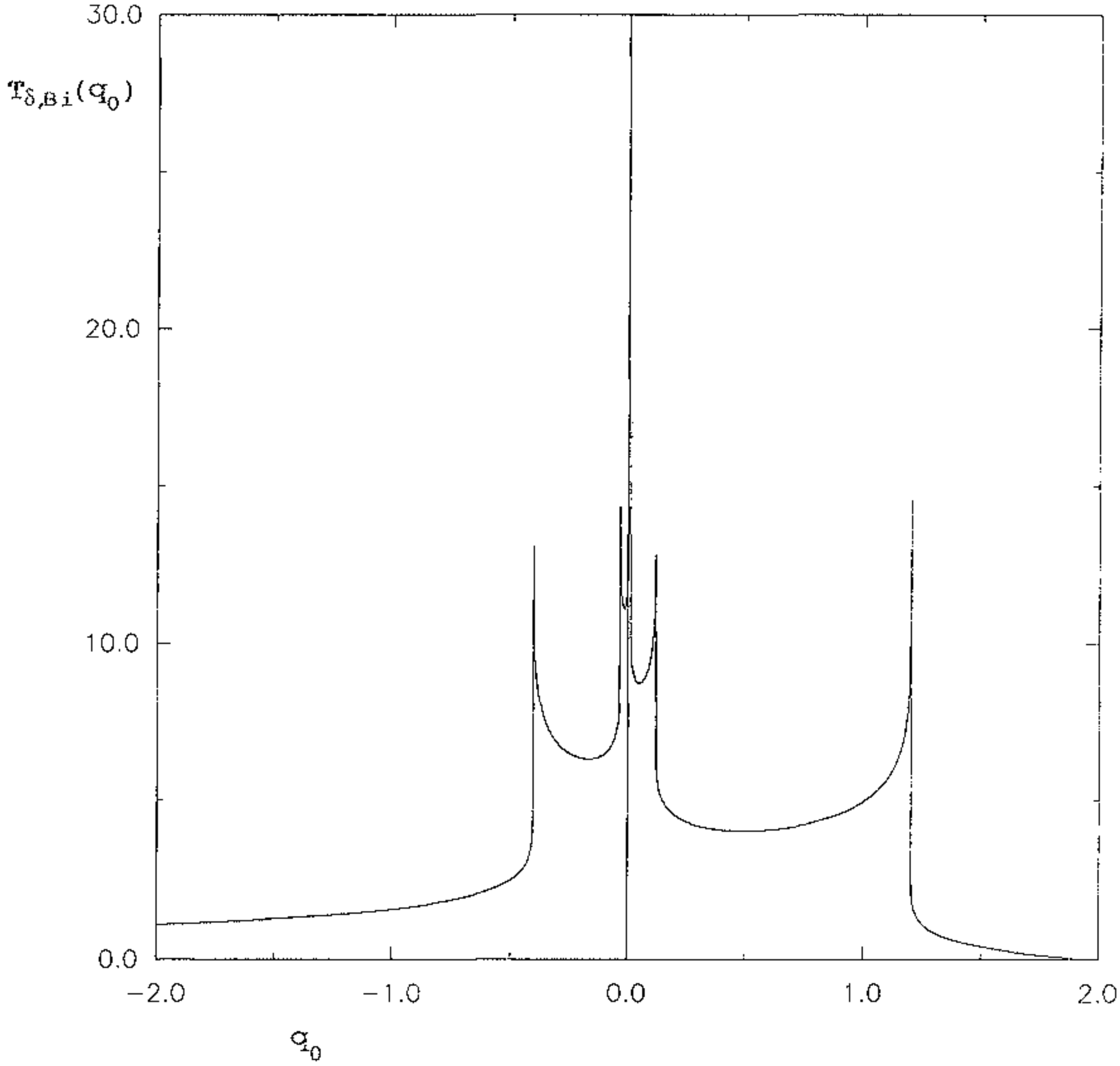


Figure C5.

$Bi = \infty$
$A = 0$
$\delta = 2$

Graph of the Function $T_{\delta,Bi}$.

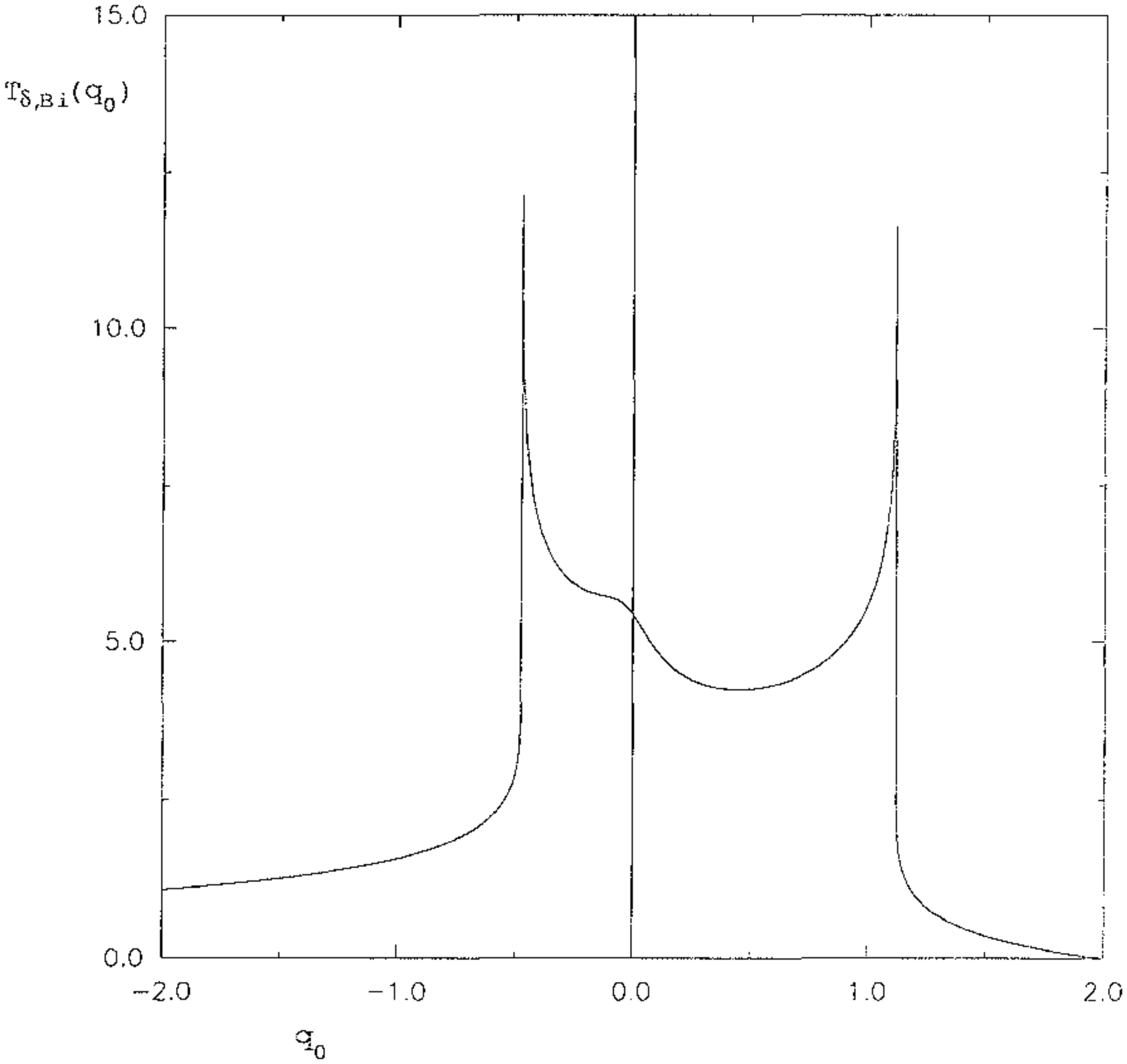


Figure C6.

$Bi = \infty$
$A = 0$
$\delta = 2.15$

Graph of the Function $T_{\delta,Bi}$.

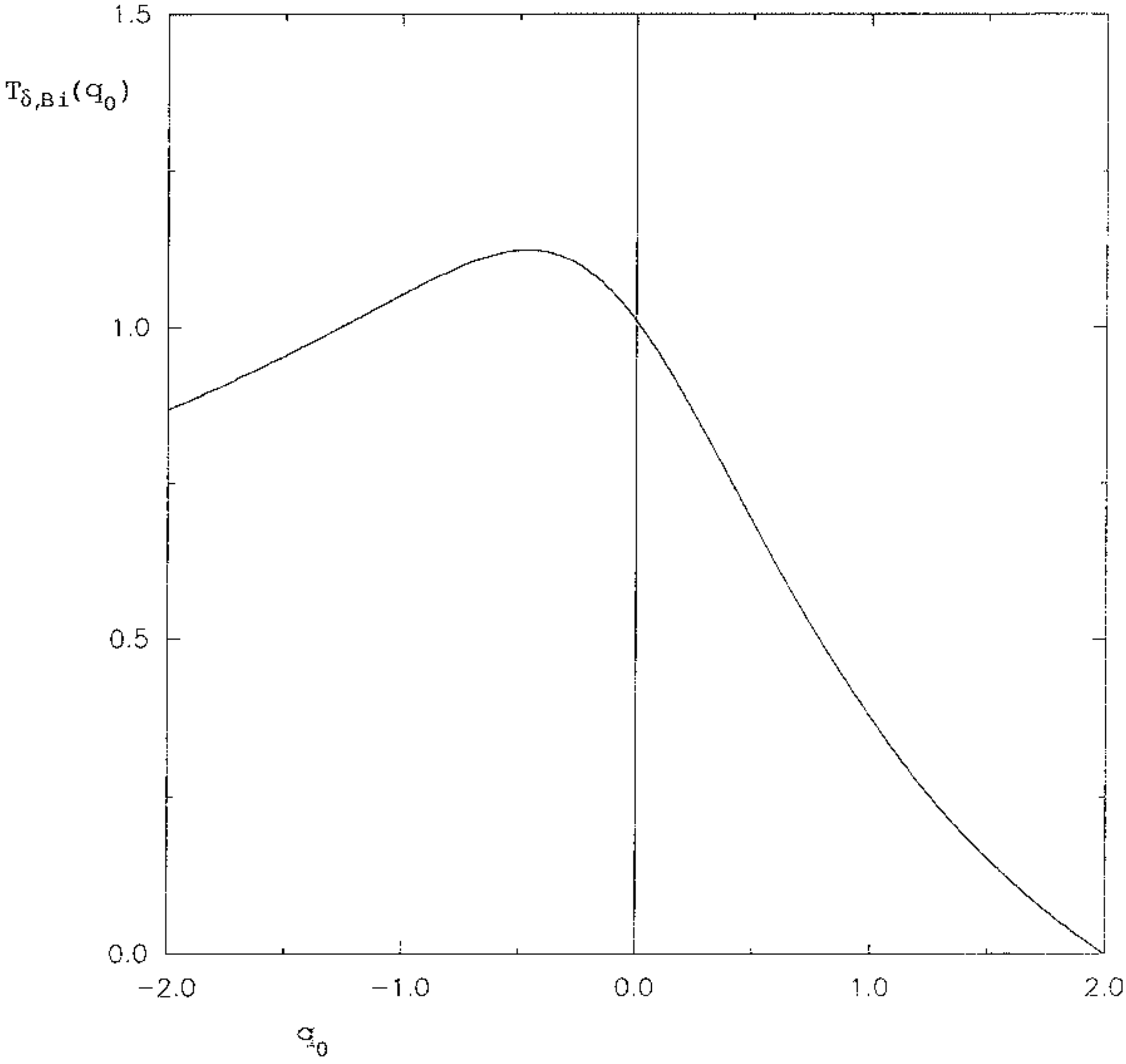


Figure C7.

$Bi = \infty$
$A = 0$
$\delta = 4$

Appendix D.

Bifurcation Diagrams.

Bifurcation Diagram.

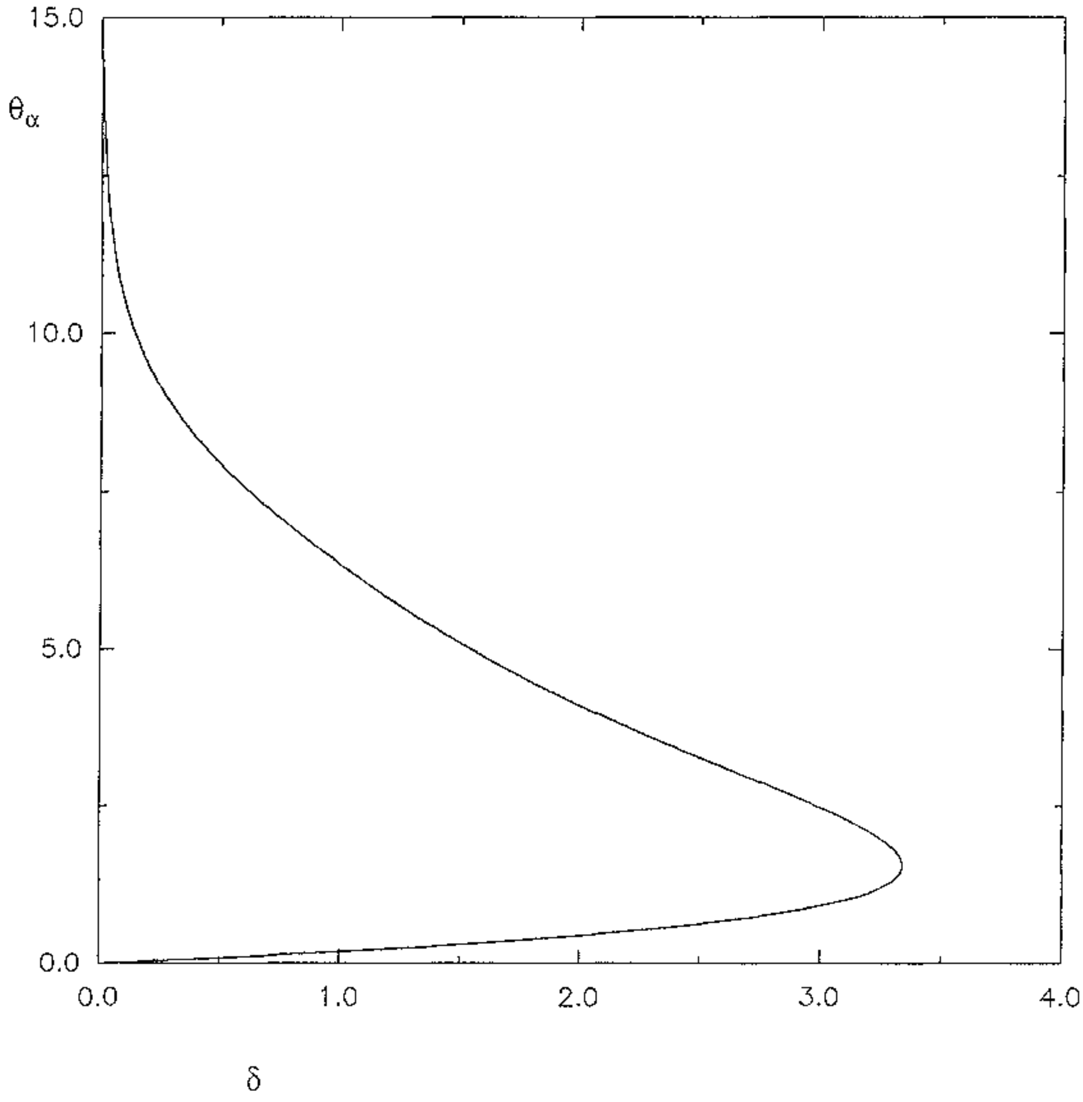


Figure D.1.0

A	= 0
Bi	= ∞
α	= .1

Bifurcation Diagram.

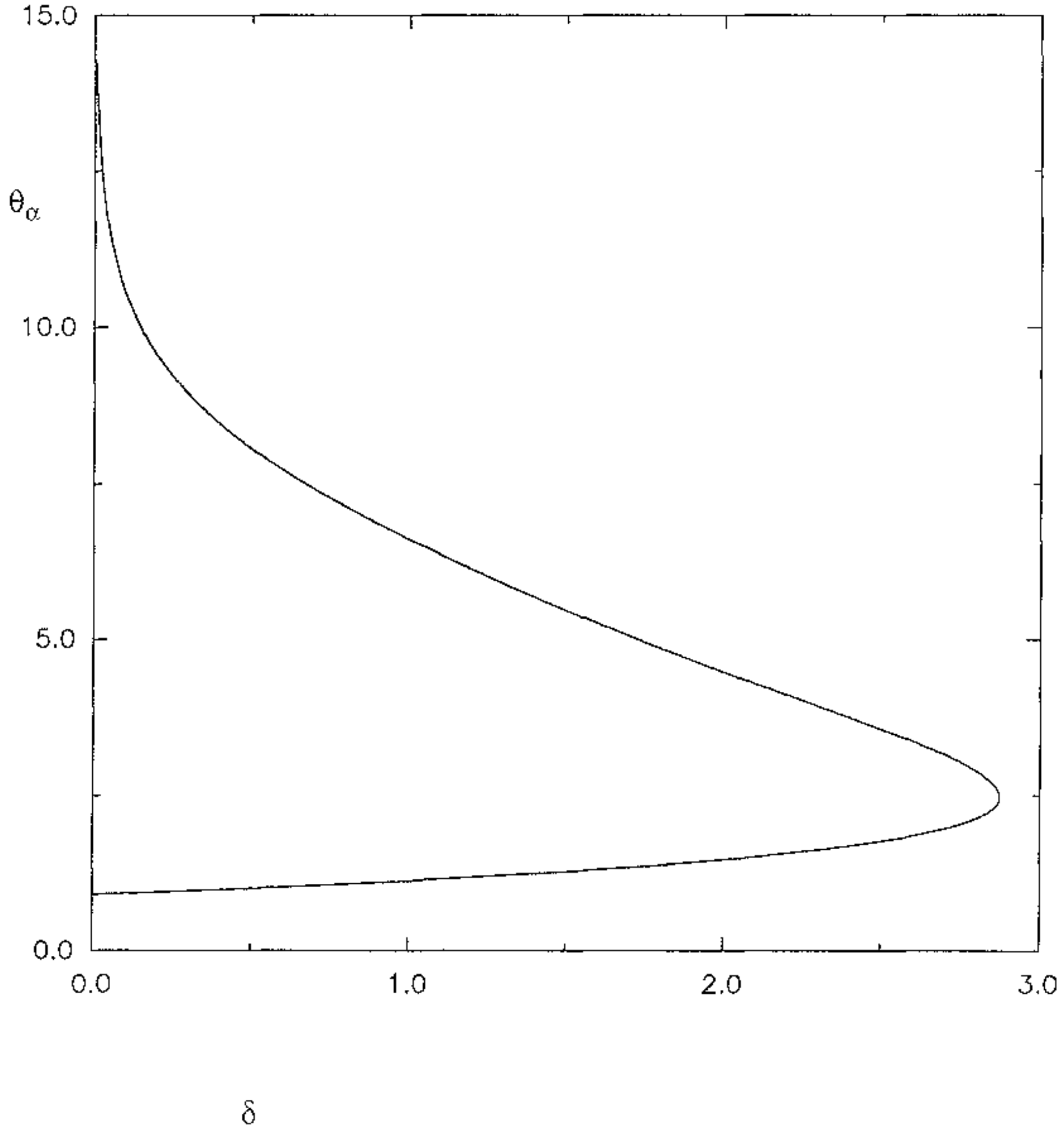


Figure D.1.1

A	= -10
Bi	= ∞
α	= .1

Bifurcation Diagram.

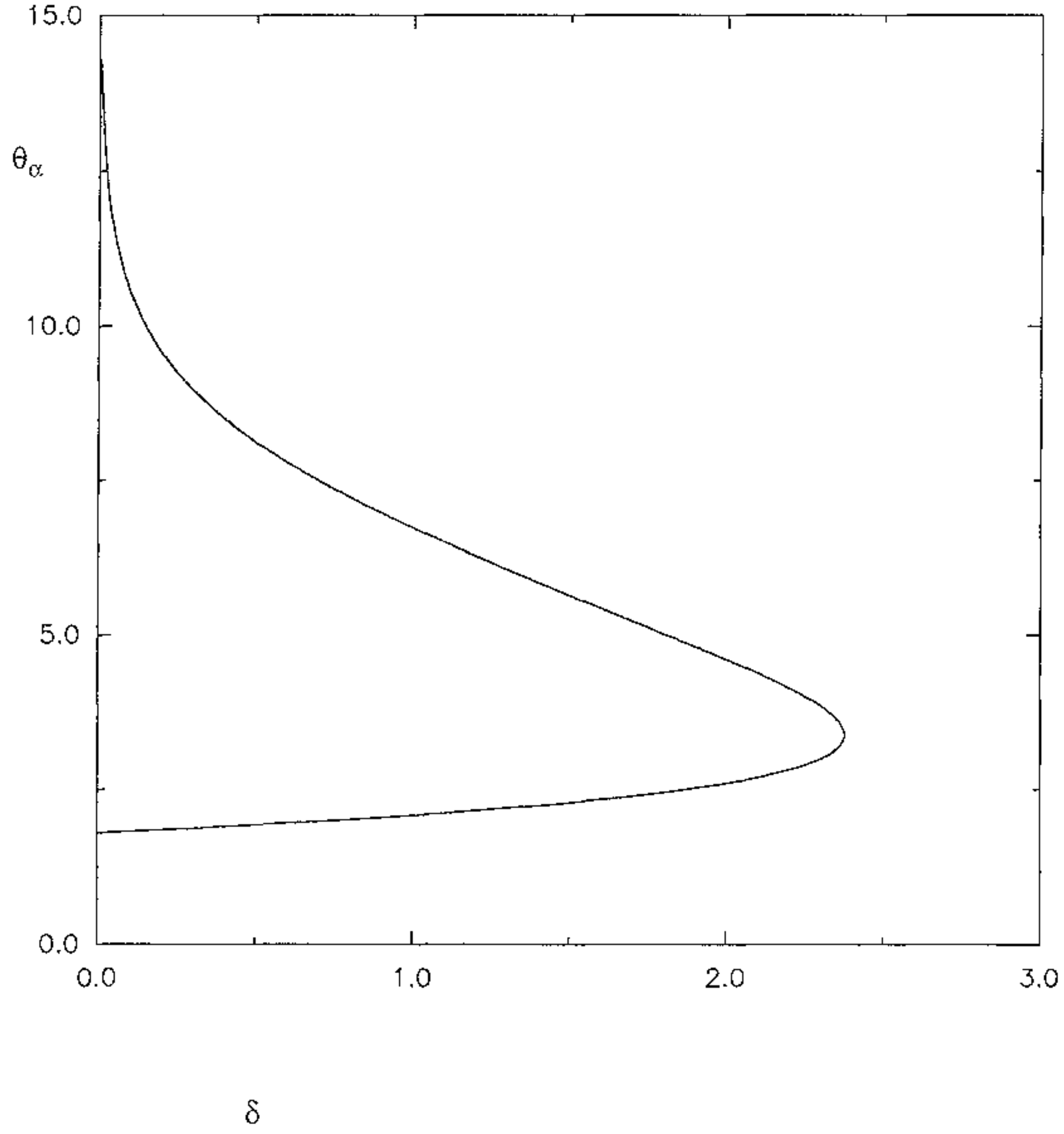


Figure D.1.2

A	= -20
Bi	= ∞
α	= .1

Bifurcation Diagram.

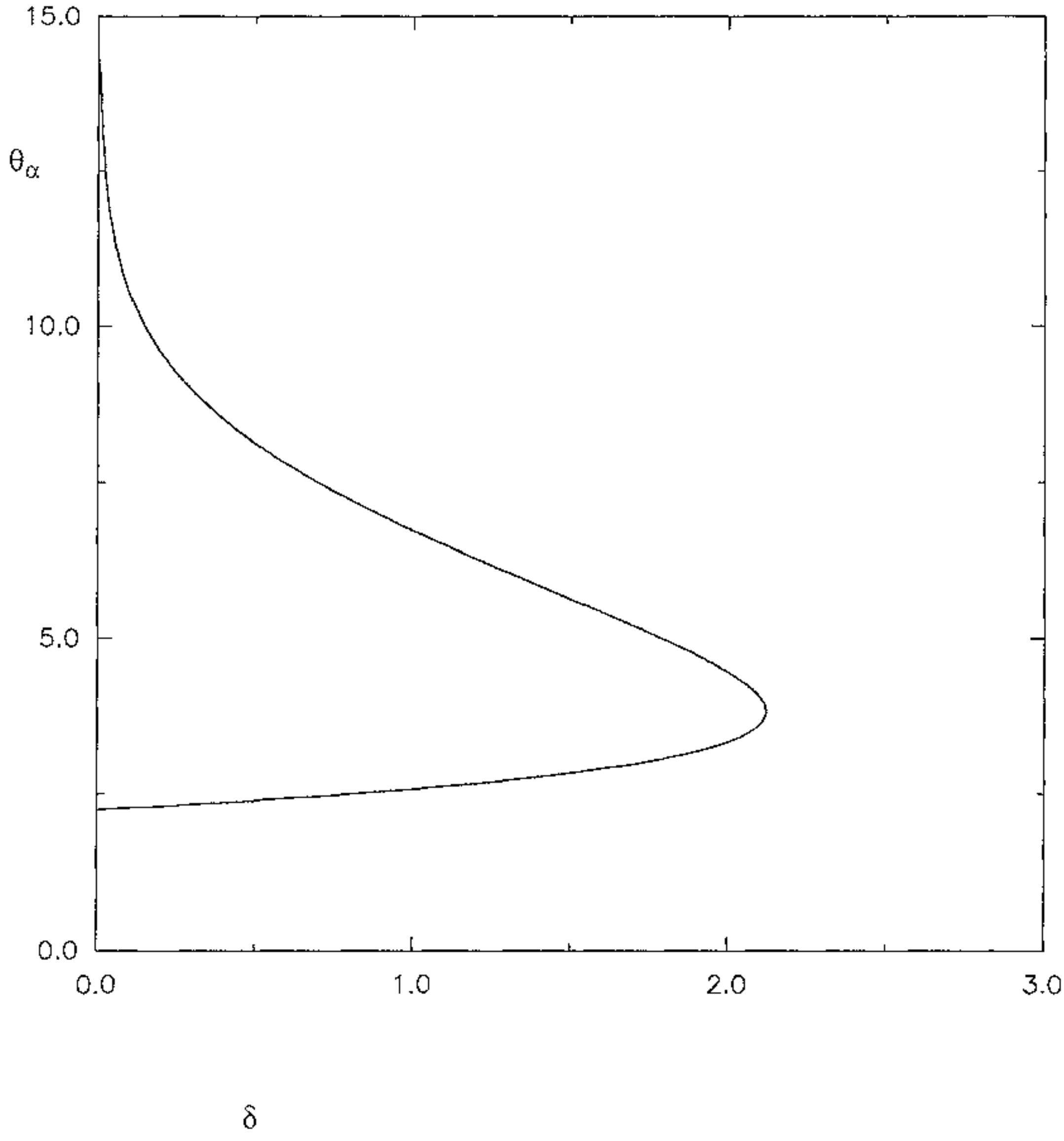


Figure D.1.3

A	= -25
Bi	= ∞
α	= .1

Bifurcation Diagram.

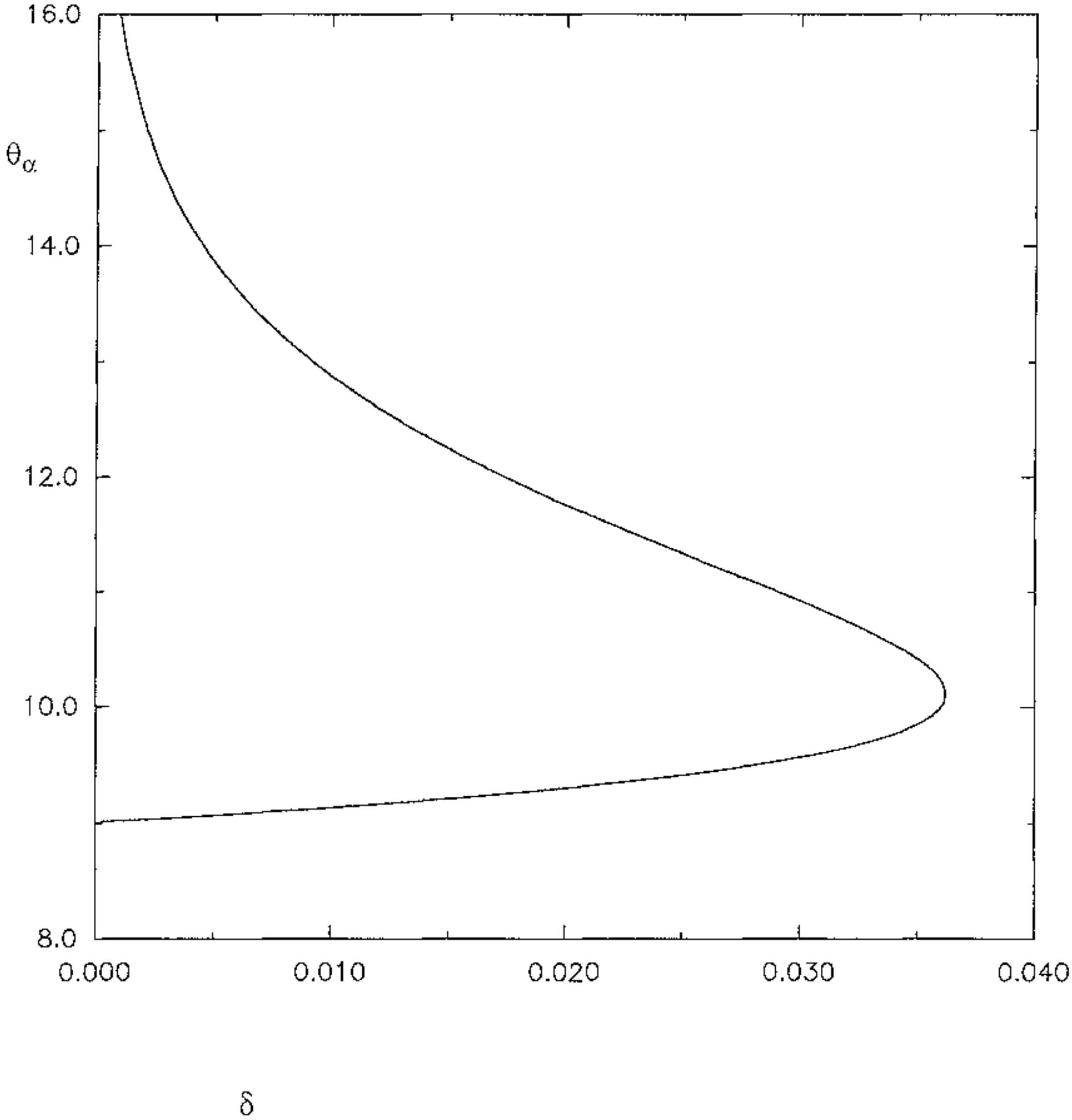


Figure D.1.4

A = -100
Bi = ∞
α = .1

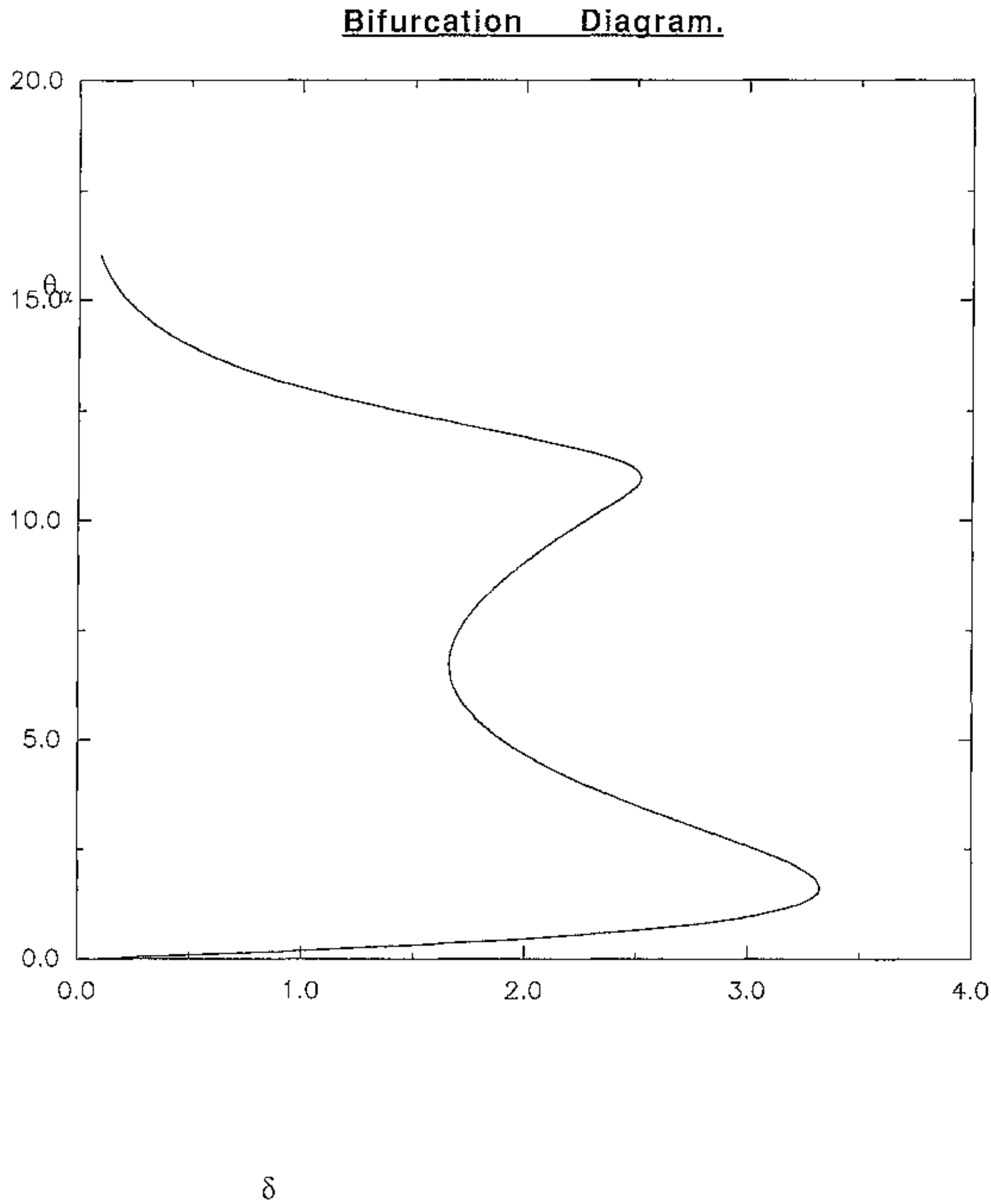


Figure D.2.0

A	= 0
Bi	= ∞
α	= .01

Bifurcation Diagram.

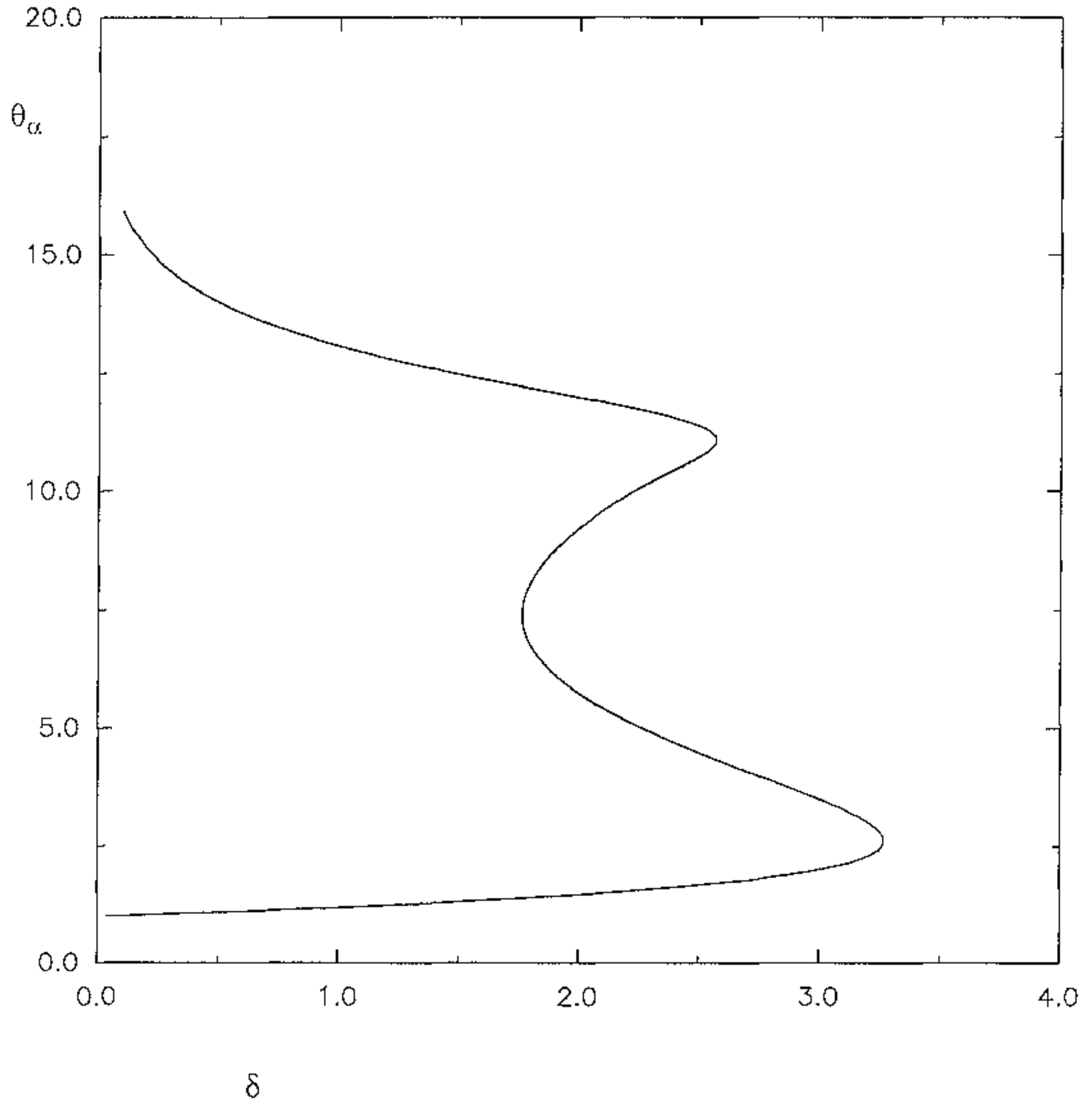


Figure D.2.1

A = -50
Bi = ∞
α = .01

Bifurcation Diagram.

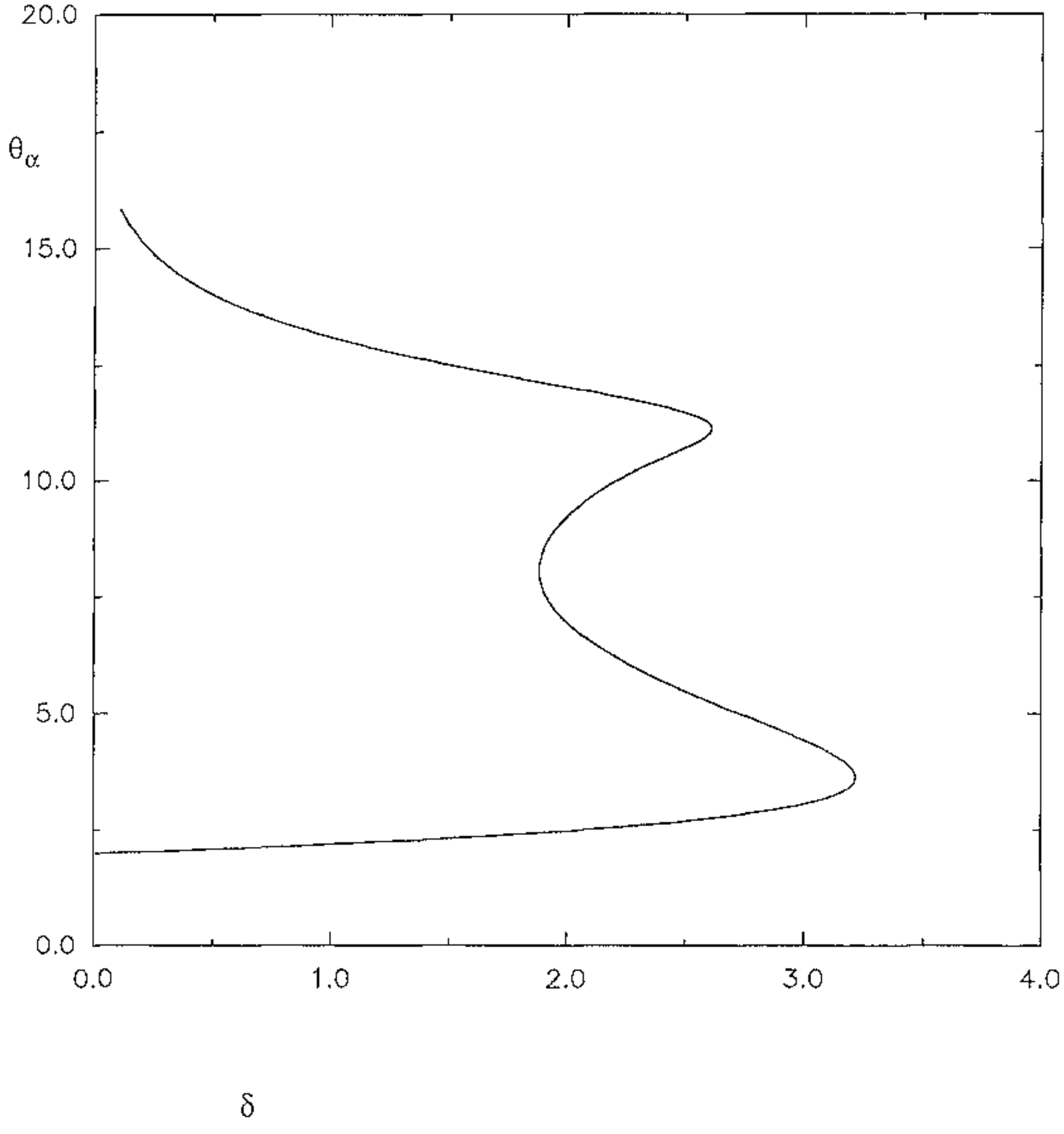


Figure D.2.2

A = -200
Bi = ∞
α = .01

Bifurcation Diagram.

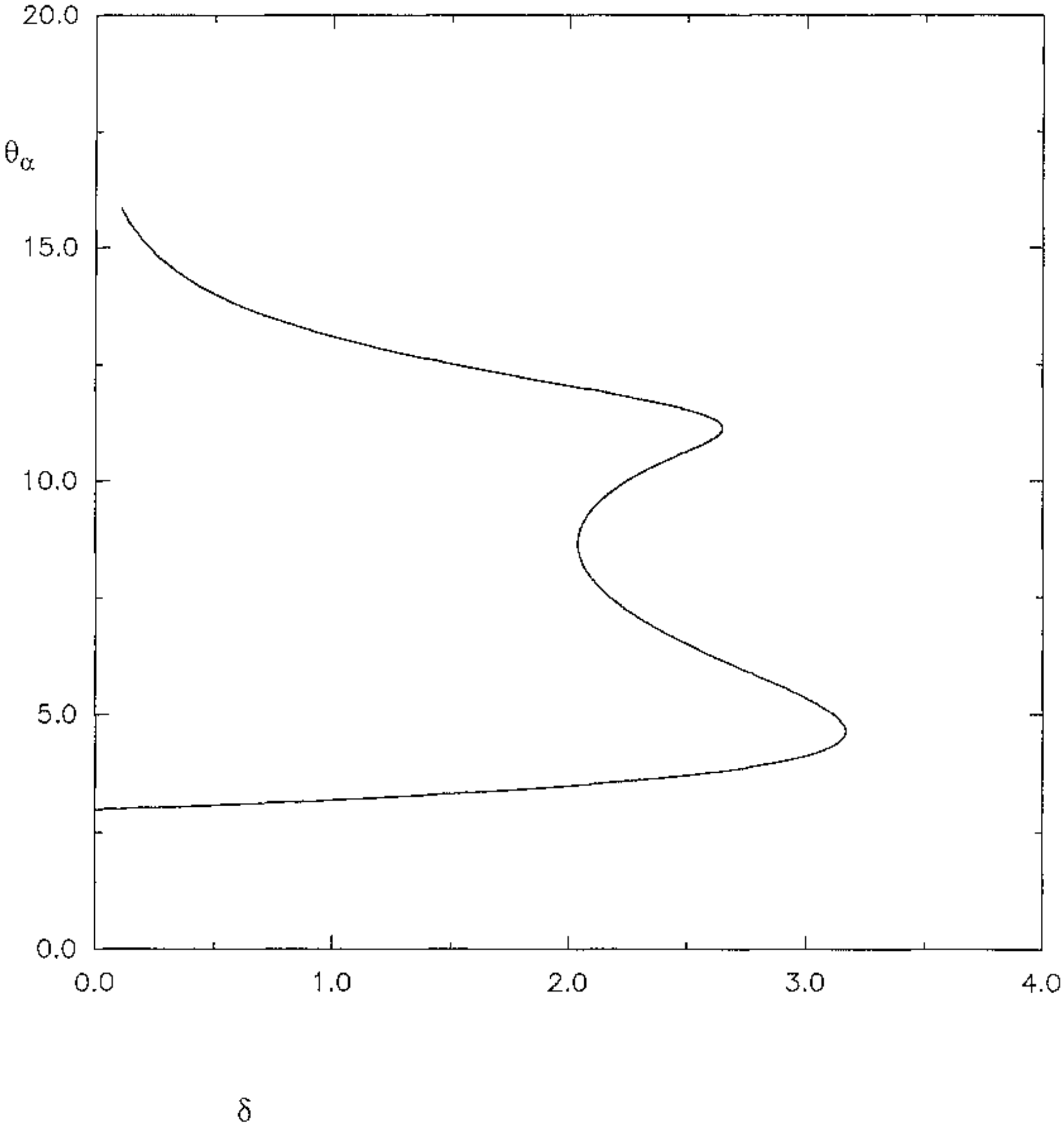


Figure D.2.3

A	= -300
Bi	= ∞
α	= .01

Bifurcation Diagram.

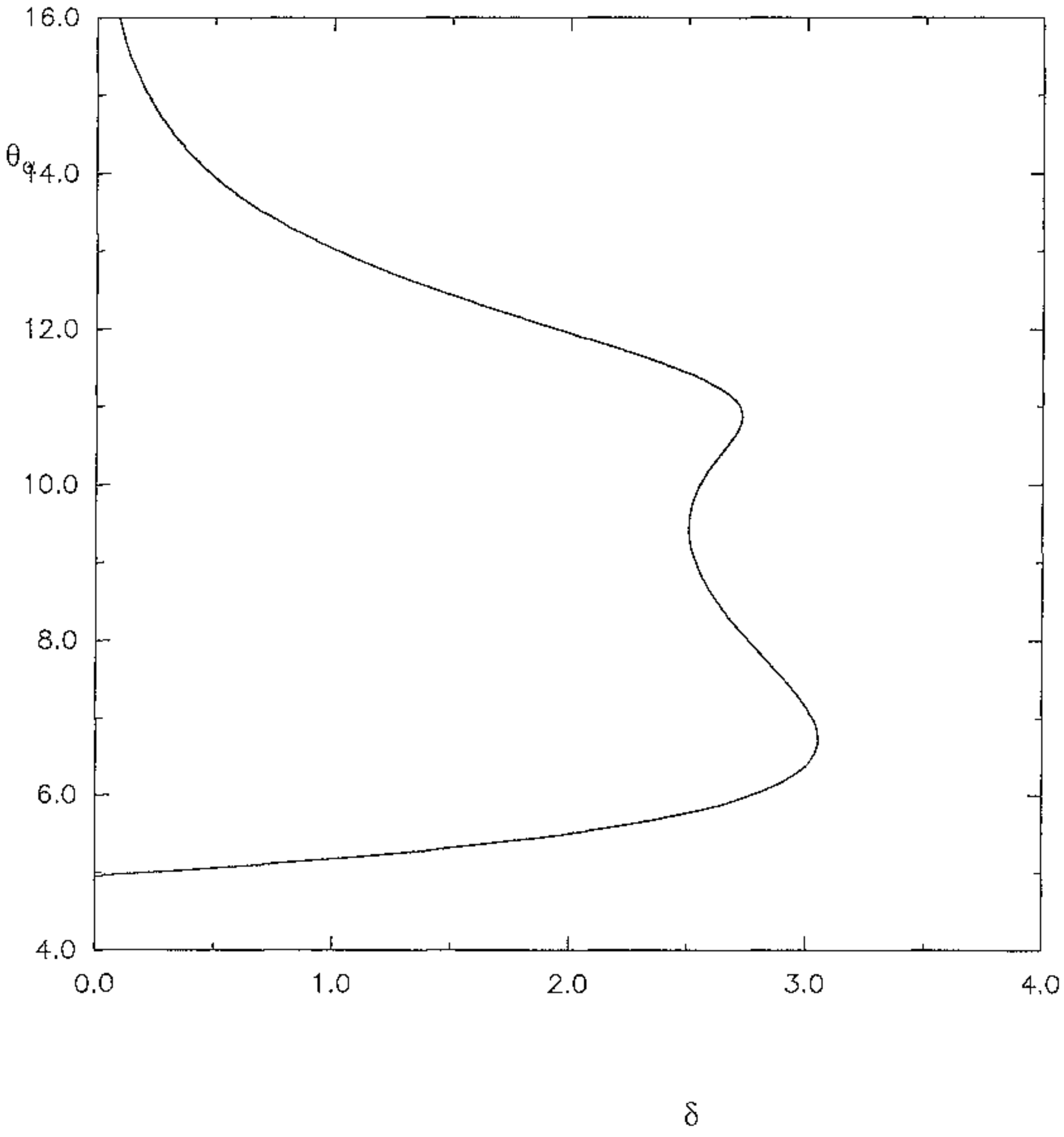


Figure D.2.4

A	= -500
Bi	= ∞
α	= .01

Bifurcation Diagram.

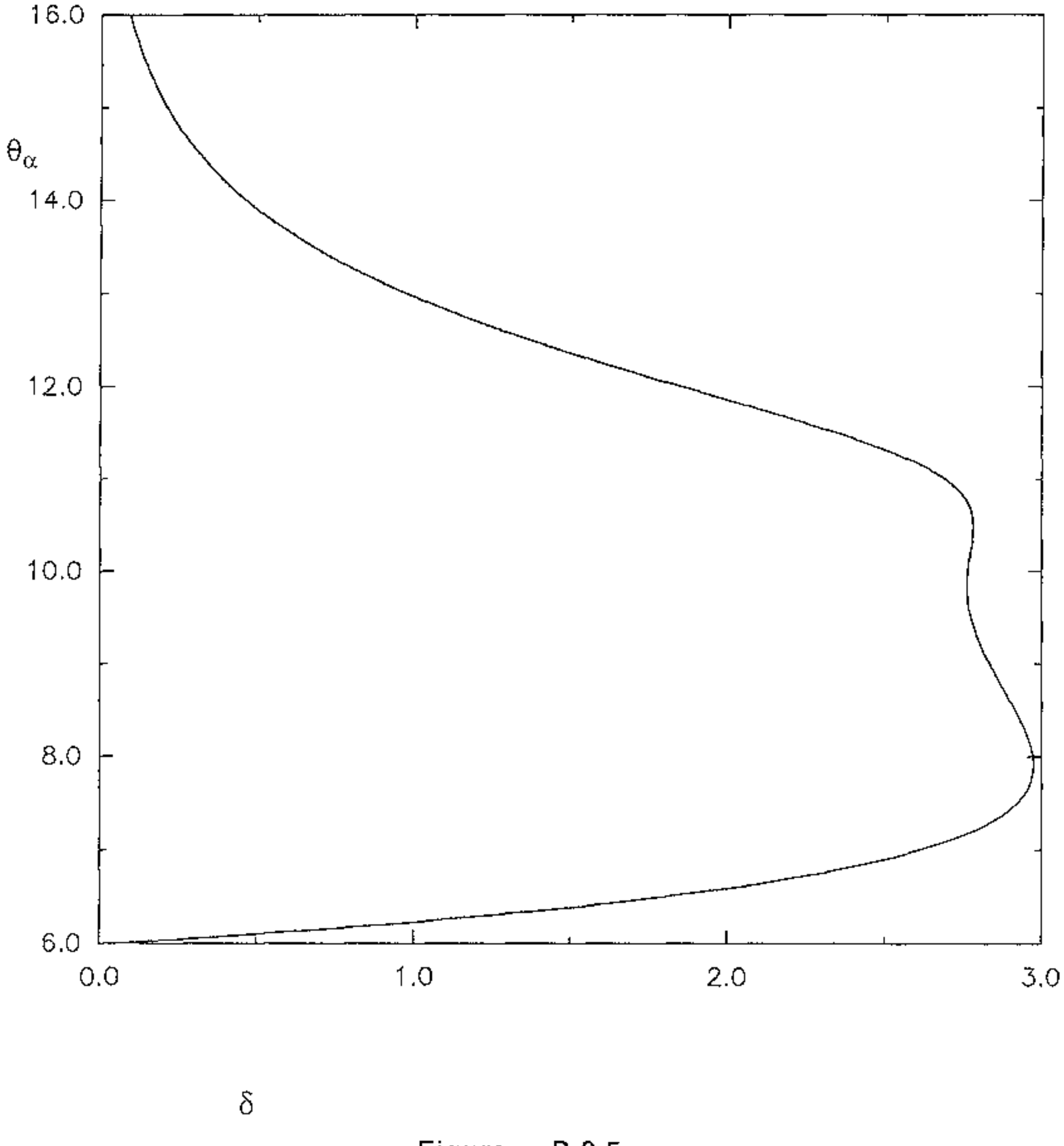


Figure D.2.5

A = -600
Bi = ∞
α = .01

Bifurcation Diagram.

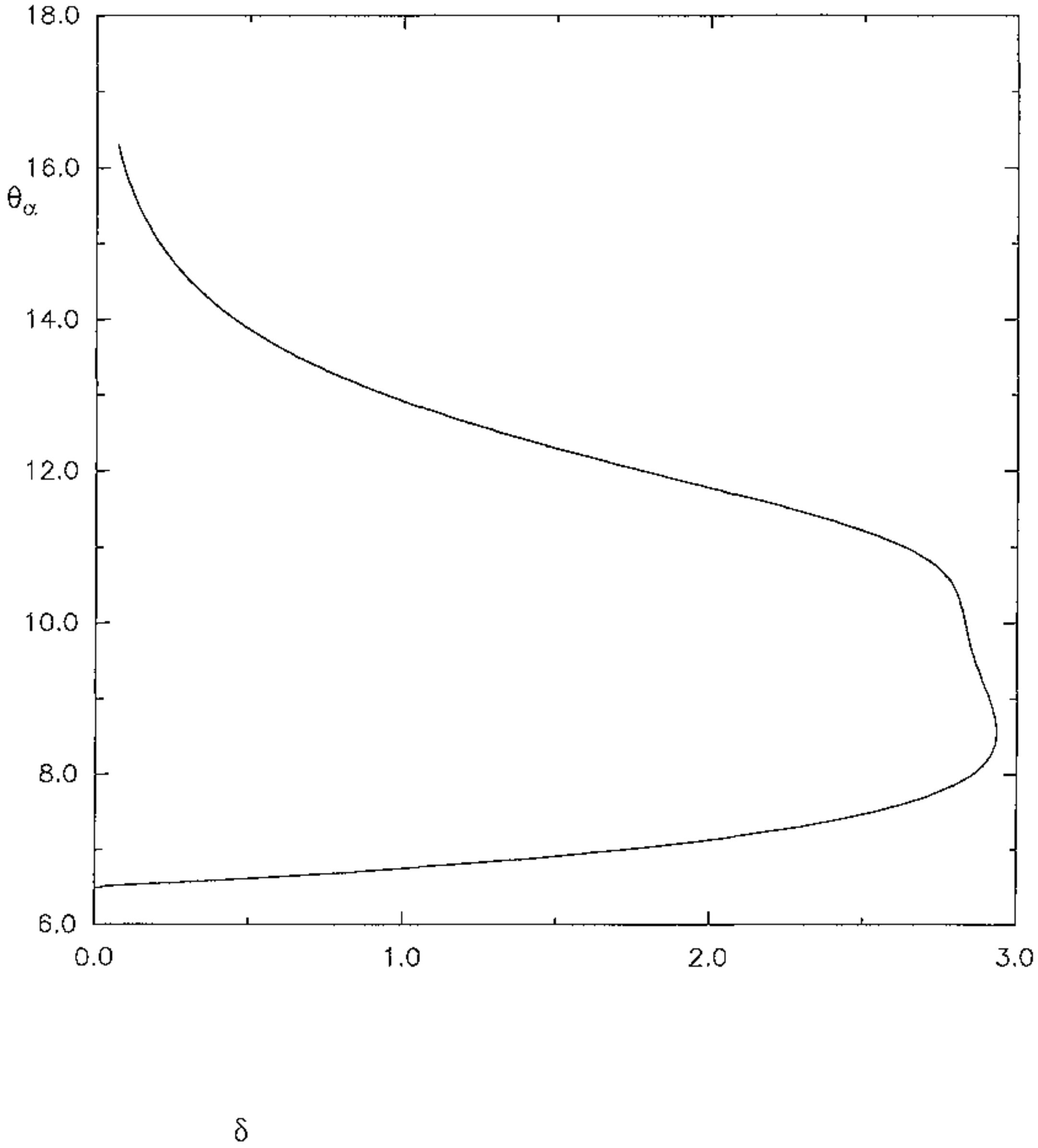


Figure D.2.6

A	= -650
Bi	= ∞
α	= .01

Bifurcation Diagram.

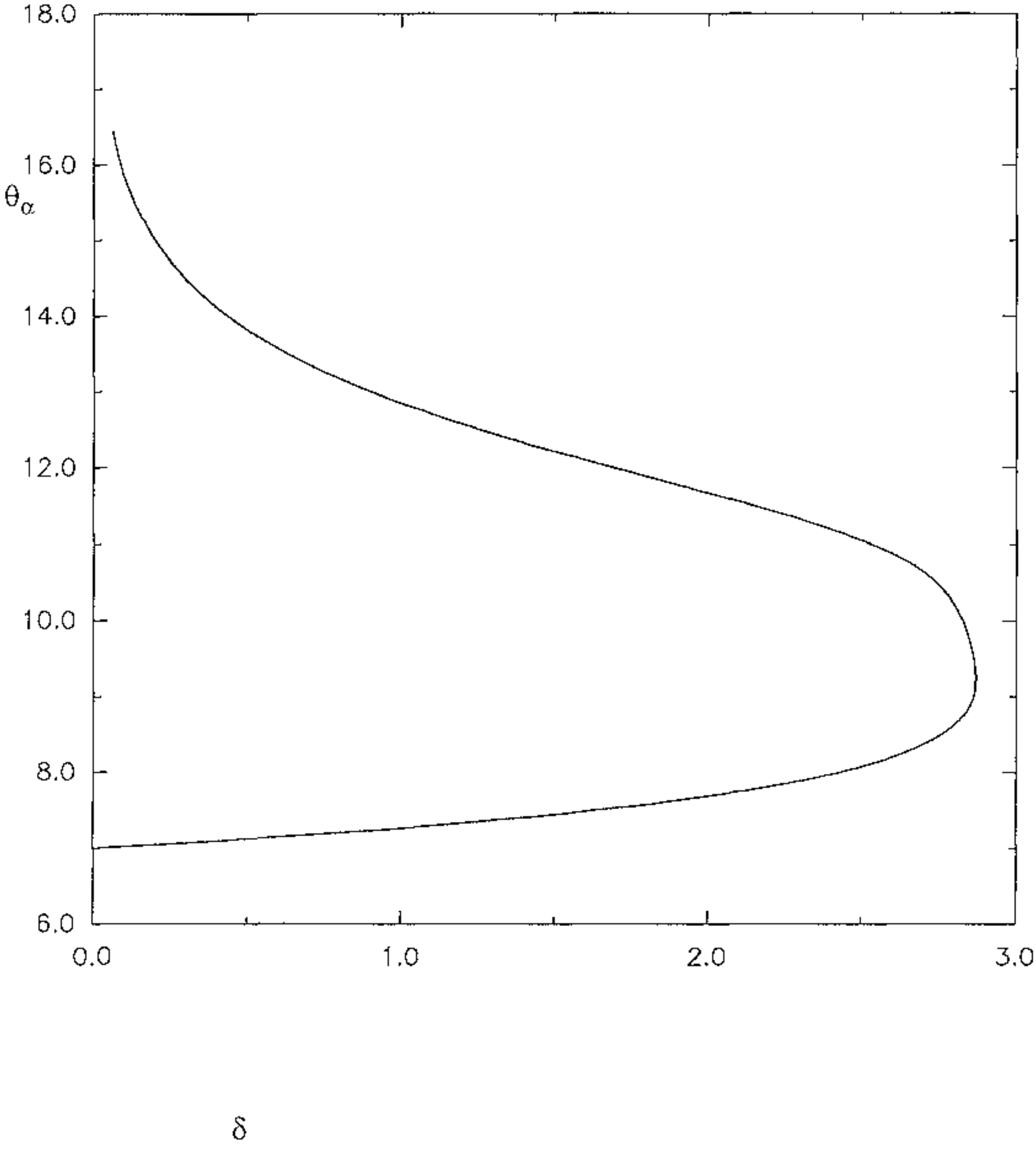


Figure D.2.7

A = -700
Bi = ∞
α = .01

Bifurcation Diagram.

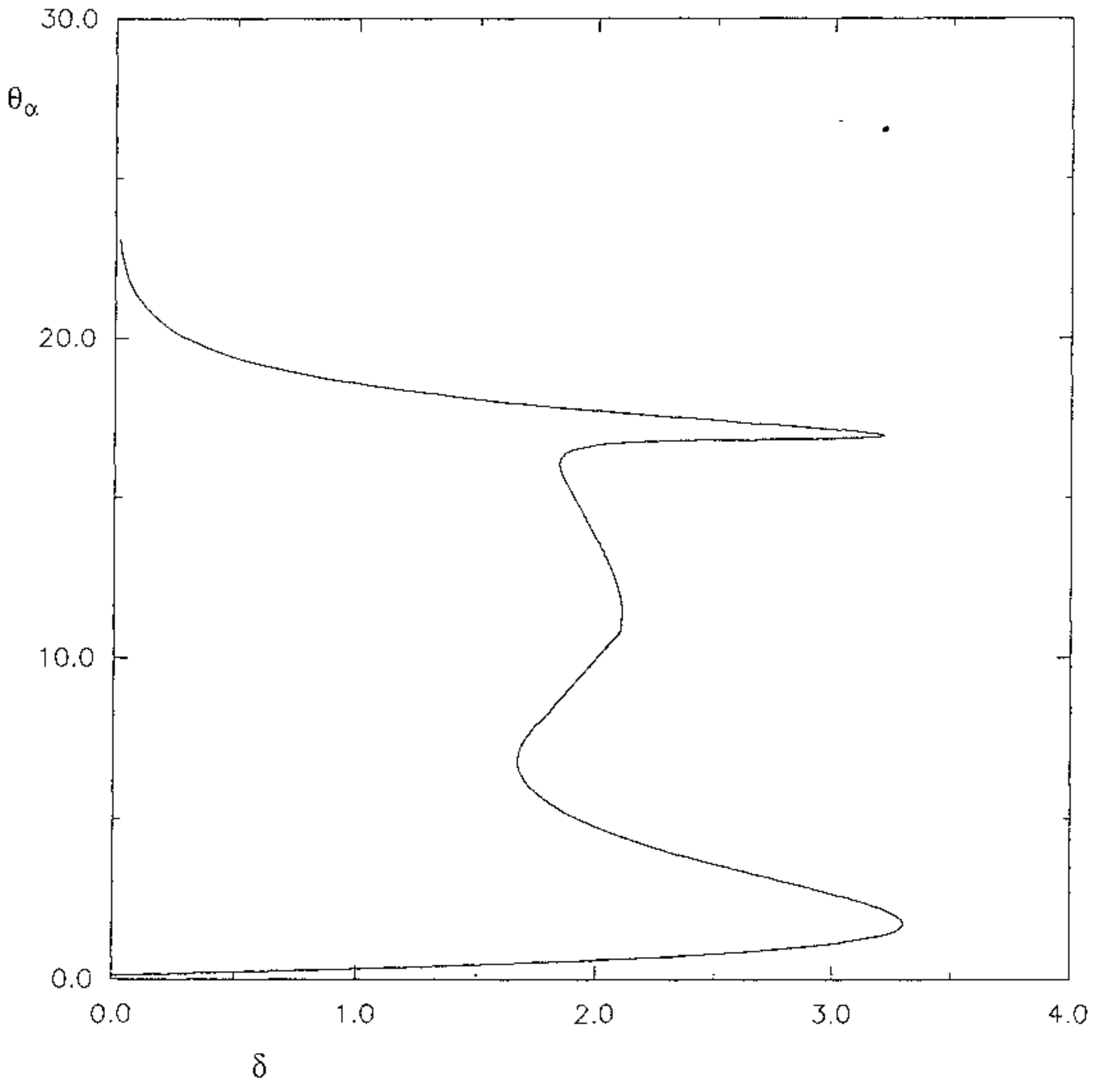


Figure D.3.0

A	= 0
Bi	= ∞
α	=.001

Bifurcation Diagram.

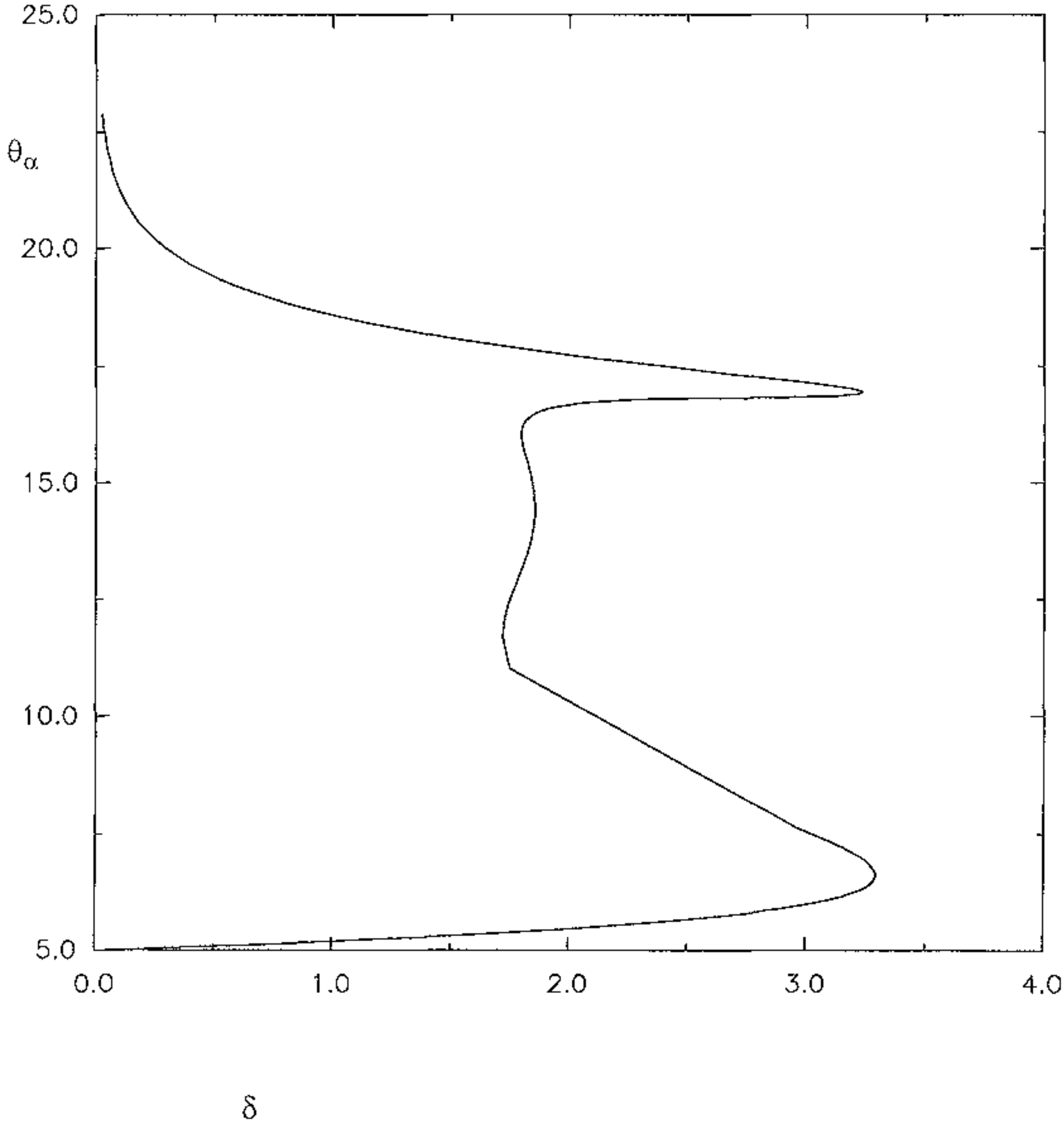


Figure D.3.1

A =-5000
Bi = ∞
α = .001

Bifurcation Diagram.

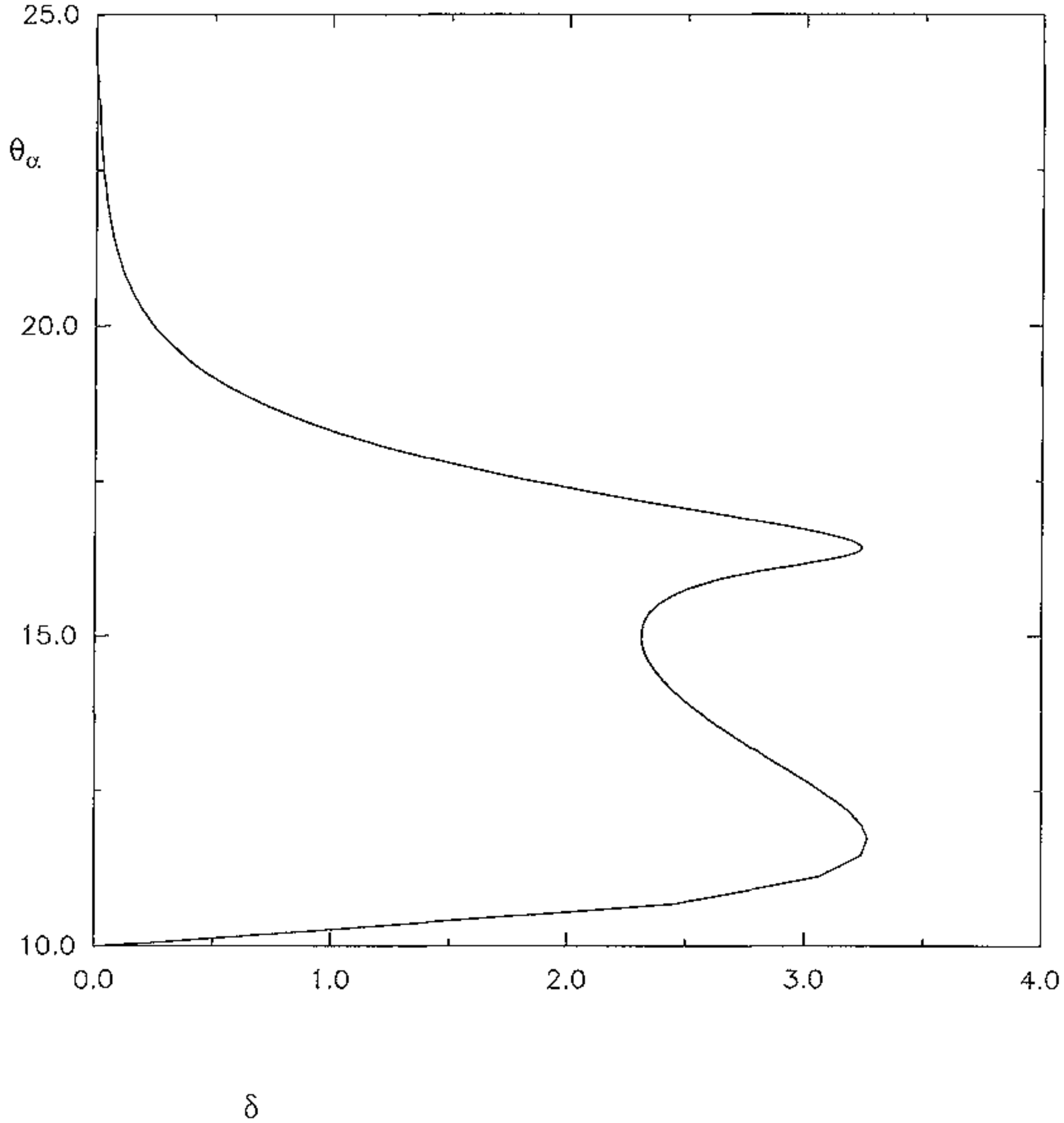


Figure D.3.2

A	=-10000
Bi	= ∞
α	= .001

Bifurcation Diagram.

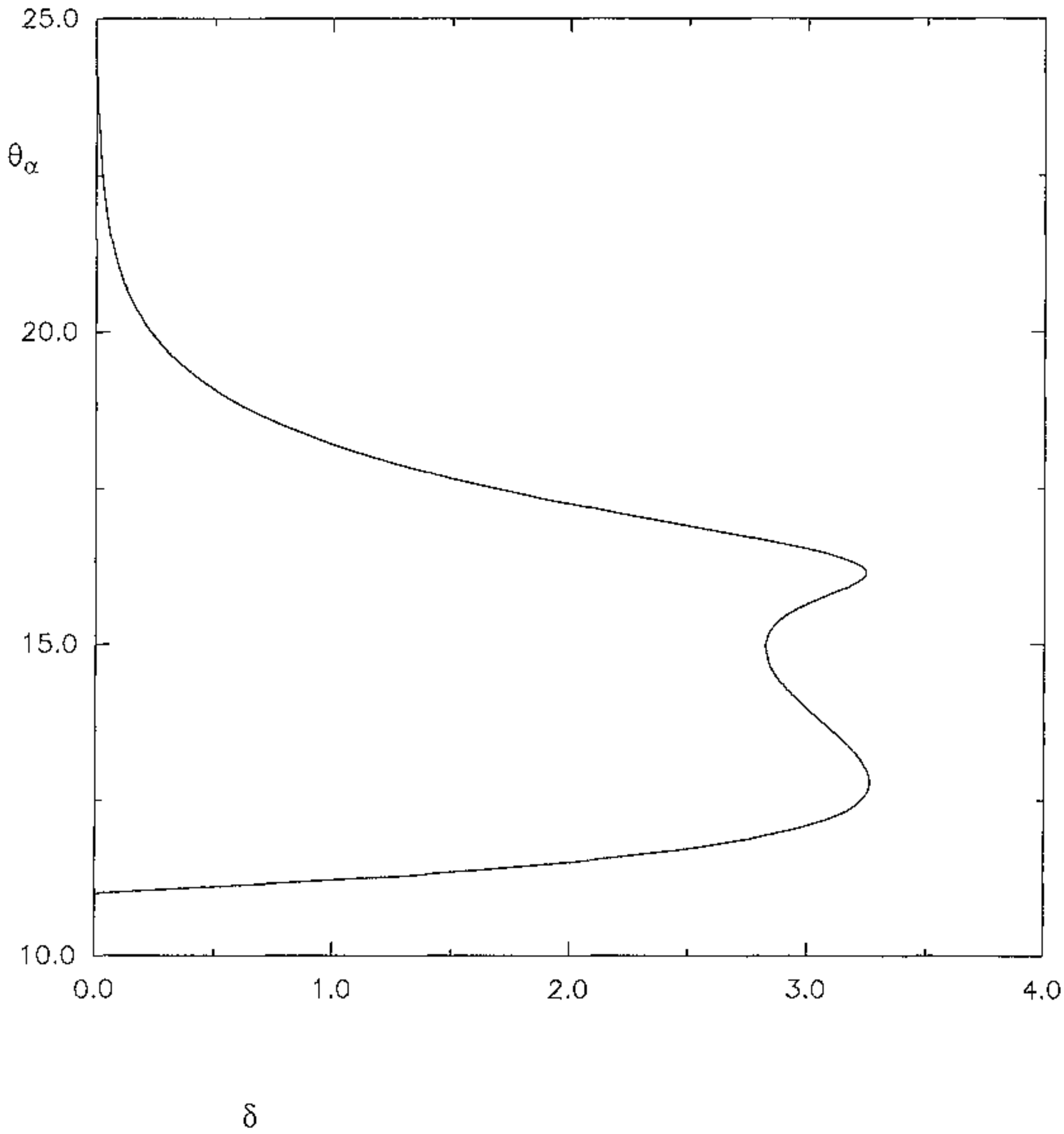


Figure D.3.3

A =-11000
Bi = ∞
α = .001

Bifurcation Diagram.

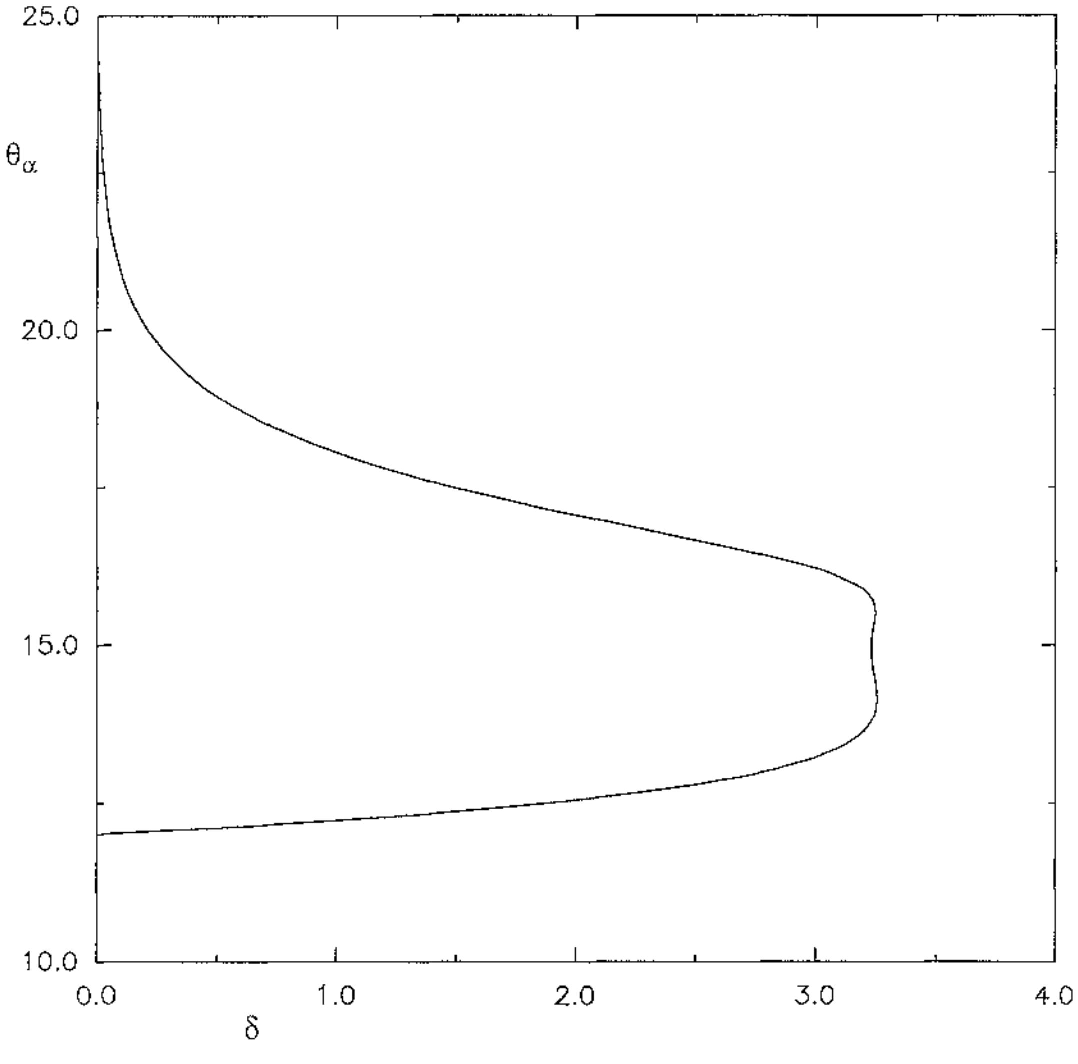
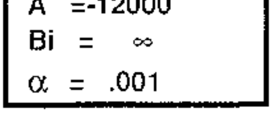


Figure D.3.4



Bifurcation Diagram.

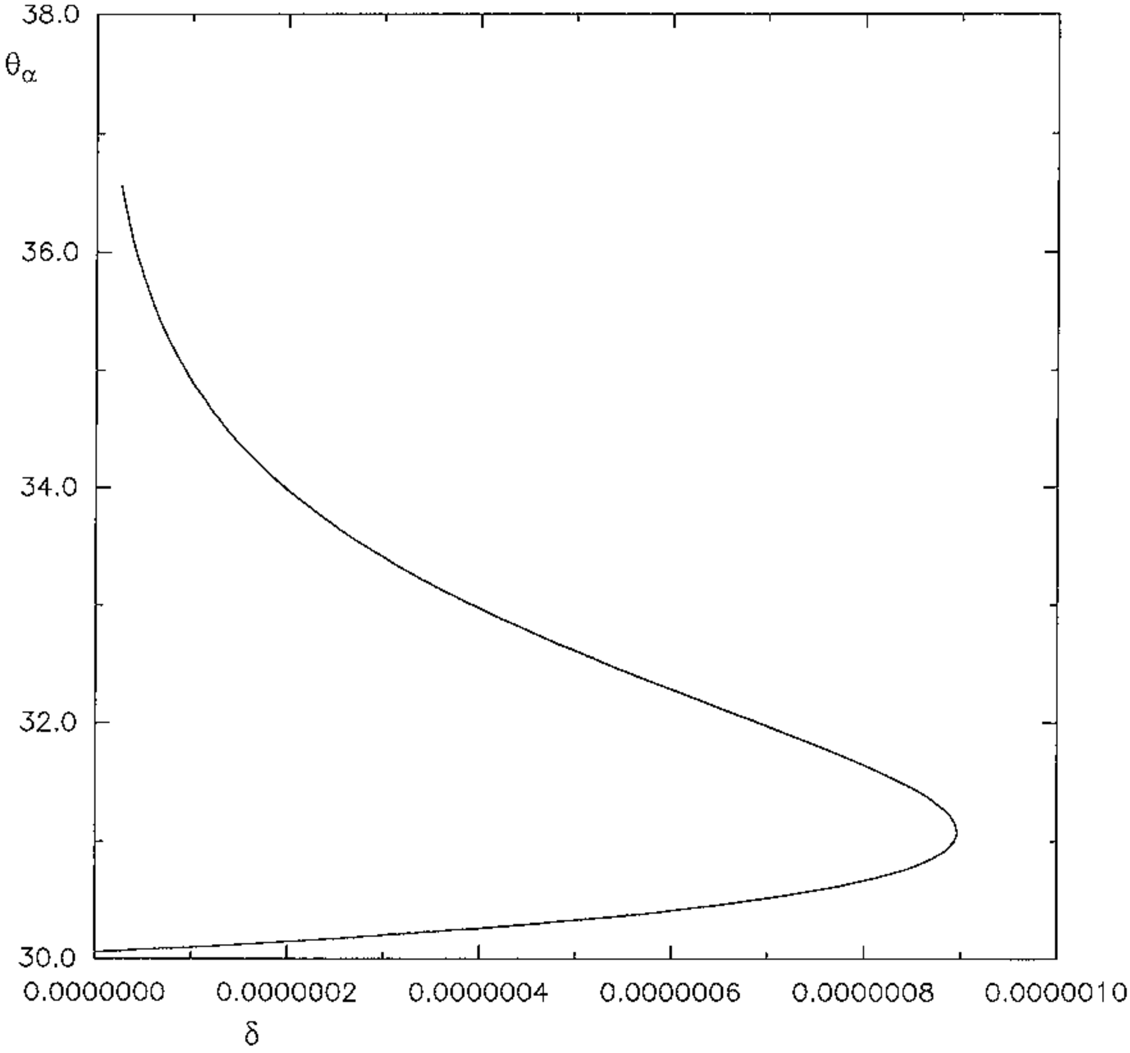


Figure D.3.5

A	=-30000
Bi	= ∞
α	= .001