STABILITY AND BIFURCATION PHENOMENA IN CHEMICAL REACTOR THEORY

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ABSTRACT

We investigate the nonlinear parabolic equations of chemical tubular reactors. For various ranges of certain physical parameters perturbation procedures are applied to reduce the problem to various questions involving periodicity of solutions of ordinary and partial differential equations, multiplicity of solutions, bifurcation phenomena, existence, and stability of solutions. The main results include an investigation of the implications of the direction and stability of bifurcating branches and the multiplicity of periodic solutions for nonlinear diffusive systems. For the non-adiabatic chemical reactors the response diagrams are given for all relevant ranges of all physical parameters.

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Chapter 1

INTRODUCTION

Section 1. Introduction - Physical Motivation

The nonlinear diffusion processes which we investigate are of the type that are mathematically expressed as

$$\text{(1.1.1)}\qquad \begin{aligned} \frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} &= h\,(T, \frac{\partial T}{\partial x}, C; \underset{\sim}{\lambda})\,, \\ \frac{\partial C}{\partial t} - \alpha \frac{\partial^2 C}{\partial x^2} &= g(C, \frac{\partial C}{\partial x}, T, \underset{\sim}{\lambda})\,, \end{aligned}$$

and a set of initial and boundary conditions where $\underset{\sim}{\lambda}$ is a vector of physical parameters in the problem and h and g depend nonlinearly on T and C. This type of nonlinear diffusion process is a commonly occurring one in chemical reactor theory where the main objective is to answer the questions of existence, multiplicity, stability, and oscillatory behavior of the solutions as some physical parameter in the problem is changed.

The particular problem from chemical reactor theory of the form (1.1.1) which we investigate is the problem of a simple, first order, exothermic reaction processed in a nonadiabatic tubular reactor. The governing equations for axial heat and mass transfer in this problem may be expressed in the dimensionless form (see H. Hlavacek and H. Hofmann [12]):

$$\frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} - \frac{1}{Pe}\frac{\partial^2 T}{\partial x^2} = -\beta(T - T_c) + DaBf(T,C),$$

$$\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} - \frac{1}{Pe}\frac{\partial^2 C}{\partial x^2} = Daf(T,C),$$

(1.1.2) $$\frac{\partial T}{\partial x}(0,t) = PeT(0,t), \quad \frac{\partial C}{\partial x}(0,t) = PeC(0,t),$$

$$\frac{\partial T}{\partial x}(1,t) = 0, \qquad \frac{\partial C}{\partial x}(1,t) = 0,$$

$$T(x,0) = \phi(x), \qquad C(x,0) = \psi(x).$$

The nonlinearity $f(T,C)$ is given by

(1.1.3) $$f(T,C) = (1 - C)\exp\left(\frac{T}{1 + \frac{1}{\gamma}T}\right) .$$

T_c is a constant and Pe, β, B, Da, and $\frac{1}{\gamma}$ are nonnegative constants. T is a dimensionless temperature while C is the conversion or product concentration. The term $-\beta(T-T_c)$ represents heat removed from the reactor due to the heat exchanger surrounding the reactor and $DaBf(T,C)$ the heat added to the reactor due to the chemical reaction.

For the case $\beta = 0$ the investigation of the time independent solutions of (1.1.2) reduces to the study of

$$\frac{1}{Pe}\frac{\partial^2 T}{\partial x^2} - \frac{\partial T}{\partial x} = Da\,(B - T)\exp\left(\frac{T}{1 + \frac{1}{\gamma}T}\right),$$

(1.1.4) $$\frac{\partial T}{\partial x}(0) = PeT(0),$$

$$\frac{\partial T}{\partial x}(1) = 0$$

where the concentration, C, is given by $C = T/B$. The questions of multiplicity and stability were investigated by Cohen [4].

For $\beta > 0$ the problem (1.1.2) has been investigated numerically by C. R. McGowin and D. D. Perlmutter [16], V. Hlavacek and H. Hofmann [13], and V. Hlavacek, H. Hofmann, and M. Kubicek [14]. References to other literature on problem (1.1.2) can be found in these references. The existence of one, three, and five steady states and the existence of oscillatory solutions are reported. Physically, the oscillatory behavior seems to occur because of the balance or imbalance of the heat added through $DaBf(T, C)$ and heat removed through $-\beta(T - T_c)$ in the system (1.1.2). We shall show for certain combinations of the parameters this is indeed the case.

Our investigation of the problem (1.1.2) will be for the case $0 < Pe \ll 1$ which means physically that the diffusion coefficients are "large." We will treat all constant values of β, B, Da, and T_c of physical interest. By the formal methods of singular perturbations we show in Chapter 2 that the problem (1.1.2) can be reduced to the study of a far more tractable set of nonlinear ordinary differential equations.

This set of nonlinear ordinary differential equations governs the enthalpy and mass balances for a simple, first order, exothermic reaction being processed in a CSTR (continuously stirred tank reactor). Mathematically, this problem can be written in the dimensionless form (see V. Hlavacek, M. Kubicek, J. Jelinek [11]):

$$\frac{dx_1}{dt} = -\lambda x_1 - \beta(x_1 - x_c) + DaBf(x_1, x_2),$$

(1.1.5) $$\frac{dx_2}{dt} = -\lambda x_2 + Daf(x_1, x_2),$$

$$x_1(0) = A_o, \quad \text{and} \quad x_2(0) = B_o,$$

where x_1 is the dimensionless temperature, x_2 is the dimensionless concentration of the product, and $x_c = T_c$. The variable λ represents a recycle factor with $0 < \lambda \leq 1$ where $\lambda = 1$ means no recycle. As for the tubular reactor problem, the term $DaBf(x_1, x_2)$ represents heat added and $-\beta(x_1 - x_c)$ represents heat removed. x_c is the temperature of the heat exchanger and $f(x_1, x_2)$ is the same as in (1.1.3) for $x_1 = T$ and $x_2 = C$.

The investigation of the system (1.1.5) has been quite intensive in the last ten years culminating with the article by V. Hlavacek, M. Kubicek, and J. Jelinek [11]. The pertinent chemical engineering literature is given there. It is known that changing the feed temperature can cause oscillations large enough to make the produce undesirable. These oscillations can also cause the temperature to surpass the limitations of the reactor (see R. Luus and L. Lapidus [15]). Thus, the question of how these large oscillations occur is important from the applied point of view. An answer is given in Section 5.5 and Chapter 6.

The problem of a chemical reaction along a long wire is another problem which has been intensely investigated in the last decade by Frank-Kameneteskii[7] and M. F. Cardoso and D. Luss [21]. We include this example not only because the governing equations are identical for most parameter ranges with the equations of the CSTR under an appropriate change of variables but also to show how the oscillatory behavior (flickering) is also present in the constant flow system during the ignition process. Recently, D. Luss and M. A. Erwin [20] concluded that these oscillations are possibly due to the unsteady flow velocity along the wire. We are able to show that this same flickering phenomena can be accomplished in a constant flow system. The mechanism by which we achieve the ignition or extinction process is through a change in the temperature of the gas surrounding the wire as opposed to changing the flow velocity used by Luss. For the CSTR, this is equivalent to a change in the feed temperature when the bath temperature and the feed temperature are the same. We shall, however, examine only the CSTR.

Section 2. Introduction - Mathematical Questions

We should point out that the techniques we use to study the specific problem (1.1.2) apply also to the study of the more general nonlinear diffusion problem of the form (1.1.1).

The equivalence between the tubular reactor and the CSTR is a problem that has been intensely investigated. The paper by V. Hlavacek and H. Hofmann [12] list most of the chemical reactor literature. The technique ascribed to this equivalence is called the "lumping approach" [12]. We use a singular perturbations procedure in Chapter 2 to show that the temperature $T(x,t)$ and concentration $C(x,t)$ are given formally by

$$(1.2.1)\qquad T(x,t) \sim x_1(t) + \sum_{n=1}^{\infty} A_n \exp\left(-n^2\pi^2\frac{t}{\epsilon}\right) \cos n\pi x + O(\epsilon) \quad \text{as } \epsilon \to 0,$$

$$(1.2.2)\qquad C(x,t) \sim x_2(t) + \sum_{n=1}^{\infty} B_n \exp\left(-n^2\pi^2\frac{t}{\epsilon}\right) \cos n\pi x + O(\epsilon) \quad \text{as } \epsilon \to 0,$$

where

$$(1.2.3)\qquad A_o = \int_0^1 \phi(\xi)\, d\xi, \qquad A_n = 2\int_0^1 \phi(\xi) \cos n\pi\xi \, d\xi,$$

$$(1.2.4)\qquad B_o = \int_0^1 \psi(\xi)\, d\xi, \qquad B_n = 2\int_0^1 \psi(\xi) \cos n\pi\xi \, d\xi,$$

$$(1.2.5)\qquad x_1(0) = A_o, \qquad x_2(0) = B_o,$$

and $x_1(t)$ and $x_2(t)$ satisfy the equation (1.1.5) for the CSTR with $\lambda = 1$. We have set $T_c \equiv x_c$ in these equations. It is in this sense that the two are equivalent.

The remainder of the work focuses on the study of the CSTR. In Chapter 3 we dispose of the questions of uniqueness, boundedness, and existence in the large. The "long time" behavior of the solution of the problem (1.1.5) is characterized in Theorem 3.2.1. In Section 2.2 we discuss the approximation

$$\exp\left(\frac{T}{1+\frac{1}{\gamma}T}\right) \approx \exp T$$

and use this in Chapters 4 through 6.

The main results in this thesis begin in Chapter 4 where we give the necessary and sufficient conditions for multiplicity, stability, index, and type of the critical point (steady state). The main achievement here is in Section 5 where we give an exhaustive classification of the relations between stability and multiplicity. We believe that we have some new and surprising results here. In the last section we invoke results of Chapter 3 to prove existence and nonexistence of periodic solutions.

Chapter 5 contains the major achievements of this thesis. We prove that when there is a change in the stability of the critical point of index $+1$ as the parameter Da varies that there is an associated bifurcation of periodic orbits. The stability of these bifurcating periodic orbits and the connection with the direction of bifurcation are rigorously established. We shall see that the direction of a bifurcating branch of periodic orbits and its stability can have some surprising implications concerning both the number of periodic orbits and the stability of various segments of the response diagram for the reactor process.

In Chapter 6 we exploit the direction of bifurcation and its connection with oscillatory instabilities occurring in reactor problems. We first discuss the classical "jump" phenomena and then show two new types of "jump" phenomena in which there is a "jump" into oscillatory steady states.

Chapter 2

THE REDUCED PROBLEM AND THE EXPONENTIAL APPROXIMATION

Section 1. Introduction

In Section 2 we give the singular perturbation procedure which reduces the tubular reactor problem to the consideration of the CSTR through equation (1.2.1) and (1.2.2). In Section 3 we briefly discuss the exponential approximation used so extensively in the literature and here.

Section 2. The Singular Perturbation Procedure

By a singular perturbation procedure we now reduce the problem of the tubular reactor to considerations of the CSTR. This procedure is for small Pecket numbers.

Set $Pe = \epsilon$. The tubular reactor problem discussed in Chapter 1 is formulated mathematically as

$$T_{,t} - \frac{1}{\epsilon} T_{,xx} + T_{,x} = -\beta(T - T_c) + DaB(1 - C) \exp\left(\frac{T}{1 + \frac{1}{\gamma}T}\right),$$

$$C_{,t} - \frac{1}{\epsilon} C_{,xx} + C_{,x} = Da(1 - C) \exp\left(\frac{T}{1 + \frac{1}{\gamma}T}\right),$$

(2.2.1)
$$T_{,x}(0,t) = \epsilon T(0,t), \qquad T_{,x}(1,t) = 0,$$

$$C_{,x}(0,t) = \epsilon C(0,t), \qquad C_{,x}(1,t) = 0,$$

$$T(x,0) = \phi(x), \qquad C(x,0) = \psi(x).$$

Assume $0 < \epsilon << 1$. By the methods of singular perturbations (see Cole [5]) there is an initial boundary layer at $t = 0$ for $0 \leq x \leq 1$ of thickness $O(\epsilon)$. Away from this layer the asymptotic expansion (outer expansion) is of the form

(2.2.2) $$T(x,t) \sim \sum_{n=0}^{\infty} T_n(x,t)\epsilon^n \quad \text{and} \quad C(x,t) \sim \sum_{n=0}^{\infty} C_n(x,t)\epsilon^n .$$

By substituting (2.2.2) into (2.2.1) and equating coefficients of the like powers of ϵ, we generate a sequence of problems which to first order in ϵ is given by

(2.2.3) $$\begin{cases} \dfrac{\partial^2 T_o}{\partial x^2} = 0 , & \dfrac{\partial^2 C_o}{\partial x^2} = 0 , \\ \dfrac{\partial T_o}{\partial x}(0,t) = 0 , & \dfrac{\partial C_o}{\partial x}(0,t) = 0 , \\ \dfrac{\partial T_o}{\partial x}(1,t) = 0 , & \dfrac{\partial C_o}{\partial x}(1,t) = 0 , \end{cases}$$

(2.2.4) $$\begin{cases} \dfrac{\partial^2 T_1}{\partial x^2} = \dfrac{\partial T_o}{\partial t} + \dfrac{\partial T_o}{\partial x} + \beta(T_o - T_c) - DaB(1-C_o)\exp\left(\dfrac{T_o}{1+\frac{1}{\gamma}T_o}\right), \\ \dfrac{\partial^2 C_1}{\partial x^2} = \dfrac{\partial C_o}{\partial t} + \dfrac{\partial C_o}{\partial x} - Da(1-C_o)\exp\left(\dfrac{T_o}{1+\frac{1}{\gamma}T_o}\right), \\ \dfrac{\partial T_1}{\partial x}(0,t) = T_o(0,t) , \qquad \dfrac{\partial C_1}{\partial x}(0,t) = C_o(0,t) , \\ \dfrac{\partial T_1}{\partial x}(1,t) = 0 , \qquad \dfrac{\partial C_1}{\partial x}(1,t) = 0 . \end{cases}$$

The solution of problem (2.2.3) is

$$T_o(x,t) = x_1(t) \qquad \text{and} \qquad C_o(x,t) = x_2(t) \ ,$$

where at this stage $x_1(t)$ and $x_2(t)$ are arbitrary functions of time. To generate a self-consistent perturbation scheme, the functions $x_1(t)$ and $x_2(t)$ must be determined from a consistency condition in problem (2.2.4).

We now proceed to solve problem (2.2.4). The problem (2.2.4) is solvable only if a consistency condition is satisfied (see Stakgold [18]). This consistency condition is equivalent to integrating the equations in (2.2.4) from zero to one and using the boundary conditions. Since $T_o(x,t) = x_1(t)$ and $C_o(x,t) = x_2(t)$, this yields

(2.2.5)
$$-x_1(t) = \frac{dx_1}{dt} + \beta(x_1 - T_c) - DaB(1-x_2)\exp\left(\frac{x_1}{1+\frac{1}{\gamma}x_1}\right),$$
$$-x_2(t) = \frac{dx_2}{dt} - Da(1-x_2)\exp\left(\frac{x_1}{1+\frac{1}{\gamma}x_1}\right),$$

or, equivalently,

(2.2.6)
$$\frac{dx_1}{dt} = -x_1 - \beta(x_1 - T_c) + DaB(1-x_2)\exp\left(\frac{x_1}{1+\frac{1}{\gamma}x_1}\right),$$
$$\frac{dx_2}{dt} = -x_2 + Da(1-x_2)\exp\left(\frac{x_1}{1+\frac{1}{\gamma}x_1}\right).$$

The solution to problem (2.2.4) is then

$$T_1(x,t) = -\frac{1}{2}(x-1)^2 x_1(t) + x_3(t) ,$$

(2.2.7)

$$C_1(x,t) = -\frac{1}{2}(x-1)^2 x_2(t) + x_4(t) ,$$

where x_3 and x_4 are arbitrary functions of time and must be determined from a consistency condition in the $O(\epsilon^2)$ problem. At this stage we determine the initial conditions for the problem (2.2.6).

Make the change of variables $\tau = t/\epsilon$; then the problem (2.2.1) is

$$T_{,\tau} - T_{,xx} = \epsilon\left(-T_{,x} - \beta(T-T_c) + DaB(1-C)\exp\left(\frac{T}{1+\frac{1}{\gamma}T}\right)\right) ,$$

$$C_{,\tau} - C_{,xx} = \epsilon\left(-C_{,x} + Da(1-C)\exp\left(\frac{T}{1+\frac{1}{\gamma}T}\right)\right) ,$$

(2.2.8)

$$T_{,x}(0,\epsilon\tau) = \epsilon T(0,\epsilon\tau), \qquad C_{,x}(0,\epsilon\tau) = \epsilon C(0,\epsilon\tau) ,$$

$$T_{,x}(1,\epsilon\tau) = 0 \qquad C_{,x}(1,\epsilon\tau) = 0 ,$$

$$T(x,0) = \phi(x), \quad \text{and} \quad C(x,0) = \psi(x) .$$

The inner asymptotic expansion (the asymptotic expansion in the boundary layer) is

$$T(x,\epsilon\tau) \sim \sum_{n=0}^{\infty} \overline{T}_n(x,\tau)\epsilon^n \quad \text{and} \quad C(x,\epsilon\tau) \sim \sum_{n=0}^{\infty} C_n(x,\tau)\epsilon^n .$$

Within first order in ϵ we obtain

(2.2.9)
$$\frac{\partial \overline{T}_o}{\partial \tau} - \frac{\partial \overline{T}_o}{\partial x^2} = 0 , \qquad \frac{\partial \overline{C}_o}{\partial \tau} - \frac{\partial \overline{C}_o}{\partial x^2} = 0 ,$$
$$\frac{\partial \overline{T}_o}{\partial x}(0,\tau) = 0, \qquad \frac{\partial \overline{C}_o}{\partial x}(0,\tau) = 0 ,$$
$$\frac{\partial \overline{T}_o}{\partial x}(1,\tau) = 0 , \qquad \frac{\partial \overline{C}_o}{\partial x}(1,\tau) = 0 ,$$
$$\overline{T}_o(x,0) = \phi(x) , \qquad \overline{C}_o(x,0) = \psi(x) .$$

The solution of this linear diffusion problem is

(2.2.10)
$$\overline{T}_o(x,\tau) = A_o + \sum_{n=1}^{\infty} A_n \exp(-n^2\pi^2\tau) \cos n\pi x ,$$
$$\overline{C}_o(x,\tau) = B_o + \sum_{n=1}^{\infty} B_n \exp(-n^2\pi^2\tau) \cos n\pi x ,$$

where

(2.2.11)
$$A_o = \int_0^1 \phi(\xi)\, d\xi , \qquad A_n = 2\int_0^1 \phi(\xi) \cos n\pi\xi\, d\xi ,$$
$$B_o = \int_0^1 \psi(\xi)\, d\xi , \qquad B_n = 2\int_0^1 \psi(\xi) \cos n\pi\xi\, d\xi .$$

To match the inner expansion and outer expansion, it is required that

(3.2.12)
$$\lim_{t \to 0^+} T_o(x,t) = \lim_{\tau \to \infty} \overline{T}_o(x,\tau) \qquad \text{and}$$
$$\lim_{t \to 0^+} C_o(x,t) = \lim_{\tau \to \infty} \overline{C}_o(x,\tau) .$$

Therefore, we obtain the following initial conditions for the problem (2.2.6)

$$x_1(0) = A_o = \int_0^1 \phi(\xi)\, d\xi \quad \text{and}$$

(2.2.13)

$$x_2(0) = B_o = \int_0^1 \psi(\xi)\, d\xi \ .$$

Subtracting off that part of the expansion common to both expansions [5], we obtain an expansion which is uniformly valid within first order in ϵ:

$$T(x,t) \sim x_1(t) + \sum_{n=1}^{\infty} A_n \exp\left(-n^2\pi^2 \frac{t}{\epsilon}\right) \cos n\pi x + O(\epsilon) \quad \text{as } \epsilon \to 0,$$

(2.2.14)

$$C(x,t) \sim x_2(t) + \sum_{n=1}^{\infty} B_n \exp\left(-n^2\pi^2 \frac{t}{\epsilon}\right) \cos n\pi x + O(\epsilon) \quad \text{as } \epsilon \to 0,$$

where $x_1(t)$ and $x_2(t)$ satisfy (2.2.6) and (2.2.13) and A_n and B_n are given by (2.2.11).

Section 3. The Exponential Approximation

In Chapters 4 through 6 we use the exponential approximation

$$\exp\left(\frac{T}{1 + \frac{1}{\gamma} T}\right) \approx \exp(T)$$

which is used so extensively in the chemical engineering literature (for example, see V. Hlavacek and H. Hofmann [12], V. Hlavacek, M. Kubicek, and J. Jelinek [11], and the references in these two papers). A discussion of this approximation can be found in Frank-Kamenetskii [7]. The main support for this approximation is that

$1/\gamma$ is small so that the qualitative features for both forms should be the same. We use this approximation because without it the algebra would become hopelessly complicated and we wish to see what qualitative features this approximation produces.

Chapter 3

PROPERTIES OF THE SOLUTION OF THE REDUCED PROBLEM

Section 1. Existence, Uniqueness, and Boundedness

In this chapter we present all the theoretical results conerning questions of existence, uniqueness, and boundedness of the solutions of the CSTR problem whenever the initial conditions are physically meaningful. In Section 2 we characterize the "long-time" behavior of these solutions. All the results in this chapter apply to a CSTR in which the reaction is simple but of arbitrary order regardless of the exponential approximation made in the Arrhenius rate constant. The main results are contained in Theorems 3.1.1 and 3.2.1. The information is necessary for our later analysis, but the results and proofs are relatively straightforward. We include them here for the sake of completeness. The principal results of this dissertation actually start in Chapter 4.

Recall (see equations (2.2.6) and (2.2.13)) that we have reduced our investigation to a special case of

$$\frac{dx_1}{dt} = -\lambda x_1 - \beta(x_1 - x_c) + Bf(x_1,x_2) \equiv F_1(x_1,x_2),$$

$$\frac{dx_2}{dt} = -\lambda x_2 + f(x_1,x_2) \equiv F_2(x_1,x_2), \tag{3.1.1}$$

$$x_1(0) \in (-\gamma,\infty) \text{ for } -\infty \leq -\gamma < x_c, \quad x_2(0) \in (0,1).$$

The nonlinearity $f(x_1,x_2)$ is given by

$$(3.1.2) \qquad f(x_1, x_2) = Da(1 - x_2)^n \exp\left(\frac{x_1}{1 + \frac{1}{\gamma} x_1}\right),$$

where the n denotes the order of the reaction. When $\gamma = +\infty$, we have the approximation discussed in Chapter 2.

The domain on which the problem is to be analyzed is

$$(3.1.3) \qquad D = \left\{(x_1, x_2) \mid -\gamma < x_1 < \infty,\ 0 < x_2 < 1\right\}.$$

We will show that for $(x_1(0), x_2(0)) \in D$ and for all $t > 0$ there exists a unique solution $(x_1(t), x_2(t))$ of (3.1.1) which remains in a compact subset of D. This compact subset depends on $(x_1(0), x_2(0))$ and the parameters in the problem. We assume that λ and Da are positive and β and B are non-negative.

Since F_1 and F_2 are analytic in all variables, F_1 and F_2 satisfy a Lipschitz condition on both x_1 and x_2 in some neighborhood of every point of the domain D. Therefore we can conclude that (see Hurewicz [22]) there exists a unique solution to the problem (3.1.1) with the further properties that

(1) the solution is defined for all real values of $t \geq 0$; or

(2) if the solution is not defined for $t > t_1$ for some $t_1 > 0$, then either the point $(x_1(t), x_2(t))$ approaches the boundary of D or either $x_1(t)$ or $x_2(t)$ becomes unbounded as $t \to t_1^-$.

We first show that (2) cannot occur. Note that for $x_2 = 1$, $dx_2/dt = -\lambda < 0$ and for $x_2 = 0$, $dx_2/dt = f(x_1, 0) > 0$ so that no solution can enter that part of the boundary of D at which $x_2 = 0$ or $x_2 = 1$. Thus $x_2(t) \in (0,1)$ whenever $x_2(0) \in (0,1)$. For

$-\infty < -\gamma < 0$ we note that as $x_1 \to -\gamma$, $f \to 0$ so that $dx_1/dt \to \lambda\gamma - \beta(-\gamma - x_c) > 0$ if $x_c > -\gamma$. Thus (x_1, x_2) cannot enter that part of the boundary $x_1 = -\gamma$ when $-\gamma$ is finite. Next we show that $x_1(t)$ remains bounded; this resolves the case $-\gamma = -\infty$. First assume $t < t_1$, then the differential equations (3.1.1) can be written as

$$(3.1.4) \qquad \begin{cases} \frac{d}{dt}(e^{(\lambda+\beta)t}x_1) = e^{(\lambda+\beta)t}\beta x_c + Be^{(\lambda+\beta)t}f(x_1,x_2), \\[2ex] \frac{d}{dt}(e^{\lambda t}x_1) = e^{\lambda t}f(x_1,x_2). \end{cases}$$

Using the second of these equations in the first we obtain

$$(3.1.5) \qquad \frac{d}{dt}(e^{(\lambda+\beta)t}x_1) = e^{(\lambda+\beta)t}\beta x_c + Be^{\beta t}\frac{d}{dt}(e^{\lambda t}x_1) .$$

Integrating (3.1.5) from zero to $t < t_1$, we obtain

$$(3.1.6) \qquad e^{(\lambda+\beta)t}x_1(t) \quad - x_1(0) = \frac{\beta x_c}{\beta+\lambda}(e^{(\lambda+\beta)t} - 1)$$

$$+ B\int_0^t e^{\beta\tau}\frac{d}{d\tau}(e^{\lambda\tau}x_1(\tau))\, d\tau .$$

By performing integration by parts on the last integral in (3.1.4) and by multiplying through by $e^{-(\lambda+\beta)t}$, we obtain

$$(3.1.7) \qquad x_1(t) - Bx_2(t) - \frac{\beta x_c}{\beta+\lambda} - \left(x_1(0) - Bx_2(0) - \frac{\beta x_c}{\beta+\lambda}\right) e^{-(\lambda+\beta)t}$$

$$= -B\beta\int_0^t e^{(\lambda+\beta)(\tau-t)}x_2(\tau)\, d\tau .$$

Since $x_2(t) \in (0,1)$ for all $t \in [0,t_1]$, every term in (3.15) remains bounded except possibly $x_1(t)$ as $t \to t_1^-$. It follows that $x_1(t)$

remains bounded as $t \to t_1^-$. Hence, there exists no $t_1 > 0$ such that $|x_1(t)| \to \infty$ as $t \to t_1^-$. We can conclude, therefore, that only (1) is possible, that is, the unique solution $(x_1(t), x_2(t))$ of (3.1.1) exists for all $t \geq 0$ and remains in D. It remains to show that $(x_1(t), x_2(t))$ is contained in a compact subset of D which will depend upon $(x_1(0), x_2(0)) \in D$ and the parameters in the problem.

From (3.1.5), the fact that $\lambda + \beta > 0$, and $x_2(t) \in (0,1)$ it follows that every term in (3.1.5), except possibly $x_1(t)$, remains bounded as $t \to +\infty$. Consequently, $x_1(t)$ must remain bounded as $t \to +\infty$. The solution $(x_1(t), x_2(t))$ which is initially in D remains in a bounded subset of D for all $t > 0$. Thus $M = M(x_1(0), x_2(0))$ such that $|x_1(t)| \leq M$ for all $t \geq 0$. We now show that x_2 is bounded away from that part of the boundary on which $x_2 = 0$ or $x_2 = 1$. By continuity of f it follows that $dx_2/dt > 0$ for all x_1 and x_2 satisfying $|x_2| \leq M$ and $0 \leq x_1 \leq \epsilon_1$, and $dx_2/dt < 0$ for all x_1 and x_2 satisfying $|x_2| \leq M$ and $1 - \epsilon_2 \leq x_1 \leq 1$ for some sufficiently small positive numbers ϵ_1 and ϵ_2. Consequently, the solution $(x_1(t), x_2(t))$ is bounded away from the boundary $x_2 = 0$ or $x_2 = 1$. We can now claim that for $(x_1(0), x_2(0)) \in D$ the solution, $(x_1(t), x_2(t))$, of (3.1.1) is contained in some compact subset of D for all $t \geq 0$.

We define a positive semiorbit as (see J. Hale [9])

$$\gamma^+ = \left\{ (x_1, x_2) \,|\, (x_1, x_2) = (x_1(t), x_2(t)) \text{ where } (x_1(t), x_2(t)) \text{ is the unique solution of (3.1.1)}, \; t \geq 0 \right\}$$

Then, we can summarize all the preceding information in

Theorem 3.1.1. If

(i) $\lambda > 0$, $\beta \geq 0$, $Da > 0$, $B \geq 0$ and $x_c > -\gamma$,

and

(ii) $f(x_1, x_2) = Da(1 - x_2)^n \exp\left(\frac{x_1}{1 + \frac{1}{\gamma} x_1}\right)$,

there exists a unique solution of (3.1.1) which is defined for all $t \geq 0$. The positive semiorbit, γ^+, is contained in the interior of a compact subset of D. This compact subset depends on $(x_1, 0), x_2(0))$ and the parameters in assumption (i).

Section 2. Preliminaries Concerning Periodic Solutions

The previous theorem mentions only the positive semiorbit. In order to apply certain classical theorems to establish the existence of periodic solutions we shall need to consider the negative semiorbit, γ^-. If it is known, a priori, that there exists a compact set, say K, of D such that $(x_1(t), x_2(t))$ is contained in the interior of K for $t < 0$ and cannot approach the boundary of K as $t \to t_1^+$ for any $t_1 < 0$, then it follows in a manner similar to the argument in Theorem 3.1.1 that the solution of (3.1.1) is unique and exists for all $t < 0$. In this case we define

$$\gamma^- = \Big\{(x_1, x_2) \,\Big|\, (x_1, x_2) = (x_1(t), x_2(t)) \text{ where } (x_1(t), x_2(t)) \text{ is the unique solution of (3.1.1) for } t < 0,\ t \leq 0\Big\}$$

and the α-limit set or negative limit set of the negative semiorbit γ^-

as

$$\alpha(\gamma^-) = \Big\{(x_1, x_2) \mid \exists \text{ a sequence } \{t_k\} \text{ such that } \lim_{k\to\infty} t_k = -\infty$$
$$\text{and } (x_1, x_2) = \lim_{k\to\infty} (x_1(t_k), x_2(t_k))\Big\}.$$

The positive semiorbit is always defined for our problem (3.1.1) and so we define the ω-limit set or positive limit set (see J. Hale [9]) as

$$\omega(\gamma^+) = \Big\{(x_1, x_2) \mid \exists \text{ a sequence } \{t_k\} \text{ such that } \lim_{k\to\infty} t_k = +\infty$$
$$\text{and } \lim_{k\to\infty} (x_1(t_k), x_2(t_k)) = (x_1, x_2)\Big\}.$$

We now classify all the possible cases of $\alpha(\gamma^-)$ and $\omega(\gamma^+)$ in Theorem 3.2.1 below (see J. Hale [9]).

Theorem 3.2.1. Let γ^+ be a positive semiorbit (γ^- a negative semiorbit) contained in a compact subset, say K, of D and suppose K has only a finite number of critical points. Then one of the following is satisfied:

(i) $\omega(\gamma^+)$ ($\alpha(\gamma^-)$) is a critical point;

(ii) $\omega(\gamma^+)$ ($\alpha(\gamma^-)$) is a periodic orbit with either $\gamma^+ = \omega(\gamma^+)$ ($\gamma^- = \alpha(\gamma^-)$) or $\omega(\gamma^+) = \overline{\gamma^+} \setminus \gamma^+$ ($\alpha(\gamma^-) = \overline{\gamma^-} \setminus \gamma^-$) where the bar denotes closure;

(iii) $\omega(\gamma^+)$ ($\alpha(\gamma^-)$) consists of a finite number of critical points and a set of orbits γ_i with $\alpha(\gamma_i)$ and $\omega(\gamma_i)$ consisting of a critical point for each orbit γ_i.

In the next chapter we will analyze the local structure of the critical points of the autonomous system (3.1.1). Theorems 3.1.1 and 3.2.1 will then be useful in establishing global behavior of the problem (3.1.1). In particular, when there is only one critical point and it is unstable, we can prove that only case (ii) of Theorem 3.2.1 is applicable. This then establishes the existence of periodic solutions in the large.

Chapter 4

ANALYSIS OF THE STEADY STATES

Section 1. Introduction

In this and the remaining chapters we consider the case of a simple first order reaction with the approximation

$$\exp\left(\frac{x_1}{1+\frac{1}{\gamma}x_1}\right) \approx \exp(x_1) . \tag{4.1.1}$$

This means that the differential equations in (3.1.1) now becomes

$$\begin{aligned} \frac{dx_1}{dt} &= -\lambda x_1 - \beta(x_1 - x_c) + DaB(1-x_2)\exp(x_1), \\ \frac{dx_2}{dt} &= -\lambda x_2 + Da(1-x_2)\exp(x_1), \\ x_1(0) &\in (-\infty,\infty), \quad x_2(0) \in (0,1) . \end{aligned} \tag{4.1.2}$$

By the change of variables $\lambda t \rightarrow t$, $\beta/\lambda \rightarrow \beta$, and $Da/\lambda \rightarrow Da$ the system (4.1.2) becomes

$$\begin{aligned} \frac{dx_1}{dt} &= -x_1 - \beta(x_1 - x_c) + DaB(1-x_2)\exp(x_1) \\ &\equiv F_1(x_1, x_2; \beta, Da, B), \\ \frac{dx_2}{dt} &= -x_2 + Da(1-x_2)\exp(x_1) \equiv F_2(x_1, x_2; \beta, Da, B), \\ x_1(0) &\in (-\infty,\infty), \quad x_2(0) \in (0,1). \end{aligned} \tag{4.1.3}$$

It is this system (4.1.3) on which we now focus all of our attention. In the first sections of this chapter we will examine the local structure of the critical points of the autonomous system (4.1.3). This will include necessary and sufficient conditions for uniqueness and multiplicity, index, type, and stability of the critical points. Within the context of reactor theory these critical points are steady states. In Section 4 we define the concepts of stability as used in this study; several theorems giving various conditions for stability are then stated. In Section 5 the relationship between stability and multiplicity is examined. We believe that we have some new and surprising results here. In the last section we invoke the results of Chapter 3 to prove existence and nonexistence of periodic solutions.

Section 2. Multiplicity and Index of the Steady States

We state and then prove the necessary and sufficient conditions for uniqueness and multiplicity of the critical points (steady states). The index of the steady states is also given (Figure 1 should help to illustrate the context of Theorem 4.2.1.)

Theorem 4.2.1. Let

(4.2.1) $$m_1 = \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}},$$

(4.2.2) $$m_2 = \frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}},$$

(4.2.3) $$Da_i = Da(m_i) = \frac{m_i}{1-m_i}\exp\left(\frac{-Bm_i}{1+\beta} - \frac{\beta x_c}{1+\beta}\right)$$

for $i = 1, 2$. *Let* (a_1, a_2) *denote a critical point of the autonomous system* (4.1.3). *Then,*

1. *When* $B \leq 4(1+\beta)$ *or when* $B > 4(1+\beta)$ *and* $Da \in (0, Da_2) \cup (Da_1, 1)$ *there exists one and only one critical point of the autonomous system* (4.1.3). *The index* $\mathcal{J}(a_1, a_2) = +1$ *except when* $B = 4(1+\beta)$ *and* $a_2 = \frac{1}{2} = m_1 = m_2$.
2. *When* $B > 4(1+\beta)$ *and* $Da = Da_1$ *or* Da_2 *there exists two critical points.*
3. *When* $B > 4(1+\beta)$ *and* $Da \in (Da_2, Da_1)$ *there exist three critical points for each such* Da, B, *and* β. *The index* $\mathcal{J}(z_1, a_2) = +1$ *when* $a_2 \in (0, m_1) \cup (m_2, 1)$ *and* $\mathcal{J}(a_1, a_2) = -1$ *when* $a_2 \in (m_1, m_2)$.

Remark. When one does not use the approximation (4.1.1), there still remain at most three steady states for certain values of the parameters regardless of the value of $1/\gamma \geq 0$.

Proof: The necessary and sufficient conditions for multiplicity of the critical points for the system (4.1.3) are contained in the survey paper of V. Hlavacek, M. Kubicek, and J. Jelinek [11]. We shall use an argument similar to the one used by Cohen [4]. The index of the steady states is examined in the book by Gavalas [17]; however, we give an independent argument.

We first settle the questions of multiplicity and uniqueness of the critical points. The critical points (a_1, a_2) are by definition solutions of the algebraic equations

(4.2.4) $\qquad F_1(a_1, a_2; \beta, B, Da) = 0 \quad$ and

(4.2.5) $$F_2(a_1, a_2; Da) = 0$$

where F_1 and F_2 are given by (4.1.3). Using (4.2.5) in (4.2.4), we obtain an equivalent set of equations:

(4.2.6) $$a_1 = \frac{Ba_2}{1+\beta} + \frac{\beta x_c}{1+\beta} \quad \text{and}$$

(4.2.7) $$Da = \frac{a_2}{1-a_2} \exp\left(-\frac{Ba_2}{1+\beta} - \frac{\beta x_c}{1+\beta}\right).$$

Note that $Da > 0$ implies $a_2 \in (0,1)$, a fact which we have already used in Chapter 3. Since a_1 is linearly related to a_2 through (4.2.6), the multiplicity conditions can be obtained from equation (4.2.7). From (4.2.7) note that Da varies from zero to $+\infty$ as a_2 varies from 0 to 1. If Da increases monotonically with a_2, then we have uniqueness, i.e., for a fixed β, B, x_c, and Da there exists one and only one solution of (4.2.7). If Da does not increase monotonically with a_2, then for some fixed Da there still exist more than one a_2 satisfying (4.2.7). This is the way we investigate the multiplicity conditions. From (4.2.7) we obtain

(4.2.8) $$\frac{dDa}{da_2} = \frac{(Ba_2^2 - Ba_2 + 1 + \beta)}{(1+\beta)(1-a_2)^2} \exp\left(-\frac{Ba_2}{1+\beta} - \frac{\beta x_c}{1+\beta}\right).$$

Let m_1 and m_2 be roots of

(4.2.9) $$Ba_2^2 - Ba_2 + (1+\beta) = 0, \quad \text{i.e.,}$$

(4.2.10) $$m_1 = \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}} \quad \text{and} \quad m_2 = \frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}}.$$

Note that $B < 4(1+\beta)$ implies m_1 and m_2 are complex which implies

$dDa/da_2 > 0$ for $a_2 \in (0,1)$. $B = 4(1+\beta)$ implies $dDa/da_2 > 0$ except for $a_2 = m_1 = m_2 = \frac{1}{2}$ where $dDa/da_2 = 0$. Thus for $B \leq 4(1+\beta)$ we have a unique correspondence between Da and a_2. Let $B > 4(1+\beta)$ then $dDa/da_2 > 0$ for $a_2 \in (0,m_1) \cup (m_2,1)$ and $dDa/da_2 < 0$ for $a_2 \in (m_1,m_2)$. Let Da_i be defined by (4.2.3). Then the situation is as in Figure 1. For $B > 4(1+\beta)$ we have uniqueness for $Da \in (0,Da_2) \cup (Da_1,\infty)$. When $Da \in (Da_2,Da_1)$ there exist three solutions of (4.2.7). For $Da = Da_1$ or Da_2 there exist exactly two critical points. This completes the multiplicity conditions in Theorem 4.2.1.

We now determine index of the steady states. The index $\mathcal{J}$ of a critical point is given by

$$\mathcal{J}(a_1,a_2) = \frac{\det A}{|\det A|}$$

if $\det A \neq 0$ and where $A = \underset{\sim}{F},_{\underset{\sim}{x}}(a_1,a_2)$. (See K. O. Friedrichs [8] or Coddington and Levinson [3].) Now

$$A = \underset{\sim}{F},_x = \begin{pmatrix} DaB(1-a_2)\exp(a_1)-1-\beta & -DaB\exp(a_1) \\ Da(1-a_2)\exp(a_1) & -1-Da\exp(a_1) \end{pmatrix}. \tag{4.2.11}$$

Using (4.2.6) and (4.2.7), (4.2.11) simplifies to

$$A = \begin{pmatrix} Ba_2-1-\beta & -Ba_2/(1-a_2) \\ a_2 & -1/(1-a_2) \end{pmatrix}. \tag{4.2.12}$$

Therefore

$$\text{(4.2.13)} \qquad \det A = \frac{1}{1-a_2}(Ba_2^2 - Ba_2 + 1 + \beta) .$$

Using (4.2.8) in (4.2.13), we obtain

$$\text{(4.2.14)} \qquad \det A = (1+\beta)(1-a_2)\exp\left(\frac{Ba_2}{1+\beta} + \frac{\beta x_c}{1+\beta}\right)\frac{dDa}{da_2} .$$

By the definition of $\vartheta(a_1, a_2)$ we obtain

$$\text{(4.2.15)} \qquad \vartheta(a_1,a_2) = \begin{cases} +1 & \text{whenever} \quad dDa/da_2 > 0 \\ -1 & \text{whenever} \quad dDa/da_2 < 0 . \end{cases}$$

The results on the index in the theorem now follow immediately from our previous considerations of dDa/da_2. Q.E.D.

Section 3. Classification of the Types of Steady States

The results of this section all follow from classical theorems on ordinary differential equations. The most important facts which will be used later are contained in the remarks following Theorem 4.3.1.

Write system (4.1.3) as

$$\text{(4.3.1)} \qquad \frac{d}{dt}\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix} = \begin{pmatrix} Ba_2 - 1 - \beta & -\dfrac{Ba_2}{1-a_2} \\ a_2 & -\dfrac{1}{1-a_2} \end{pmatrix}\begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix} + \begin{Bmatrix} DaBe^{a_1}\left((1-e^{y_1})y_2 + (1-a_2)(e^{y_1}-1-y_1)\right) \\ Dae^{a_1}\left((1-e^{y_1})y_2 + (1-a_2)(e^{y_1}-1-y_1)\right) \end{Bmatrix}$$

where (a_1, a_2) is a critical point and $y_i = x_i - a_i$ for $i = 1, 2$. The associated linearized problem is

(4.3.2) $$\frac{dy}{dt} = Ay$$

where A has the obvious meaning. We now state the following theorem:

Theorem 4.3.1. For (4.3.1) and (4.3.2) we have

$$\det A = \frac{1}{1-a_2}(Ba_2^2 - Ba_2 + (1+\beta)) ,$$

and

$$\text{tr } A = -\frac{1}{1-a_2}(Ba_2^2 - (B+1+\beta)a_2 + (2+\beta)) .$$

Let $\Delta = (\text{tr } A)^2 - 4 \det A$. Then, the critical points of the linear system (4.3.2) are classified as follows:

1. If $\det A < 0$, then the critical point is a saddle point.

2. Let $\det A > 0$. The steady state is a spiral if $\Delta < 0$ and $\text{tr } A \neq 0$, a center if $\Delta < 0$ and $\text{tr } A = 0$, a proper node (I) if $\Delta = 0$, and an improper node (II) if $\Delta > 0$.

3. Let $\det A = 0$. The critical point is an improper node (III) if $\Delta > 0$ and a degenerate point if $\Delta = 0$.

The type of critical point for the nonlinear problem (4.3.1) is the same as that for the linear problem in cases 1 and 2 above except in the case of the center. This critical point is either a center or a spiral for the nonlinear problem.

Remark 1. One of the interesting features of our autonomous system is that for some combination of the parameters β, Da, and B each of the cases in (1) - (3) actually occurs.

Remark 2. Given the parameters Da, B, β, and x_c, one must first examine a_2 through

$$Da = \frac{a_2}{1 - a_2} \exp\left(- \frac{Ba_2}{1+\beta} - \frac{\beta x_c}{1+\beta} \right)$$

paying particular attention to the multiplicity question. In case $B > 4(1+\beta)$ and $a_2 \in (m_1, m_2)$, the critical point (a_1, a_2) is a saddle point. Thus for the case of three critical points we can say that the middle critical point is always a saddle point with two trajectories entering and two trajectories leaving the critical point.

Remark 3. Let $B > 3 + \beta + 2\sqrt{2 + \beta}$ and

$$s_1 = \frac{B + 1 + \beta}{2B} - \frac{1}{2B} \sqrt{(B + 1 + \beta)^2 - 4B(2 + \beta)}$$

and

$$s_2 = \frac{B + 1 + \beta}{2B} + \frac{1}{2B} \sqrt{(B + 1 + \beta)^2 - 4B(2 + \beta)} .$$

Then s_1 and s_2 are roots of $\operatorname{tr} A = 0$ and $0 < s_1 < s_2 < 1$. Let Da_o be the corresponding Da defined through (4.2.7). For β and B fixed, assume $\det A > 0$ for $a_2 = s_1$ or s_2. Then tr A changes sign as a_2 passes through s_1 or s_2 and $\det A > 0$ for a_2 in some sufficiently small interval about s_1 or s_2. In this case we note that $(\operatorname{tr} A)^2 - 4 \det A < 0$ for a_2 in some sufficiently small interval about s_1 or s_2 which means that all the critical points are spirals except when $a_2 = s_1$ or s_2. For $a_2 = s_1$ or s_2 the critical point is either a center or a spiral. An equivalent way of saying this is that when the index of a critical point is $+1$ and there is a change in sign of $\mathrm{tr}\, A$ as Da varies through some point Da_o for fixed β, B, and x_c, the point Da_o corresponds to a center in the linearized problem (4.3.2). For Da in some sufficiently small interval about Da_o all the corresponding critical points are spirals except at Da_o which will correspond to either a center or spiral.

Proof of Theorem 4.3.1: The classification given is standard and may be found in Coddington and Levinson [3]. Since the nonlinearity in (4.3.1) is $O(r^2)$ as $r = \sqrt{y_1^2 + y_2^2} \to 0$, the second part of the theorem regarding the persistence of the local structure of the critical points follows from classical theorems in Coddington and Levinson [3] or Struble [19].

Section 4. Preliminary Stability Considerations

In this section we define those types of stability which will be used in this study and which are physically important for the CSTR. Several theorems are then stated. These definitions can be found in J. Hale [9], P. Hartman [10], W. Coppel [6], Coddington and Levinson [3], or most any book on ordinary differential equations. Since we shall study only the stability of the critical points and the periodic orbits of the autonomous system (3.1.1), our definitions are restricted to these cases. For the autonomous system

$$(4.4.1) \qquad \frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{F}(\underset{\sim}{x})$$

the critical point $\underset{\sim}{a}$ is said to be

(i) stable if for each $\epsilon > 0$, there exists a $\delta > 0$ such that any solution $\underset{\sim}{x}(t)$ of (4.4.1) which satisfies $||\underset{\sim}{x}(t) - \underset{\sim}{a}|| < \delta$ exists and satisfies the inequality $||\underset{\sim}{x}(t) - \underset{\sim}{a}|| < \epsilon$ for all $t \geq 0$,

(ii) asymptotically stable if in addition to being stable $||\underset{\sim}{x}(t) - \underset{\sim}{a}|| \to 0$ as $t \to \infty$ whenever $||\underset{\sim}{x}(0) - \underset{\sim}{a}||$ is sufficiently small,

(iii) unstable if it is not stable.

For the definition of orbital stability let $\underset{\sim}{p}(t)$ be a non-constant periodic solution of the autonomous system $\underset{\sim}{x}' = \underset{\sim}{F}(x)$. Let Γ be the closed path $\underset{\sim}{x} = \underset{\sim}{p}(t)$ in $\underset{\sim}{x}$ space. The periodic solution $\underset{\sim}{p}(t)$ is said to be

(i) orbitally stable if for each $\epsilon > 0$ there exists a $\delta > 0$ such that every solution $\underset{\sim}{x}(t)$ of $\underset{\sim}{x}' = \underset{\sim}{F}(\underset{\sim}{x})$ whose distance from Γ is less than δ for $t = 0$ is defined and remains at a distance less than ϵ from Γ for all $t \to 0$,

(ii) orbitally asymptotically stable if in addition the distance of $\underset{\sim}{x}(t)$ from Γ tends to zero as $t \to \infty$,

and

(iii) unstable if it is not orbitally stable.

We state below three theorems needed for our stability analysis:

<u>Theorem 4.4.1.</u> (<u>Coppel</u> [6]). <u>The solution of $\underset{\sim}{y}' = A\underset{\sim}{y}$ is stable if every eigenvalue of the matrix A has real part not greater than zero, and those with zero real part are of the simple type. It is asymptotically stable if every eigenvalue of A has negative real part.</u>

Theorem 4.4.2. (Birkhoff and Rota [2]). If the critical point $\underset{\sim}{o}$ of the linear autonomous system

$$(4.4.2) \qquad \underset{\sim}{y}' = A\underset{\sim}{y}$$

is asymptotically stable then so is that of the perturbed system

$$(4.4.3) \qquad \underset{\sim}{y}' = A\underset{\sim}{y} + \underset{\sim}{G}(\underset{\sim}{y})$$

provided $\|\underset{\sim}{G}(\underset{\sim}{y})\| = O(\|\underset{\sim}{y}\|^2)$ as $\underset{\sim}{y} \to 0$.

Theorem 4.4.3. (J. Hale [9]). Let $\underset{\sim}{p}(t)$ be a T^o-periodic solution of $\underset{\sim}{x}' = \underset{\sim}{F}(\underset{\sim}{x})$. $\underset{\sim}{p}(t)$ is asymptotically orbitally stable if

$$(4.4.4) \qquad \int_0^{T^o} \nabla \cdot \underset{\sim}{F}(\underset{\sim}{p}(t))\, dt < 0$$

and is unstable if

$$(4.4.5) \qquad \int_0^{T^o} \nabla \cdot \underset{\sim}{F}(\underset{\sim}{p}(t))\, dt > 0 .$$

Remark 1. The norm used in the above definitions will be used to mean

$$\|\underset{\sim}{y}\| = \sqrt{y_1^2 + y_2^2} .$$

Remark 2. The instability in theorem 4.5.3 is actually quite strong. It implies that all trajectories sufficiently close lead away from $\underset{\sim}{p}(t)$.

Section 5. Steady State Response Diagram for the Chemical Reactors

Some of the main results of this dissertation are contained in this section. We completely characterize the stability and number of critical points (steady states in reactor theory) for all parameters in the problem. Our classification is exhaustive; that is, we have classified all possible cases of multiplicity and stability relationships into six mutually exclusive cases.

It will be convenient to refer simultaneously to Figures 2 through 14 and Table I which give examples of the six mutually exclusive cases. The author considers the most useful way to use these figures is to pick a β and B from one of the six regions in Figure 2 and then read Theorem 4.5.1 for precisely what happens. The Figures 3 through 14 are two dimensional views of the critical point (a_1, a_2) and Da. The a_1 axis is taken to be into the paper. As an example let (β, B) be in region V. Then, Figures 13 and 14 show schematically what happens. There is a unique correspondence between Da and (a_1, a_2). For all values of Da the critical point (a_1, a_2) has an index of +1. For $Da \in (Da_3, Da_4)$, where Da_3 and Da_4 are given in Theorem 4.5.1, the critical point (a_1, a_2) is an unstable spiral or node. For $Da \in (0, D_3) \cup (D_4, \infty)$ the critical point is an asymptotically stable node or spiral.

The analytical description of the six regions — I through VI — follows Theorem 4.5.1. We now state Theorem 4.5.1 which describes in detail the relation between stability and multiplicity of the critical points:

<u>Theorem 4.5.1.</u> <u>Let</u>

(4.5.1) $$s_1 = \frac{B+1+\beta}{2B} - \frac{1}{2B}\sqrt{(B+1+\beta)^2 - 4B(2+\beta)} \ ,$$

(4.5.2) $$s_2 = \frac{B+1+\beta}{2B} + \frac{1}{2B}\sqrt{(B+1+\beta)^2 - 4B(2+\beta)} \ ,$$

(4.5.3) $$m_1 = \frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}} ,$$

(4.5.4) $$m_2 = \frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}} .$$

Let $Da_1 = Da(m_1)$ and $Da_2 = Da(m_2)$ for $B \geq 4(1+\beta)$ and $Da_3 = Da(s_1)$ and $Da_4 = Da(s_2)$ for $B \geq 3 + \beta + 2\sqrt{2+\beta}$ where

$$Da(x) = \frac{x}{1-x} \exp\left(- \frac{Bx}{1+\beta} - \frac{\beta x_c}{1+\beta}\right)$$

Assume that x_c is fixed but arbitrary. Then we have the following six cases.

I. For β and B in this region m_1 and m_2 are imaginary while either s_1 and s_2 are imaginary or $s_2 > s_1 > 1$. There is a unique correspondence between Da and the critical point (a_1, a_2) which is an asymptotically stable node or spiral. Furthermore, all trajectories in the domain D tend to the critical point. (See Figure 3.)

II. In this region $0 < m_1 < m_2 < 1$ and for $B < 3 + \beta + 2\sqrt{2+\beta}$ s_1 and s_2 are imaginary, but for $B \geq 3 + \beta + 2\sqrt{2+\beta}$ s_1 and s_2 are real and $0 < m_1 < s_1 < s_2 < m_2 < 1$. The critical point is an asymptotically stable spiral or node for $a_2 > m_2$ or $a_2 < m_1$ and is an unstable saddle point for $m_1 < a_2 < m_2$. For $Da \in (Da_2, Da_1)$ there exists three critical points with the middle one the saddle while for $Da \in (0, Da_2) \cup (Da_1, \infty)$ there is exactly one critical point. (See Figure 4.)

III. For β and B in this region there are three critical points for

$Da \in (Da_2, Da_1)$ and one critical point for $Da \in (0, Da_2) \cup (Da_1, \infty)$. We have $0 < m_1 < s_1 < m_2 < s_2 < 1$. The critical point is an asymptotically stable node or spiral for $a_2 \in (0, m_1) \cup (s_2, 1)$, an unstable saddle for $a_2 \in (m_1, m_2)$, and an unstable node or spiral for $a_2 \in (m_2, s_2)$. (For a typical case see Figure 5, 6, or 7 and Table I.)

IV. In this region there are three critical points for $Da \in (Da_2, Da_1)$ and one for $Da \in (0, Da_2) \cup (Da_1, \infty)$. We have $0 < s_1 < m_1 < m_2 < s_2 < 1$. The critical point is an asymptotically stable node or spiral for $a_2 \in (0, s_1) \cup (s_2, 1)$, a saddle point for $a_2 \in (m_1, m_2)$, and an unstable spiral or node for $a_2 \in (s_1, m_1) \cup (m_2, s_2)$. (See Figures 8 and 9 and Table I for typical cases.)

V. In this region there is exactly one critical point for all $Da > 0$. m_1 and m_2 are imaginary, but s_1 and s_2 are real and $0 < s_1 < s_2 < 1$. For $a_2 \in (0, s_1) \cup (s_2, 1)$ the critical point is a stable node or spiral and for $a_2 \in (s_1, s_2)$ the critical point is an unstable node or spiral. (See Figures 13 and 14 and Table I for typical cases.)

VI. For β and B in this region there are three critical points for $Da \in (Da_2, Da_1)$ and one for $Da \in (0, Da_2) \cup (Da_1, \infty)$. We have $0 < m_1 < m_2 < s_1 < s_2 < 1$. The critical point is a stable spiral or node for $a_2 \in (0, m_1) \cup (m_2, s_1) \cup (s_2, 1)$, an unstable spiral or node for $a_2 \in (s_1, s_2)$, and a saddle for $a_2 \in (m_1, m_2)$. (A typical case is shown in Figures 10, 11, and 12 and Table I.)

Remark 1. Before describing analytically the six regions we note that there are three curves separating the six regions:

(4.5.5) $$B = f_1(\beta) = 4(1+\beta),$$

(4.5.6) $$B = f_2(\beta) = 3 + \beta + 2\sqrt{2+\beta}\ ,$$

(4.5.7) $$B = f_3(\beta) = (1+\beta)^3/\beta\ .$$

f_1 and f_2 intersect at $\beta = 7/9$. f_3 is tangent to f_2 at $\beta = (\sqrt{5}-1)/2$ and to f_1 and $\beta = 1$. The regions I through VI are defined as the set of β and B satisfying $\beta \geq 0$, $B \geq 0$, and

I: $0 \leq B < \min\left\{4(1+\beta),\ 3+\beta+2\sqrt{2+\beta}\right\}$,

II: $4(1+\beta < B < \frac{(1+\beta)^3}{\beta}$ for $0 < \beta \leq \frac{\sqrt{5}-1}{2}$ and $4(1+\beta) < B <$ $3+\beta+2\sqrt{2+\beta}$ for $\frac{\sqrt{5}-1}{2} \leq \beta < \frac{7}{9}$.

III: $\frac{(1+\beta)^3}{\beta} < B$ for $0 \leq \beta < \infty$,

IV: $4(1+\beta) < B < \frac{(1+\beta)^3}{\beta}$ for $\beta > 1$,

V: $3+\beta+2\sqrt{2+\beta} < B < 4(1+|)$ for $\beta > \frac{7}{9}$,

VI: $3+\beta+2\sqrt{2+\beta} < B < \frac{(1+\beta)^3}{\beta}$ for $\frac{\sqrt{5}-1}{2} < \beta \leq \frac{7}{9}$ or $4(1+\beta) < B <$ $\frac{(1+\beta)^3}{\beta}$ for $\frac{7}{9} \leq \beta < 1$.

Proof of Theorem 4.5.1. The multiplicity question has been settled in Theorem 4.2.1 and we shall not repeat it here except to say that for $B > 4(1+\beta)$ (regions II, III, IV, and VI) we have multiplicity and for $B < 4(1+\beta)$ (regions I and V) we have only one critical point.

We now turn to the question of stability and emphasize that the stability analysis is for the nonlinear problem (4.3.1) as well as for the associated linear problem (4.3.2).

Recall from (4.3.1) and (4.3.2) that

$$\frac{d\underset{\sim}{y}}{dt} = A\underset{\sim}{y} + G(\underset{\sim}{y}, \underset{\sim}{a}) \tag{4.5.8}$$

where G is the nonlinear part of (4.3.1) and

$$A = \begin{bmatrix} Ba_2 - 1 - \beta & -\dfrac{Ba_2}{1 - a_2} \\ a_2 & -\dfrac{1}{1 - a_2} \end{bmatrix} . \tag{4.5.9}$$

Since $G = O(||\underset{\sim}{y}||)$ as $\underset{\sim}{y} \to 0$ $(||\underset{\sim}{y}|| = \sqrt{y_1^2 + y_2^2})$, we can conclude that the critical point is a uniformly asymptotically stable node or spiral if $\det A > 0$ and $\operatorname{tr} A < 0$. The critical point will be a saddle if $\det A < 0$ and an unstable node or spiral if $\det A > 0$ and $\operatorname{tr} A > 0$. From (4.5.9) we have

$$\operatorname{tr} A = -\frac{1}{1 - a_2}(Ba_2^2 - (B + 1 + \beta)a_2 + (2 + \beta)) \tag{4.5.10}$$

$$\det A = \frac{1}{1 - a_2}(Ba_2^2 - Ba_2 + (1 + \beta)) . \tag{4.5.11}$$

Let s_1 and s_2 be roots of $\operatorname{tr} A = 0$ and m_1 and m_2 roots of $\det A = 0$. These roots are then given by (4.5.1) through (4.5.4). For $B < 4(1 + \beta)$, m_1 and m_2 are imaginary which implies that $\det A > 0$ for all values of $Da > 0$ and $a_2 \in (0, 1)$ since $\det A > 0$ for $a_2 = 0$. Thus the stability in this case is determined by the sign of $\operatorname{tr} A$. For $B < 3 + \beta + 2\sqrt{2 + \beta}$ either s_1 and s_2 are imaginary or $s_2 > s_1 > 1$ so that $\operatorname{tr} A < 0$ for all $Da > 0$ and $a_2 \in (0,1)$. Thus all critical points are uniformly asymptotically stable spirals or nodes when $B < 4(1+\beta)$ and $B < 3+\beta+2\sqrt{2+\beta}$. This is case of region I. In region II $\det A > 0$ and $\operatorname{tr} A > 0$ for $a_2 \in (s_1, s_2)$ and $\operatorname{tr} A < 0$ for $a_2 \in (0, s_1) \cup (s_2, 1)$. This completes the case of region V. For $B > 4(1+\beta)$ and $B < 3+\beta+2\sqrt{2+\beta})$ $)0 \leq \beta < \frac{7}{9})$, s_1 and s_2 are imaginary but m_1 and m_2 are real. For $a_2 \in (0, m_1) \cup (m_2, 1)$ $\det A > 0$ and $\operatorname{tr} A < 0$ while for $a_2 \in (m_1, m_2)$ $\det A < 0$. This completes part of region II. Now assume $B > \max\{4(1+\beta), 3+\beta+2\sqrt{2+\beta}\}$. Then m_1, m_2, s_1, and s_2 are real and $\operatorname{tr} A < 0$ for $a_2 \in (0, s_1) \cup (s_2, 1)$, $\operatorname{tr} A > 0$ for $a_2 \in (s_1, s_2)$, $\det A < 0$ for $a_2 \in (m_1, m_2)$, and $\det A > 0$ for $a_2 \in (0, m_1) \cup (m_2, 1)$. By comparing the roots m_1, m_2, s_1, and s_2 we can determine the relationships between stability and multiplicity. This comparison is done in the Appendix A to give the remaining cases in the theorem.

The fact that all trajectories in D tend to the critical point for (β, B) in region I will be proved in Section 6. Q.E.D.

Section 6. Existence and Nonexistence of Periodic Solutions

Having analyzed the critical points with respect to multiplicity, type, index, and stability, we now turn to the question of periodic solutions. We shall divide the analysis into two parts. In the first part, still very much within the spirit of the present chapter, we shall continue to use the classical phase-plane techniques to obtain existence of periodic solutions via the Poincare-Bendixson type analysis. Finally in the second part, which we reserve for Chapter 5, we come to some of the main results of this paper, namely the study of bifurcating periodic solutions via the implicit function theorem and the implications and relationships between multiplicity, stability, bifurcation, and periodicity.

First, we note that if a periodic solution exists then the periodic solution must encircle those critical points the sum of whose indices must be $+1$. We have shown in Section 4.2 that when we have a unique critical point, the index is always $+1$. For the case of three critical points, we have shown that the upper and lower critical points have index $+1$, while the middle critical point has an index of -1. Thus, the periodic solution must encircle only the lower critical point, only the upper critical point, or all three critical points. It cannot happen that the periodic solution encircles 2 of the 3 critical points.

We shall now show that if there is only one critical point and it is unstable then a periodic orbit exists and encircles this unique unstable critical point. In Theorem 3.2.1 we characterized the ω-limit points of any positive half-trajectory γ^+ lying in D. Any critical point of index $+1$ is either a node, spiral, or center. Thus, in case of a unique unstable critical point, the critical point must be an unstable node or an unstable spiral. (The center has special significance and is examined in greater detail in Chapter 6.) Hence, all trajectories must leave the unique unstable critical point. This implies that neither case (i) nor case (iii) can occur in Theorem 3.2.1 so long as the initial conditions for γ^+ are not the critical point itself. Consequently, we have the following theorem:

Theorem 4.6.1. For β, B and Da chosen so that there is but one critical point and it is unstable, then a periodic orbit must encircle this unstable critical point. This unstable critical point must be either a node or a spiral.

At the present we can say no more about the existence of periodic orbits. We will, however, return to this in Chapter 5. For β and B in Region I and for β and B in that part of Region II where $B \leq 3 + \beta + 2\sqrt{2} + \beta$ and $Da \in (0, Da_2) \cup (Da_1, \infty)$ we now show that there are no periodic orbits; in fact, $\omega(\gamma^+)$ is the unique stable critical point for all γ^+ in D. To prove this we need the following lemma:

Lemma 4.6.2. If $B \leq 3 + \beta + 2\sqrt{2+\beta}$ and there exists a periodic orbit, then it must be orbitally asymptotically stable.

Proof: Assume there is a periodic orbit of period T^o. We examine Poincares Criterion (Theorem 4.4.3):

$$\oint \nabla \cdot \underset{\sim}{F}\, d\tau = \int_0^{T^o} \nabla \cdot \underset{\sim}{F}\, d\tau$$

$$= \int_0^{T^0} [-(1+\beta) + DaB(1-x_2)e^{x_1} - 1 - Dae^{x_1}]\, d\tau$$

$$= -\int_0^{T^o} \frac{(Bx_2^2 - (B+1+\beta)x_2 + 2 + \beta)}{1 - x_2}\, d\tau$$

$$+ \int_0^{T^o} B\dot{x}_2 - \frac{\dot{x}_2}{1 - x_2}\, d\tau \; .$$

The last integral is zero by periodicity so that

$$\oint \nabla \cdot \underset{\sim}{F}\, d\tau = -\int_0^{T^0} \frac{(Bx_2^2 - (B+1+\beta)x_2 + 2 + \beta}{1 - x_2}\, d\tau \, .$$

But for $B \leq 3 + \beta + 2\sqrt{2+\beta}$ we have $Bx_2^2 - (B+1+\beta)x_2 + 2 + \beta > 0$ for $x_2 \in (0,1)$ except for one point $x_2 = (B+1+\beta)/2B$ when $B = 3 + \beta + 2\sqrt{2+\beta}$. Thus we have $\oint \nabla \cdot \underset{\sim}{F}\, d\tau < 0$; so, by Poincaris Criterion the assumed periodic orbit is asymptotically orbitally stable. (In the above proof we have used the fact that any periodic orbit is contained in D so that $x_2 \subset (0,1)$). Q.E.D.

With this lemma we are ready now to prove

<u>Theorem 4.6.3.</u> <u>For β and B in region I or in that part of region II where $B \leq 3 + \beta + 2\sqrt{2+\beta}$ and $Da \in (0, Da_2) \cup (Da_1, \infty)$, $\omega(\gamma^+)$ is the unique stable critical point for each γ^+ for which $(x_1(0), x_2(0)) \in D$. In other words, all trajectories go into the critical point.</u>

<u>Proof:</u> Since we know that for β, B, and Da chosen as in the theorem the unique critical point is asymptotically stable, $\omega(\gamma^+)$ must be either the critical point or a periodic orbit from Theorem 3.2.1. Assume that $\omega(\gamma^+)$ is a periodic orbit. By Lemma 4.6.2 this periodic orbit must be asymptotically orbitally stable. Consider now an initial value problem with $(x_1,(0), x_2(0))$ in the interior of the periodic orbit but distinct from the critical point. Choose $(x_1(0), x_2(0))$ so close to the periodic orbit that $\omega(\gamma^+)$ is this periodic orbit. By our remark at the end of Theorem 3.1.1 and by the stability of our periodic solution it follows that γ_o^- is defined and does not enter this stable periodic solution. By Theorem 3.2.7

$\alpha(\gamma_o^-)$ must be either a critical point or a periodic orbit. It cannot be the critical point since the critical point is asymptotically stable. Thus it must be a periodic orbit. This periodic orbit must then be unstable contradicting Lemma 4.6.2. Thus the assumption that $\omega(\gamma^+)$ is a periodic orbit is untenable. Q.E.D.

Chapter 5

BIFURCATION OF PERIODIC SOLUTIONS

Section 1. Introduction

In Section 3 of the previous chapter we found that when the index of a critical point is +1 and there is a change in stability as Da varies for β and B fixed, the point, say Da_0, at which the stability changes corresponds to a center in the linearized problem associated with the autonomous system

$$\frac{dx_1}{dt} = -x_1 - \beta(x_1 - x_c) + DaB(1-x_2)\exp(x_1) \equiv F_1(x_1, x_2; \beta, B, Da)$$

(5.1.1)

and $$\frac{dx_2}{dt} = -x_2 + Da(1-x_2)\exp(x_1) \equiv F_2(x_1, x_2; Da).$$

Furthermore, for Da in a sufficiently small interval about Da_0 all critical points are spirals. On one side of Da_0 they are stable and on the other side, unstable. These centers correspond to the points (a_1, a_2) when $a_2 = s_i$ and $\mathcal{J}(a_1(s_i), s_i) = +1$ for $i = 1$ or 2. We shall prove that from each of these centers there is an associated bifurcation of periodic orbits. The stability of these bifurcating periodic orbits and the connection with the direction of bifurcation are rigorously established.

We shall see that the direction of a bifurcating branch and its stability can have some surprising implications concerning both the number of periodic solutions which exist and the stability of various segments of the response diagram for the reactor process.

One of the results of knowing the direction and stability of the bifurcating periodic solutions is that we can determine the type and stability of that critical point of the nonlinear system (5.1.1) which is a center for the linearized problem associated with (5.1.1). Recall that the linear analysis was unable to predict this.

Section 2. Friedrichs' Theory for Bifurcating Periodic Solutions.

It will be convenient to write (5.1.1) in the form

$$\frac{d\underset{\sim}{y}}{ds} = A\underset{\sim}{y} + \mu\underset{\sim}{G}(\underset{\sim}{y}, \mu) ,$$

where μ is a small parameter and where the system

$$\frac{d\underset{\sim}{y}}{ds} = A\underset{\sim}{y}$$

has period solutions. (This is the case when the eigenvalues of A are purely imaginary or one and only one of the eigenvalues is zero. We shall consider only the first case and leave the latter one to further investigation. So we will consider only the case where the matrix A comes from the linearization about the center.) In order to achieve such a reformulation we shall adopt a general theory due to K. O. Friedrichs [8]. For our purposes we shall formulate the necessary general theory in this section and apply it in Section 3.

For the two dimensional autonomous system

(5.2.2) $$\frac{d\underset{\sim}{x}}{dt} = \hat{\underset{\sim}{F}}(\underset{\sim}{x}, \gamma) \ ,$$

let $\hat{\underset{\sim}{a}}^{\gamma}$ be defined by $\hat{\underset{\sim}{F}}(\hat{\underset{\sim}{a}}^{\gamma}, \gamma) = 0$. Introduce the following change of variables:

$$\gamma = \gamma_0 + \varepsilon \ , \quad \underset{\sim}{a}^{\varepsilon} = \hat{\underset{\sim}{a}}^{\gamma_0 + \varepsilon} \ , \quad s = \frac{T^0}{T^{\varepsilon}} t \ , \quad \varepsilon = \mu\delta \ ,$$

(5.2.3)
$$T^{\varepsilon} = T^0(1+\mu\eta) \ , \quad \underset{\sim}{x}^{\varepsilon} = \underset{\sim}{a}^{\varepsilon} + \mu\underset{\sim}{y}(s,\mu) \ ,$$

$$A^{\varepsilon} = \underset{\sim}{F}_{,\underset{\sim}{x}}(\underset{\sim}{a}^{\varepsilon}, \varepsilon) \ , \quad \varepsilon C^{\varepsilon} = A^{\varepsilon} - A^0 \ , \quad C^0 = \left.\frac{dA^{\varepsilon}}{d\varepsilon}\right|_{\varepsilon=0} \ ,$$

$$\mu^2 Q^{\varepsilon}(\underset{\sim}{y}, \mu) = \underset{\sim}{F}(\underset{\sim}{a}^{\varepsilon} + \mu\underset{\sim}{y}, \varepsilon) - \mu A^{\varepsilon}\underset{\sim}{y}$$

where T^0, δ, η, and $\underset{\sim}{a}^0$ are to be determined and μ is an auxiliary parameter. Under this change of variables, the problem (5.2.2) becomes

(5.2.4) $$\frac{d\underset{\sim}{y}}{ds} = A^0\underset{\sim}{y} + \mu\left\{\delta C^{(\mu\delta)}\underset{\sim}{y} + \eta A^{(\mu\delta)}\underset{\sim}{y} + (1+\mu\eta)Q^{(\mu\delta)}(\underset{\sim}{y},\mu)\right\}.$$

Then we have

<u>Theorem 5.2.1</u>. (<u>Modification of Friedrichs</u> [8], p. 94, <u>Theorem</u> 6.) <u>Suppose the two dimensional vector</u> $\underset{\sim}{F}(\underset{\sim}{x}, \varepsilon) \in C^2[D \times (-\varepsilon_0, \varepsilon_0)]$ <u>where</u> D <u>is a domain in</u> $\mathbb{R}^2$ <u>and</u> ε_0 <u>is a positive number</u>. <u>Assume that the equation</u> $\frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{F}(\underset{\sim}{x}, \varepsilon)$ <u>has a constant solution</u> $\underset{\sim}{x} = \underset{\sim}{a}^{\varepsilon}$ <u>such that</u>

for the value $\varepsilon = 0$ the matrix $A^0 = \underset{\sim}{F},_{\underset{\sim}{x}}(\underset{\sim}{a}^0, 0)$ has purely imaginary eigenvalues $\pm i\omega_0$ with $\omega_0 \neq 0$. Suppose further that the trace of the matrix C^0 does not vanish. Then there exists functions $\eta = \eta(\mu)$ and $\delta = \delta(\mu)$ with $\varepsilon = \mu\delta(\mu)$, $T^\varepsilon = T^0(1+\mu\eta(\mu))$, $\delta(0) = 0$, $\eta(0) = 0$, and $\delta(\mu)$ and $\eta(\mu)$ ε $C^1[0,\mu_0)$ for some sufficiently small $\mu_0 > 0$ and a function $\underset{\sim}{\chi}(s,\mu)$ with period T^0 in s assuming an arbitrarily prescribed initial value $\underset{\sim}{\chi}(0,\mu) = \underset{\sim}{b}_0$ such that

(5.2.5) $$\underset{\sim}{x}^\varepsilon = \underset{\sim}{a}^{\varepsilon(\mu)} + \mu\underset{\sim}{\chi}\left(\frac{T^0}{T^{\varepsilon(\mu)}}t, \mu\right)$$

is a solution of the differential equation

(5.2.6) $$\frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{F}(\underset{\sim}{x}, \varepsilon(\mu)) .$$

In the above theorem, the case $T^\varepsilon \equiv T^0$ and $\varepsilon \equiv 0$ is not excluded. In this case, the point $\underset{\sim}{a}^0$ which is a center for the linearized problem is also a center for the nonlinear problem. Contained in the proof of Theorem 5.2.1 is the following fact:

Corollary 5.2.2. Bifurcation from the critical point $\hat{\underset{\sim}{a}}^\gamma$ of $\frac{d\underset{\sim}{x}}{dt} = \hat{\underset{\sim}{F}}(\underset{\sim}{x}, \gamma)$ can occur only from those $\hat{\underset{\sim}{a}}^{\gamma_0}$ which are centers in the associated linearized problem or possibly when one and only one of the eigenvalues of the matrix A is zero.

To determine the local behavior of the solution $\underset{\sim}{\chi}$ and the functions η and δ on μ, we first note that $\delta, \eta \in C^1[0, \mu_0)$. Using $\delta(0) = \eta(0) = 0$, we have

$$\eta(\mu) = \mu\eta^1 + \mu \frac{d\eta}{d\mu}(\theta_1 \mu) \text{ for } \mu \in [0, \mu_0) \text{ and some } 0 < \theta_1 < 1 \text{ and}$$

$$\delta(\mu) = \mu\delta^1 + \mu \frac{d\delta}{d\mu}(\theta_2 \mu) \text{ for } \mu \in [0, \mu_0) \text{ and some } 0 < \theta_2 < 1 .$$

Note that $\mu \frac{d\eta}{d\mu}(\theta_1\mu)$ and $\mu \frac{d\delta}{d\mu}(\theta_2 \mu)$ are $o(\mu)$ as $\mu \to 0$. Since $\varepsilon = \mu\delta(\mu) = \delta^1\mu^2 + o(\mu^2)$ as $\mu \to 0$, the sign of ε is determined by the sign of δ^1 for μ sufficiently small if $\delta^1 \neq 0$. Similarly, the sign of $T^\varepsilon - T^0$ is determined by the sign of η^1. The most important point here is that the direction of bifurcation is determined by δ^1. Since $\gamma - \gamma_0 = \delta^1\mu^2 + o(\mu^2)$ as $\mu \to 0$, the sign of $\gamma - \gamma_0$ is determined by δ^1 for μ sufficiently. If $\delta^1 > 0$, then a small periodic solution grows from $\hat{\underset{\sim}{a}}^{\gamma_0}$ as γ increases beyond γ_0. If $\delta^1 < 0$, then a small periodic solution grows from $\hat{\underset{\sim}{a}}^{\gamma_0}$ as γ decreases below γ_0. It is in this sense that we say δ^1 determines the direction of bifurcation.

To determine δ^1 and η^1 we need the following continuity properties of $\underset{\sim}{y}$:

Theorem 5.2.3. *Under the assumed continuity assumptions on $\underset{\sim}{F}$ in Theorem 5.2.1 and the derived continuity properties of $\delta(\mu)$ and $\eta(\mu)$, we have*

$$(5.2.7) \qquad \underset{\sim}{y}(s,\mu) = \underset{\sim}{y}^0(s) + \mu y^1(s) + \mu \overline{\underset{\sim}{y}}(s,\mu)$$

where $\mu\overline{\underset{\sim}{y}}(s,\mu) = o(\mu)$ as $\mu \to 0$ uniformly for $s \in [0, \infty)$. The functions $y^0(s)$, $y^1(s)$, and $\overline{\underset{\sim}{y}}(s,\mu)$ are periodic of period T^0 for μ sufficiently small. The functions $y^0(s)$ and $y^1(s)$ are given by

(5.2.8) $$\underset{\sim}{y}^0(s) = Y(s)\underset{\sim}{b}_0$$

(5.2.9) and $$\underset{\sim}{y}^1(s) = Y(s)\int_0^s Y^{-1}(\tau)Q^0(y^0(\tau), 0)d\tau$$

where Y(s) is the matrix solution of

(5.7.10) $$\frac{dY}{ds} = A^0 Y \text{ and } Y(0) = I.$$

Proof: An equivalent formulation of the problem (5.2.4) with initial conditions $\underset{\sim}{y}(0,\mu) = \underset{\sim}{b}_0$ is

(5.2.11) $$\underset{\sim}{y} = Y(s)\underset{\sim}{b}_0 + \mu Y(s)\int_0^s Y^{-1}(\tau)\{\delta B^\varepsilon \underset{\sim}{y} + \eta A^\varepsilon \underset{\sim}{y} + (1+\mu\eta)Q^\varepsilon(\underset{\sim}{y},\mu)\}\, d\tau$$

where $\delta = \delta(\mu)$, $\eta = \eta(\mu)$, $\varepsilon = \mu\delta(\mu)$, and Y(s) satisfies (5.2.10). From Theorems 2.3 and 2.4 of M. Urabe [23] it follows that

(5.2.12) $$y = Y(s)\underset{\sim}{b}_0 + \mu Y(s)\int_0^s Y^{-1}(\mu)\, Q^0\Big(\underset{\sim}{y}(\tau,0), 0\Big)d\tau$$
$$+ \mu\, \bar{\underset{\sim}{y}}(s,\mu)$$

where $\bar{\underset{\sim}{y}}(s,\mu) = o(1)$ as $\mu \to 0$ uniformly on any finite interval and $\underset{\sim}{y}(s,0) = Y(s)\underset{\sim}{b}_0$. Y(s) is T^0 periodic by the definition of A^0 and (5.2.10). Assuming for the moment that $\int_0^s Y^{-1}(\tau)Q^0\Big(\underset{\sim}{y}(\tau,0), 0\Big)d\tau$ is T^0-periodic, $\bar{\underset{\sim}{y}}(s,\mu)$ is T^0-periodic since every other term in (5.2.12) is T^0-periodic. From periodicity of each term in (5.2.12) it follows that (5.2.12) is uniformly valid on $[0, \infty)$ as $\mu \to 0$.

We now prove that $\int_0^s Y^{-1}(\tau) Q^0(\underset{\sim}{y}(\tau, 0), 0) d\tau$ is T^0-periodic. From the definition of $Y(\tau)$ it follows that $Y(\tau)$ and $Y^{-1}(\tau)$ are matrices of linear combinations of $\sin \omega_0 \tau$ and $\cos \omega_0 \tau$ where $\omega_0 = \frac{2\pi}{T^0}$. Since $Q^0(\underset{\sim}{y}^0(\tau, 0), 0)$ is quadratic in $y_1^0(\tau)$ and $y_2^0(\tau)$ where $\underset{\sim}{y}(\tau, 0) = \left\{ \begin{matrix} y_1^0 \\ y_2^0 \end{matrix} \right\}$, the expression $Y^{-1}(\tau) Q^0(\underset{\sim}{y}^0(\tau, 0), 0)$ is a vector whose components are linear combinations of the terms $\cos^3 \omega_0 \tau$, $\cos^2 \omega_0 \tau \sin \omega_0 \tau$, $\cos \omega_0 \tau \sin^2 \omega_0 \tau$, and $\sin^3 \omega_0 \tau$. Consequently, $\int_0^s Y^{-1}(\tau) Q^0(\underset{\sim}{y}(\tau, 0), 0) d\tau$ is T^0-periodic and $\int_0^{T^0} Y^{-1}(\mu) Q^0(\underset{\sim}{y}(\tau, 0), 0) d\tau = 0$.

Using Theorems 5.2.1 and 5.2.3 we obtain the following information about $\delta(\mu)$, $\eta(\mu)$, δ^1, and η^1 :

<u>Theorem 5.2.4</u>. <u>The functions $\eta(\mu)$ and $\delta(\mu)$ are obtained implicitly from</u>

(5.2.13) $$0 = \eta \int_0^{T^0} Y^{-1}(\tau) A^{(\mu\delta)} \underset{\sim}{y}(\tau, \mu) d\tau + \delta \int_0^{T^0} Y^{-1}(\tau) B^{(\mu\delta)} \underset{\sim}{y}(\tau, \mu) d\tau$$
$$+ \int_0^{T^0} Y^{-1}(\tau)(1 + \mu\eta) Q^{(\mu\delta)}(\underset{\sim}{y}(\tau, \mu), \mu) d\tau.$$

<u>δ^1 and η^1 are determined explicitly from</u>

(5.2.14) $$0 = \eta^1 \int_0^{T^0} Y^{-1}(\tau) A^0 \underset{\sim}{y}^0 d\tau + \delta^1 \int_0^{T^0} Y^{-1}(\tau) B^0 \underset{\sim}{y}^0 d\tau$$
$$+ \int_0^{T^0} Y^{-1}(\tau) \left(\frac{dQ^{(\mu\delta)}}{d\mu} (\underset{\sim}{y}(\tau, \mu), \mu) \right) \Bigg|_{\mu = 0} d\tau$$

where $\underset{\sim}{y}^0$ is given in Theorem 5.2.3 and Y(s) is the fundamental matrix solution mentioned in Theorem 5.2.3.

Proof. The expression (5.2.13) is contained in the proof of Theorem 6, p. 94 of K. O. Friedrichs [8]. We now derive the expression (5.2.14). Divide expression (5.2.13) by μ and recall from the proof of Theorem 5.2.3 that $\int_0^{T^0} Y^{-1}(\tau)\, Q^0(\underset{\sim}{y}(\tau,0),0)d\tau = 0$; we obtain

$$(5.2.15)\qquad 0 = \frac{\eta(\mu)}{\mu}\int_0^{T^0} Y^{-1}(\tau)A^{\varepsilon}\underset{\sim}{y}(\tau,\mu)d\tau + \frac{\delta(\mu)}{\mu}\int_0^{T^0} Y^{-1}(\tau)B^{\varepsilon}\underset{\sim}{y}(\tau,\mu)d\tau$$
$$+\int_0^{T^0} Y^{-1}(\tau)\left\{\frac{Q^{\varepsilon}(\underset{\sim}{y}(\tau,\mu),\mu)-Q^0(\underset{\sim}{y}(\tau,0),0)}{\mu}\right\}d\tau$$
$$+\int_0^{T^0} Y^{-1}(\tau)\eta(\mu)Q^{\varepsilon}(\underset{\sim}{y}(\tau,\mu),\mu)d\tau$$

where $\varepsilon = \mu\delta(\mu)$. By the uniformity of the convergence of $\underset{\sim}{y}(s,\mu)$ as $\mu \to 0$ we obtain

$$(5.2.16)\qquad \lim_{\mu\to 0}\frac{\eta(\mu)}{\mu}\int_0^{T^0} Y^{-1}A^{\varepsilon}\underset{\sim}{y}(\tau,\mu)d\tau = \eta^1\int_0^{T^0} Y^{-1}(\tau)\lim_{\mu\to 0}A^{\varepsilon}\underset{\sim}{y}(\tau,\mu)d\tau$$
$$= \eta^1\int_0^{T^0} Y^{-1}(\tau)A^0\underset{\sim}{y}(\tau,0)d\tau,$$

$$(5.2.17)\qquad \lim_{\mu\to 0}\frac{\delta(\mu)}{\mu}\int_0^{T^0} Y^{-1}(\tau)B^{\varepsilon}\underset{\sim}{y}(\tau,\mu)d\tau = \delta^1\int_0^{T^0} Y^{-1}(\tau)\lim_{\mu\to 0}B^{\varepsilon}\underset{\sim}{y}(\tau,\mu)d\tau$$
$$= \delta^1\int_0^{T^0} Y^{-1}(\tau)B^0\underset{\sim}{y}(\tau,0)d\tau,$$

$$(5.2.18)\qquad \lim_{\mu\to 0}\int_0^{T^0} Y^{-1}(\tau)\eta(\mu)Q^{\varepsilon}(\underset{\sim}{y}(\tau,\mu),\mu)dT = \int_0^{T^0} Y^{-1}(\tau)\eta(0)Q^0(\underset{\sim}{y}(\tau,0),\mu)d\tau = 0.$$

From the continuity properties of $Q^{\varepsilon}(\underset{\sim}{y}(\tau,\mu),\mu)$ and the expression (5.2.7) for $\underset{\sim}{y}(\tau,\mu)$ we can interchange the limit process and integration in the third integral in expression (5.2.15) to obtain

$$\lim_{\mu\to 0}\int_0^{T^0} Y^{-1}(\tau)\left\{\frac{Q^{\varepsilon}(\underset{\sim}{y}(\tau,\mu),\mu)-Q^0(\underset{\sim}{y}(\tau,0),0)}{\mu}\right\}d\tau$$

$$=\int_0^{T^0} Y^{-1}(\tau)\left(\frac{dQ^{\varepsilon}}{d\mu}\quad(\underset{\sim}{y}(\tau,\mu),\mu)\right)\Big|_{\mu=0}\,d\tau\,.$$

Thus, the expressions (5.2.15) through (5.2.19) yield the desired result (5.2.14). Q.E.D.

<u>Section 3. Application to Reactor Equations.</u>

We now wish to apply the results of the previous section to the system (5.1.1). By Corollary (5.2.2) bifurcation of periodic solutions can occur only from the center or possibly at those points at which one and only one eigenvalue of the matrix A is zero. This latter case can happen only when $B > 4(1+\beta)$ and $a_2 = m_1$ or m_2. However, we shall investiage only the first case. For the system (5.1.1), let β and B be restricted to one of the regions III through VI in which case there is a Da, say Da_0, and a corresponding $\underset{\sim}{a}^0$ such that $\underset{\sim}{a}^0$ is a center in the linearized problem. Let $Da = Da_0 + \varepsilon$. Recall from (4.2.6) and (4.2.7) that the critical points are defined through

(5.3.1) $$a_1^{\varepsilon} = \frac{Ba_2^{\varepsilon}}{1+\beta} + \frac{\beta x_c}{1+\beta}$$

and

$$(5.3.2) \qquad Da_0 + \epsilon = \frac{a^\varepsilon_2}{1-a^\varepsilon_2} \exp(-a^\varepsilon_1).$$

We now proceed to reformulate our problem and show that Theorem 5.2.1 applies. With the definition of $\underset{\sim}{F}$ given in (5.1.1) we find that

$$(5.3.3) \qquad \underset{\sim}{F}_{,\underset{\sim}{x}}(\underset{\sim}{a}^\varepsilon, \varepsilon) = \begin{pmatrix} -1-\beta+B(Da_0+\varepsilon)\exp(a^\varepsilon_1) & -(Da_0+\varepsilon)B\exp(a^\varepsilon_1) \\ (Da_0+\varepsilon)(1-a^\varepsilon_2)\exp(a^\varepsilon_1) & -1-(Da_0+\varepsilon)\exp(a^\varepsilon_1) \end{pmatrix}.$$

Using (5.3.2), we obtain

$$(5.3.4) \qquad A^\varepsilon = \begin{pmatrix} Ba^\varepsilon_2 -1-\beta & \frac{-Ba^\varepsilon_2}{1-a^\varepsilon_2} \\ a^\varepsilon_2 & \frac{-1}{1-a^\varepsilon_2} \end{pmatrix}$$

and

$$(5.3.5) \qquad C^0 = \frac{dA^\varepsilon}{d\varepsilon}\bigg|_{\varepsilon=0} = \begin{pmatrix} B & \frac{-1}{(1-a^0_2)^2} \\ 1 & \frac{-1}{(1-a^0_2)^2} \end{pmatrix} \left(\frac{da^\varepsilon_2}{d\varepsilon}\bigg|_{\varepsilon=0}\right).$$

Using (5.3.1) and (5.3.2), we obtain

$$(5.3.6) \qquad \left(\frac{da^\varepsilon_2}{d\varepsilon}\right)\bigg|_{\varepsilon=0} = \frac{(1+\beta)a^0_2}{Da_0 \det A^0} .$$

Furthermore,

$$(5.3.7) \qquad \underset{\sim}{F}(\underset{\sim}{a}^{\varepsilon} + \mu \underset{\sim}{y}, \varepsilon) = \mu A^{\varepsilon} + \mu^2 Q^{\varepsilon}(\underset{\sim}{y}, \mu)$$

where

$$(5.3.8) \quad Q^{\varepsilon}(\underset{\sim}{y}, \mu) = \frac{a_2^{\varepsilon}}{1-a_2^{\varepsilon}} \begin{Bmatrix} B\left\{\frac{1-a_2^{\varepsilon}}{\mu^2}\left(\exp(\mu y_1)-1-\mu y_1\right) - \frac{y_2}{\mu}\left(\exp(\mu y_1)-1\right)\right\} \\ \left\{\frac{(1-a_2^{\varepsilon})}{\mu^2}\left(\exp(\mu y_1)-1-\mu y_1\right) - \frac{y}{\mu}\left(\exp(\mu y_1)-1\right)\right\} \end{Bmatrix}.$$

The matrix A^0 has eigenvalues

$$(5.3.9) \qquad \lambda_{1,2} = \frac{\operatorname{tr} A^0}{2} \pm \frac{1}{2}\sqrt{(\operatorname{tr} A^0)^2 - 4 \det A^0}$$

The requirement that the eigenvalues of A^0 be purely imaginary is satisfied if and only if

$$(5.3.10) \qquad \operatorname{tr} A^0 = 0 \quad \text{and} \quad \det A^0 > 0$$

Note that this is the case if and only if the critical point (a_1^0, a_2^0) is a center for the linearized problem associated with (5.1.1). Then

$$(5.3.11) \qquad \lambda_{1,2} = \pm i\omega_0$$

where $\omega_0 = \sqrt{\det A^0}$. Now $\operatorname{tr} A^0 = 0$ means $Ba^0_2 - 1 - \beta = \frac{1}{1-a^0_2}$ or, in an equivalent form, (5.3.12) $$B(a^0_2)^2 - (B+1+\beta)a^0_2 + 2+\beta = 0 .$$

Recall from Section 4.5 that the roots of (5.3.12) are

(5.3.13) $$s_1 = \frac{B+1+\beta}{2B} - \frac{1}{2B}\sqrt{(B+1+\beta)^2 - 4B(2+\beta)}$$

and

(5.3.14) $$s_2 = \frac{B+1+\beta}{2B} + \frac{1}{2B}\sqrt{(B+1+\beta)^2 - 4B(2+\beta)} .$$

From Theorem 4.5.1 we know that for β and B in Regions III through VI the roots s_1 and s_2 are real and $0 < s_1 < s_2 < 1$. For (β, B) in any one of the regions IV through VI $\det A^0 > 0$ for $a^0_2 = s_1$ and for (β, B) in any one of the Regions III through VI $\det A^0 > 0$ for $a^0_2 = s_2$. We now proceed to show that in each such case $\operatorname{tr} C^0 \neq 0$. From (5.3.5) and (5.3.6) we have

(5.3.15) $$\operatorname{tr} C^0 = \left[B - \frac{1}{(1-a^0_2)^2}\right]\left[\frac{(1+\beta)a^0_2}{Da_0 \det A^0}\right] = \left[\frac{B(1-a^0_2)^2 - 1}{(1-a^0_2)^2}\right]\left[\frac{(1+\beta)a^0_2}{Da_0 \det A^0}\right] .$$

Using (5.3.13) and (5.3.14) we obtain

(5.3.16) $$B(1-a^0_2)^2 - 1 = \frac{1}{2B}\sqrt{(B-1-\beta)^2 - 4B}\left(\sqrt{(B+1-\beta)^2 - 4B} \mp (B-1-\beta)\right)$$

where the minus corresponds to s_1 and the + to s_2. Thus for $\det A^0 > 0$ we have

(5.3.17) $\quad tr\, C^0 > 0 \quad$ for $\quad a^0_2 = s_1$

and

(5.3.18) $\quad tr\, C^0 < 0 \quad$ for $\quad a^0_2 = s_2$

when β and B are in Regions III through VI. Since our autonomous system (5.1.1) certainly satisfies the continuity requirements in Theorem 5.2.1, we have

Theorem 5.3.1. Bifurcation of periodic solutions occurs from the critical points $(a^0_1, a^0_2) = (\frac{Bs_1}{1+\beta} + \frac{\beta x_c}{1+\beta}, s_1)$ when β and B are in any one of the Regions IV, V or VI and from the critical points $(a^0_1, a^0_2) = (\frac{Bs_2}{1+\beta} + \frac{\beta x_c}{1+\beta}, s_2)$ when β and B are in any one of the Regions III, IV, V, or VI. That is, Theorem 5.2.1 applies in each of these cases.

Our next aim will be to use Theorems 5.2.3 and 5.2.4 to determine the direction of bifurcation and the local structure of the periodic solution. We first determine $\chi^0(s)$ and $\chi^1(s)$. For convenience we introduce the notation

(5.3.19) $\quad a = a^0_2 \quad$ and $\quad b = Ba^0_2 - 1 - \beta$.

Since $tr A^0 = 0$ and $\det A^0 = \omega_0^2 > 0$, we have

(5.3.20) $$A^0 = \begin{pmatrix} b & -Bab \\ a & -b \end{pmatrix}$$

and

(5.3.21) $$\omega_0^2 = Ba^2 b - b^2 > 0 \ .$$

The fundamental matrix solution, $Y(s)$, of $\frac{d\underset{\sim}{y}}{ds} = A^0 \underset{\sim}{y}$ satisfies

(5.3.22) $$\frac{dY}{ds} = A^0 Y \qquad \text{and} \qquad Y(0) = I.$$

By using (5.3.21), it is easily verified that

(5.3.23) $$Y(s) = (\cos \omega_0 s) I + \left(\frac{\sin \omega_0 s}{\omega_0}\right) A^0$$

and

(5.3.24) $$Y^{-1}(s) = \cos \omega_0 s I - \left(\frac{\sin \omega_0 s}{\omega_0}\right) A^0 .$$

In the expansion

(5.3.25) $$\underset{\sim}{y}(s, \mu) = \underset{\sim}{y}^0(s) + \mu \underset{\sim}{y}^1(s) + \mu \bar{\underset{\sim}{y}}(s, \mu)$$

we have from Theorem 5.2.3 that

(5.3.26) $$\underset{\sim}{y}^0(s) = Y(s) \underset{\sim}{b}_0$$

and

$$\chi^1(s) = Y(s)\int_0^s Y^{-1}(\tau)Q^0(y^0(\tau),0)d\tau \,. \tag{5.3.27}$$

Since $\underset{\sim}{b}_0$ is arbitrary (see p. 90 of K.O. Friedrichs [8]), we take $\underset{\sim}{b}_0 = \begin{Bmatrix}0\\1\end{Bmatrix}$ without loss of generality. This particular choice of $\underset{\sim}{b}_0$ makes the algebra simpler in the succeeding determination of $y^1(s)$ and δ^1. Thus

$$y^0(s) = Y(s)\begin{Bmatrix}0\\1\end{Bmatrix} = \begin{Bmatrix} \dfrac{-Bab}{\omega_0}\sin\omega_0 s \\ \cos\omega_0 s - \dfrac{b}{\omega_0}\sin\omega_0 s \end{Bmatrix} . \tag{5.3.28}$$

Next we find that (see Appendix B for the calculations)

$$\begin{aligned} y^1(s) = {} & \frac{Ba^2b^2}{6\omega_0^{\,3}}\begin{Bmatrix} B\Big((Ba-2b)(2\sin\omega_0 s-\sin 2\omega_0 s)+2\omega_0(\cos\omega_0 s-\cos 2\omega_0 s)\Big) \\ (Ba-2b)(2\sin\omega_0 s-\sin 2\omega_0 s)+2\omega_0(\cos\omega_0 s-\cos 2\omega_0 s) \end{Bmatrix} \\ & + \frac{Ba^2b^2}{6\omega_0^{\,4}}\begin{Bmatrix} B\Big((Ba-2b)(1-2\cos\omega_0 s+\cos^2\omega_0 s)-\omega_0(\sin 2\omega_0 s-2\sin\omega_0 s)\Big) \\ (Ba-2b)(1-2\cos\omega_0 s+\cos^2\omega_0 s)-\omega_0(\sin 2\omega_0 s)-2\sin\omega_0 s) \end{Bmatrix} \end{aligned} \tag{5.3.29}$$

From equation (5.2.12) in Theorem 5.2.4 we have

$$\eta^1\widetilde{A}\underset{\sim}{b}_0 + \delta^1\widetilde{B}\,\underset{\sim}{b}_0 = -\frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\left.\frac{dQ}{d\mu}\right|_{\mu=0} d\tau \tag{5.3.30}$$

where

$$\widetilde{A} = \frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)A^0\,Y(\tau)d\tau = A^0 \ , \tag{5.3.31}$$

(5.3.32) $$\tilde{B} = \frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)B^0Y(\tau)d\tau = \frac{1}{2}(B^0 - \frac{1}{\omega^2}A^0B^0A^0),$$

(5.3.33) $$C^0 = \begin{pmatrix} B & -Bb^2 \\ 1 & -b^2 \end{pmatrix}\frac{da_2{}^0}{d\varepsilon} .$$

(See Appendix C for the calculations of (5.3.31) and (5.3.32.) For $\underset{\sim}{b}_0 = \left\{\begin{matrix}0\\1\end{matrix}\right\}$ (5.4.30) becomes

(5.3.34) $$b\left\{\begin{matrix}Ba\\1\end{matrix}\right\}\eta' + \frac{b}{2\omega_0{}^2}\left(\frac{da_2{}^0}{d\varepsilon}\right)\left\{\begin{matrix}B(b\omega_0{}^2+b^2-Ba)\\ \omega^2 b+(Ba-b)(b^2-Ba)\end{matrix}\right\}\delta'$$

$$= \frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\left.\frac{dQ}{d\mu}\right|_{\mu=0} d\tau .$$

Let Δ be the determinant of the coefficient matrix of η^1 and δ^1, then (see Appendix D)

(5.3.35) $$\Delta = -\frac{Bab}{2}\,trC^0 ,$$

From (5.3.17), (5.3.18), (5.3.19) and (5.3.21) we know that $\Delta \neq 0$. We can, therefore, solve for δ^1 (see Appendix D for the calculations) to obtain

(5.3.36) $$\delta^1 = \frac{Ba^2b^2}{8\omega_0{}^4 tr\,C^0}\left\{\omega_0{}^2(b-1) + (2b-Ba) - (2b-Ba)^2\right\}$$

where

(5.3.37) $$b = Bs_i - 1 - \beta \qquad \text{for} \qquad i = 1 \text{ or } 2,$$

(5.3.38) $a = s_i$ for $i = 1$ or 2,

(5.3.39) $\omega_0^2 = Ba^2b - b^2$,

and s_1 and s_2 are given by (5.3.13) or (5.3.14).

Thus, in the light of the remarks on direction of bifurcation following Corollary (5.2.2) we have determined the direction of bifurcation through the formula

$$Da - Da_0 = \delta^1\mu^2 + o(\mu^2) .$$

It did not appear to the author that this expression (5.3.36) would simplify further. Thus, we will evaluate it numerically for various choices of β and B. Before investigating (5.3.36) numerically, we will prove the stability (or instability) of the bifurcating branch of periodic solutions and its relation to the sign of δ^1.

Section 4. Stability of the Bifurcating Branch of Periodic Solutions.

The stability of the bifurcating periodic solutions is determined for sufficiently small μ by using Poincare's criterion (see Section 4.4). We note that the periodic solution $\underset{\sim}{a}^\varepsilon + \mu\underset{\sim}{y}(s,\mu)$ is asymptotically orbitally stable if

(5.4.1) $$\frac{1}{T^0}\int_0^{T^0} \nabla \cdot \underset{\sim}{F}(\underset{\sim}{a}^\varepsilon + \mu\tilde{y}(\tau,\mu))d\tau < 0$$

and is unstable if

(5.4.2) $$\frac{1}{T^0}\int_0^{T^0} \nabla \cdot \underset{\sim}{F}(\underset{\sim}{a} + \mu\widetilde{y}(\tau,\mu))d\tau > 0 \;.$$

In Appendix E it is shown that

(5.4.3) $$\frac{1}{T^0}\int_0^{T^0} \nabla \cdot \underset{\sim}{F} d\tau = \mu^2 \Lambda + o(\mu^2) \quad \text{as} \quad \mu \to 0$$

where

(5.4.4) $$\Lambda = \frac{B^2 a^2 b^2}{8\omega_0^4}\{\omega_0^2(1-b) + (Ba-2b)^2 + Ba-2b\} \;.$$

Recall that

(5.4.5) $$\delta^1 = -\frac{B^2 a^2 b^2}{8\omega_0^4 \operatorname{tr} C^0}\{\omega_0^2(1-b) + (Ba-2b)^2 + (Ba-2b)\} \;.$$

Now $\operatorname{tr}C^0 > 0$ for $a^0_2 = s_1$ and $\operatorname{tr}C^0 < 0$ for $a^0_2 = s_2$. Consider first the case $a^0_1 = s_1$ and β and B in any of the Regions IV through VI. If $\Lambda > 0$ (< 0) then $\delta^1 < 0$ (> 0). Thus δ^1 positive implies asymptotic orbital stability, and δ^1 negative implies instability. For $a^0_2 = s_2$ and β and B in anyone of the Regions III through VI we have $\Lambda > 0$ (< 0) iff $\delta^1 > 0$ (< 0). In this case δ^1 positive implies instability and δ^1 negative implies asymptotic orbital stability of the bifurcating periodic solutions.

Thus, the direction of bifurcation determines the stability. An easy way to remember the foregoing remarks is that if a bifurcated periodic solution surrounds an unstable critical point, the periodic solution is asymptotically orbitally stable. If it surrounds a stable critical point, it is unstable. Of course, these remarks hold true only for μ sufficiently small.

Section 5. Bifurcation of Periodic Orbits and the Response Diagram.

In this section and in Chapter 6 we will present some of the most important results of this study. Some of these results are presented in Figures 5 through 14 to which we will refer later.

Since the direction of bifurcation determines the stability, we need to examine the expression (5.3.36) for different values of β and B. δ^1 is a function of β and B so that in principle we could numerically solve for $\delta^1(\beta, B) = 0$. This would divide the six βB regions into further regions where $\delta^1(\beta, B) > 0$ and $\delta^1(\beta, B) < 0$. However, we shall content ourselves with a few numerical examples which the author believes contain all the qualitative features of this bifurcation problem. We first set $x_c = 0$. (It only scales Da if $x_c \neq 0$.)

We will use Theorems 4.5.1 and 5.3.1 and the expression (5.3.36) for the direction of bifurcation. The expressions for s_1, s_2, m_1, m_2, and the corresponding value of Da have been evaluated numerically for different values of β and B and the results are contained in Table I and Figures 5 through 14. The expression for δ^1 has been evaluated in each case but only the direction is shown. The stability of these bifurcating periodic solutions is also indicated. Let

$$P_1 = (Da_1, m_1), \quad P_2 = (Da_2, m_2),$$

$$P_3 = (Da_3, s_1), \quad P_4 = (Da_4, s_2)$$

where the Da in each case is given by

$$Da(a_2) = \frac{a_2}{1-a_2} \exp\left(-\frac{Ba_2}{1+\beta}\right).$$

The "S" shaped curves have been exaggerated to present the qualitative features. Recall from Theorem 4.6.1 that in any case in which there is a unique unstable critical point for a value of β, B and Da there is a periodic orbit surrounding this unstable critical point. In Figure 8 this means that there is a periodic orbit for each $Da \in (Da_1, Da_4)$. A similar remark applies to Figures 8, 9, 11, 12, 13, 14. This information comes entirely from the Poincaré-Bendixison type analysis.

The results on bifurcation of periodic orbits give different information. In Figure 5 the bifurcated branch means that for $Da > Da_4$ but sufficiently close to Da_4 there is a small unstable periodic orbit surrounding the upper asymptotically stable critical point. In Figures 6 through 14 the bifurcated branch from $(\frac{Ba^0_2}{1+\beta}, a^0_2)$ means that for $Da < Da_4$ but sufficiently close to Da_4 there is a small asymptotically orbitally stable periodic orbit surrounding the unstable critical point $(\frac{Ba^\varepsilon_2}{1+\beta}, a^\varepsilon_2)$ where $\varepsilon = Da - Da_4$ and $\varepsilon < 0$ here.

A similar remark applies to Figures 10, 11, 12 and 13 but the asymptotically orbitally stable periodic orbit bifurcates as Da increases beyond Da_3. In Figures 8, 9, and 14 there are unstable periodic orbits surrounding the asymptotically stable critical point for Da sufficiently close to Da_3 but less than Da_3. Of these latter three, we can say more about the two cases in Figures 9 and 14. For these two cases there is a unique asymptotically stable critical point surrounded by an unstable periodic orbit for each $Da < Da_3$ but sufficiently close. By Theorem 3.2.1 and Remark 2 following Theorem 4.4.3 there exists a second (presumably stable) period orbit surrounding this small unstable periodic orbit. Thus in these two cases we have proved the existence of two periodic orbits. This situation has been observed numerically by V. Hlavacek, M. Kubicek, and J. Jelinek [11] for the case in Figure 14 (for different parameters) but not for the situation in Figure 9. More specifically, Hlavacek considers the case $(\beta, B) = (3.14)$ and $x_c = 0$. Our results show that $(\beta, B) = (3,14)$ is in Region V in which case there is a unique critical point for all $Da > 0$. The critical point is unstable for $Da \in (.1650, .3366)$ and is asymptotically stable for $Da \in (0, .1650) \cup (.3366, \infty)$. The situation is as in Figure 14 with the above appropriate number changes. By numerically integrating the autonomous system for $(\beta, B) = (3,14)$ and ranges of $Da < .1650$, Hlavacek shows that for $.1620 < Da < .1650$ there is a stable critical point surrounded by an unstable periodic orbit which is in turn surrounded by a stable periodic orbit. For $Da < .1620^-$ there are no periodic orbits. This leads us to conjecture that the branch of periodic orbits meet as in Figure 15. We take $Da^* = .1620$, $Da_3 = .1650$, and $Da_4 = .3366$. We also conjecture that the branches emanating from points P_3 and P_4 in Figures 10, 11, 12 and 13 connect and that there are only stable periodic orbits in each case.

For the cases in Figures 5, 6 and 7 we conjecture that the branch of periodic solutions emanating from point P_4 meet a branch of bifurcating periodic orbits emanating from the point P_2. One reason for this conjecture is that Hlavacek [11] has shown that for a particular $Da \in (Da_2, Da_4)$ there is a stable periodic orbit surrounding only the upper unstable branch. Secondly, the point P_2 corresponds to a critical point with the property that the matrix, A, associated with linearized problem (4.3.2) has zero as a simple eigenvalue. Recall from Corollary 5.2.2 that this is a possible point of bifurcation of periodic orbits and a case that has not been investigated to the author's knowledge.

We now discuss the above mentioned example of Hlavacek [11] since the correspondence between the parameters is exact only after a transformation. He uses the parameters $\lambda = 0.5$, $Da = 0.0505$, $\beta = 0.8$, $B = 12.5$, and $x_c = 0$. The transformation we made in Section 4.1 was $\frac{Da}{\lambda} \to Da$, $\beta/\lambda \to \beta$, and $\lambda \to 1$. The phase plane portraits are the same. For the parameters $Da = .101$, $\beta = 1.6$, $B = 12.5$ our results show that $(\beta, B) = (1.6, 12.5)$ places us in Region III. We have

$$P_1 = (Da_1, m_1) = (.1013, \ .2951) ,$$

$$P_2 = (Da_2, m_2) = (.0806, \ .7049) ,$$

$$P_4 = (Da_4, \delta_2) = (.1072, \ .8816),$$

$$\delta^1(P_4) < 0 .$$

Qualitatively, this is the same as in Figure 7. Thus, there is a period orbit surrounding the upper unstable critical point for $Da^* = .1010 \in (Da_2, Da_1)$. Consequently, our conjecture is tantamount to Figure 16.

Finally, for the case of β and B in Region IV (Figures 8 and 9) we conjecture that the branch emanating from P_3 connects with the branch emanating from P_4. Hlavacek [11] shows an example where there is a large stable periodic orbit surrounding three unstable critical points. Our conjecture is tantamount to saying that this is always the case. When the situation is as in Figure 8 there would be two periodic orbits for $Da < Da_3$ but sufficiently close to Da_3. A small unstable periodic orbit would encircle the corresponding stable critical point on the lower branch and a large periodic orbit, presumably stable, surrounding all three critical points and the unstable critical point.

Chapter 6

JUMP PHENOMENA

Section 1. Introduction

In this chapter we use the response diagrams discussed in Section 5.6 to show how "jumps" into periodic orbits occur as the Damkohler is changed. We first discuss (for completeness) the classical "jump" between steady states and then show two new types of "jump" phenomena in which there is a "jump" into oscillatory steady states.

Section 2. Oscillatory Instabilities and Ignition and Extinction Processes.

By an oscillatory instability we shall not mean an unstable limit cycle but instead a "jump" into a large limit cycle (usually stable) from a steady state as some parameter changes. Before discussing these instabilities we focus our attention on another instability —the ignition and extinction processes. Crudely speaking, an ignition process is said to occur when the temperature "jumps" from one steady state to a much higher steady state as some parameter changes. The extinction process is the reverse process. A discussion of these processes can be found in Aris [1]. The above mentioned paramter is usually the feed temperature —the temperature of the chemicals entering the reactor—or the flow velocity of the entering chemicals. We consider variations of the first parameter, the feed temperature, since the Damkohler number Da $\propto \exp(\frac{-E}{RT_0})$ where E and R are physical constants and T_0 is the feed temperature. We note that Da is a strictly increasing function of T_0. As we vary T_0, we will require that β, B and x_c remain constant. In terms of the concentration, C_0, and temperature of the feed this requires that $C_0/T_0{}^2$ remain constant and that the temperature of the heat exchanger in the reactor be the same as the temperature of the chemicals (see V. Hlavacek, M. Kubicek, and J. Jelinek [11]). Throughout the remainder of this section we assume that these conditions are satisfied. We will first discuss the "jump" between steady states or, in physical terms, the extinction and ignition processes.

For β and B in that part of Region II in which $B < 3 + \beta + 2\sqrt{2+\beta}$ we know by Theorem 4.6.1 that for all Da such that there is a unique critical point all trajectories tend to the critical point. In Figure 17 we have a typical "S" shaped curve.

Suppose we are at a steady state at point 1. As Da increases we assume that the initial conditions $(x_1(0), x_2(0))$ are changed so that $(x_1(0), x_2(0))$ is a small perturbation from $(a_1(Da), a_2(Da))$. In this case the solution will quickly settle to the steady state $(a_1(Da), a_2(Da))$. As Da increases we traverse the "S" shaped curve from 1 to 2 to 3 to 4. Any further increase in Da beyond Da_I causes the steady state to "jump" to a much higher value at 5. We have in fact proved that this jump occurs by our previous remark that all trajectories must tend to the unique steady state.

This "jump" is called an ignition process and we say that the feed temperature has become sufficiently high to ignite the reactor. Increasing Da further carries the steady state to point 6. As we decrease Da we pass through points 5 to 7 to 8. Any further decrease in Da at point 8 causes another "jump" downward. In this case the reactor has been extinguished by too cold a feed.

Thus for β and B in that part of Region II where $B \leq 3 + \beta + 2\sqrt{2+\beta}$ we have proved that this "jump" to a lower or higher steady state actually occurs. When $\beta = 0$, one can also prove this; for β and B in the remaining part of Region II we conjecture that it also is true.

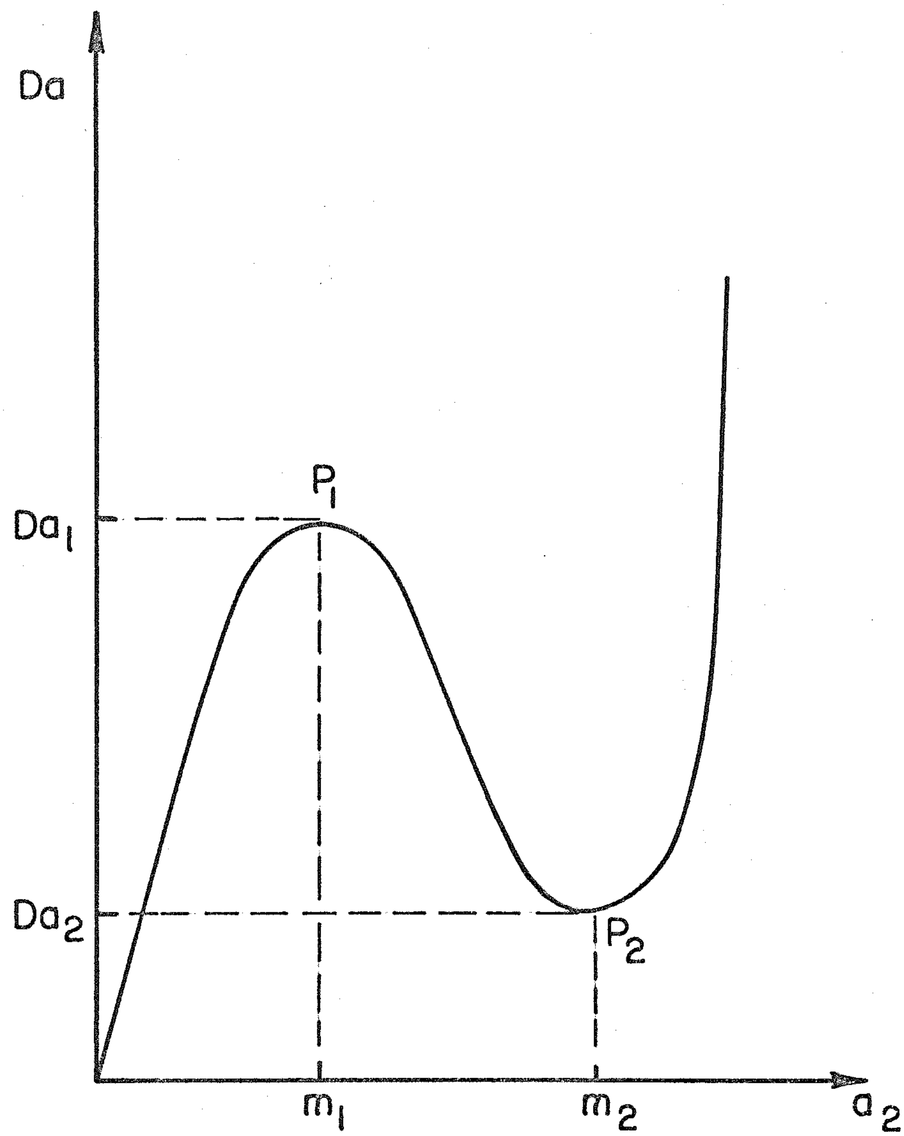
Consider next the "S" shaped response curve, Figure 18. Suppose we start at point 1. As the feed temperature increases the steady state passes to point 2. Any further increase in Da will cause a "jump" but now into a periodic orbit around the critical point at point 3. This same phenomenon occurs whenever a situation like Figure 11 occurs.

Finally consider the response curve as in Figure 19. Suppose we start at position 1 and increase Da; we pass from 1 to 2 to 3. A slight perturbation of the initial conditions at point 3 causes the solution to jump into a large periodic orbit at this point. By changing Da now we only change the size of the large periodic orbit by a small amount. In this case there is a loss in the control of the reactor. Suppose we start at point 5 and decrease Da. When we reach point 4, a slight perturbation in the initial condition causes no trouble since the solution settles back to the steady state. Decreasing Da further causes the slow growth of a stable periodic orbit. In this case we can control the size of the periodic orbit by increasing Da. Thus the direction of bifurcation tells us when we will lose control of the reactor by changing the feed temperature. A similar phenomena occurs in Figures 8 and 9.

TABLE I

FIGURE NO.	(β, B)	$P_1 = (m_1, Da_1)$	$P_2 = (m_2, Da_2)$	$P_3 = (s_1, Da_3)$	$P_4 = (s_1, Da_4)$	Sign of δ^1
5	(.72, 10.0)	(.2027, .07849)	(.7793, .03804)		(.8532, .04074)	$\delta^1(P_4) > 0$
6	(.72, 7.3)	(.3801, .1222)	(.6199, .1174)		(.7131, .1205)	$\delta^1(P_4) < 0$
7	(.78, 7.3)	(.4215, .1293)	(.5785, .1280)		(.6991, .1321)	$\delta^1(P_4) < 0$
	(1.6, 12.5)	(.2951, .1013)	(.7049, .0806)		(.8812, .1072)	$\delta^1(P_4) < 0$
8	(1.4, 9.8)	(.4286, .1303)	(.5714, .1293)	(.4212, .1304)	(.8237, .1617)	$\delta^1(P_3) < 0$, $\delta^1(P_4) < 0$
9	(1.44, 9.8)	(.4681, .1343)	(.5319, .1342)	(.4271, .1341)	(.8219, .1700)	$\delta^1(P_3) < 0$, $\delta^1(P_4) < 0$
10	(.72, 7.02)	(.4294, .1304)	(.5706, .1294)	(.6154, .1298)	(.6296, .1301)	$\delta^1(P_3) > 0$, $\delta^1(P_4) < 0$
11	(.74, 7.06)	(.4405, .1318)	(.5595, .1312)	(.6055, .1316)	(.6409, .1325)	$\delta^1(P_3) > 0$, $\delta^1(P_4) < 0$
12	(.82, 7.3)	(.4738, .13462)	(.5262, .13457)	(.5622, .1347)	(.6870, .1395)	$\delta^1(P_3) > 0$, $\delta^1(P_4) < 0$
13	(.9, 7.4)			(.5739, .1441)	(.6829, .1507)	$\delta^1(P_3) > 0$, $\delta^1(P_4) < 0$
14	(1.34, 9.0)			(.4694, .1454)	(.7906, .1805)	$\delta^1(P_3) < 0$, $\delta^1(P_4) < 0$
	(3.0, 14.0)			(.4060, .1650)	(.8798, .3366)	$\delta^1(P_3) < 0$, $\delta^1(P_4) < 0$

Numerical Examples for Figures 5-14



$B > 4(1+\beta)$

$P_1 = (m_1, Da_1)$

$P_2 = (m_2, Da_2)$

FIGURE 1

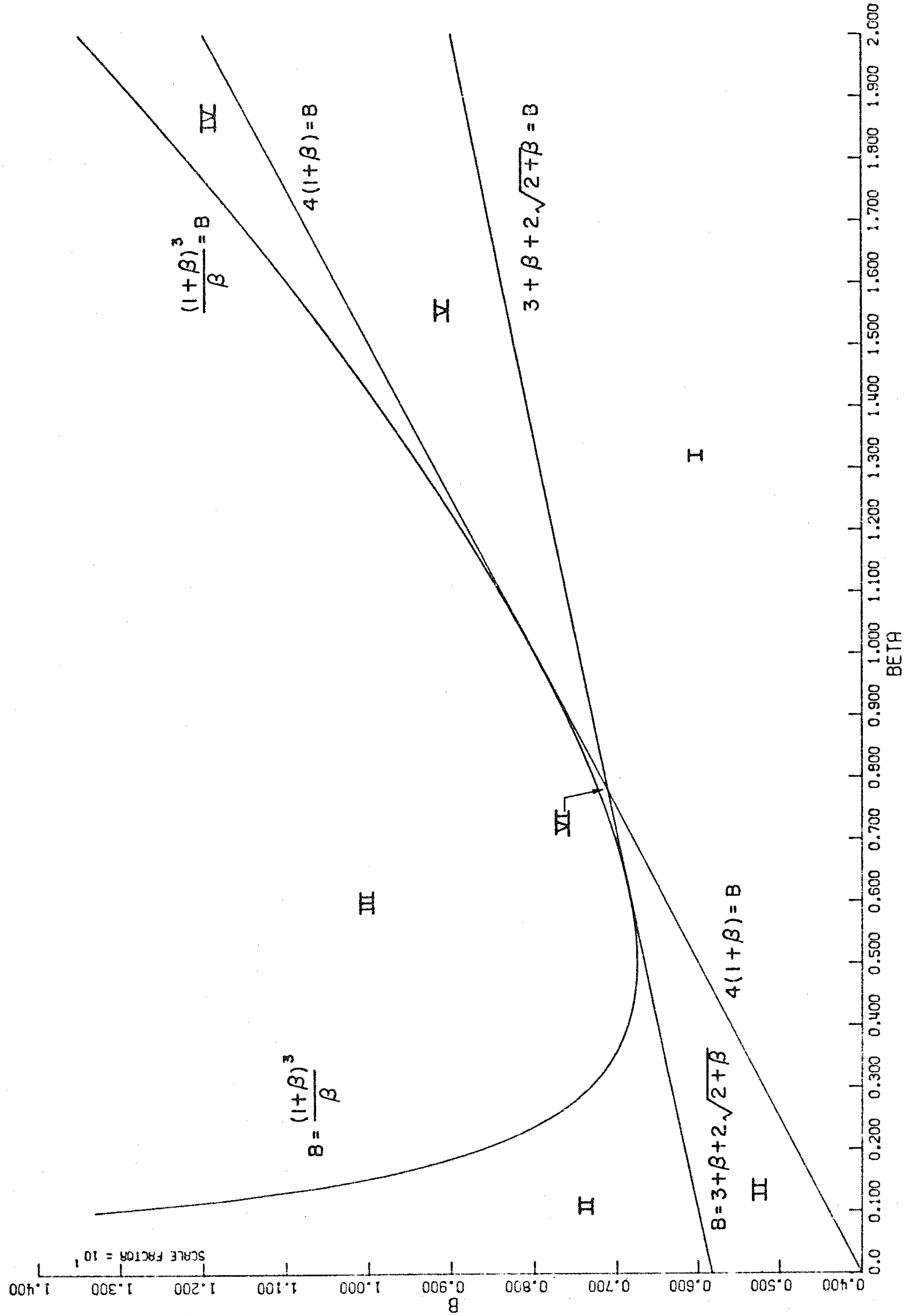

B
BETA
SCALE FACTOR = 10^1
0.0
0.100
0.200
0.300
0.400
0.500
0.600
0.700
0.800
0.900
1.000
1.100
1.200
1.300
1.400
1.500
1.600
1.700
1.800
1.900
2.000
0.400
0.500
0.600
0.700
0.800
0.900
1.000
1.100
1.200
1.300
1.400
I
II
III
IV
V
VI
$\frac{(1+\beta)^3}{\beta} = B$
$4(1+\beta) = B$
$3+\beta+2\sqrt{2+\beta} = B$
$B = \frac{(1+\beta)^3}{\beta}$
$B = 3+\beta+2\sqrt{2+\beta}$
$4(1+\beta) = B$

FIGURE 2

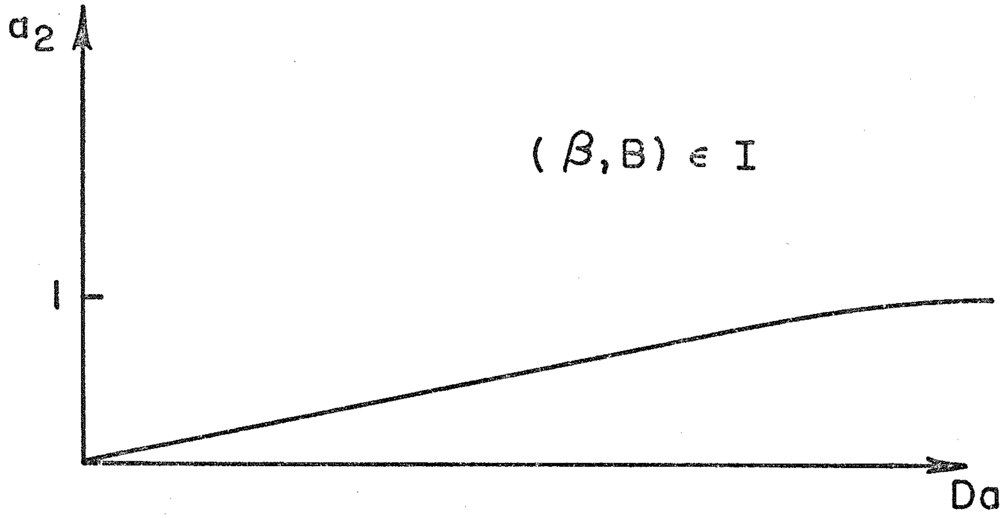


FIGURE 3

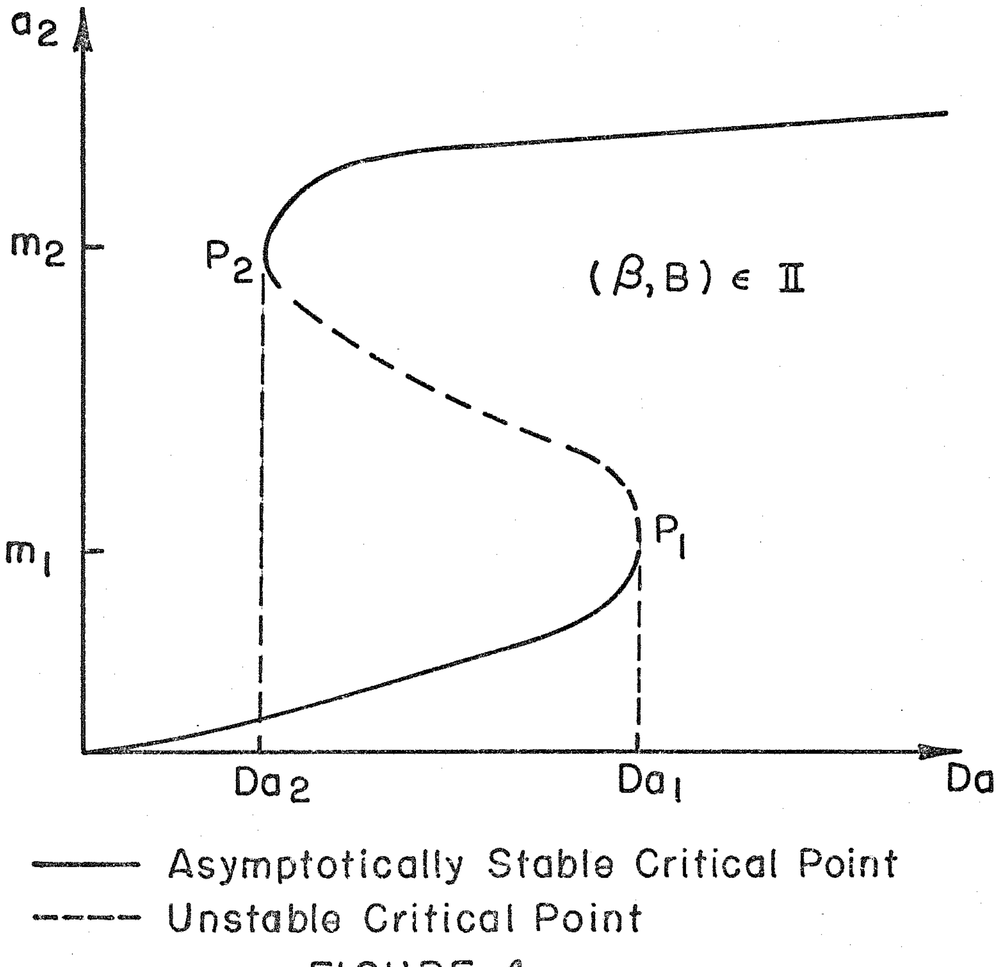
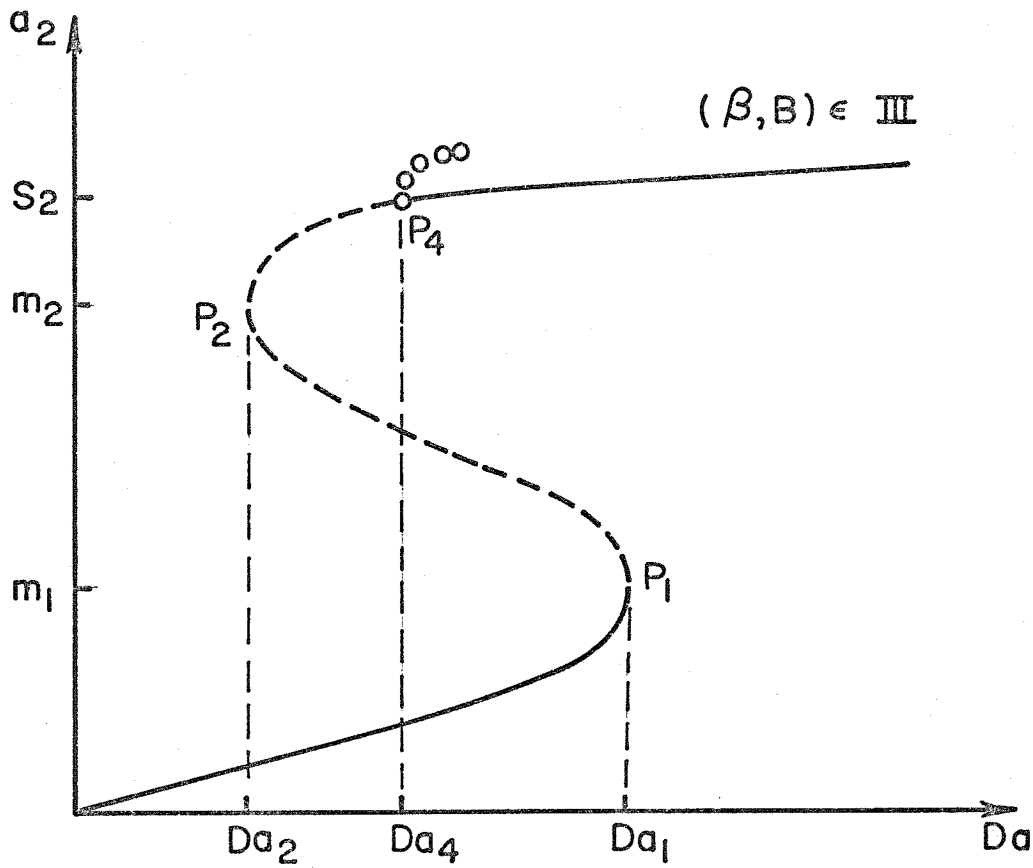


FIGURE 4



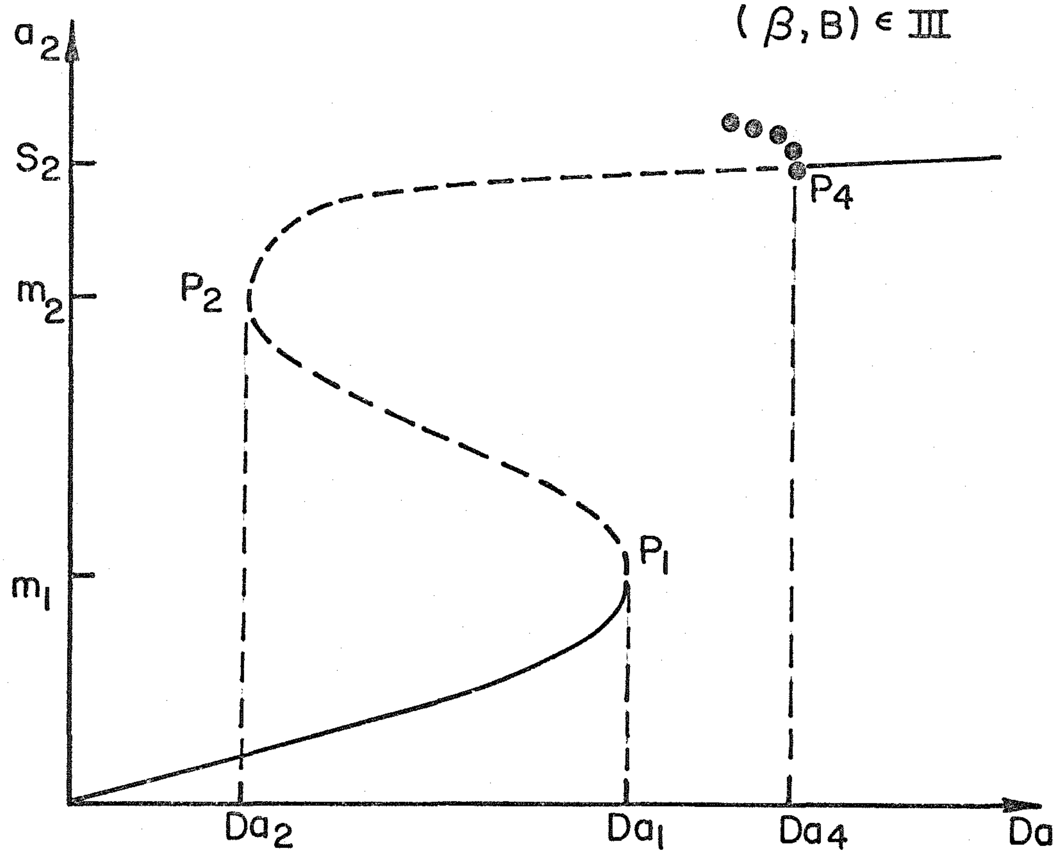
——— Asymptotically Stable Critical Point

- - - - - Unstable Critical Point

o o o o Unstable Periodic Orbit

$\delta'(P_4) > 0$

FIGURE 5



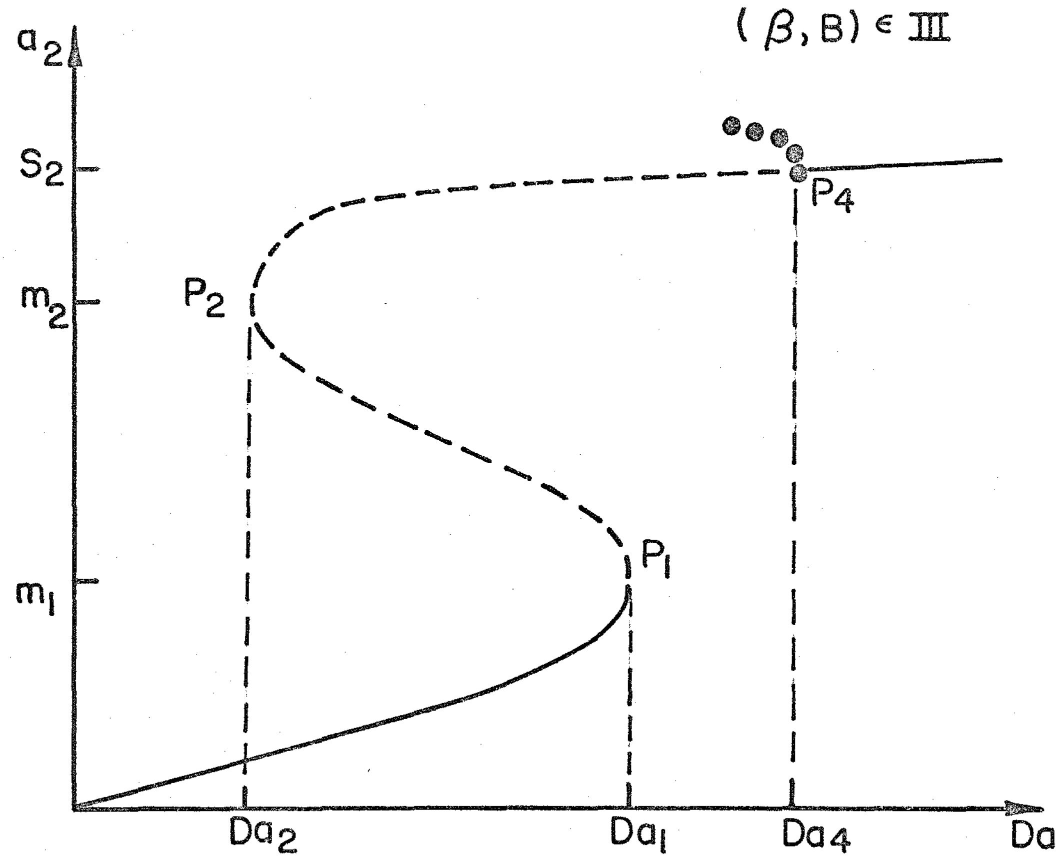
—— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_4) < 0$

FIGURE 7



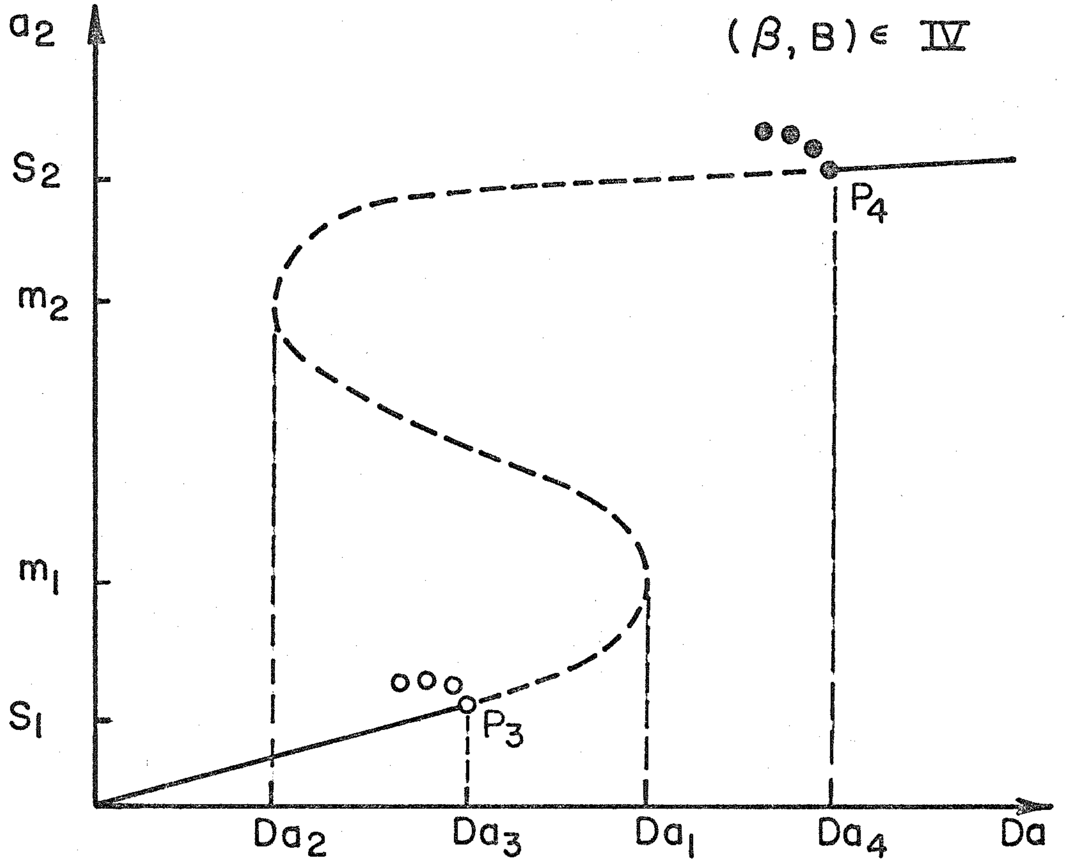
——— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_4) < 0$

FIGURE 7



——— Asymptotically Stable Critical Point

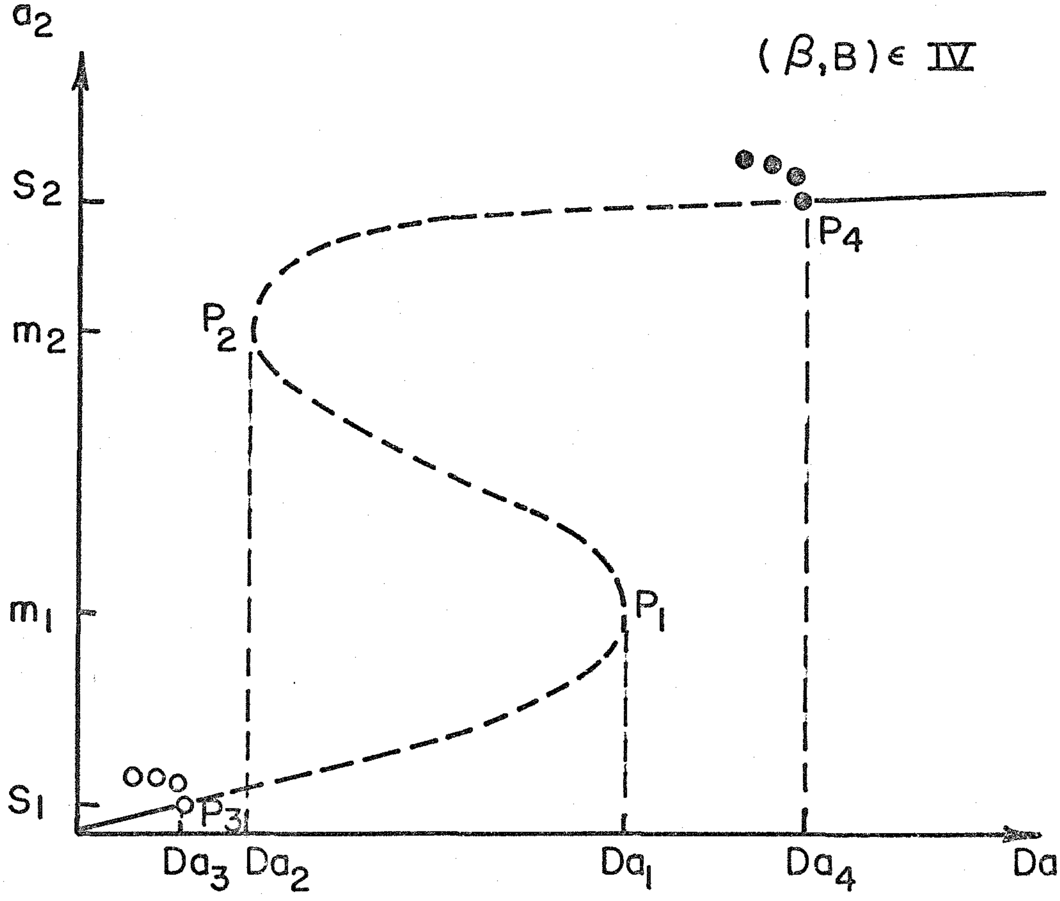
– – – – Unstable Critical Point

○○○ Unstable Periodic Orbit

●●● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_3) < 0, \ \delta'(P_4) < 0$

FIGURE 8



—— Asymptotically Stable Critical Point

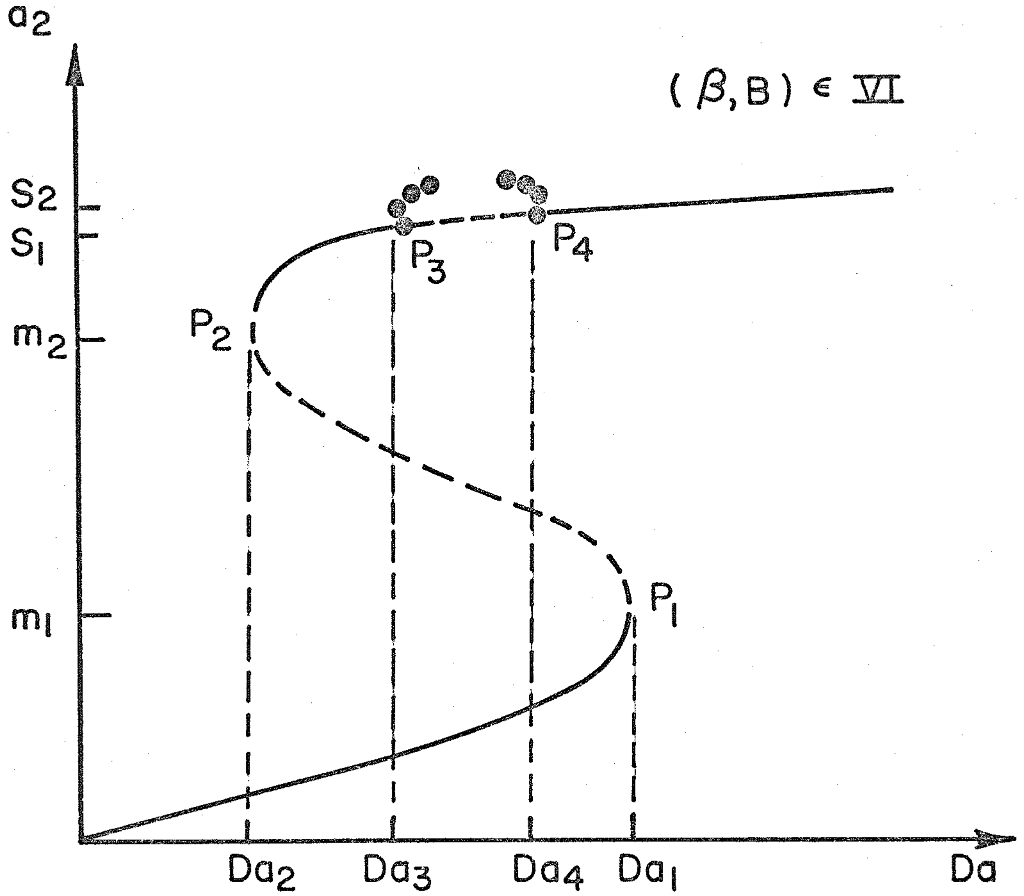
- - - - Unstable Critical Point

o o o Unstable Periodic Orbit

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_4) < 0, \; \delta'(P_3) < 0$

FIGURE 9



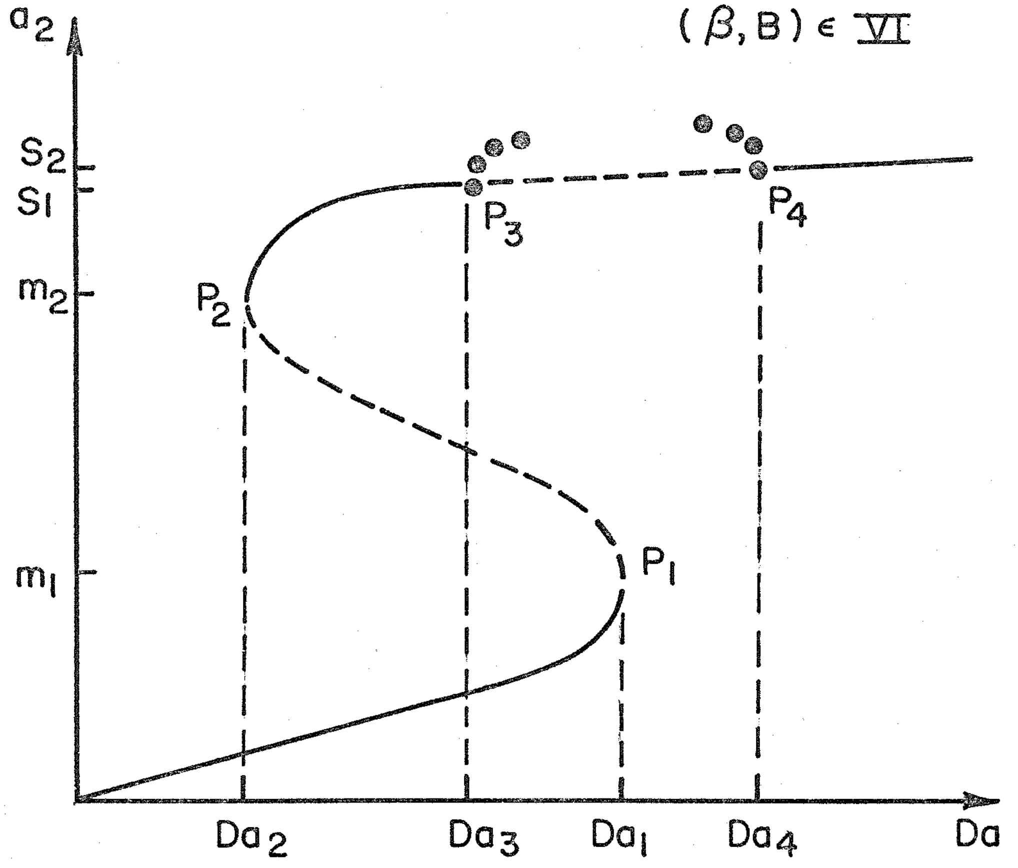
—— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

●●● Asymptotically Orbitally Stable Periodic Orbit

* $\delta'(P_3) > 0$, $\delta'(P_4) < 0$

FIGURE 10



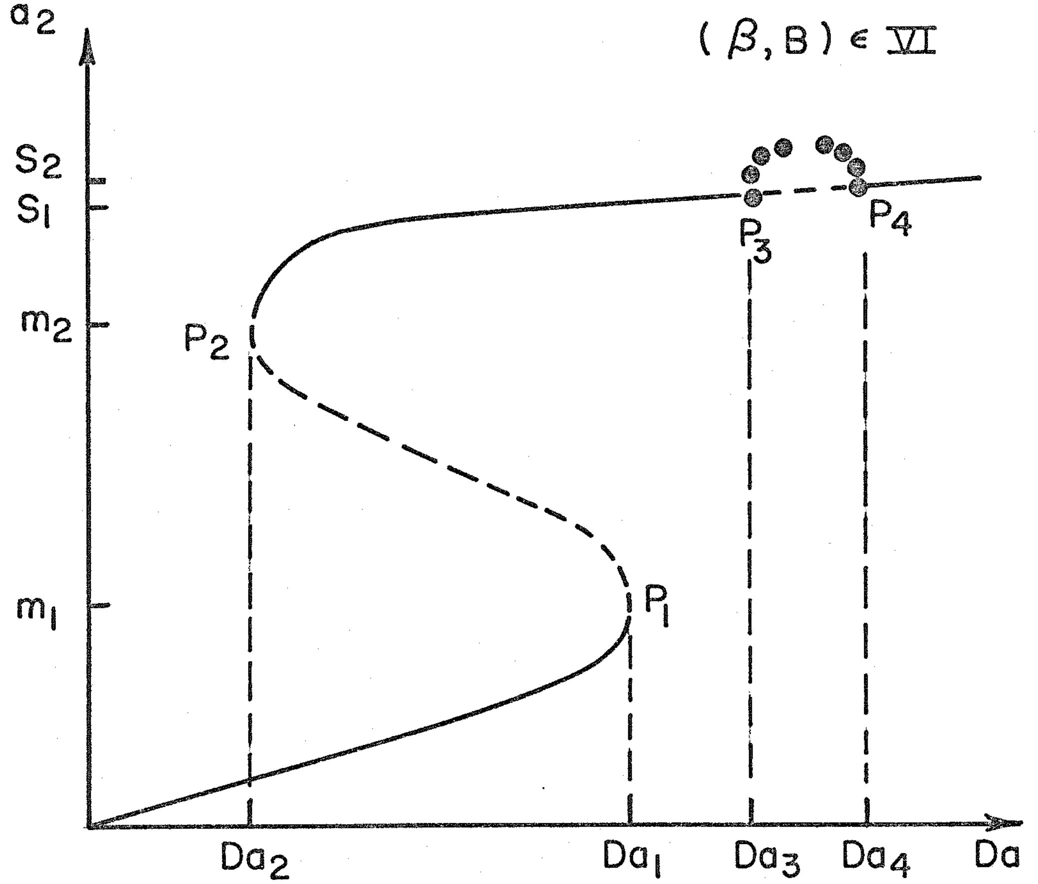
——— Asymptotically Stable Critical Point

– – – Unstable Critical Point

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_3) > 0$, $\delta'(P_4) < 0$

FIGURE II



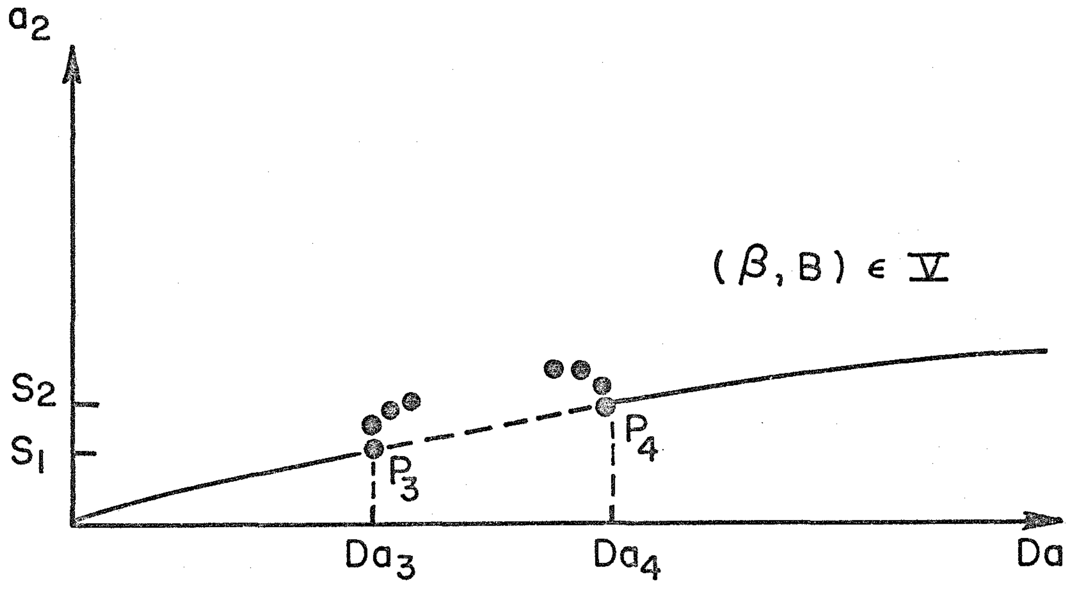
—— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_3) > 0, \ \delta'(P_4) < 0$

FIGURE 12



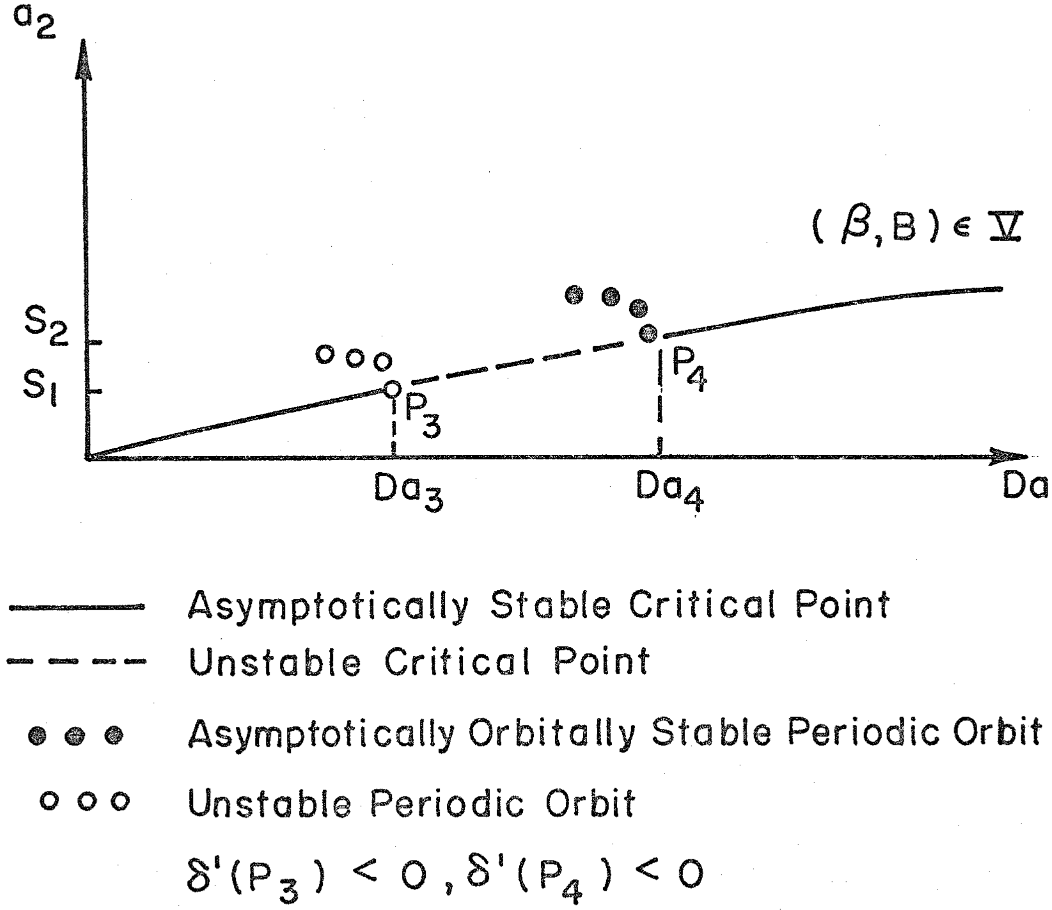
——— Asymptotically Stable Critical Point

– – – – Unstable Critical Point

● ● ● Asymptotically Orbitally Stable Periodic Orbit

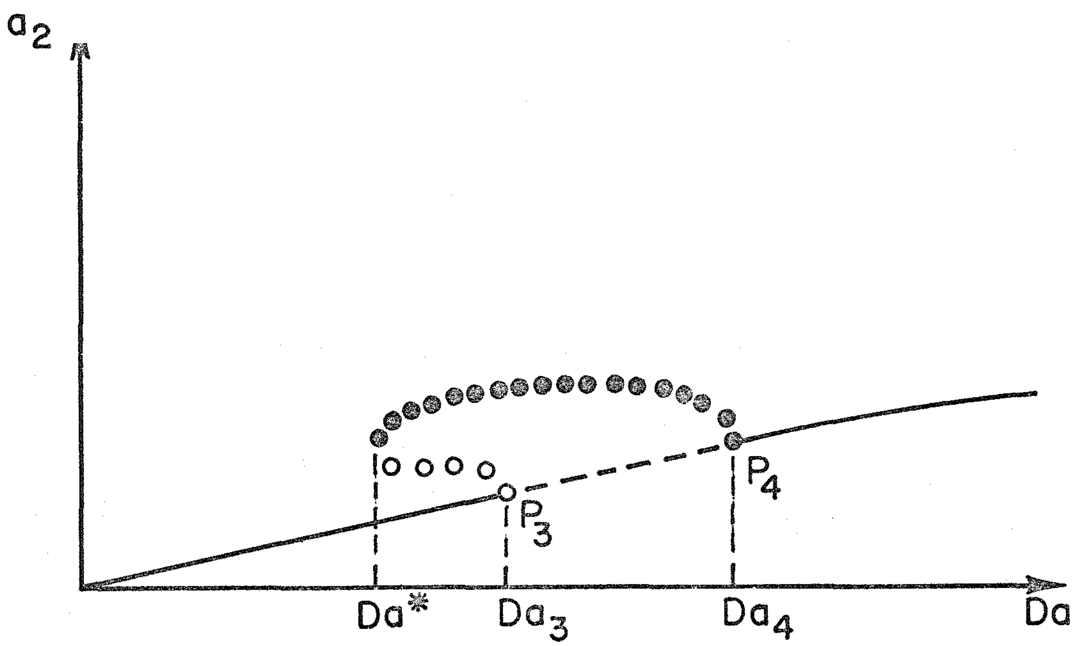
$\delta'(P_3) > 0 , \ \delta'(P_4) < 0$

FIGURE 13



a_2
$(\beta, B) \in \mathrm{V}$
S_2
S_1
P_3
P_4
Da_3
Da_4
Da
Asymptotically Stable Critical Point
Unstable Critical Point
Asymptotically Orbitally Stable Periodic Orbit
Unstable Periodic Orbit
$\delta'(P_3) < 0, \delta'(P_4) < 0$

FIGURE 14



—— Asymptotically Stable Critical Point

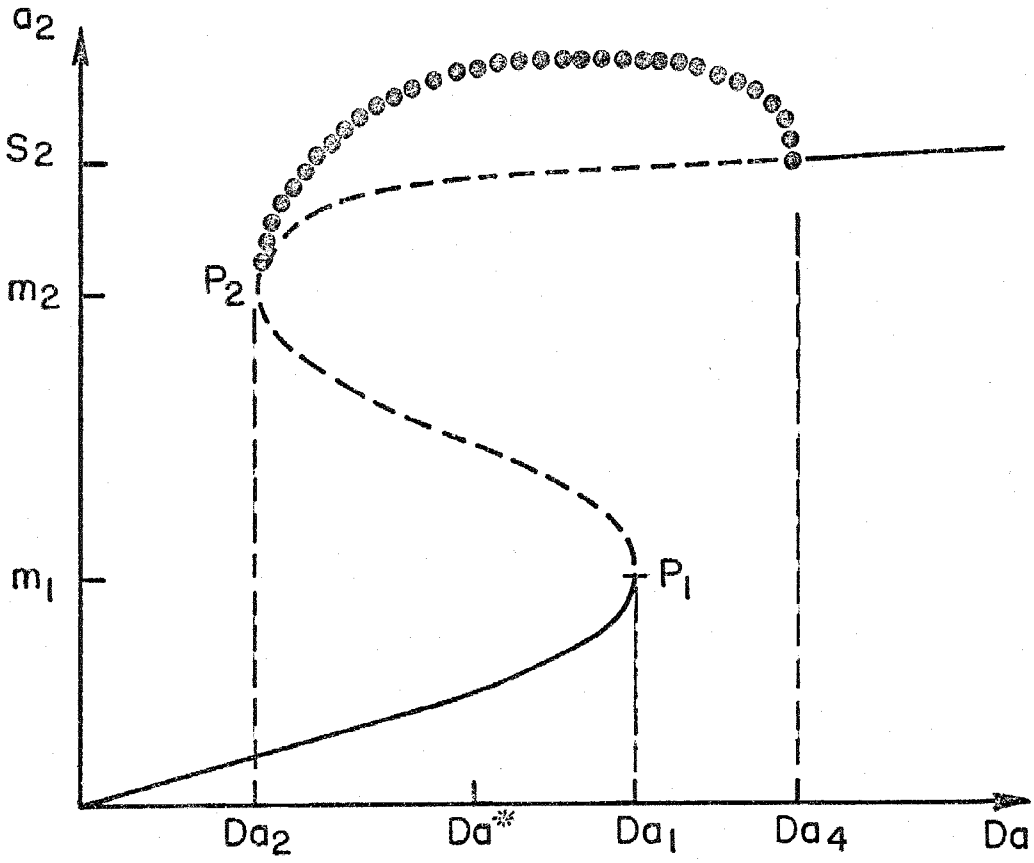
- - - - Unstable Critical Point

○ ○ ○ Unstable Periodic Orbit

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_3) < 0, \ \delta'(P_4) < 0$

FIGURE 15



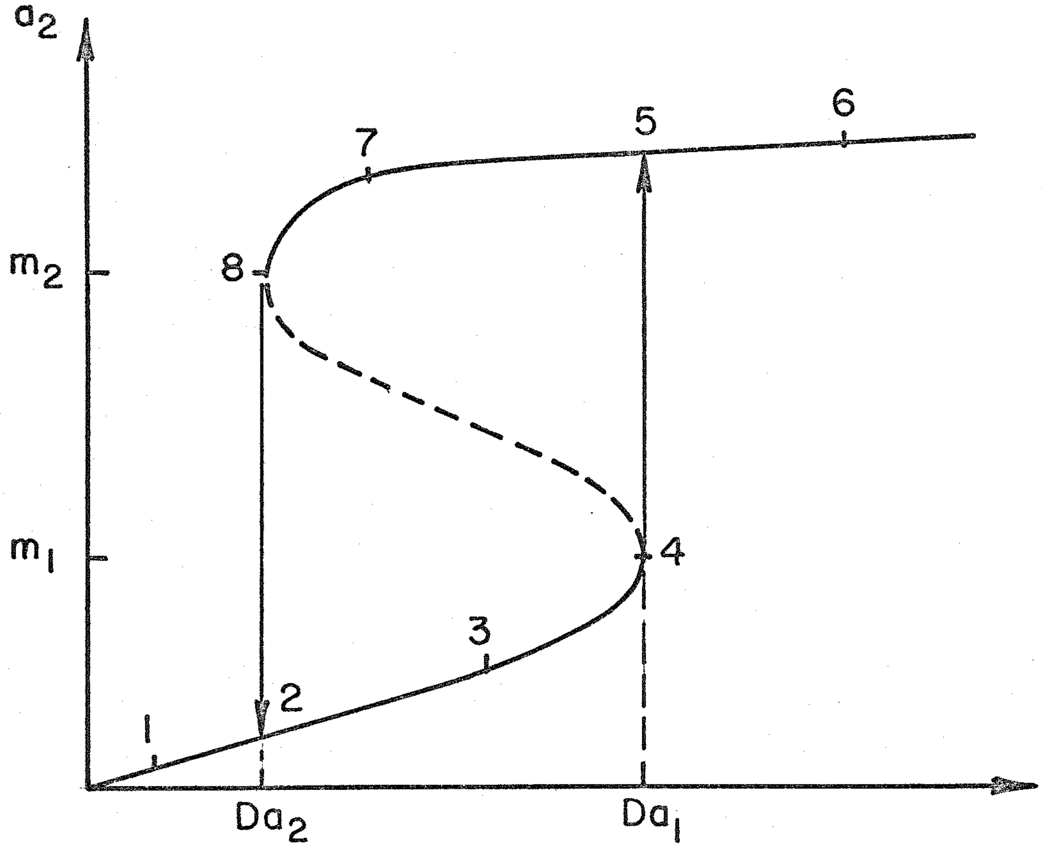
——— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_4) < 0$

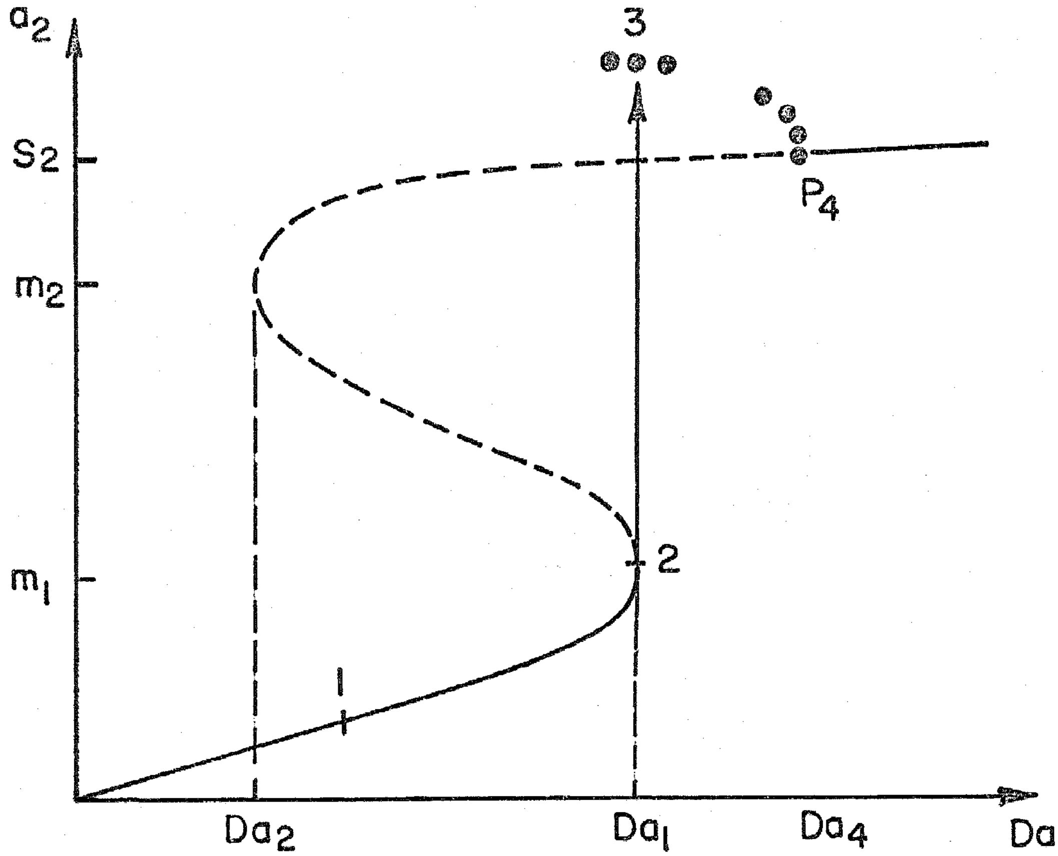
FIGURE 16



——— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

FIGURE 17



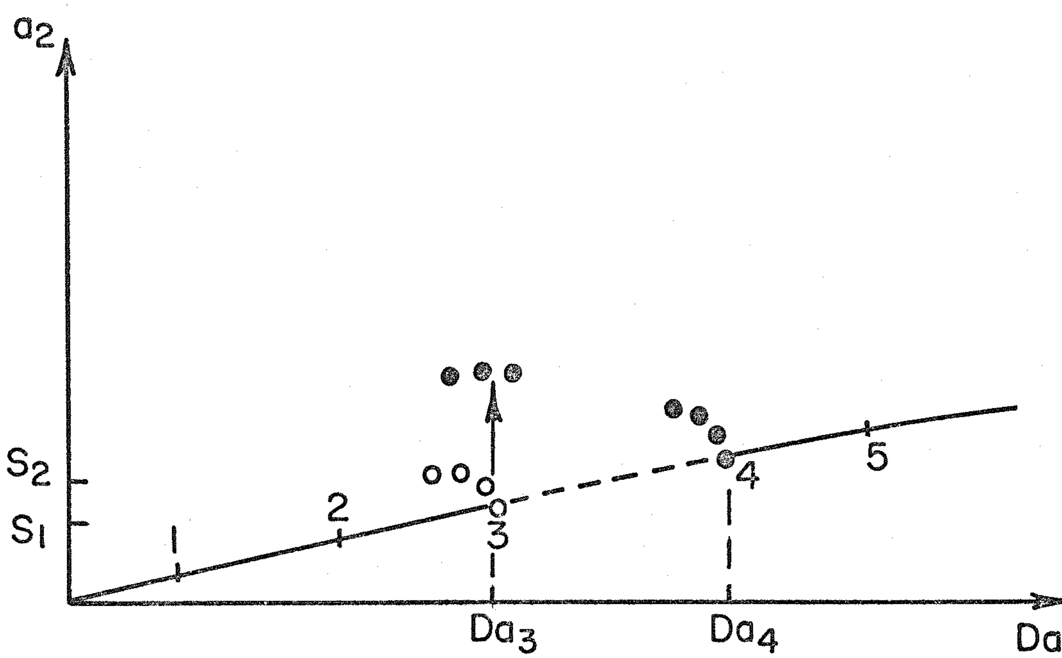
—— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

••• Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_4) < 0$

FIGURE 18



——— Asymptotically Stable Critical Point

- - - - Unstable Critical Point

o o o Unstable Periodic Orbit

● ● ● Asymptotically Orbitally Stable Periodic Orbit

$\delta'(P_3) < 0$, $\delta'(P_4) < 0$

FIGURE 19

Appendix A

We compare the roots m_1, m_2, s_1, and s_2 for the various values of β and B restricted to $B > 4(1+\beta)$ and $B > 3 + \beta + 2\sqrt{2+\beta}$ (this implies that m_1, m_2, s_1, and s_2 are real). In this comparison there are four curves which arise. They are

(A-1) $$B = f_1(\beta) = 4(1+\beta) \ ,$$

(A-2) $$B = f_2(\beta) = 3 + \beta + 2\sqrt{2+\beta} \ ,$$

(A-3) $$B = f_3(\beta) = \frac{(1+\beta)^3}{\beta} \ ,$$

(A-4) $$B = f_4(\beta) = (\sqrt{5} + 2)(1+\beta) \ .$$

It is easy to show that $f_1(\beta)$ and $f_3(\beta)$ have a point of tangency at $\beta = 1$ and $f_2(\beta)$ and $f_3(\beta)$, at $\beta = \frac{\sqrt{5}-1}{2}$. $f_1(\beta)$ intersects $f_2(\beta)$ at $\beta = {}^7/9$ and f_4 intersects f_2 and f_3 at $\beta = \frac{\sqrt{5}-1}{2}$. The roots m_1, m_2, s_2, s_2 are defined through

(A-5) $$m_1 = \tfrac{1}{2} - \tfrac{1}{2}\sqrt{1 - \frac{4(1+\beta)}{B}} \ ,$$

(A-6) $$m_2 = \tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - 4(1+\beta)} \ ,$$

(A-7) $$s_1 = \frac{B+1+\beta}{2B} - \frac{1}{2B}\sqrt{(B-1-\beta)^2 - 4B} \ ,$$

(A-8) $$s_2 = \frac{B+1+\beta}{2B} + \frac{1}{2B}\sqrt{(B-1-\beta)^2-4B} \ .$$

We seek those values of β and B which satisfy

(i) $s_1 < m_1$, (ii) $s_1 > m_2$,

(iii) $s_2 < m_1$, (iv) $s_2 > m_2$.

Since the algebra is straightforward, we give only the results:

Re(i): $s_1 < m_1$ iff $\beta > 1$, $B > 4(1+\beta)$, and $B < \frac{(1+\beta)^3}{\beta}$.

Re(ii): $s_1 > m_2$ iff $\beta < 1$, $B < 2(\beta+3)$, $B < (2+\sqrt{5})(1+\beta)$,

$B < \frac{(1+\beta)^3}{\beta}$, $B > 4(1+\beta)$, and $B > 3+\beta+2\sqrt{2+\beta}$.

Re(iii): $s_2 < m_1$ never occurs for $B > 4(1+\beta)$ and $B > 3+\beta+2\sqrt{2+\beta}$

Re(iv): $s_2 > m_2$ iff $\beta \geq 1$ and $B > 4(1+\beta)$, or

$\beta < 1$ and $B > (1+\beta)^3/\beta$, or

$B < (2+\sqrt{5})(1+\beta)$, $B > 4(1+\beta)$, and

$B > 3+\beta+2\sqrt{2+\beta}$.

From our definition of $f_i(\beta)$ $(i = 1, 2, 3, 4)$ and remarks about the intersections of these curves it follows that (see the definitions of the various regions in Section 4.5.)

$$s_1 < m_1 \text{ iff } (\beta, B) \in IV ,$$

$$s_1 > m_2 \text{ iff } (\beta, B) \in VI ,$$

$$s_2 > m_2 \text{ iff } (\beta, B) \in III, IV, \text{ or } VI.$$

Consequently, for $B > \max\left\{4(1+\beta),\ 3+\beta+2\sqrt{2+\beta}\right\}$

$$m_1 < s_1 < m_2 \text{ iff } (\beta, B) \in II \text{ or } III ,$$

$$m_1 < s_2 < m_2 \text{ iff } (\beta, B) \in II .$$

This completes the comparison of the roots m_1, m_2, s_1, and s_2.

Appendix B

We determine

(B-1) $$\underset{\sim}{y}^1 = Y(s)\int_0^s Y^{-1}(\tau)Q^0(\underset{\sim}{y}^0(\tau),0)d\tau = \int_0^s Y(s-\tau)Q^0(\underset{\sim}{y}^0(\tau),0)d\tau \ .$$

where

(B-2) $$\underset{\sim}{y}^0 = \begin{Bmatrix} y^0{}_1 \\ y^0{}_2 \end{Bmatrix} = \begin{Bmatrix} -\dfrac{Bab}{\omega_0}\sin\omega_0 s \\ \cos\omega_0 s - \dfrac{b}{\omega_0}\sin\omega_0 s \end{Bmatrix} ,$$

(B-3) $$Q^0(\underset{\sim}{y}^0,0) = \frac{ab}{2}\begin{Bmatrix} B(1-a)(y^0{}_1)^2 - 2y^0{}_2\, y^0{}_1) \\ (1-a)(y^0{}_1)^2 - 2y^0{}_2\, y^0{}_1) \end{Bmatrix} , \text{ and}$$

(B-4) $$Y(s) = (\cos\omega_0 s)I + \left(\frac{\sin\omega_0 s}{\omega_0}\right)A^0 .$$

Using (B-3) and (B-4), we obtain

(B-5) $$\begin{aligned} Y(s-\tau)Q^0(y^0,0) = {} & \frac{ab}{2}\cos\omega_0 s \begin{Bmatrix} B(((1-a)(y^0{}_1)^2 - 2y^0{}_1 y^0{}_2)\sin\omega_0 \tau) \\ (\quad '' \quad\quad '' \quad) \end{Bmatrix} \\ & + \frac{ab}{2}\sin\omega_0 s \begin{Bmatrix} B(((1-a)(y^0{}_1)^2 - 2y^0{}_2 y^0{}_2)\sin\omega_0 \tau) \\ (\quad '' \quad\quad '' \quad) \end{Bmatrix} \\ & + \frac{ab}{2\omega_0}\sin\omega_0 s \begin{Bmatrix} B(((1-a)(y^0{}_1)^2 - 2y^0{}_2 y^0{}_1)\cos\omega_0 \tau) \\ (Ba-b)(\quad '' \quad\quad '' \quad\quad '' \quad) \end{Bmatrix} \\ & - \frac{ab}{2\omega_0}\cos\omega_0 s \begin{Bmatrix} B(((1-a)(y^0{}_1)^2 - 2y^0{}_1 y^0{}_2)\sin\omega_0 \tau) \\ (Ba-b)(\quad '' \quad\quad '' \quad\quad '' \quad) \end{Bmatrix} . \end{aligned}$$

Using (B-2), we obtain

$$\text{(B-6)} \quad \int_0^s (y^0{}_1)^2 \cos\omega_0 \tau d\tau = \frac{B^2 b^2 a^2}{3\omega_0^3} \sin^3 \omega_0 s \ ,$$

$$\text{(B-7)} \quad \int_0^s (y^0{}_1)^2 \sin\omega_0 \tau d\tau = \frac{B^2 b^2 a^2}{3\omega_0^3} (2 - \cos\omega_0 s(2 + \sin^2 \omega_0 s)) \ ,$$

$$\text{(B-8)} \quad \int_0^s y^0{}_1 y^0{}_2 \cos\omega_0 \tau d\tau = \frac{Bab}{3\omega_0^2} (\cos^3 \omega_0 s - 1) + \frac{Bb^2 a}{3\omega_0^2} \sin^3 \omega_0 s \ ,$$

$$\text{(B-9)} \quad \int_0^s y^0{}_1 y^0{}_2 \sin\omega_0 \tau d\tau = -\frac{Bab}{3\omega_0^2} \sin^3 \omega_0 s + \frac{Bb^2 a}{3\omega_0^3} (2 - \cos\omega_0 s(2 + \sin^2 \omega_0 s)) \ .$$

Using $(1-a)^{-1} = b$ (this is the fact that $\operatorname{tr} A^0 = b - \frac{1}{(1-a)} = 0$), equations (B-1) and (B-5) through (B-9), we obtain

$$\text{(B-10)} \quad y^1(\tau) = \int_0^s Q^0(\underset{\sim}{y}^0(\tau), 0) d\tau$$

$$= \frac{Ba^2 b^2}{6\omega_0^3} \begin{Bmatrix} B\{(Ba-2b)\sin^3\omega_0 s \cos\omega_0 s - 2\omega_0(\cos^4\omega_0 s - \cos\omega_0 s)\} \\ \{ \quad '' \qquad\qquad '' \quad \} \end{Bmatrix}$$

$$+ \frac{Ba^2 b^2}{6\omega_0^3} \begin{Bmatrix} B\{(Ba-2b)\left(2\sin\omega_0 s - \sin\omega_0 s \cos\omega_0 s (2 + \sin^2 \omega_0 s)\right) + 2\omega_0 \sin^4 \omega_0 s\} \\ \{ \quad '' \qquad '' \qquad '' \qquad '' \quad \} \end{Bmatrix}$$

$$+ \frac{Ba^2 b^2}{6\omega_0^4} \begin{Bmatrix} B\{(Ba-2b)\sin^4 \omega_0 s - 2\omega_0 (\cos^3 \omega_0 s \sin\omega_0 s - \sin\omega_0 s)\} \\ (Ba-b)\{ \quad '' \qquad '' \qquad '' \quad \} \end{Bmatrix}$$

$$- \frac{Ba^2 b^2}{6\omega_0^4} \begin{Bmatrix} B\{(Ba-2b)\left(2\cos\omega_0 s - \cos^2\omega_0 s(2 + \sin^2\omega_0 s)\right) + 2\omega_0 \sin^3 \omega_0 s \cos\omega_0 s\} \\ (Ba-b)\{ \quad '' \qquad '' \qquad '' \quad \} \end{Bmatrix}$$

This simplifies to

$$y^1(s) = \frac{Ba^2b^2}{6\omega_0^3}\left[\begin{array}{l} B\{(Ba-2b)(2\sin\omega_0 s - \sin 2\omega_0 s \;\; + 2\omega_0(\cos\omega_0 s - \cos 2\omega_0 s)\} \\ \;\{ \quad \text{''} \qquad\qquad \text{''} \qquad\qquad\qquad\qquad \text{''} \qquad\qquad\qquad \} \end{array}\right]$$

$$+ \frac{Ba^2b^2}{6\omega_0^4}\left\{\begin{array}{l} B\{(Ba-2b)(1-2\cos\omega_0 s + \cos^2\omega_0 s) - \omega_0(\sin 2\omega_0 s - 2\sin\omega_0 s)\} \\ (Ba-b)\{\text{''} \qquad\qquad \text{''} \qquad\qquad\qquad\qquad \text{''} \qquad\qquad \} \end{array}\right\} .$$

Appendix C

We show that

$$\text{(C-1)} \qquad \tilde{A} = \frac{1}{T^0} \int_0^{T^0} Y^{-1}(\tau)\, A^0\, Y(\tau)\, d\tau = A^0$$

and

$$\text{(C-2)} \qquad \tilde{C} = \frac{1}{T^0} \int_0^{T^0} Y^{-1}(\tau)\, C^0\, Y(\tau)\, d\tau = \tfrac{1}{2}\left(C^0 \; \frac{1}{\omega_0^2} A^0 C^0 A^0\right) .$$

Recall that

$$\text{(C-3)} \qquad Y(\tau) = \cos\omega_0 \tau I + \left(\frac{\sin\omega_0 \tau}{\omega_0}\right) A^0$$

and

$$\text{(C-4)} \qquad Y^{-1}(\tau) = Y(-\tau) .$$

Therefore,

$$\text{(C-5)} \quad Y^{-1}(\tau) A^0 Y(\tau) = \left((\cos\omega_0 \tau) I - \frac{\sin\omega_0 \tau}{\omega_0} A^0\right) A^0 \left((\cos\omega_0 \tau) I + \frac{\sin\omega_0 \tau}{\omega_0} A^0\right)$$

$$= A^0 Y^{-1}(\tau) Y(\tau) = A^0$$

and

$$\text{(C-6)} \quad Y^{-1}(\tau)C^0Y(\tau) = \left(\cos\omega_0\tau C^0 - \frac{\sin\omega_0\tau}{\omega_0} A^0 C^0\right)\left(\cos\omega_0 I + \frac{\sin\omega_0\tau}{\omega_0} A^0\right)$$

$$= \cos^2\omega_0\tau C^0 - \frac{\sin^2\omega_0\tau}{\omega_0^2} A^0 C^0 A^0 + \frac{1}{2}\frac{\sin 2\omega_0\tau}{\omega_0}(C^0A^0 - A^0C^0).$$

(C-1) and (C-2) immediately follow from (C-5), (C-6) and the fact that $\omega = \frac{2\pi}{T^0}$.

Appendix D

Starting with

$$\text{(D-1)} \qquad \eta^1 \tilde{A}\underset{\sim}{b}_0 + \delta^1 \tilde{C}\underset{\sim}{b}_0 = -\frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\left.\frac{dQ^\varepsilon}{d\mu}\right|_{\mu=0} d\tau \ ,$$

we shall show that the determinant of the coefficient matrix, Δ, is given by

$$\text{(D-2)} \qquad \Delta = -\frac{Bab}{2}\, trC^0$$

and the expression for δ^1 is given by

$$\text{(D-3)} \qquad \delta^1 = \frac{Ba^2 b^2}{8\omega_0{}^4\, trC^0}\left(\omega_0^2(b-1) + (2b-Ba) - (2b-Ba)^2\right)$$

when $\underset{\sim}{b}_0 = \left\{ {0 \atop 1} \right\}$.

Recall from (5.3.20) and (5.3.33) that

$$\text{(D-4)} \qquad A^0 = \begin{pmatrix} b & -Bab \\ a & -b \end{pmatrix}$$

and

$$\text{(D-5)} \qquad C^0 = \begin{pmatrix} B & -Bb^2 \\ 1 & -b^2 \end{pmatrix} \frac{da^0_2}{d\varepsilon} .$$

Consequently,

(D-6) $$\tilde{A}\underset{\sim}{b}_0 = A^0\begin{Bmatrix}0\\1\end{Bmatrix} = \begin{Bmatrix}-Bab\\-b\end{Bmatrix}$$

and

(D-7) $$\tilde{B}\underset{\sim}{b}_0 = \tfrac{1}{2}(C^0 - \frac{1}{\omega_0^2} A^0 C^0 A^0)\begin{Bmatrix}0\\1\end{Bmatrix} = - \frac{b}{2\omega_0^2}\frac{da^0_2}{d\varepsilon}\begin{Bmatrix} B(b\omega_0^2+b^2-Ba) \\ \omega_0^2 b+(Ba-b)(b^2-Ba)\end{Bmatrix}$$

At this stage we have (5.3.34):

(D-8) $$b\begin{Bmatrix}Ba\\1\end{Bmatrix}\eta^1 + \frac{b\,da_2^0}{2\omega_0^2\,d\varepsilon}\begin{Bmatrix} B(b\omega_0^2+b^2-Ba) \\ \omega_0^2 b+(Ba-b)(b^2-Ba)\end{Bmatrix}\delta^1 = \frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\frac{dQ^\varepsilon}{d\mu}\bigg|_{\mu=0} d\tau .$$

Let Δ be the determinant of the coefficient matrix of δ^1 and η^1 in (C-8). Then

(D-9) $$\Delta = \frac{b^2}{2\omega_0^2}\frac{da_2^0}{d\varepsilon}\Big(Ba(\omega_0^2 b + (Ba-b)(b^2-Ba) - B(b\omega_0^2 + b^2-Ba)\Big) .$$

To simplify the expression (D-9) we will use

(D-10) $$\omega_0^2 = Ba^2 b - b^2 \quad \text{and} \quad (1-a)b = 1.$$

Now

(D-11) $Ba\left(\omega_0^2 b + (Ba-b)(b^2-Ba)\right) - B(b\omega_0^2 + b^2 - Ba)$

$$= B\{a(Ba^2b^2 - b^3 + Bab^2 - B^2a^2 - b^3 + Bab) - Ba^2b^2 + b^3 - b^2 + Ba\}$$

$$= B\{Ba^2b^2(a-1) + b^3(1-a) + Ba^2b^2 - B^2a^3 - ab^3 + Ba^2b - b^2 + Ba\} \ .$$

In this last expression we have

(D-12) $Ba^2b + Ba = Ba(ab+1) = Bab, \quad Ba^2b^2(a-1) = -Ba^2b, \quad b^3(1-a) = b^2 \ .$

Using (D-12) in (D-11), we obtain

(D-13) $B\{Ba^2b^2(a-1) + b^3(1-a) + Ba^2b^2 - B^2a^3 - ab^3 + Ba^2 - b^2 + Ba\}$

$$= B\{-Ba^2b + b^2 + Ba^2b^2 - B^2a^3 - ab^3 + Ba^2b - b^2 + Ba\}$$

$$= B\{Ba^2b^2 - B^2a^3 - ab^3 + Ba\}$$

$$= -Ba(-Bab^2 + B^2a^2 + b^3 - B) = -Ba((B-b^2)(Ba^2 - b))$$

$$= -\frac{Ba\omega_0^2}{b}(B-b^2) \ .$$

(D-13) and (D-9) imply that

$$\Delta = \frac{b^2}{2\omega_0^2}\frac{da^0_2}{d\varepsilon}\left(-\frac{Ba\omega_0^2}{b}(B-b^2)\right) = -\frac{Bab}{2}\left(\frac{da^0_2}{d\varepsilon}(B-b^2)\right) \ .$$

Recall that $\mathrm{tr}C^0 = \dfrac{da^0_2}{d\varepsilon}(B-b^2)$ so that

(D-14) $$\Delta = -\frac{Bab}{2}\,\mathrm{tr}C^0 \ .$$

This then establishes (D-2) or (5.3.35) .

We now turn to the expression (D-3).

Since we have established that $\Delta \neq 0$, we can solve for δ^1:

(D-15) $$\delta^1 = \frac{1}{\Delta}\det\begin{pmatrix} Bab & \dfrac{1}{T^0}\displaystyle\int_0^{T^0} Y^{-1}(\tau)\,\dfrac{dQ^\varepsilon}{d\mu}\Big|_{\mu=0} d\tau \\ b & \end{pmatrix} .$$

We must determine $\frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\,\frac{dQ^\varepsilon}{d\mu}\Big|_{\mu=0} d\tau$. First, we note that

(D-16) $$\frac{dQ^\varepsilon}{d\mu}\Big|_{\mu=0} = ab\begin{Bmatrix} B\left\{(1-a)\left(y_1^0 y_1^1 + \dfrac{(y_1^0)^3}{3!}\right) - \left(y_2^1 y_1^0 + y_2^0 y_1^1 + \dfrac{y_2^0 (y_1^0)^2}{2!}\right)\right\} \\ \left\{(1-a)\left(y_1^0 y_1^1 + \dfrac{(y_1^0)^3}{3!}\right) - \left(y_2^1 y_1^0 + y_2^0 y_1^1 + \dfrac{y_2^0 (y_1^0)^2}{2!}\right)\right\} \end{Bmatrix}$$

$$= ab\begin{Bmatrix} B\left\{1-a)\,\dfrac{(y_1^0)^3}{3!} - \dfrac{y_2^0 y_1^0}{2!}\right\} \\ \left\{(1-a)\,\dfrac{(y_1^0)^3}{3!} - \dfrac{y_2^0 u_1^0}{2!}\right\} \end{Bmatrix}$$

$$+ ab\begin{pmatrix} B(1-a)y_1^0 - By_2^0 & -By_1^0 \\ (1-a)y_1^0 - y_2^0 & -y_1^0 \end{pmatrix}\begin{Bmatrix} y_1^1 \\ y_2^1 \end{Bmatrix} .$$

In the expression $\frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\,\frac{dQ^\varepsilon}{d\mu}\Big|_{\mu=0} d\tau$ we make the change of variables $\theta = \omega_0 \tau$ to obtain

(D-17) $$\frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\,\frac{dQ^\varepsilon}{d\mu}\Big|_{\mu=0} d\tau = \frac{1}{2\pi}\int_0^{2\pi} Y^{-1}(\theta)\,\frac{dQ^\varepsilon}{d\mu}\Big|_{\mu=0} d\theta \ .$$

Note that $Y^{-1}(\tau)$ is actually a function of $\omega_0 \tau$. Consequently, we have used the same notation for $Y^{-1}(\tau)$ and $Y^{-1}(\omega_0 \tau) = Y^{-1}(\theta)$.

We first examine the expression

$$\text{(D-18)} \quad \frac{1}{2\pi}\int_0^{2\pi} Y^{-1}(\theta)\cdot\frac{ab}{3!}\begin{Bmatrix} B(1-a)(y_1^0)^3 - 3By_2^0(y_1^0)^2 \\ (1-a)(y_1^0)^3 - 3y_2^0(y_1^0)^2 \end{Bmatrix} d\theta$$

$$= \frac{B^2a^3b^3}{12\pi\omega_0^4}\int_0^{2\pi}(\omega_0\cos\theta I - \sin\theta A^0)\begin{Bmatrix} B^2a\sin^3\theta + 3B(\omega_0\sin^2\theta\cos\theta - b\sin^3\theta) \\ Ba\sin^3\theta + 3(\omega_0\sin^2\theta\cos\theta - b\sin^3\theta) \end{Bmatrix} d\theta$$

$$= \frac{-B^2a^3b^3}{12\pi\omega_0^4}\int_0^{2\pi}\begin{Bmatrix} 3B\omega_0^2\sin^2\theta\cos^2\theta \\ 3\omega_0^2\sin^2\theta\cos^2\theta \end{Bmatrix} d\theta$$

$$+ \frac{B^2a^3b^3}{12\pi\omega_0^4}\int_0^{2\pi}\begin{Bmatrix} B(Ba-3b)\sin^4\theta \\ (Ba-b)(Ba-3b)\sin^4\theta \end{Bmatrix} d\theta$$

$$= \frac{-B^2a^3b^3}{48\omega_0^4}\begin{Bmatrix} 3B\omega_0^2 \\ 3\omega_0^2 \end{Bmatrix} + \frac{B^2a^3b^3}{48\omega_0^4}\begin{Bmatrix} 3B(Ba-3b) \\ 3(Ba-b)(Ba-3b) \end{Bmatrix}$$

$$= \frac{B^2a^3b^3}{16\omega_0^4}\begin{Bmatrix} B\omega_0^2 - B(Ba-3b) \\ \omega_0^2 - (Ba-b)(Ba-3b) \end{Bmatrix} .$$

Next,

$$(D\text{-}19)\quad Y^{-1}(\theta)ab\begin{pmatrix} B(1-a)y_1{}^0-By_2{}^0 & -By_1{}^0 \\ (1-a)y_1{}^0-y_2{}^0 & -y_1{}^0 \end{pmatrix}$$

$$= Y^{-1}(\theta)ab\begin{pmatrix} \frac{-B^2a}{\omega_0}\sin\theta-B\cos\theta+\frac{Bb}{\omega_0}\sin\theta & \frac{B^2ab}{\omega_0}\sin\theta \\ \frac{-Ba}{\omega_0}\sin\theta-\cos\theta+\frac{b}{\omega_0}\sin\theta & \frac{Bab}{\omega_0}\sin\theta \end{pmatrix}$$

$$= \frac{ab}{\omega^2}(\omega_0\cos\theta I-\sin\theta A^0)\begin{pmatrix} -B(Ba-b)\sin\theta-B\omega_0\cos\theta, B^2ab\sin\theta \\ -(Ba-b)\sin\theta-\omega_0\cos\theta,\ Bab\sin\theta \end{pmatrix}$$

$$= \frac{ab}{\omega_0}\begin{pmatrix} -B(Ba-b)\sin\theta\cos\theta-B\omega_0\cos^2\theta & B^2ab\sin\theta\cos\theta \\ -(Ba-b)\sin\theta\cos\theta-\omega_0\cos^2\theta & Bab\sin\theta\cos\theta \end{pmatrix}$$

$$+\frac{ab}{\omega_0{}^2}\begin{pmatrix} B(Ba-b)\sin^2\theta+B\omega_0\sin\theta\cos\theta, & -B^2ab\sin^2\theta \\ (Ba-b)^2\sin^2\theta+(Ba-b)\omega_0\sin\theta\cos\theta, & -B(Ba-b)ab\sin^2\theta \end{pmatrix}$$

$\equiv Y_1 + Y_2$, respectively.

Now define

$$(D\text{-}20)\quad \underset{\sim}{Z}_1 = \frac{Ba^2b^2}{6\,\omega_0{}^3}\begin{Bmatrix} B\Big((Ba-2b)(2\sin\theta-\sin 2\theta)+2\omega_0(\cos\theta-\cos 2\theta)\Big) \\ \Big((Ba-2b)(2\sin\theta-\sin 2\theta)+2\omega_0(\cos\theta-\cos 2\theta)\Big) \end{Bmatrix},$$

$$\underset{\sim}{Z}_2 = \frac{Ba^2b^2}{6\omega_0{}^4}\begin{Bmatrix} B\Big((Ba-2b)(1-2\cos\theta+\cos^2\theta)-2\omega_0(\cos\theta\sin\theta-\sin\theta)\Big) \\ (Ba-b)\Big((Ba-2b)(1-2\cos\theta+\cos^2\theta)-2\omega_0(\cos\theta\sin\theta-\sin\theta)\Big) \end{Bmatrix},$$

then $\underset{\sim}{y}^1 = \underset{\sim}{Z}_1+\underset{\sim}{Z}_2$.

Therefore,

$$\text{(D-22)}\quad \frac{1}{2\pi}\int_0^{2\pi} Y^{-1}(\theta)ab\begin{pmatrix} B(1-a)y_1^0 - By_2^0 & -By_1^0 \\ (1-a)y_1^0 - y_2^0 & -y_1^0 \end{pmatrix} \chi^1 d\theta$$

$$= \frac{1}{2\pi}\int_0^{2\pi}\Big(Y_1(\theta)+Y_1(\theta)\Big)\Big(\underset{\sim}{Z}_1(\theta)+\underset{\sim}{Z}_2(\theta)\Big)d\theta \;.$$

$$= \frac{1}{2\pi}\int_0^{2\pi} Y_1(\theta)\underset{\sim}{Z}_1(\theta)d\theta + \frac{1}{2\pi}\int_0^{2\pi} Y_1(\theta)\underset{\sim}{Z}_2(\theta)d\theta + \frac{1}{2\pi}\int_0^{2\pi} Y_2(\theta)\underset{\sim}{Z}_1(\theta)d\theta$$

$$+ \frac{1}{2\pi}\int_0^{2\pi} Y_2(\theta)\underset{\sim}{Z}_2(\theta)d\theta \;.$$

Since the evaluation of the last four integrals in (D-22) is straightforward, we give only the results:

$$\text{(D-23)}\quad \frac{1}{2\pi}\int_0^{2\pi} Y_1(\theta)\underset{\sim}{Z}_1(\theta)d\theta = \frac{B^2a^3b^3}{48\omega_0^4}\begin{Bmatrix} 2B(Ba-2b)(Ba-b-ab)+4B\omega_0^2 \\ 2(Ba-2b)(Ba-b-ab)+4\omega_0^2 \end{Bmatrix},$$

$$\text{(D-24)}\quad \frac{1}{2\pi}\int_0^{2\pi} Y_1(\theta)\underset{\sim}{Z}_2(\theta)d\theta = \frac{B^2a\ b}{48\omega_0^4}\begin{Bmatrix} B\Big(2(Ba-b)-7(Ba-2b)-2ab(Ba-b)\Big) \\ \Big(2(Ba-b)-7(Ba-2b)-2ab(Ba-b)\Big) \end{Bmatrix},$$

$$\text{(D-25)}\quad \frac{1}{2\pi}\int_0^{2\pi} Y_2(\theta)\underset{\sim}{Z}_1(\theta)d\theta = \frac{B^2a^3b^3}{48\,\omega_0^4}\begin{Bmatrix} 2B(Ba-2b)+4B \\ (Ba-b)(2(Ba-2b)+4) \end{Bmatrix},$$

$$\text{(D-26)}\quad \frac{1}{2\pi}\int_0^{2\pi} Y_2(\theta)\underset{\sim}{Z}_2(\theta)d\theta = \frac{B^2a^3b^3}{48\omega_0^6}\begin{Bmatrix} B(5(Ba-b)(Ba-2b)(1-ab)-2\omega_0^2) \\ (Ba-b)(5(Ba-b)(Ba-2b)(1-ab)-2\omega_0^2) \end{Bmatrix}.$$

Now, the expression $\frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\left.\frac{dQ^2}{d\mu}\right|_{\mu=0} d\tau$ is the sum of the five expressions (D-18) and (D-23) through (D-26). Using $Ba - B = -\frac{B}{b}$ and $Ba(Ba-b) - B = \frac{B\omega_0^2}{b}$, we obtain

$$(D\text{-}27) \quad \delta^1 = \frac{B^2 a^3 b^4}{\omega_0^4 \Delta\, 48} \left[\frac{3B}{b}\,\omega_0^2 + \frac{3B\omega_0^2}{b}(Ba-3b) - \frac{B}{b}\Big(2(Ba-2b)(Ba-b-ba)+4\omega_0^2\Big) \right.$$

$$- \frac{B}{b}\Big(2(Ba-b) - 7(Ba-2b) - 2ab(Ba-b)\Big) + \frac{B\omega_0^2}{b}\Big(2(Ba-2b)+4\Big)$$

$$\left. + \frac{B}{b}\Big(5(Ba-2b)(Ba-b)(1-ab) - 2\omega_0^2\Big)\right]$$

$$= \frac{B^3 a^3 b^3}{48\Delta\omega_0^4}\Big[3\omega_0^2 + 3\omega_0^2(Ba-3b) - 2(Ba-2b)(Ba-b-ab)$$

$$-4\omega_0^2 - 2(Ba-b) + 7(Ba-2b) + 2ab(Ba-b)$$

$$+2\omega_0^2(Ba-2b) + 4\omega_0^2 + 5(Ba-2b)(Ba-b)(1-ab) - 2\omega_0^2\Big] \quad .$$

Now

$$(D\text{-}28) \quad 3\omega_0^2(Ba-3b) + 2\omega_0^2(Ba-2b) + 5(Ba-2b)(Ba-b)(1-ab)$$

$$= 5(Ba-2b)(Ba-b-Ba^2b+ab^2+Ba^2b-b^2) - 3\omega_0^2 b$$

$$= 5(Ba-2b)(Ba-2b) - 3\omega_0^2 b,$$

$$(D\text{-}29) \quad (Ba-2b)(Ba-b-ab) = (Ba-2b)(Ba-2b + b(1-a)) = (Ba-2b)^2 + (Ba-2b).$$

Using (D-28) and (D-29) in (D-27), we obtain

$$\text{(D-30)} \quad \delta^1 = \frac{B^3 a^3 b^3}{48\Delta\omega_0^4}\left(\omega_0^2 + 3(Ba-2b)^2 + 5(Ba-2b) + 2(ab-1)(Ba-b) - 3b\omega_0^2\right) .$$

But

$$\text{(D-31)} \quad 2(ab-1)(Ba-b) = 2Ba^2b - 2ab^2 - 2(Ba-b)$$

$$= 2\omega_0^2 + 2b^2(1-a) - 2(Ba-b) = 2\omega_0^2 - 2(Ba-2b).$$

So, (D-30) and (D-31) imply

$$\text{(D-32)} \quad \delta^1 = \frac{+B^3 a^3 b^3}{48\omega_0^4\Delta}\left(3\omega_0^2(1-b) + 3(Ba-2b)^2 + (Ba-2b)\right)$$

$$= \frac{+B^3 a^3 b^3}{16\omega_0^4\Delta}\left(\omega_0^2(1-b) + (Ba-2b)^2 + (Ba-2b)\right) .$$

Using the expression for Δ in (D-2) we have

$$\delta^1 = \frac{-B^2 a^2 b^2}{8\omega_0^4 \operatorname{tr} C^0}\left(\omega_0^2(1-b) + (Ba-2b)^2 + (Ba-2b)\right) .$$

This is the desired expression (D-3).

Appendix E

We shall now show that

$$\text{(E-1)}\quad \frac{1}{T^o}\int_o^{T^o} \nabla\cdot \underset{\sim}{F}(\underset{\sim}{a}^{\epsilon} + \mu\, y(s,\mu))\,ds = \Lambda\,\mu^2 + o(\mu^2) \text{ as } \mu \to 0$$

where

$$\text{(E-2)}\quad \Lambda = \frac{B^2 a^2 b^2}{8\,\omega_o^4}\left\{\omega_o^2(1-b) + (Ba-2b)^2 + (Ba-2b)\right\},$$

$$\underset{\sim}{F} = A^o y + \mu\left\{\eta(\mu)\, A^{\epsilon} y + \delta(\mu)\, C^{\epsilon} y + (1+\mu\,\eta(\mu))\, \underset{\sim}{Q}^{\epsilon}(y,\mu)\right\}.$$

Now

$$\text{(E-3)}\quad \nabla\cdot\underset{\sim}{F} = \text{tr } A^o + \mu\,\eta(\mu)\text{ tr } A^{\epsilon} + \mu\,\delta(\mu)\text{ tr } C^{\epsilon}$$

$$+ \mu(1 + \mu\,\eta(\mu))\,\nabla\cdot\underset{\sim}{Q}^{\epsilon}(y,\mu)$$

where

$$\text{(E-4)}\quad \mu\,\nabla\cdot Q^{\epsilon}(y,\mu) = \frac{a_2^{\epsilon}}{1-a_2^{\epsilon}}\left\{B(1-a_2^{\epsilon})(\exp(\mu y_1)-1 - B\,\mu\, y_2 \exp(\mu\, y_1)\right.$$

$$\left. - (\exp(\mu\, y_1) - 1)\right\}.$$

By definition $\text{tr } A^o = 0$ and $\text{tr } A^{\epsilon} = \text{tr } A^o + \mu\,\delta(\mu)\text{ tr } C^{\epsilon}$. Thus, using the continuity properties of C^{ϵ}, $\epsilon(\mu) = \mu\,\delta(\mu)$, $\eta(\mu)$, and $y(s,\mu)$ in Theorems 5.2.1 and 5.2.3, we obtain

$$\text{(E-5)}\quad \nabla\cdot\underset{\sim}{F} = \mu^2\,\delta^1\text{ tr } C^o + \mu\,\nabla\cdot\underset{\sim}{Q}^{\epsilon(\mu)}(y(s,\mu),\ \mu)$$

$$+ o(\mu^2) \text{ as } \mu \to 0.$$

Next we examine $\mu \nabla \cdot \underset{\sim}{Q}^{\epsilon}$:

$$a_2^{\epsilon} = a_2^{o} + O(\mu^2) \qquad \text{as} \qquad \mu \to 0$$

$$\text{(E-6)} \quad e^{\mu y_1} - 1 = \mu\, y_1{}^{o} + \mu^2\, y_1{}^{1} + \mu^2 \frac{(y_1{}^{o})^2}{2} + o(\mu^2) \ \text{ as } \mu \to 0$$

$$\mu\, y_2\, e^{\mu y_1} = \mu\, y_2^{o} + \mu^2(y_2^{1} + y_1^{o}\, y_2^{o}) + o(\mu^2) \ \text{ as } \mu \to 0$$

where we have used Theorem 5.2.3.

Therefore, using (E-6) in (E-5), we obtain

$$\text{(E-7)} \quad \mu\, \nabla \cdot \underset{\sim}{Q}^{\epsilon} = B\, a_2^{o}\, (\mu\, y_1^{o} + \frac{\mu^2}{2}\, (2\, y_1^{1} + (y_1{}^{o})^2))$$

$$- \frac{B\, a_2^{o}}{1 - a_2^{o}}\, (\mu\, y_2^{o} + \mu^2(y_2^{1} + y_1^{o}\, y_2{}^{o}))$$

$$- \frac{a_2^{o}}{1 - a_2^{o}}\, (\mu\, y_1^{o} + \frac{\mu^2}{2}\, (2\, y_1^{1} + (y_1^{o})^2))$$

$$+ o(\mu^2) \text{ as } \mu \to 0 \ .$$

At this point we change notation:

$$a = a_2^{o} \quad \text{and} \quad b = B\, a_2^{o} - 1 - \beta =$$

Then, using $b = \dfrac{1}{1 - a_2^{o}}$, we have

$$\text{(E-8)} \quad \frac{1}{T^{o}} \int_{o}^{T^{o}} \nabla \cdot \underset{\sim}{F}\, ds = \mu\, \delta^1\, \text{tr}\, C^{o}$$

$$+ \frac{\mu^2 a}{T^{o}} \int_{o}^{T^{o}} (B - b)(y_2^{1} + \frac{(y_1{}^{o})^2}{2}) - Bb(y_2^{1} + y_1^{o}\, y_2^{o}\, ds$$

$$+ \frac{\mu\, a}{T^{o}} \int_{o}^{T^{o}} (B - b) y_1^{o} - B\, b\, y_2^{o}\, ds + o(\mu^2) \text{ as } \mu \to 0 \ .$$

From the expressions (5.3.28) and (5.3.29) for

y^o and y^1 we obtain

(E-9) $$\frac{1}{T^o} \int_o^{T^o} (B-b)y_1^o - B\,b\,y_2^o\, ds = O \quad ,$$

(E-10) $$\frac{a}{T^o} \int_o^{T^o} (B-b)\,(y_1^1 + \frac{(y_1^o)}{2}) - B\,b(y_2^1 + y_1^o\, y_2^o)\, ds$$

$$= 3\,a\,(B-b)\,\frac{B\,a^2b^2\,B(Ba-2b)}{12\,\omega_o^4} - \frac{B^2a^3b^3}{4\,\omega_o^4}(Ba-b)(Ba-2b)$$

$$+ \frac{(B-b)B\,a^3b^2}{4\,\omega_o^2} - \frac{B^2a^2b^3}{2\,\omega_o^2}$$

$$= \frac{B^2a^2b^2}{4\,\omega_o^4}\Big\{b(Ba-2b)(B-b) - (Ba-b)(Ba-2b)ab$$

$$-a(B-b)\omega_o^2 - 2\,b\,\omega_o^2\Big\}$$

$$= \frac{B^2a^2b^2}{4\,\omega_o^4}\Big\{(Ba-2b)\,\omega_o^2 + \omega_o^2(1-b) + (Ba-ab)\,(Ba-2b)$$

$$-ab(Ba-b)\,(Ba-2b)\Big\}$$

$$= \frac{B^2a^2b^2}{4\,\omega_o^4}\Big\{(Ba-2b+b+b(1-a))\,(Ba-2b)$$

$$+ (Ba-2b)\,\omega_o^2 + \omega_o^2(1-a) - (Ba^2b-b^2a)(Ba-2b)\Big\}$$

$$= \frac{B^2a^2b^2}{4\,\omega_o^4}\Big\{(Ba-2b)\,\omega_o^2 + \omega_o^2(1-b) + (Ba-2b)^2$$

$$+ b(Ba-2b) + (Ba-2b) - (\omega_o^2+b)\,(Ba-2b)\Big\}$$

$$= \frac{B^2a^2b^2}{4\,\omega_o^4}\left\{\omega_o^2(1-b) + (Ba-2b)^2 + (Ba-2b)\right\}$$

where we have used $\omega_o^2 = Ba^2b - b^2$ and $b(1-a) = 1$.

Substitution of (E-9), (E-10), and (5.3.3) into (E-8) yields

$$\frac{1}{T^o}\int_o^{T^o} \nabla\cdot\underset{\sim}{F}\,ds = \mu^2\,\frac{B^2a^2b^2}{\omega_o^4}\left(\frac{1}{4} - \frac{1}{8}\right)\left(\omega_o^2(1-b) + (Ba-2b)^2 + (BA-2b)\right)$$

$$+ o(\mu^2)$$

$$= \mu^2\,\frac{B^2a^2b^2}{8\,\omega_o^4}\left\{\omega_o^2(1-b) + (Ba-2b)^2 + (Ba-2b)\right\}$$

$$+ o(\mu^2) \qquad \text{as} \qquad \mu \to 0 \quad .$$

This establishes (E-1) and (E-2).

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