A Model Equation Arising from Chemical Reactor Theory

AUBREY B. POORE

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1. Introduction

During the last two decades extensive efforts have been extended to the investigation of multiplicity and stability of steady states, periodic phenomena, bifurcation and the closely related jump phenomena in problems arising from chemical reactor theory. One of the most intensely studied of these problems is the following system of ordinary differential equations:

$$
\begin{aligned}
\frac{dx_1}{dt} &= -\lambda x_1 - \beta(x_1 - x_c) + BDaf(x_1, x_2),\\
\frac{dx_2}{dt} &= -\lambda x_2 + Daf(x_1, x_2),
\end{aligned}
\tag{1.1}
$$

where λ, β, x_c, Da, and B are physical parameters: $(1-\lambda)$ is the proportion of chemical recycled into the reactor; β is a measure of the heat transfer coefficient between reactor and coolant whose normalized, dimensionless temperature is x_c; B is a measure of the heat generated by the reaction; and Da, the so-called Damköhler number, is the reaction rate at $x_1 = x_2 = 0$. Thus $\lambda \in (0, 1)$, and Da and B are positive and β nonnegative, $\beta = 0$ corresponding to an adiabatic reactor. x_1 is a dimensionless temperature of a product chemical whose concentration is x_2 and $f(x_1, x_2)$ is a nonlinearity involving the chemical kinetics and rate function. The equations in (1.1) are exact for the CSTR (continuously stirred tank reactor) without control (see R. ARIS & N. AMUNDSON [2], R. ARIS [1], or V. HLAVÁČEK, M. KUBÍČEK & J. JELÍNEK [13]) and a chemical reaction on an infinite catalytic wire (see D. LUSS & M. CARDOSO [3]). Using an appropriate singular perturbations method, the author and D. S. COHEN [6], [7], [17] have shown that these equations are a first approximation to the system of parabolic partial differential equations which govern the nonadiabatic tubular reactor problem.

Various aspects of the problem (1.1) have been observed (experimentally, computationally, and theoretically) by many different investigators for special cases and parameters for problem (1.1). Most of these results and references to the extensive chemical engineering literature on the problem (1.1) can be found in the recent review paper by V. HLAVÁČEK, M. KUBÍČEK & J. JELÍNEK [13]. For the problem (1.1) with control the reader is referred to the papers of ARIS & AMUNDSON [2] and more recently J. C. HYUN & R. ARIS [15].

Our present analysis is for the nonlinearity

$$f(x_1, x_2) = (1 - x_2)\, e^{x_1}. \tag{1.2}$$

This specific form is not necessary; our analysis applies equally well to more general nonlinearities which "resemble" f. We mention, in particular, nonlinearities of the form

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

where $n \geqq 1$ and $\varepsilon > 0$. We confine our attention to the specific form (1.2) here for algebraic simplicity. Indeed, most of the numerical calculations for the CSTR are for this case.

By dividing both equations in (1.1) by λ and making the transformation $\lambda t \to t$, $Da/\lambda \to Da$, and $\beta/\lambda \to \beta$, we may assume without any loss of generality that $\lambda = 1$ in equation (1.1). Thus we investigate

$$\begin{aligned} \frac{dx_1}{dt} &= -x_1 - \beta(x_1 - x_c) + DaB(1 - x_2)\, e^{x_1} = F_1(x_1, x_2), \\ \frac{dx_2}{dt} &= -x_2 + Da(1 - x_2)\, e^{x_1} \equiv F_2(x_1, x_2). \end{aligned} \tag{1.3}$$

In Section 2 we present all the theoretical results concerning questions of existence, uniqueness, boundedness, and the "long-time" behavior of the solutions of (1.3). Section 3 contains the necessary and sufficient conditions for uniqueness and multiplicity, index, and type of the critical points. We exhaustively classify all relations between multiplicity and stability of the critical points in Section 4. In Section 5 we prove the existence of periodic orbits for various parameter ranges and for others we establish global asymptotic stability.

Several investigators (see HLAVÁČEK [13]) have used various approximate techniques to obtain more information about periodic solutions. R. ARIS & N. AMUNDSON [2] were the first to make use of the bifurcation of periodic orbits following POINCARÉ'S bifurcation theory as is described by N. MINORSKY [16]. The work of ARIS & AMUNDSON [2] considers bifurcation as a control parameter changes – a parameter not included in our system (1.3). Our present approach to the bifurcation problem follows a general theory of bifurcating periodic orbits as is described by K. O. FRIEDRICHS [9]. For β, B, and Da, say Da_0, chosen so that there is a corresponding critical point which is a center for the linearized problem associated with (1.3), we prove that there bifurcates a periodic orbit as Da increases above Da_0 or decreases below Da_0 when β and B are held fixed. 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. In particular, we prove the existence of unstable periodic orbits surrounding a stable critical point and the existence of multiple periodic orbits. Several new cases of jump phenomena are established.

We formulate the necessary general theory of K. O. FRIEDRICHS [9] and derive the necessary information from this theory in Section 6, and apply it in Section 7 to (1.3). In Section 8 we rigorously establish the connection between the stability and direction of bifurcating periods orbits and discuss the relation to the response diagram. The implications to jump phenomena are contained in Section 9.

2. General Properties

In this section we present all the theoretical results concerning questions of existence, uniqueness, boundedness, and the "long-time" behavior of the solutions of (1.3) whenever the initial conditions are physically meaningful. These results are contained in Theorems 2.1 and 2.2. This information is necessary for our later analysis; however, the results and proofs are relatively straightforward. The principal results actually start in Section 3.

For the system (1.3) let the domain, D, be defined by

$$D=\{(x_1, x_2) \mid x_1 \in(-\infty, \infty), x_2 \in(0, 1)\}. \tag{2.1}$$

We could restrict the domain D to the set

$$D=\left\{(x_1, x_2) \mid x_2 \in(0, 1), x_1 \geqq \frac{\beta x_c}{1+\beta}\right\}$$

or enlarge it to include all of $\mathbb{R}^2$; however, we content ourselves with D given by (2.1). When they exist, we define the positive semiorbit $\gamma^+(p)$, the negative semiorbit $\gamma^-(p)$, the ω-limit set $\omega(\gamma^+)$, and the α-limit set $\alpha(\gamma^-)$ as in J. HALE [11]. Then we have

Theorem 2.1. *If $\beta+1>0$, $Da>0$, and $B\geqq 0$, then there is a unique solution which exists for all $t\geqq 0$ to the problem* (1.3) *for $(x_1(0), x_2(0))=p\in D$. The positive semiorbit $\gamma^+(p)$ through p is contained in a compact subset of D for any $p\in D$. This compact subset is such that x_1 is bounded independent of Da. Furthermore, all existing periodic orbits can be uniformly bounded in such a way that the x_1-bound is dependent only on β, B, and x_c, and independent of Da and the initial conditions.*

Proof. An outline of this relatively straightforward proof is given in the appendix. Q.E.D.

Theorem 2.2. *If $\gamma^+(p)$ for $p\in D$ is any positive semiorbit of* (1.3) *or if $\gamma^+(p)$ is a negative semiorbit contained in a compact subset of D, then one of the following is satisfied for problem* (1.3):

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

(ii) *$\omega(\gamma^+)(\alpha(\gamma^-))$ is a periodic orbit with either*

$$\gamma^+=\omega(\gamma^+)(\gamma^-=\alpha(\gamma^-)) \quad or \quad \omega(\gamma^+)=\overline{\gamma^+}\backslash\gamma^+(\alpha(\gamma^-)=\overline{\gamma^-}\backslash\gamma^-)$$

where the bar denotes closure;

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

Proof. For any $p \in D$, Theorem 2.1 implies that $\gamma^+(p)$ is contained in a compact subset of D. It is shown that there are at most three critical points in D for the system (1.3) in Theorem 3.1. Since we have assumed that any existing $\gamma^-(p)$ is contained in a compact subset of D, the conclusion of the theorem now follows from classical theorems such as those in J. HALE [11]. Q.E.D.

3. Critical Points: Multiplicity, Index, and Type

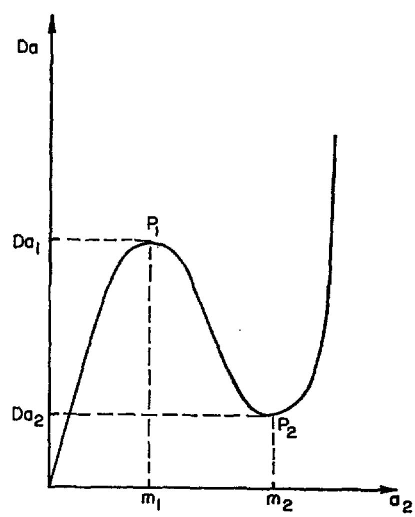
In this section the necessary and sufficient conditions for uniqueness and multiplicity, index, and type of the critical points are examined. These facts are contained in Theorems 3.1 and 3.2. Figure 1 should help illustrate the context of Theorem 3.1.

Theorem 3.1. Let

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

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

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



$B > 4(1+\beta)$
$P_1 = (m_1, Da_1)$
$P_2 = (m_2, Da_2)$

Fig. 1

for $i=1,2$. Let (a_1, a_2) denote a critical point of the autonomous system (1.3). *Then we have the following*:

1. *When $B \leqq 4(1+\beta)$ or when $B>4(1+\beta)$ and $Da \in (0, Da_2) \cup (Da_1, \infty)$, there exists one and only one critical point of the autonomous system* (1.3). *The index $\mathscr{I}(a_1, a_2)=+1$.*

2. *When $B>4(1+\beta)$ and $Da=Da_1$ or Da_2, there exist exactly two critical points. One critical point has an index of plus one and the other ($a_2=m_1$ and $Da=Da_1$ or $a_2=m_2$ and $Da=Da_2$) has an index of zero.*

3. *When $B>4(1+\beta)$ and $Da \in (Da_2, Da_1)$, there exist exactly three critical points for each such Da, B, and β. The index $\mathscr{I}(a_1, a_2)=+1$ when $a_2 \in (0, m_1) \cup (m_2, 1)$ and $\mathscr{I}(a_1, a_2)=-1$ when $a_2 \in (m_1, m_2)$.*

Proof. The necessary and sufficient conditions for multiplicity of the critical points for the system (1.3) are contained in the survey paper of V. HLAVÁČEK, M. KUBÍČEK & J. JELÍNEK [13]. We shall use an argument similar to the one used by COHEN [5]. The index of the steady states is examined in the book by GAVALAS [10]; 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

$$F_1(a_1, a_2; \beta, B, Da)=0 \tag{3.4}$$

and

$$F_2(a_1, a_2; Da)=0 \tag{3.5}$$

where F_1 and F_2 are given by (1.3). Using (3.5) in (3.4), we obtain an equivalent set of equations:

$$a_1=\frac{B a_2}{1+\beta}+\frac{\beta x_c}{1+\beta} \tag{3.6}$$

and

$$Da=\frac{a_2}{1-a_2} \exp\left(-\frac{B a_2}{1+\beta}-\frac{\beta x_c}{1+\beta}\right). \tag{3.7}$$

Note that $Da>0$ if and only if $a_2 \in (0, 1)$. Since a_1 is linearly related to a_2 through (3.6), the multiplicity conditions can be obtained from equations (3.7). From (3.7) 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 (3.7). If Da does not increase monotonically with a_2, then for some fixed Da there exists more than one a_2 satisfying (3.7). In this way we investigate the multiplicity conditions. From (3.7) we obtain

$$\frac{dDa}{da_2}=\frac{(B a_2^2-B a_2+1+\beta)}{(1+\beta)(1-a_2)^2} \exp\left(-\frac{B a_2}{1+\beta}-\frac{\beta x_c}{1+\beta}\right). \tag{3.8}$$

Let m_1 and m_2 be roots of

$$B a_2^2-B a_2+(1+\beta)=0, \text{ i.e.,} \tag{3.9}$$

$$m_1=\frac{1}{2}-\frac{1}{2}\sqrt{1-\frac{4(1+\beta)}{B}} \quad \text{and} \quad m_2=\frac{1}{2}+\frac{1}{2}\sqrt{1-\frac{4(1+\beta)}{B}}. \tag{3.10}$$

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 $B\leqq 4(1+\beta)$ 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 (3.3); then, the situation is as in Figure 1. For $B>4(1+\beta)$, we have uniqueness whenever $Da\in(0,Da_2)\cup(Da_1,\infty)$ and three solutions of (3.7) whenever $Da\in(Da_2,Da_1)$. For $Da=Da_1$ or Da_2, there exist exactly two critical points. This completes the multiplicity conditions in Theorem 3.1.

We now determine index of the steady states. By using the concept of rotation of the vector field associated with (1.3) (see [4]) and calculating the rotation on a circle enclosing the critical point (a_1, a_2), one easily concludes that $\mathscr{I}(a_1,a_2)=+1$ for $a_2=m_1=m_2$ when $B=4(1+\beta)$ and $\mathscr{I}=0$ for $a_2=m_1$ or m_2 when $B>4(1+\beta)$. In these cases $\det A=0$ where $A=F_x(a_1,a_2)$. For $\det A\neq 0$, the index is given by (see K. O. FRIEDRICHS [9] or CODDINGTON & LEVINSON [4])

$$\mathscr{I}=\frac{\det A}{|\det A|}$$

where

$$A=F_x=\begin{pmatrix} Da\,B(1-a_2)\exp(a_1)-1-\beta & -Da\,B\exp(a_1) \\ Da(1-a_2)\exp(a_1) & -1-Da\exp(a_1)\end{pmatrix}. \tag{3.11}$$

By use of (3.6) and (3.7), (3.11) simplifies to

$$A=\begin{pmatrix} Ba_2-1-\beta & -Ba_2/(1-a_2) \\ a_2 & -1/(1-a_2)\end{pmatrix}. \tag{3.12}$$

Therefore

$$\det A=\frac{1}{1-a_2}(Ba_2^2-Ba_2+1+\beta). \tag{3.13}$$

Using (3.8) in (3.13), we obtain

$$\det A=(1+\beta)(1-a_2)\exp\left(\frac{Ba_2}{1+\beta}+\frac{\beta x_c}{1+\beta}\right)\frac{dDa}{da_2}. \tag{3.14}$$

By the definition of $\mathscr{I}(a_1,a_2)$ we obtain

$$\mathscr{I}(a_1,a_2)=\begin{cases}+1 & \text{whenever } dDa/da_2>0\\ -1 & \text{whenever } dDa/da_2<0.\end{cases} \tag{3.15}$$

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

Write system (1.3) as

$$\frac{d}{dt}\begin{Bmatrix} y_1\\ y_2\end{Bmatrix}=\begin{pmatrix} Ba_2-1-\beta & -\dfrac{Ba_2}{1-a_2} \\ a_2 & -\dfrac{1}{1-a_2}\end{pmatrix}\begin{Bmatrix} y_1\\ y_2\end{Bmatrix} \tag{3.16}$$
$$+\begin{Bmatrix} Da\,B e^{a_1}((1-e^{y_1})y_2+(1-a_2)(e^{y_1}-1-y_1))\\ Da\,e^{a_1}((1-e^{y_1})y_2+(1-a_2)(e^{y_1}-1-y_1))\end{Bmatrix}$$

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

$$\frac{dy}{dt} = Ay \tag{3.17}$$

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

Theorem 3.2. *For* (3.17) *we have*

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

and

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

Let $\Delta = (\operatorname{tr} A)^2 - 4\det A$. *Then, the critical points of the linear system* (3.17) *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* $\operatorname{tr} A \neq 0$, *a center if* $\Delta < 0$ *and* $\operatorname{tr} A = 0$, *a proper node or an improper node if* $\Delta = 0$, *and an improper node if* $\Delta > 0$.

3. *Let* $\det A = 0$. *The critical point is degenerate in the sense that the phase plane consists entirely of critical points or entirely of parallel straight lines and critical points.*

The type of critical point for the nonlinear problem (3.16) *is the same as that for the linear problem in cases 1 and 2 above except in the case of the center. The 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 determine 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 orbits entering and two orbits leaving the critical point.

Remark 3. The roots of $\operatorname{tr} A = 0$ are given by

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

and

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

Let $B>3+\beta+2\sqrt{2+\beta}$ (β and B fixed) so that s_1 and s_2 are real and $0<s_1<s_2<1$. If $\det A>0$ for $a_2=s_1(s_2)$ with Da, say Da_0, defined through the equation in the second remark, the implicit function theorem can be used to show that the critical point $\boldsymbol{a}$ is a function of Da for Da in a sufficiently small interval about Da_0. Furthermore, $(\operatorname{tr} A)^2-4\det A<0$ for Da in some sufficiently small interval about Da_0 (a_2 close to $s_1(s_2)$), which implies that these critical points are spirals except at $a_2=s_1(s_2)$ which corresponds to a center or spiral.

Proof of Theorem 3.2. The classification given is standard and may be found in CODDINGTON & LEVINSON [4]. Since the nonlinearity in (3.16) 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 [4]. Q.E.D.

4. Steady State Response Diagram for the Chemical Reactors

Some of the main results of this paper begin 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 1 (at the end of the paper) 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 Figures 2 and then read Theorem 4.1 for the precise facts. The Figures 3 through 14 are two dimensional projections into the (Da, a_2) plane of the curve defined by (3.6) and (3.7) in (Da, a_1, a_2) parameter space. The a_1 axis is taken to be out of the paper. As an example, let (β, B) be in Region V; then, Figure 10 or 11 shows schematically what occurs. 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 4.1, the critical point (a_1, a_2) is an unstable spiral or node. For

$$Da\in(0, Da_3)\cup(Da_4, \infty)$$

the critical point is an asymptotically stable node or spiral.

The analytic description of the six regions – I through VI – follows Theorem 4.1. We now state Theorem 4.1 which describes in detail the relation between stability and multiplicity of the critical points:

Theorem 4.1. *Let*

$$s_1=\frac{B+1+\beta}{2B}-\frac{1}{2B}\sqrt{(B+1+\beta)^2-4B(2+\beta)}, \tag{4.1}$$

$$s_2=\frac{B+1+\beta}{2B}+\frac{1}{2B}\sqrt{(B+1+\beta)^2-4B(2+\beta)}, \tag{4.2}$$

$$m_1=\frac{1}{2}-\frac{1}{2}\sqrt{4-\frac{4(1+\beta)}{B}}, \tag{4.3}$$

$$m_2=\frac{1}{2}+\frac{1}{2}\sqrt{1-\frac{4(1+\beta)}{B}}. \tag{4.4}$$

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

$$Da(x) = \frac{x}{1-x} \exp\left(-\frac{Bx}{1+\beta} - \frac{Bx_c}{1+\beta}\right). \tag{4.5}$$

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

(i) *For* β *and* B *in Region* I, 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 orbits in the domain* D *tend to the critical point. (See Figure 3.)*

(ii) *For* β *and* B *in Region* II, $0 < m_1 < m_2 < 1$ *and for* $B < 3+\beta+2\sqrt{2+\beta}$, s_1 *and* s_2 *are imaginary, but for* $B \geqq 3+\beta+2\sqrt{2+\beta}$, 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 exist 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 Region* III, *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 Figures 5, 6, or 7 and Table 1.)*

(iv) *For* β *and* B *in Region* IV, *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 1 for typical cases.)*

(v) *For* β *and* B *in Region* V, *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 Figure 10 or 11 and Table 1 for a typical case.)*

(vi) *For* β *and* B *in Region* VI, *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 12, 13, and 14 and Table 1.)*

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

$$B = f_1(\beta) = 4(1+\beta), \tag{4.6}$$

$$B = f_2(\beta) = 3+\beta+2\sqrt{2+\beta}, \tag{4.7}$$

$$B = f_3(\beta) = (1+\beta)^3/\beta. \tag{4.8}$$

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

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

II: $\quad 4(1+\beta)<B<\dfrac{(1+\beta)^3}{\beta} \quad$ for $0<\beta\leqq\dfrac{\sqrt{5}-1}{2}$

and $4(1+\beta)<B<3+\beta+2\sqrt{2+\beta} \quad$ for $\dfrac{\sqrt{5}-1}{2}\leqq\beta<\dfrac{7}{9}$,

III: $\quad \dfrac{(1+\beta)^3}{\beta}<B \quad$ for $0\leqq\beta<\infty$,

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

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

VI: $\quad 3+\beta+2\sqrt{2+\beta}<B<\dfrac{(1+\beta)^3}{\beta} \quad$ for $\dfrac{\sqrt{5}-1}{2}<\beta\leqq\dfrac{7}{9}$

or $4(1+\beta)<B<\dfrac{(1+\beta)^3}{\beta} \quad$ for $\frac{7}{9}\leqq\beta<1$.

Proof of Theorem 4.1. The multiplicity question has been settled in Theorem 3.1 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 (3.16) as well as for the associated linear problem (3.17).

Recall from (3.16) and (3.17) that

$$\frac{dy}{dt}=Ay+G(y,a) \tag{4.9}$$

where G is the nonlinear part of (3.16) and

$$A=\begin{bmatrix} Ba_2-1-\beta & -\dfrac{Ba_2}{1-a_2} \\ a_2 & -\dfrac{1}{1-a_2} \end{bmatrix}. \tag{4.10}$$

Since $G=O(\|y\|^2)$ as $\|y\|\to O(\|y\|=\sqrt{y_1^2+y_2^2})$, we can conclude that the critical point is an 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 $\operatorname{tr} A>0$. (These facts follow from classical theorems in [4].) From (4.10) we have

$$\operatorname{tr} A=\frac{-1}{1-a_2}\left(Ba_2^2-(B+1+\beta)a_2+(2+\beta)\right) \tag{4.11}$$

and

$$\det A = \frac{1}{1-a_2}\left(B a_2^2 - B a_2 + (1+\beta)\right). \tag{4.12}$$

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 (4.1) through (4.4). 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 asymptotically stable spirals or nodes when $B<4(1+\beta)$ and $B<3+\beta+2\sqrt{2+\beta}$. This completes Region I. In Region V $\det A>0$ 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 $B<3+\beta+2\sqrt{2+\beta}$ $(0 \leqq \beta < \frac{7}{9})$, 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 and m_2, s_1, and s_2 we can determine all relationships between stability and multiplicity and the remaining Regions II, III, IV, VI. Since the algebra is straightforward, we forgo this comparison.

The fact that all orbits in D tend to the critical point for (β, B) in Region I will be proved in Section 5. Q.E.D.

5. Periodic Phenomena and Global Asymptotic Stability

Having analyzed the critical points with respect to multiplicity, type, index, and stability, we now turn to the question of periodic orbits and global asymptotic stability (see P. HARTMAN [12] for the definition). We separate the analysis into two parts. In the first part, still very much within the present spirit, we continue to use the classical phase-plane techniques to examine periodic orbits via the Poincaré-Bendixson type analysis. In the second part, which begins in Section 6, we study bifurcating periodic orbits via the implicit function theorem and the implications and relationships between multiplicity, stability, bifurcation, and periodicity. The main results of this section appear in Theorems 5.1 and 5.3.

First, we note that if a periodic solution exists, it must encircle those critical points the sum of whose indices must be $+1$. We have shown in Section 3 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 unstable unique critical point. In Theorem 2.2 we characterized 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 an unstable unique critical point, the critical point must be an unstable node or an unstable spiral. (The center has special significance and is examined in great detail in Section 6.) Hence, all orbits must leave the unique unstable critical point. This implies that neither case (i) nor case (iii) can occur in Theorem 2.2 so long as the initial conditions for γ^+ are not the critical point itself. Consequently, we have the following theorem:

Theorem 5.1. *When β, B and Da are chosen so that there is but one critical point and it is an unstable node or spiral, a periodic orbit exists and encircles this critical point.*

Remark. In the Appendix it is shown that for any periodic orbit

$$\min\left\{x_1(0), \frac{\beta x_c}{1+\beta}\right\} \leqq x_1(t) < B + \frac{\beta x_c}{1+\beta} + \{\exp(-(1+\beta)t)\}\left\{x_1(0) - Bx_2(0) - \frac{\beta x_c}{1+\beta}\right\}.$$

Since $\omega(\gamma^+) = \gamma^+(p)$ when p is a point of the periodic orbit, it follows that $x_1(t) \leqq B + \frac{\beta x_c}{1+\beta}$. Next observe that $\frac{dx_1}{dt} > 0$ for $x_1 = \frac{\beta x_c}{1+\beta}$ except at $x_2 = 1$ where $\frac{dx_2}{dt} < 0$ and thus $x_1(0)$ can be chosen to satisfy $x_1(0) \geqq \frac{\beta x_c}{1+\beta}$ for a periodic orbit.

We immediately have

$$\frac{\beta x_c}{1+\beta} \leqq x_1(t) \leqq B + \frac{\beta x_c}{1+\beta}$$

whenever $(x_1(t), x_2(t))$ is a periodic orbit. One could derive estimates for $x_2(t)$ and further refine the estimate on the magnitude of x_1 or the temperature in reactor theory.

At present we can say no more about the existence of periodic orbits. We will, however, return to this in Section 7. For β and B in Region I, for β and B in that part of Region II where $B \leqq 3 + \beta + 2\sqrt{2+\beta}$ and $Da \in (0, Da_2) \cup (Da_1, \infty)$, and for any fixed β and B with Da sufficiently small or large 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 5.2. *If $B \leqq 3 + \beta + 2\sqrt{2+\beta}$ or if Da is sufficiently small or large with β and B fixed, then any existing periodic orbit must be asymptotically orbitally stable.*

Proof. We examine Poincaré's Criterion (see W. A. Coppel [15]):

$$\oint \nabla \cdot \boldsymbol{F}\, d\tau = \int_0^{T^0} \nabla \cdot \boldsymbol{F}\, d\tau = \int_0^{T^0} [-(1+\beta) + Da\,B(1-x_2)e^{x_1} - 1 - Da\, e^{x_1}]\, d\tau. \tag{5.1}$$

Recall from Theorem 2.1 that for any existing periodic solution, x_1 is bounded independently of Da; thus, the integrand, $\nabla \cdot \boldsymbol{F}$, in (5.1) can be made negative by requiring that Da be small and positive. This implies the result in this case.

Next, we use $\dot{x}_2+x_2=Da(1-x_2)\,e^{x_1}$ from (1.3) to obtain from (5.1)

$$\oint \nabla\cdot \boldsymbol{F}\,d\tau=\int_0^{T^0}\big(-(2+\beta)-Da\,e^{x_1}+Bx_2\big)\,d\tau+\int_0^{T^0} B\dot{x}_2\,d\tau \tag{5.2}$$
$$=\int_0^{T^0}\big(-(2+\beta)-Da\,e^{x_1}+Bx_2\big)\,d\tau,$$

where $\int_0^{T^0} B\dot{x}_2\,d\tau$ is zero by periodicity. Since $x_2\in(0,1)$ and x_1 is bounded independently of Da by Theorem 2.1, the integrand of the last integral in (5.2) can be made negative by requiring that Da be sufficiently large. This implies the result in this case.

Finally, using $\dot{x}_2+x_2=Da(1-x_2)\,e^{x_1}$ and $\frac{\dot{x}_2+x_2}{1-x_2}=Da\,e^{x_1}$ in (5.1), we obtain

$$\oint \nabla\cdot \boldsymbol{F}\,d\tau=-\int_0^{T^0}\frac{\big(Bx_2^2-(B+1+\beta)\,x_2+2+\beta\big)}{1-x_2}\,d\tau+\int_0^{T^0}\left(B\dot{x}_2-\frac{\dot{x}_2}{1-x_2}\right)d\tau. \tag{5.3}$$

The last integral is zero by periodicity so that

$$\oint \nabla\cdot \boldsymbol{F}\,d\tau=-\int_0^{T^0}\frac{\big(Bx_2^2-(B+1+\beta)\,x_2+2+\beta\big)}{1-x_2}\,d\tau. \tag{5.4}$$

When $B\leqq 3+\beta+2\sqrt{2+\beta}$, 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 $\oint \nabla\cdot \boldsymbol{F}\,d\tau<0$. Poincaré's Criterion implies that the assumed periodic orbit is asymptotically orbitally stable for $B\leqq 3+\beta+2\sqrt{2+\beta}$. Q.E.D.

With this lemma we can prove

Theorem 5.3. *If*

(i) *β and B are in Region* I,

(ii) *β and B are in that part of Region* II *where $B\leqq 3+\beta+2\sqrt{2+\beta}$ and $Da\in(0, Da_2)\cup(Da_1,\infty)$, or*

(iii) *β and B are fixed and Da is either sufficiently small or large,*

then $\omega(\gamma^+)$ is the unique stable critical point for each $\gamma^+(p)$ for which $p=(x_1(0), x_2(0))\in D$. In other words, we have the property of global asymptotic stability in each case (i), (ii), *and* (iii). *Furthermore, for $\beta=0$ there can be no periodic orbits.*

Proof. The nonexistence of periodic orbits for $\beta=0$ follows easily by an examination of the path directions along the straight line $x_1=Bx_2$ in the phase plane and the fact that any existing periodic orbits must encircle one or more of the critical points which must lie on this line.

It follows from Theorem 4.1 that for β, B, and Da chosen as in the hypotheses, there is a unique asymptotically stable critical point. From Theorem 2.2 $\omega(\gamma^+)$ must be either a periodic orbit or the critical point for any $\gamma^+(p)$ whenever $p\in D$. Assume that $\omega(\gamma^+)$ is a periodic orbit. By Lemma 5.2 this assumed periodic orbit must be asymptotically orbitally stable and also must encircle the critical point which has index $+1$ by Theorem 3.1. Consider now the initial value problem (1.3) with $(x_1(0), x_2(0))=q$ in the interior of this periodic orbit but distinct from the critical point. By the techniques similar to the ones used in the proof of Theorem 2.1 one can establish the existence of the full orbit $\gamma(q)$ through q. Thus $\gamma^-(q)$ is contained in the interior of the periodic orbit. Since the periodic orbit is asymptotically orbitally stable and the critical point orbit is asymptotically stable, it follows from Theorem 2.2 that $\alpha(\gamma^-(q))$ must be a periodic orbit which must then be unstable. This is a contradiction since all existing periodic orbits must be asymptotically orbitally stable by Lemma 5.2. Q.E.D.

6. Friedrichs' Bifurcation Theory

It will be convenient to write (1.3) in the form

$$\frac{dy}{ds} = Ay + \mu\, G(y, \mu) \tag{6.1}$$

where μ is a small parameter, A is a constant matrix, and where the system

$$\frac{dy}{ds} = Ay \tag{6.2}$$

has periodic solutions. (This is the case when A has purely imaginary eigenvalues or possibly when one of the eigenvalues of A is zero.) We consider only the case where A has purely imaginary eigenvalues. This is the case if and only if the critical point of the linearized problem (6.2) is a center. In order to achieve such a reformulation we shall adopt a general theory due to K. O. Friedrichs [9]. For our purposes we shall formulate the necessary general theory in this section and apply it in Section 7.

For the two dimensional autonomous system

$$\frac{dx}{dt} = \hat{F}(x, \gamma), \tag{6.3}$$

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

$$\begin{gathered}
\gamma = \gamma_0 + \varepsilon, \qquad a^\varepsilon = \hat{a}^{\gamma_0 + \varepsilon}, \qquad s = \frac{T^0}{T^\varepsilon}\, t, \qquad \varepsilon = \mu\delta, \\
T^\varepsilon = T^0(1 + \mu\eta), \qquad x^\varepsilon = a^\varepsilon + \mu\, y(s, \mu), \qquad \hat{F}(\hat{a}^\gamma, \gamma) = F(a^\varepsilon, \varepsilon), \\
A^\varepsilon = F_x(a^\varepsilon, \varepsilon), \qquad \varepsilon C^\varepsilon = A^\varepsilon - A^0, \qquad C^0 = \left.\frac{dA^\varepsilon}{d\varepsilon}\right|_{\varepsilon=0}, \\
\mu^2 Q^\varepsilon(y, \mu) = F(a^\varepsilon + \mu y, \varepsilon) - \mu A^\varepsilon y
\end{gathered} \tag{6.4}$$

where T^0, δ, η, and a^0 are to be determined and μ is an auxiliary parameter. Under this change of variables, the problem (6.3) becomes

$$\frac{dy}{ds} = A^0 y + \mu\{\delta\, C^{(\mu\delta)} y + \eta A^{(\mu\delta)} y + (1 + \mu\eta)\, Q^{(\mu\delta)}(y, \mu)\}. \tag{6.5}$$

Then we have

Theorem 6.1. (*Modification of* Friedrichs [9], p. 94, *Theorem 6.*) *Suppose the two dimensional vector* $F(x, \varepsilon) \in C^2[D \times (-\varepsilon_0, \varepsilon_0)]$ *where* D *is a domain in* $\mathbb{R}^2$ *and* ε_0

is a positive number. Assume that the equation $\frac{dx}{dt}=F(x,\varepsilon)$ *has a constant solution* $x=a^{\varepsilon}$ *such that for the value* $\varepsilon=0$ *the matrix* $A^0=F_x(a^0,0)$ *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 exist 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* $\eta(\mu)\in C^1(-\mu^0,\mu^0)$ *for some sufficiently small* $\mu_0>0$ *and a function* $y(s,\mu)$ *with period* T^0 *in* s *assuming an arbitrarily prescribed initial value* $y(0,\mu)=b_0$ *such that*

$$x^{\varepsilon}=a^{\varepsilon(\mu)}+\mu y\left(\frac{T^0}{T^{\varepsilon(\mu)}}t,\mu\right) \tag{6.6}$$

is a solution of the differential equation

$$\frac{dx}{dt}=F(x,\varepsilon(\mu)). \tag{6.7}$$

Contained in the proof of Theorem 6.1 is the following fact:

Corollary 6.2. *Bifurcation from the critical point* $\hat{a}^{\gamma}$ *of* $\frac{dx}{dt}=\hat{F}(x,\gamma)$ *can occur only from those* $\hat{a}^{\gamma_0}$ *which are centers in the associated linearized problem or possibly when one of the eigenvalues of the matrix* A *is zero.*

To determine the local behavior of the solution y and the dependence of the functions η and δ on μ, we first note that $\delta,\eta\in C^1(-\mu^0,\mu^0)$. Using

$$\delta(0)=\eta(0)=0,\quad \delta^1\equiv\frac{d\delta}{d\mu}(0),\quad\text{and}\quad \eta^1=\frac{d\eta}{d\mu}(0),$$

we have

$$\eta(\mu)=\mu\eta^1+\mu\left(\frac{d\eta}{d\mu}(\theta_1\mu)-\eta^1\right)\qquad\text{for some } 0<\theta_1<1 \tag{3.8}$$

and

$$\delta(\mu)=\mu\delta^1+\mu\left(\frac{d\delta}{d\mu}(\theta_2\mu)-\delta^1\right)\qquad\text{for some } 0<\theta_2<1,\ \mu\in(-\mu_0,\mu_0). \tag{3.9}$$

Note that

$$\mu\left(\frac{d\eta}{d\mu}(\theta_1\mu)-\eta^1\right)\quad\text{and}\quad\mu\left(\frac{d\delta}{d\mu}(\theta_2\mu)-\delta^1\right)$$

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 $|\mu|$ sufficiently small. If $\delta^1>0$, then a small periodic solution grows from $\hat{a}^{\gamma_0}$ as γ increases beyond γ_0. If $\delta^1<0$, then a small periodic solution grows from $\hat{a}^{\gamma_0}$ 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 $\boldsymbol{y}$:

Theorem 6.3. *Under the assumed continuity properties of $\boldsymbol{F}$ and the derived continuity properties of $\delta(\mu)$ and $\eta(\mu)$ in Theorem 6.1, we have*

$$\boldsymbol{y}(s,\mu)=\boldsymbol{y}^0(s)+\mu\,\boldsymbol{y}^1(s)+\mu\,\bar{\boldsymbol{y}}(s,\mu) \tag{6.10}$$

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

$$\boldsymbol{y}^0(s)=Y(s)\,\boldsymbol{b}_0 \tag{6.11}$$

and

$$\boldsymbol{y}^1(s)=Y(s)\int_0^s Y^{-1}(\tau)\,Q^0(y^0(\tau),0)\,d\tau \tag{6.12}$$

where $Y(s)$ is the matrix solution of

$$\frac{dY}{ds}=A^0\,Y \quad \text{and} \quad Y(0)=I. \tag{6.13}$$

Proof. An equivalent formulation of the problem (6.5) with initial conditions $\boldsymbol{y}(0,\mu)=\boldsymbol{b}_0$ is

$$\boldsymbol{y}=Y(s)\,\boldsymbol{b}_0+\mu Y(s)\int_0^s Y^{-1}(\tau)\,\{\delta C^\varepsilon\,\boldsymbol{y}+\eta A^\varepsilon\,y+(1+\mu\eta)\,Q^\varepsilon(y,\mu)\}\,d\tau \tag{6.14}$$

where $\delta=\delta(\mu)$, $\eta=\eta(\mu)$, $\varepsilon=\mu\delta(\mu)$, and $Y(s)$ satisfies (6.13). From Theorems 2.3 and 2.4 of M. Urabe [19] or from similar theorems in [4], it follows that

$$y=Y(s)\,\boldsymbol{b}_0+\mu Y(s)\int_0^s Y^{-1}(\tau)\,Q^0(\boldsymbol{y}(\tau,0),0)\,d\tau+\mu\,\bar{\boldsymbol{y}}(s,\mu) \tag{6.15}$$

where $\bar{\boldsymbol{y}}(s,\mu)=o(1)$ as $\mu\to 0$ uniformly on any finite interval and $\boldsymbol{y}(s,0)=Y(s)\,\boldsymbol{b}_0$. $Y(s)$ is T^0-periodic by the definition of A^0 and (6.13). Assuming for the moment that $\int_0^s Y^{-1}(\tau)\,Q^0(\boldsymbol{y}(\tau,0),0)\,d\tau$ is T^0-periodic, $\bar{\boldsymbol{y}}(s,\mu)$ is T^0-periodic since every other term in (6.15) is T^0-periodic. From periodicity of each term in (6.15) it follows that (6.15) is uniformly valid on $[0,\infty)$ as $\mu\to 0$.

We now prove that $\int_0^s Y^{-1}(\tau)\,Q^0(\boldsymbol{y}(\tau,0),0)\,d\tau$ 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 $Q^0(\boldsymbol{y}^0(\tau,0),0)$ is quadratic in $y_1^0(\tau)$ and $y_2^0(\tau)$ where $\boldsymbol{y}^0(\tau,0)=\begin{Bmatrix} y_1^0 \\ y_2^0 \end{Bmatrix}$, the expression $Y^{-1}(\tau)\,Q^0(\boldsymbol{y}^0(\tau,0),0)$ 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,

$$\int_0 Y^{-1}(\tau)\, Q^0(y(\tau, 0), 0)\, d\tau$$

is T^0-periodic and $\int_0^{T^0} Y^{-1}(\tau)\, Q^0(y(\tau, 0), 0)\, d\tau = 0$. Q.E.D.

Using Theorems 6.1 and 6.3, we obtain the following information about $\delta(\mu)$, $\eta(\mu)$, δ^1, and η^1:

Theorem 6.4. *The functions $\eta(\mu)$ and $\delta(\mu)$ are obtained implicitly from*

$$\begin{aligned} 0 = \eta \int_0^{T^0} Y^{-1}(\tau)\, A^{(\mu\delta)}\, y(\tau, \mu)\, d\tau + \delta \int_0^{T^0} Y^{-1}(\tau)\, C^{(\mu\delta)}\, y(\tau, \mu)\, d\tau \\ + \int_0^{T^0} Y^{-1}(\tau)(1 + \mu\eta)\, Q^{(\mu\delta)}(y(\tau, \mu), \mu)\, d\tau. \end{aligned} \tag{6.16}$$

δ^1 and η^1 are determined explicitly from

$$\begin{aligned} 0 = \eta^1 \int_0^{T^0} Y^{-1}(\tau)\, A^0\, y^0\, d\tau + \delta^1 \int_0^{T^0} Y^{-1}(\tau)\, C^0\, y^0\, d\tau \\ + \int_0^{T^0} Y^{-1}(\tau) \left(\frac{dQ^{(\mu\delta)}}{d\mu}(y(\tau, \mu), \mu) \right) \Bigg|_{\mu=0} d\tau \end{aligned} \tag{6.17}$$

where y^0 and $Y^{-1}(\tau)$ are defined from Theorem 6.3.

Proof. The expression (6.16) is contained in the proof of Theorem 6, p. 94 of K. O. FRIEDRICHS [9]. We now derive the expression (6.17). Divide expression (6.16) by μ and recall from the proof of Theorem (6.3) that

$$\int_0^{T^0} Y^{-1}(\tau)\, Q^0(y(\tau, 0), 0)\, d\tau = 0;$$

we obtain

$$\begin{aligned} 0 = \frac{\eta(\mu)}{\mu} \int_0^{T^0} Y^{-1}(\tau)\, A^\varepsilon\, y(\tau, \mu)\, d\tau + \frac{\delta(\mu)}{\mu} \int_0^{T^0} Y^{-1}(\tau)\, C^\varepsilon\, y(\tau, \mu)\, d\tau \\ + \int_0^{T^0} Y^{-1}(\tau) \left\{ \frac{Q^\varepsilon(y(\tau, \mu), \mu) - Q^0(y(\tau, 0), 0)}{\mu} \right\} d\tau \\ + \int_0^{T^0} Y^{-1}(\tau)\, \eta(\mu)\, Q^\varepsilon(y(\tau, \mu), \mu)\, d\tau \end{aligned} \tag{6.18}$$

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

$$\begin{aligned} \lim_{\mu \to 0} \frac{\eta(\mu)}{\mu} \int_0^{T^0} Y^{-1} A^\varepsilon\, y(\tau, \mu)\, d\tau &= \eta^1 \int_0^{T^0} Y^{-1}(\tau) \lim_{\mu \to 0} A^\varepsilon\, y(\tau, \mu)\, d\tau \\ &= \eta^1 \int_0^{T^0} Y^{-1}(\tau)\, A^0\, y(\tau, 0)\, d\tau, \end{aligned} \tag{6.19}$$

$$\begin{aligned}\lim_{\mu\to 0}\frac{\delta(\mu)}{\mu}\int_0^{T^0} Y^{-1}(\tau)\,C^\varepsilon y(\tau,\mu)\,d\tau &= \delta^1\int_0^{T^0} Y^{-1}(\tau)\lim_{\mu\to 0} C^\varepsilon y(\tau,\mu)\,d\tau\\ &= \delta^1\int_0^{T^0} Y^{-1}(\tau)\,C^0\,y(\tau,0)\,d\tau,\end{aligned}\tag{6.20}$$

$$\lim_{\mu\to 0}\int_0^{T^0} Y^{-1}(\tau)\,\eta(\mu)\,Q^\varepsilon(y(\tau,\mu),\mu)\,dT=\int_0^{T^0} Y^{-1}(\tau)\,\eta(0)\,Q^0(y(\tau,0),\mu)\,d\tau=0.\tag{6.21}$$

From the continuity properties of $Q^\varepsilon(y(\tau,\mu),\mu)$ and the expression (6.14) for $y(\tau,\mu)$ we can interchange the limit process and integration in the third integral in expression (6.18) to obtain

$$\begin{aligned}&\lim_{\mu\to 0}\int_0^{T^0} Y^{-1}(\tau)\left\{\frac{Q^\varepsilon(y(\tau,\mu),\mu)-Q^0(y(\tau,0),0)}{\mu}\right\}d\tau\\ &\quad=\int_0^{T^0} Y(\tau)\left(\frac{dQ^\varepsilon}{d\mu}(y(\tau,\mu),\mu)\right)\bigg|_{\mu=0}d\tau.\end{aligned}\tag{6.22}$$

Thus, the expressions (6.18) through (6.22) yield the desired result (6.17). Q.E.D.

7. Application to Reactor Equations

Since the bifurcation theorem (Theorem 6.1) is concerned with the variation of a single parameter and three parameters are at our disposal, we can choose which parameters to hold fixed while one is varied. However, the parameter which we choose to vary should be one that can be varied in chemical experiments. One possibility, and the one we shall follow, is to vary the Damköhler number, Da, since it is a monotone function of the temperature of the chemicals entering a reactor for the CSTR problem or of the temperature of the gas surrounding the wire in the catalytic wire problem ([13], [3]). Such a choice leads naturally to a discussion of the ignition and extinction processes in Section 9. Another possibility arises from the fact that $Da=Da_0\tau$ and $\beta=\beta_0\tau$ where $\tau=1/\lambda v$, $(1-\lambda)$ is the proportion of chemicals recycled into the reactor, and v is the velocity of the chemicals entering a reactor. Although we shall consider only variations of Da, the analysis of bifurcation for variations of τ could be carried out along similar lines.

We now proceed with the application of the results of the previous section to the system (1.3). By Corollary 6.2 bifurcation of periodic solutions can occur only from the center or possibly at those points at which one of the eigenvalues of the matrix A is zero. This latter case can happen only when $B\geqq 4(1+\beta)$ and $a_2=m_1$ or m_2. However, we shall investigate only the first case. Let β and B be fixed and restricted to one of the Regions III through VI so that there is a Da, say Da_0, and a corresponding $\boldsymbol{a}^0$ such that $\boldsymbol{a}^0$ is a center for the linearized problem. Let $Da=Da_0+\varepsilon$; then, the critical points are given by

$$a_1^\varepsilon=\frac{B a_2^\varepsilon}{1+\beta}+\frac{\beta x_c}{1+\beta}\tag{7.1}$$

and

$$Da_0+\varepsilon=\frac{a_2^\varepsilon}{1-a_2^\varepsilon}\exp(-a_1^\varepsilon).\tag{7.2}$$

We now proceed to reformulate our problem and show that Theorem 6.1 applies. With the definition of F given in (1.3), we find that

$$F_x(a^\varepsilon, \varepsilon) = \begin{pmatrix} -1-\beta+B(Da_0+\varepsilon)(1-a_2^\varepsilon)\exp(a_1^\varepsilon), & -(Da_0+\varepsilon)B\exp(a_1^\varepsilon) \\ (Da_0+\varepsilon)(1-a_2^\varepsilon)\exp(a_1^\varepsilon), & -1-(Da_0+\varepsilon)\exp(a_1^\varepsilon) \end{pmatrix}. \tag{7.3}$$

Using (7.2), we obtain

$$A^\varepsilon = \begin{pmatrix} Ba_2^\varepsilon - 1 - \beta & \dfrac{-Ba_2^\varepsilon}{1-a_2^\varepsilon} \\ a_2^\varepsilon & \dfrac{-1}{1-a_2^\varepsilon} \end{pmatrix} \tag{7.4}$$

and

$$C^0 = \left.\frac{dA^\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} = \begin{pmatrix} B & \dfrac{-B}{(1-a_2^0)^2} \\ 1 & \dfrac{-1}{(1-a_2^0)^2} \end{pmatrix} \left.\left(\frac{da_2^\varepsilon}{d\varepsilon}\right)\right|_{\varepsilon=0}. \tag{7.5}$$

By use of (7.1) and (7.2), it follows that

$$\left.\left(\frac{da_2^\varepsilon}{d\varepsilon}\right)\right|_{\varepsilon=0} = \frac{(1+\beta)a_2^0}{Da_0 \det A^0}. \tag{7.6}$$

Furthermore,

$$F(a^\varepsilon + \mu y, \varepsilon) = \mu A^\varepsilon + \mu^2 Q^\varepsilon(y, \mu) \tag{7.7}$$

where

$$Q^\varepsilon(y,\mu) = \frac{a_2^\varepsilon}{1-a_2^\varepsilon} \begin{Bmatrix} B\left\{\dfrac{1-a_2^\varepsilon}{\mu^2}(\exp(\mu y_1)-1-\mu y_1) - \dfrac{y_2}{\mu}(\exp(\mu y_1)-1)\right\} \\ \left\{\dfrac{(1-a_2^\varepsilon)}{\mu^2}(\exp(\mu y_1)-1-\mu y_1) - \dfrac{y_2}{\mu}(\exp(\mu y_1)-1)\right\} \end{Bmatrix}. \tag{7.8}$$

The matrix A^0 has eigenvalues

$$\lambda_{1,2} = \frac{\operatorname{tr} A^0}{2} \pm \frac{1}{2}\sqrt{(\operatorname{tr} A^0)^2 - 4\det A^0}. \tag{7.9}$$

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

$$\operatorname{tr} A^0 = 0 \quad \text{and} \quad \det A^0 > 0. \tag{7.10}$$

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 (1.3). Then,

$$\lambda_{1,2} = \pm i\omega_0 \tag{7.11}$$

where $\omega_0 = \sqrt{\det A^0}$. Now $\operatorname{tr} A^0 = 0$ means $Ba_2^0 - 1 - \beta = \dfrac{1}{1-a_2^0}$ or, in an equivalent form,

$$B(a_2^0)^2 - (B+1+\beta)a_2^0 + 2 + \beta = 0. \tag{7.12}$$

Recall from Section 4 that the roots of (7.12) are

$$s_1=\frac{B+1+\beta}{2B}-\frac{1}{2B}\sqrt{(B+1+\beta)^2-4B(2+\beta)} \tag{7.13}$$

and

$$s_2=\frac{B+1+\beta}{2B}+\frac{1}{2B}\sqrt{(B+1+\beta)^2-4B(2+\beta)}. \tag{7.14}$$

From Theorem 4.1 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 $a_2^0=s_1$ and for (β, B) in any one of the Regions III through VI, $\det A^0>0$ for $a_2^0=s_2$. We now proceed to show that in each such case $\operatorname{tr} C^0 \neq 0$. From (7.5) and (7.6) we have

$$\operatorname{tr} C^0=\left[B-\frac{1}{(1-a_2^0)^2}\right]\left[\frac{(1+\beta)\,a_2^0}{Da_0\det A^0}\right]=\left[\frac{B(1-a_2^0)^2-1}{(1-a_2^0)^2}\right]\left[\frac{(1+\beta)\,a_2^0}{Da_0\det A^0}\right]. \tag{7.15}$$

Using (7.13) and (7.14), we obtain

$$B(1-a_2^0)^2-1=\frac{1}{2B}\sqrt{(B-1-\beta)^2-4B}\left(\sqrt{(B-1-\beta)^2-4B}\mp(B-1-\beta)\right) \tag{7.16}$$

where the negative sign corresponds to s_1 and the positive to s_2. Thus, for $\det A^0>0$ we have

$$\operatorname{tr} C^0>0 \quad \text{for } a_2^0=s_1 \tag{7.17}$$

and

$$\operatorname{tr} C^0<0 \quad \text{for } a_2^0=s_2 \tag{7.18}$$

when β and B are in Regions III through VI. Since our autonomous system (1.3) certainly satisfies the continuity requirements in Theorem (6.1), we have

Theorem 7.1. *Bifurcation of periodic solutions occurs from the critical points* $(a_1^0, a_2^0)=(Bs_1/(1+\beta)+\beta x_c/(1+\beta), s_1)$ *when β and B are in any one of the Regions* IV, V *or* VI *and from the critical point* $(a_1^0, a_2^0)=(Bs_2/(1+\beta)+\beta x_c/(1+\beta), s_2)$ *when β and B are in any one of the Regions* III, IV, V, *or* VI. *Thus, Theorem* 6.1 *applies in each of these cases.*

Our next aim will be to use Theorems 6.3 and 6.4 to determine the direction of bifurcation and the local structure of the periodic solution. We first determine $y^0(s)$ and $y^1(s)$. For convenience we introduce the notation

$$a=a_2^0 \quad \text{and} \quad b=Ba_2^0-1-\beta. \tag{7.19}$$

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

$$A^0=\begin{pmatrix} b & -Bab \\ a & -b \end{pmatrix} \tag{7.20}$$

and

$$\omega_0^2=Ba^2b-b^2>0. \tag{7.21}$$

The fundamental matrix solution, $Y(s)$, of $dy/ds = A^0 y$ satisfies

$$\frac{dY}{ds} = A^0 Y \quad \text{and} \quad Y(0) = I. \tag{7.22}$$

By using (7.21), it is easily verified that

$$Y(s) = (\cos\omega_0 s) I + \left(\frac{\sin\omega_0 s}{\omega_0}\right) A^0 \tag{7.23}$$

and

$$Y^{-1}(s) = \cos\omega_0 s I - \left(\frac{\sin\omega_0 s}{\omega_0}\right) A^0. \tag{7.24}$$

In the expansion

$$y(s,\mu) = y^0(s) + \mu y^1(s) + \mu \bar{y}(s,\mu) \tag{7.25}$$

we have from Theorem 6.3 that

$$y^0(s) = Y(s)\, b_0 \tag{7.26}$$

and

$$y^1(s) = Y(s) \int_0^s Y^{-1}(\tau)\, Q^0\big(y^0(\tau), 0\big)\, d\tau. \tag{7.27}$$

Since b_0 is arbitrary (see p. 90 of K. O. FRIEDRICHS [9]), we take $b_0 = \begin{Bmatrix} 0 \\ 1 \end{Bmatrix}$ without loss of generality. This particular choice of b_0 makes the algebra simpler in the succeeding determination of $y^1(s)$ and δ^1. Thus

$$y^0(s) = Y(s) \begin{Bmatrix} 0 \\ 1 \end{Bmatrix} = \begin{Bmatrix} \dfrac{-Bab}{\omega_0} \sin\omega_0 s \\ \cos\omega_0 s - \dfrac{b}{\omega_0} \sin\omega_0 s \end{Bmatrix}. \tag{7.28}$$

Using (7.8), (7.23), (7.24), (7.28) in (7.27) yields

$$\begin{aligned} y^1(s) = {} & \frac{Ba^2 b^2}{6\omega_0^3} \begin{Bmatrix} B\big((Ba-2b)(2\sin\omega_0 s - \sin 2\omega_0 s) + 2\omega_0(\cos\omega_0 s - \cos 2\omega_0 s)\big) \\ (Ba-2b)(2\sin\omega_0 s - \sin 2\omega_0 s) + 2\omega_0(\cos\omega_0 s - \cos 2\omega_0 s) \end{Bmatrix} \\ & + \frac{Ba^2 b^2}{6\omega_0^4} \begin{Bmatrix} B\big((Ba-2b)(1 - 2\cos\omega_0 s + \cos^2\omega_0 s) - \omega_0(\sin 2\omega_0 s - 2\sin\omega_0 s)\big) \\ (Ba-2b)(1 - 2\cos\omega_0 s + \cos^2\omega_0 s) - \omega_0(\sin 2\omega_0 s - 2\sin\omega_0 s) \end{Bmatrix}. \end{aligned} \tag{7.29}$$

By using the above values of y^0 and y^1 in equation (6.17), one obtains

$$\eta^1 \tilde{A} b_0 + \delta^1 \tilde{C} b_0 = -\frac{1}{T^0} \int_0^{T^0} Y^{-1}(\tau) \left.\frac{dQ}{d\mu}\right|_{\mu=0} d\tau \tag{7.30}$$

where

$$\tilde{A} = \frac{1}{T^0} \int_0^{T^0} Y^{-1}(\tau) A^0 Y(\tau)\, d\tau = A^0, \tag{7.31}$$

$$\tilde{C} = \frac{1}{T^0} \int_0^{T^0} Y^{-1}(\tau) C^0 Y(\tau)\, d\tau = \frac{1}{2}\left(C^0 - \frac{1}{\omega^2} A^0 C^0 A^0\right), \tag{7.32}$$

$$C^0 = \begin{pmatrix} B & -Bb^2 \\ 1 & -b^2 \end{pmatrix} \frac{da_2^0}{d\varepsilon}. \tag{7.33}$$

For $\boldsymbol{b}_0 = \begin{Bmatrix} 0 \\ 1 \end{Bmatrix}$, (7.30) becomes

$$\begin{aligned} b\begin{Bmatrix} Ba \\ 1 \end{Bmatrix}\eta^1 + \frac{b}{2\omega_0^2}\left(\frac{da_2^0}{d\varepsilon}\right)\begin{Bmatrix} B(b\omega_0^2 + b^2 - Ba) \\ \omega^2 b + (Ba - b)(b^2 - Ba) \end{Bmatrix}\delta^1 \\ = \frac{1}{T^0}\int_0^{T^0} Y^{-1}(\tau)\left.\frac{dQ}{d\mu}\right|_{\mu=0} d\tau. \end{aligned} \tag{7.34}$$

Let Δ be the determinant of the coefficient matrix of η^1 and δ^1; then a simple calculation shows that

$$\Delta = -\frac{Bab}{2}\operatorname{tr} C^0. \tag{7.35}$$

From (7.17), (7.18), (7.19), and (7.21) we know that $\Delta \neq 0$. We can, therefore, solve for δ^1 to obtain

$$\delta^1 = \frac{Ba^2b^2}{8\omega_0^4 \operatorname{tr} C^0}\{\omega_0^2(b-1) + (2b - Ba) - (2b - Ba)^2\} \tag{7.36}$$

where

$$b = Bs_i - 1 - \beta \quad \text{for } i = 1 \quad \text{or } 2, \tag{7.37}$$

$$a = s_i \quad \text{for } i = 1 \quad \text{or } 2, \tag{7.38}$$

$$\omega_0^2 = Ba^2b - b^2, \tag{7.39}$$

and s_1 and s_2 are given by (7.13) or (7.14).

Thus, in the light of the remarks on the direction of bifurcation following Corollary 6.2, we have determined the direction of bifurcation through the formula

$$Da - Da_0 = \delta^1\mu^2 + o(\mu^2) \quad \text{as } \mu \to 0.$$

8. Stability of the Bifurcating Period Orbits and the Response Diagram

In this section and in Section 9 we present some of the most important implications of Section 7. We first establish the stability of the bifurcating periodic orbits and its relation to the sign of δ^1 and then discuss the relations between the multiplicity and stability of the steady states and the bifurcating periodic orbits on the response diagram.

We use Poincaré's Criterion (see W. A. Coppel [8]) to establish the type of stability of the bifurcating periodic orbits for μ sufficiently small. Let $\boldsymbol{H}(\boldsymbol{y}, \mu)$ denote the right hand side of (6.5). Then the periodic orbit $\boldsymbol{a}^\varepsilon + \mu\boldsymbol{y}(s, \mu)$ is asymptotically orbitally stable if

$$\frac{1}{T^0}\int_0^{T^0} \nabla \cdot \boldsymbol{H}(\boldsymbol{y}, \mu)\, ds < 0 \tag{8.1}$$

and is unstable if

$$(8.2)\qquad \frac{1}{T^0}\int_0^{T^0} \nabla\cdot H(y,\mu)\,ds>0.$$

By expanding $\nabla\cdot H$ and y in powers of μ, one can rigorously establish that

$$(8.3)\qquad \frac{1}{T^0}\int_0^{T^0} \nabla\cdot H\,ds=\mu^2\Delta+o(\mu^2)\quad \text{as } \mu\to 0,$$

where

$$(8.4)\qquad \Delta=-(\delta^1\operatorname{tr}C^0).$$

Now $\operatorname{tr}C^0>0$ for $a_2^0=s_1$ and $\operatorname{tr}C^0<0$ for $a_2^0=s_2$. Consider first the case $a_1^0=s_1$ and β and B in any of the Regions IV through VI. We have $\Delta>0(<0)$ iff $\delta^1<0(>0)$. 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 any one of the Regions III through VI, we have $\Delta>0(<0)$ 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.

We now wish to show the relations between multiplicity and stability of the critical points and the bifurcation of periodic orbits. Theorems 3.1 and 4.1 give all relations between the multiplicity and stability of the critical points and Theorem 7.1 establishes the bifurcation of periodic orbits with the direction and stability determined by δ^1 (see (7.36), (8.3) and (8.4)). Since δ^1 is a function of β and B, we could in principle solve for $\delta^1(\beta,B)=0$. This would divide the six (β,B)-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 example which the author believes contain all the qualitative features of this bifurcation problem. We first set $x_c=0$. (It only scales Da if $x_c\neq 0$.) Let

$$P_1=(Da_1,m_1),\qquad P_2=(Da_2,m_2),$$
$$P_3=(Da_3,s_1),\qquad P_4=(Da_4,s_2),$$

where the Da_i and s_1, s_2, m_1, and m_2 are given by (4.1)–(4.5). For various values of β and B the points P_1 through P_4 and δ^1 have been evaluated numerically and the results are contained in Table 1 and on the "S" shaped curves in Figures 5 through 14. (The tables and figures are at the end of the paper.) The "S" shaped curves have been exaggerated to present the qualitative features. The reader is referred directly to these figures for the presentation of the main results.

For any set of values of β, B, and Da for which there is an unstable unique critical point, it was shown in Section 5 that there must exist a periodic orbit in the corresponding phase plane of (1.3). In Figure 7 this means that there is a periodic orbit for each $Da\in(Da_1, Da_4)$. A similar remark holds for Figures 8–11, 13, 14. This information comes entirely from the Poincaré-Bendixson 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 $(Bs_2/(1+\beta), s_2)$ 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 $(Ba_2^\varepsilon/(1+\beta), a_2^\varepsilon)$ where $a_2^0 = s_2$, $\varepsilon = Da - Da_4$ and $\varepsilon < 0$ here. A similar remark applies to Figures 10, 12, 13, and 14 but the asymptotically orbitally stable periodic orbit bifurcates as Da increases beyond Da_3. In Figures 8, 9, and 11 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 11. 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. In Section 2 it was shown that each path in the domain, D, remains in a compact subset of D. Since $\int_0^T \nabla \cdot \boldsymbol{H}\, ds < 0$ for Da sufficiently close to Da_3, all paths lead away from this unstable periodic orbit. Therefore, Theorem 2.2 implies the existence of at least one more periodic orbit. That is, for $Da < Da_3$ and Da sufficiently close to Da_3 there exist at least two periodic orbits. This situation has been observed numerically by V. HLAVÁČEK, M. KUBÍČEK & J. JELÍNEK [13] for the case in Figure 11 (for different parameters) but not for the situation as in Figure 9. More specifically, HLAVÁČEK 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 $Da \in (0.1650, 0.3366)$ and is asymptotically stable for $Da \in (0, 0.1650) \cup (0.3366, \infty)$. The situation is as in Figure 11 with the above appropriate number changes. By numerically integrating the autonomous system for $(\beta, B) = (3, 14)$ and ranges of $Da < 0.1650$, HLAVÁČEK shows that for $0.1620 < Da < 0.1650$ there is a stable critical point surrounded by an unstable periodic orbit which is in turn surrounded by a stable periodic orbit. For $Da < 0.1620^-$ there are no periodic orbits. This leads us to conjecture that the branch of periodic orbits meet as in Figure 15 where we have taken $Da_3 = 0.1650$, and $Da_4 = 0.3366$. We also conjecture that the branches emanating from points P_3 and P_4 in Figures 9, 10, 12, 13, and 14 connect and that there are only stable periodic orbits in Figures 10, 12, 13, 14.

Another interesting case is that in Figure 5. There is from the general theory an unstable bifurcated periodic orbit surrounding the upper critical point for $Da > Da_4$ but close to Da_4. Our numerical investigations [18] indicate that for Da just to the right of Da_4 there is only one periodic orbit (the unstable one). Further, this branch of unstable periodic orbits continues to the right until some value of Da, say Da^*, is reached after which all periodic orbits cease $(Da^* \in (Da_4, Da_1))$. Next, the branch of periodic orbits bifurcating from point P_4 in Figures 6 and 7 continue to the left until a value of Da, say Da^*, is reached below which periodic orbits cease. $Da^* \in (Da_2, Da_4)$ in Figure 6 and $Da^* \in (Da_2, Da_1)$ in Figure 7 (see [18]). Finally, for the case of β and B in Region IV our numerical investigations [18] indicate that two different situations occur. When β and B are chosen so that

$Da_3 < Da_2$ as in Figure 9, the branch of periodic orbits emanating from P_3 actually connects with the branch emanating from P_4. On the other hand, when β and B are chosen so that $Da_2 < Da_3$ as in Figure 8, the branches of periodic orbits emanating from P_3 and P_4 continue to the left and stop at some value of Da, say Da^*, below which there are no periodic orbits and $Da^* \in (Da_2, Da_3)$. An explanation, in terms of phase plane sketches, of how periodic orbits cease at Da^* can be found in [7].

With regard to the continuation of the branches of periodic orbits we should point out that Theorem 5.3 states that there are no periodic orbits for Da sufficiently small or large. Furthermore, Theorem 2.1 states that the temperature $x_1(t)$, can be bounded independent of Da for all periodic orbits. Thus we might note that the bifurcation results suggest how all periodic orbits develop as Da changes. In fact, by starting at the bifurcation points and numerically solving the ordinary differential equations (1.3) for various parameter ranges, we [18] have accounted for all previously observed periodic orbits and have discovered significantly many new types of periodic behavior for this problem.

9. Jump Phenomena

In this section we use the response diagrams discussed in Section 8 to show how "jumps" into periodic orbits occur as the Damköhler number 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.

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 "jump" from one steady state (periodic or time independent) to a much higher steady state as some parameter changes. The extinction process is the reverse process. A discussion of these processes and the control problem for the CSTR can be found in ARIS [1] and ARIS & AMUNDSON [2]. The above mentioned parameter 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 Damköhler number $Da \sim \exp(-E/RT_0)$ 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 feed 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. HLAVÁČEK, M. KUBÍČEK & J. JELÍNEK [13]). 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.

Let β and B be in that part of Region II in which $B \leqq 3+\beta+2\sqrt{2+\beta}$. Figure 17 shows a typical "S" shaped curve for such values of β and B. Suppose we are at

Table 1. Numerical Examples for Figures 5–14

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	(0.72, 10.0)	(0.2027, 0.07849)	(0.7793, 0.03804)		(0.8532, 0.04074)	$\delta^1(P_4)<0$
6	(0.72, 7.3)	(0.3801, 0.1222)	(0.6199, 0.1174)		(0.7131, 0.1205)	$\delta^1(P_4)<0$
7	(0.78, 7.3)	(0.4215, 0.1293)	(0.5785, 0.1280)		(0.6991, 0.1321)	$\delta^1(P_4)<0$
	(1.6, 12.5)	(0.2951, 0.1013)	(0.7049, 0.0806)		(0.8812, 0.1072)	$\delta^1(P_4)<0$
8	(1.4, 9.8)	(0.4286, 0.13033)	(0.5714, 0.1293)	(0.4212, 0.13032)	(0.8237, 0.1617)	$\delta^1(P_3)<0, \delta^1(P_4)<0$
9	(1.44, 9.8)	(0.4681, 0.1343)	(0.5319, 0.1342)	(0.4271, 0.1341)	(0.8219, 0.1700)	$\delta^1(P_3)<0, \delta^1(P_4)<0$
10	(0.9, 7.4)			(0.5739, 0.1441)	(0.6829, 0.1507)	$\delta^1(P_3)>0, \delta^1(P_4)<0$
11	(1.34, 9.0)			(0.4694, 0.1454)	(0.7906, 0.1805)	$\delta^1(P_3)<0, \delta^1(P_4)<0$
	(3.0, 14.0)			(0.4060, 0.1650)	(0.8798, 0.3366)	$\delta^1(P_3)<0, \delta^1(P_4)<0$
12	(0.72, 7.02)	(0.4294, 0.1304)	(0.5706, 0.1294)	(0.6154, 0.1298)	(0.6296, 0.1301)	$\delta^1(P_3)>0, \delta^1(P_4)<0$
13	(0.74, 7.06)	(0.4405, 0.1318)	(0.5595, 0.1312)	(0.6055, 0.1316)	(0.6409, 0.1325)	$\delta^1(P_3)>0, \delta^1(P_4)<0$
14	(0.82, 7.3)	(0.4738, 0.13462)	(0.5262, 0.13457)	(0.5622, 0.1347)	(0.6870, 0.1395)	$\delta^1(P_3)>0, \delta^1(P_4)<0$

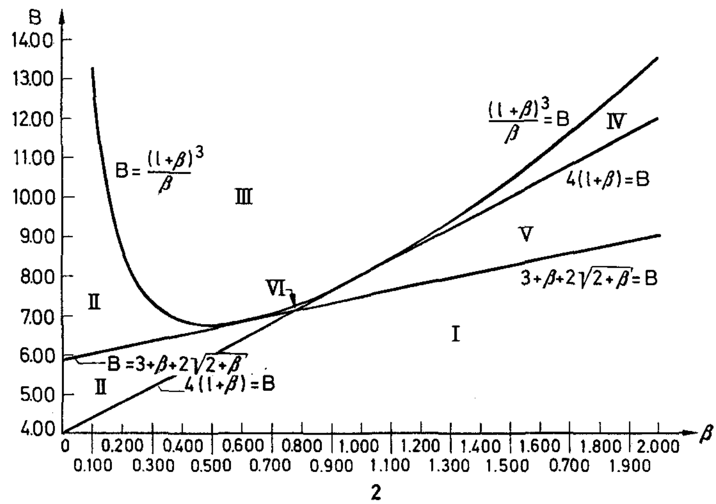


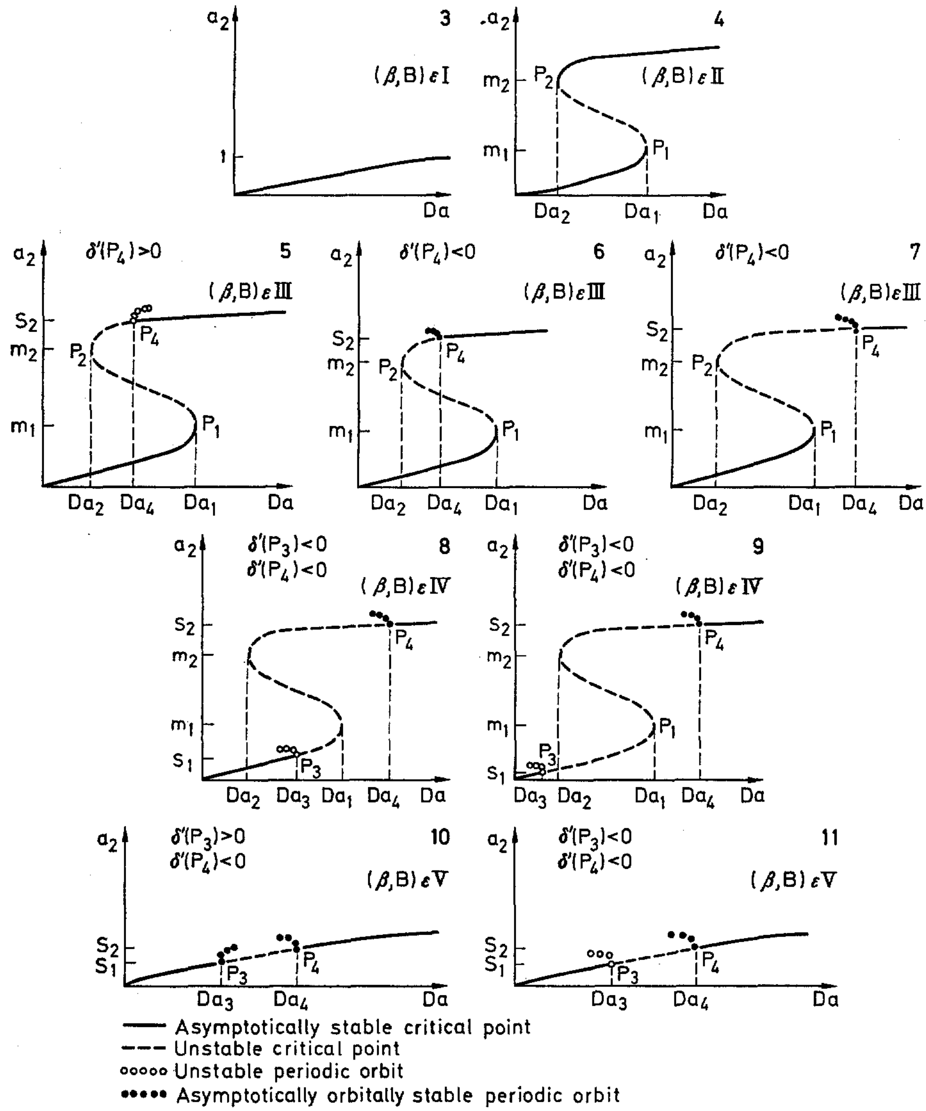
Fig. 2

a steady state at point 1. As Da increases we assume that the initial conditions $\boldsymbol{x}(0)$ are changed so that $\boldsymbol{x}(0)$ is a small perturbation from $\boldsymbol{a}(Da)$. In this case the solution will quickly settle to the steady state $\boldsymbol{a}(Da)$. As Da increases we traverse the "S" shaped curve from 1 to 2 to 3 to 4. Any further increase in Da beyond Da_1 causes the steady state to "jump" to a much higher steady state at point 5. We have, in fact, proved that this jump actually occurs by the implications of Theorem 5.3 which say that all orbits must go to this unique stable critical point. 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; the reactor has been extinguished by too cold a feed.

Thus for β and B in that part of Region II where $B \leqq 3+\beta+2\sqrt{2+\beta}$ we have proved that this "jump" to a lower or higher steady state actually occurs (again by Theorem 5.3). When $\beta=0$, one can also prove this by examination of the phase plane; for β and B in the remaining part of Region II, we conjecture that it also is true.

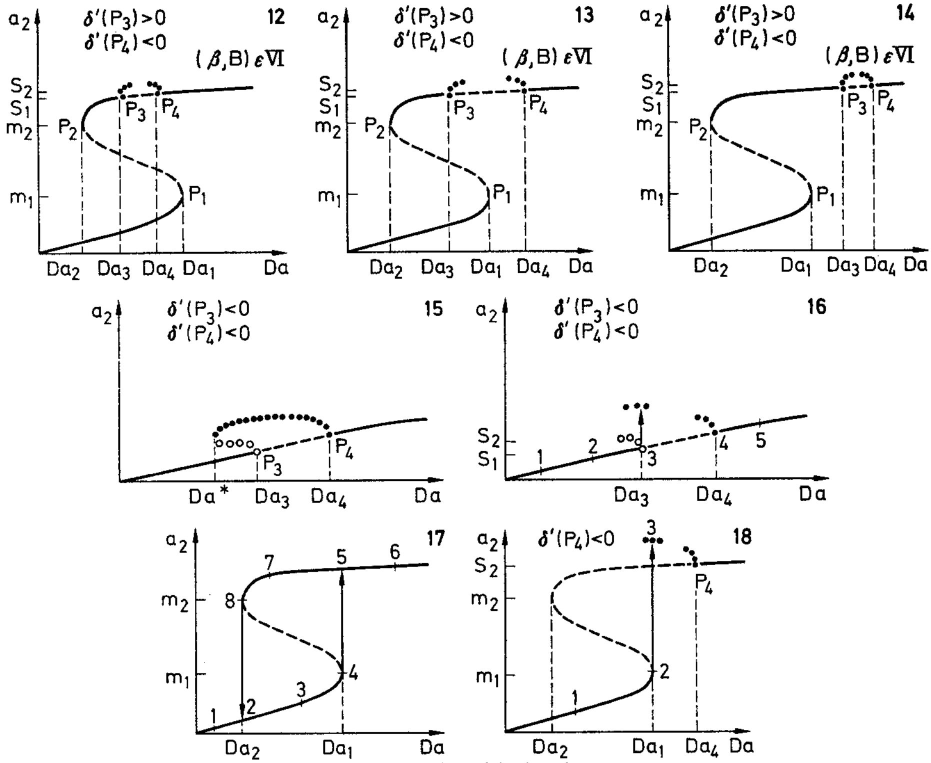
Consider next the "S" shaped response curve in Figure 18. Suppose we start at point 1. As the feed temperature increases the steady state passes to point 2. Any further increase in Da will cause a "jump" but now into a periodic orbit around the critical point at point 3. This same phenomenon occurs whenever a situation like that in Figure 13 occurs.

Next, consider the response curve as in Figure 16. 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 a small change in Da we cannot bring the temperature and concentration back to a steady state. In this case there is a loss in the control of the



Figs. 3—11

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. Similar phenomena occur in Figures 8 and 9.



—— Asymptotically stable critical point
--- Unstable critical point
ooooo Unstable periodic orbit
••••• Asymptotically orbitally stable periodic orbit

Figs. 12—18

A rather interesting phenomena, much akin to the flickering of the flame when one turns off a Bunson burner, occurs during the extinction process for a β and B chosen so that the situation is as in Figure 6. Our numerical investigations [18] indicate that the branch of periodic orbits emanating from P_4 in Figure 6 continues to the left (decreasing Da) until a value of Da, say Da^*, is reached below which there are no more periodic orbits. Furthermore, $Da^* \in (Da_2, Da_4)$ in Figure 6. Thus as Da is decreased below Da_4, there grows a stable periodic orbit until we reach Da^* at which there is a jump downward to the lower steady state. Several other cases of jump phenomena can be found in [18].

Comment. There are several equations, notably (7.29)–(7.36), (8.3), (8.4), which require considerable algebraic manipulations to establish. The author will gladly furnish these to the interested reader upon request.

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Appendix

We sketch the ideas of the proof for Theorem 2.1 since the present method is slightly different from the previous one [2] and estimates on $x_1(t)$ are needed in the proof of global asymptotic stability in Section 5.

Since $\boldsymbol{F}=(F_1, F_2)$ given in (1.3) is analytic in $\boldsymbol{x}=(x_1, x_2)$, $\boldsymbol{F}$ satisfies a Lipschitz condition in $\boldsymbol{x}$ in some neighborhood of each point of D. Therefore, we conclude (see HUREWICZ [14]) that there exists a unique solution to the initial value problem associated with (1.3) with the further properties that

(i) the solution is defined for all $t \geqq 0$; or

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

We first show that (ii) cannot occur so that the unique solution exists for all $t \geqq 0$. Note that at $x_2=1$, $dx_2/dt=-1<0$ and at $x_2=0$, $dx_2/dt=Da e^{x_1}>0$. Thus $x_2(t) \in [0, 1]$ for all $t \in [0, t_1)$. Next we observe that (1.3) can be written as

$$\frac{d}{dt}\left(e^{(1+\beta)t} x_1\right)=e^{(1+\beta)t} \beta x_c + B e^{(1+\beta)t} f(x_1 0 x_2)), \tag{1}$$

$$\frac{d}{dt}\left(e^t x_2\right)=e^t f(x_1, x_2). \tag{2}$$

By the use of (2) in (1) and integration, one obtains

$$\begin{aligned} x_1(t)-B x_2(t)-\frac{B x_c}{1+\beta}-\left(x_1(0)-B x_2(0)-\frac{B x_c}{1+\beta}\right) e^{-(1+\beta)t} \\ = -B\beta \int_0^t e^{(1+\beta)(\tau-t)} x_2(\tau)\, d\tau \end{aligned} \tag{3}$$

where $0<t<t_1$. Since $x_2(t) \in [0, 1]$, (3) immediately implies $x_1(t)$ is uniformly bounded as $t \to t_1-0$, say $|x_1(t)| \leqq M$. Clearly M can be chosen independent of Da. Since $x_1(t)$ is uniformly bounded on $[0, t_1)$, $dx_2/dt=Da e^{x_1}>0$ at $x_2=0$, $dx_2/dt=-1$ at $x_2=1$, continuity of $F_2(x_1, x_2, Da)$ (see (1.3)) implies x_2 is bounded away from the boundary for $t \in [0, t_1)$. Thus, $\boldsymbol{x}(t)$ does not become unbounded nor does it approach the boundary of D as $t \to t_1 - 0$ so that $\boldsymbol{x}(t)$ exists for all $t \geqq 0$.

We observe that the above argument is valid for t_1 replaced by ∞ so that if $\gamma^+(p)$ denotes the positive semiorbit through $p \in D$, then $\gamma^+(p)$ is contained in some compact subset of D. Since the right hand side of (3) is negative and $x_2<1$, it follows that

$$x_1(t)<B+\frac{\beta x_c}{1+\beta}+\{\exp(-(1+\beta)t)\}\left\{x_1(0)-B x_2(0)-\frac{B x_c}{1+\beta}\right\}.$$

Next, observe that on $\dfrac{\beta x_c}{1+\beta}=x_1$, $\dfrac{dx_1}{dt}>0$ except at $x_2=1$ where $\dfrac{dx_2}{dt}<0$. Thus if $x_1(0) \geqq \dfrac{\beta x_c}{1+\beta}$, then $x_1(t) \geqq \dfrac{\beta x_c}{1+\beta}$ for all $t \geqq 0$. If $x_1(0)<\dfrac{\beta x_c}{1+\beta}$, then $\dfrac{dx_1}{dt}>0$ on the line $x_1=x_1(0)$. Therefore $x_1(t) \geqq \min\left\{x_1(0), \dfrac{\beta x_c}{1+\beta}\right\}$.

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Department of Mathematics
Colorado State University
Fort Collins, Colorado

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