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BIFURCATION ANALYSIS OF NONLINEAR REACTION-DIFFUSION EQUATIONS—I. EVOLUTION EQUATIONS AND THE STEADY STATE SOLUTIONS

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A model nonlinear network involving chemical reactions and diffusion is studied. The time evolution and bounds on the steady state solutions are analyzed. Spatially ordered solutions of the equations of the dissipative structure type are found by bifurcation theory. These solutions are calculated analytically and their qualitative properties are discussed.

1. Introduction. Recent studies (Glansdorff and Prigogine, 1971; Nicolis and Portnow, 1973; Sattinger *et al.*, 1973) have shown that nonlinear chemical networks may evolve to many different stable configurations. These configurations may be uniform steady state solutions or they could be spatially or temporally organized states. Which behavior is observed depends on the parameters in the equation and/or the initial conditions of the system. As has been shown by Glansdorff and Prigogine (1971), one can only get space dependent or non-steady state solutions if one is more than a certain critical distance from thermodynamic equilibrium. These solutions have been termed *dissipative structures* and their properties may be contrasted with those on the *thermodynamic branch* which are the extrapolation of the equilibrium behavior.

There is experimental evidence for the formation of dissipative structures in both biological and nonbiological reactions. The Belousov–Zhabotinski reaction is a good, nonbiological, example (Winfree, 1974). It sustains many spatiotemporal patterns as well as uniform limit cycle type oscillations. There has been some controversy as to the role of diffusion in the formation of the horizontal bands observed in this reaction, as Kopell and Howard (1973) have argued that they may be produced through a suitable synchronization of local limit cycle-type oscillators rather than by a symmetry breaking induced by diffusion.

Several biochemical reaction sequences at the cellular level exhibit dissipative structures (Prigogine *et al.*, 1969; Goldbeter, 1973). On a more fundamental level, development and morphogenesis (Turing, 1952; Babloyantz and Hiernaux, 1974, 1975) as well as the prebiotic evolution of biopolymers (Eigen, 1971; Prigogine *et al.*, 1972) have been analyzed within the framework of dissipative structures.

The biological importance of the spontaneous emergence of order in a previously structureless system is obvious and has been well-recognized. Thermodynamic effects of self-organization have also been found. These include an increase of entropy production per unit mass upon the transition to a dissipative structure from the thermodynamic branch (Prigogine *et al.*, 1972).

In this paper we shall analyze the evolution and properties of the dissipative structures arising in nonlinear reaction–diffusion systems. Although our methods are quite general, our analysis will be limited to a particular reaction chain involving two chemical intermediates and a trimolecular step. This is the *simplest* stoichiometric reaction which has instability on the thermodynamic branch (Hanusse, 1972; Tyson, 1973; Tyson and Light, 1973). Consequently this model may be considered as a prototype of any system leading to dissipative structures in a manner analogous to the role of the harmonic oscillator as a prototype in classical or quantum mechanics or to the Volterra–Lotka model in predator–prey interactions.

The model reads:

$$\begin{aligned} \mathrm{A} &\rightarrow \mathrm{X} \\ \mathrm{B} + \mathrm{X} &\rightarrow \mathrm{Y} + \mathrm{D} \\ 2\mathrm{X} + \mathrm{Y} &\rightarrow 3\mathrm{X} \\ \mathrm{X} &\rightarrow \mathrm{E}. \end{aligned} \tag{1.1}$$

A, B, D, E are initial and final products whose concentrations are imposed throughout the system. All reaction steps are irreversible with rate constants equal to unity, and the system (1.1) will be analyzed in the case of a 1-dimensional medium.

The equations for this system are:

$$\frac{\partial X}{\partial t} = D_1 \frac{\partial^2 X}{\partial r^2} - (B + 1)X + X^2 Y + A$$
$$\frac{\partial Y}{\partial t} = D_2 \frac{\partial^2 Y}{\partial r^2} + BX - X^2 Y. \tag{1.2}$$

Here $0 \leq r \leq 1$ and $t \geq 0$. X, Y, A and B are the concentrations of the respective chemicals and D_1, D_2 are the (positive) diffusion coefficients of X and Y respectively. We are assuming that Fick's law holds.

When A, B are constant throughout the system (1.2) admits a solution on the thermodynamic branch:

$$X_0(r) = A \qquad Y_0(r) = B/A. \tag{1.3}$$

To avoid spurious boundary layer effects, one imposes the boundary conditions

$$\begin{aligned} X(0, t) &= X(1, t) = A_0 \\ Y(0, t) &= Y(1, t) = B_0/A_0 \quad \text{for } t > 0 \end{aligned} \tag{1.4}$$

and to make this a well-posed problem one adds the initial conditions

$$X(r, 0) = X_{\text{in}}(r) \qquad Y(r, 0) = Y_{\text{in}}(r). \tag{1.5}$$

Some of the results of our analysis of (1.2), together with a qualitative comparison of dissipative structures and Thom's theory of morphogenesis have already been described (Nicolis and Auchmuty, 1974). In this paper we shall give a detailed analysis of the equations.

In Section 2, it is shown that for any non-negative initial conditions, (1.2) and (1.4) have a non-negative solution $[X(r, t), Y(r, t)]$ which continues for all time. Some properties of the steady state solutions of these equations are discussed in Section 3, while Section 4 presents a linear stability analysis of the thermodynamic branch (1.3). From this analysis, one can infer the bifurcation of new steady state and time periodic solutions. Section 5 is devoted to constructing the new steady state solutions and in Section 6 we discuss the qualitative properties of the resulting dissipative structures. In Section 7, we study the bifurcation when the condition of having a uniform medium is relaxed. In this case, spatial "dispersion" leads to localized dissipative structures. The final Section 8 is devoted to some concluding remarks on the thermodynamic aspects of dissipative structures and to other comments.

Throughout this paper, many of the mathematical details will only be sketched. This has been done to avoid introducing the often elaborate machinery of the theory of partial differential equations. However it is hoped the proofs are sufficiently descriptive to enable those familiar with partial differential equations to reconstruct the complete details.

In a following paper by Mme. Herschkowitz–Kaufman (1975) the theoretical analyses of this paper are compared with the results of computer simulation. The wave-like solutions of these equations will be analyzed in a forthcoming paper. Some other results on these equations have recently been obtained by Boa (1974).

2. The Evolution Equations. In this section we shall prove some results about the nonlinear parabolic system of equations (1.2) and (1.4)–(1.5). The main result is that if the initial conditions $X_{\text{in}}(r)$ and $Y_{\text{in}}(r)$ are non-negative and if A and B both obey certain conditions, then there is a non-negative pair $(X(r, t), Y(r, t))$ of solutions of the system defined for $0 \le r \le 1$ and $0 \le t < \infty$. These solutions are infinitely-differentiable functions of both r and t on $(0, 1) \times (0, \infty)$.

For much of this paper we shall be particularly interested in the case where A and B are uniformly distributed and time-invariant so that

$$A(r, t) \equiv A_0 > 0 \qquad B(r, t) \equiv B_0 > 0 \qquad \text{for } 0 \le r \le 1,\ t \ge 0. \tag{2.1}$$

However, in this section we shall only require the following:

(i) $A(r, t) = A(r) > 0$ and $B(r, t) = B(r) \ge 0$ for $0 \le r \le 1$ and $t \ge 0$.

(ii) $A(r)$ and $B(r)$ are continuous on $[0, 1]$ and infinitely often differentiable on $(0, 1)$.

(iii) $A(0) = A(1) = A_0$ and $B(0) = B(1) = B_0$.

To treat these equations it is convenient to introduce new variables which obey homogeneous boundary conditions.

Let

$$\begin{aligned} x(r, t) &= X(r, t) - A_0 \\ y(r, t) &= Y(r, t) - B(r)/A_0. \end{aligned} \tag{2.2}$$

Then (1.2) becomes

$$\begin{aligned} \frac{\partial x}{\partial t} &= D_1 \frac{\partial^2 x}{\partial r^2} + [B(r) - 1]x + A_0^2 y + h(x, y) + [A(r) - A_0] \\ \frac{\partial y}{\partial t} &= D_2 \frac{\partial^2 y}{\partial r^2} - B(r)x - A_0^2 y - h(x, y) + b(r) \end{aligned} \tag{2.3}$$

where

$$h(x, y) = \frac{B(r)}{A_0^2} x^2 + xy(2A_0 + x) \qquad b(r) = \frac{D_2}{A_0} \frac{\mathrm{d}^2 B}{\mathrm{d}r^2}(r). \tag{2.4}$$

The boundary and initial conditions are

$$x(0, t) = x(1, t) = y(0, t) = y(1, t) = 0 \quad t \geq 0 \tag{2.5}$$

and

$$\begin{aligned} x(r, 0) &= x_0(r) = X_{\text{in}}(r) - A_0 \\ y(r, 0) &= y_0(r) = Y_{\text{in}}(r) - B(r)/A_0. \end{aligned} \quad 0 \leq r \leq 1 \tag{2.6}$$

If $w(r, t) = x(r, t) + y(r, t)$ then the equation for w is linear. Upon eliminating x from (2.3) in favor of w one gets

$$\begin{aligned} \frac{\partial w}{\partial t} &= D_1 \frac{\partial^2 w}{\partial r^2} + (D_2 - D_1) \frac{\partial^2 y}{\partial r^2} - w + y + [A(r) - A_0] + b(r) \\ \frac{\partial y}{\partial t} &= D_2 \frac{\partial^2 y}{\partial r^2} - B(r) w + [B(r) - A_0^2] y - g(w, y) + b(r) \end{aligned} \tag{2.7}$$

where

$$g(w, y) = (w - y)^2 B(r)/A_0 + (w - y + A_0)^2 y - A_0^2 y \tag{2.8}$$

w obeys the initial and boundary conditions

$$w(r, 0) = w_0(r) = x_0(r) + y_0(r) \quad 0 \leq r \leq 1 \tag{2.9}$$

$$w(0, t) = w(1, t) = 0 \qquad \text{for } t \geq 0. \tag{2.10}$$

To prove our results, we need to introduce some function spaces. $L^2(0, 1)$ is the usual Hilbert space of real-valued Lebesgue integrable functions defined on [0, 1]. The inner product is given by

$$(u, v) = \int_0^1 u(r)v(r)\,\mathrm{d}r$$

and the norm on $L^2(0, 1)$ is

$$\|u\|_2 = (u, u)^{1/2}.$$

For integral m, $C^m[0, 1]$ is the set of real-valued functions on [0, 1] which are continuously m-times differentiable on [0, 1]. It is a Banach space under the norm

$$\|u\|_m = \sum_{k=0}^{m} \max_{0 \leq r \leq 1} \left| \frac{\mathrm{d}^k u}{\mathrm{d}r^k}(r) \right|.$$

Finally $H_0^1(0, 1)$ is the Hilbert space obtained by completing the subspace $C_0^1[0, 1]$ of all functions in $C^1[0, 1]$ which obey $u(0) = u(1) = 0$ with respect to the inner product

$$((u, v)) = \int_0^1 \left[\frac{\mathrm{d}u}{\mathrm{d}r} \frac{\mathrm{d}v}{\mathrm{d}r} + uv \right] \mathrm{d}r.$$

We shall write $\|u\|_{1,2} = ((u, u))^{1/2}$.

THEOREM 2.1. *There exists $T > 0$ such that* (2.3)–(2.4) *has a solution* $(x(r, t), y(r, t))$ *defined on* $[0, 1] \times [0, T)$ *and obeying the conditions* (2.5)–(2.6). *The functions x, y are infinitely differentiable functions on* $(0, 1) \times (0, T)$.

Proof: The equations may be written

$$\frac{\partial x}{\partial t} - D_1 \frac{\partial^2 x}{\partial r^2} - [B(r) - 1]x - A_0^2 y = h(x, y) + A(r) - A_0,$$

$$\frac{\partial y}{\partial t} - D_2 \frac{\partial^2 y}{\partial r^2} + B(r)x + A_0^2 y = -h(x, y) + b(r).$$

Let $G(r, s, t, \tau)$ be the Green's function for the linear parabolic operator given by the left-hand side of this expression and the boundary conditions. Then this system may be rewritten as a nonlinear system of integral equations

$$\begin{bmatrix} x(r, t) \\ y(r, t) \end{bmatrix} = \int_0^1 G(r, s, t, 0) \begin{bmatrix} x_0(s) \\ y_0(s) \end{bmatrix} ds + \int_0^t \int_0^1 G(r, s, t, \tau) \times \begin{bmatrix} h(x(s, \tau), y(s, \tau)) + A(s) - A_0 \\ -h(x(s, \tau), y(s, \tau)) + b(s) \end{bmatrix} ds\, d\tau. \quad (2.11)$$

This Green's function is a 2×2 matrix-valued function and has the property that for each $0 \leq \tau < t$, the linear operator defined by

$$\mathscr{G}(t, \tau) \begin{bmatrix} x(r) \\ y(r) \end{bmatrix} = \int_0^1 G(r, s, t, \tau) \begin{bmatrix} x(s) \\ y(s) \end{bmatrix} ds \quad (2.12)$$

is a compact map of $C[0, 1] \times C[0, 1]$ into $C[0, 1] \times C[0, 1]$.

Using successive approximations, one can now prove that for sufficiently small $T > 0$ this equation has a solution $\begin{bmatrix} x(r, t) \\ y(r, t) \end{bmatrix}$ defined on $[0, 1] \times [0, T)$. x and y are continuous functions. Now the usual regularity methods of parabolic equations imply that x and y are infinitely often differentiable.

Letting

$$X(r, t) = A_0 + x(r, t)$$
$$Y(r, t) = B(r)/A_0 + y(r, t)$$

one gets a solution of (1.2) and (1.4)–(1.5) defined on $[0, 1] \times [0, T)$.

THEOREM 2.2. *Suppose* $(X(r, t), Y(r, t))$ *is a solution of* (1.2) *and* (1.4)–(1.5) *for* $0 \leq t \leq \tau$ *and that* $X_{\text{in}}(r) \geq 0$ *and* $Y_{\text{in}}(r) \geq 0$. Then

$$X(r, t) \geq 0, \qquad Y(r, t) \geq 0 \quad \text{for } 0 \leq r \leq 1,\ 0 \leq t \leq \tau.$$

The proof of this is sketched in the appendix on the maximum principle.

We would now like to show that one can take $T = +\infty$ in Theorem 2.1. In other words to show that the solutions of the equations can be continued for all time without "blowing up". To do this one needs to use results about "weak" solutions of (2.7)–(2.10), and the fact that they obey the *a priori* bounds given in the following lemma.

In the notation of Lions (1969) we are looking for solutions of (2.7)–(2.10) in the set

$$X = \{u = (w, y): u \in L^2[0, T; H_0^1(0, 1) \times H_0^1(0, 1)] \text{ and } \mathrm{d}u/\mathrm{d}t \in L^2[0, T; H_0^{-1}(0, 1) \times H_0^{-1}(0, 1)]\}.$$

Let

$$K = \{(w, y): w \in H_0^1(0, 1), y \in H_0^1(0, 1), y(r) \geq -B(r)/A_0, w(r) \geq -A_0 + y(r)\}.$$

We shall be particularly interested in solutions $[w(t), y(t)]$ which lie in K.

A weak solution of the system (2.7)–(2.10) on the interval $(0, \tau)$ is a pair of functions (w, y) in X obeying

$$\frac{\mathrm{d}}{\mathrm{d}t}\{(w(t), \varphi) + (y(t), \psi)\} + a(w, y, \varphi, \psi) = (A(r) - A_0, \varphi) + (b(r), \varphi + \psi) \quad \text{for } 0 < t < T$$

and

$$(w(0), \varphi) = (x_0 + y_0, \varphi)$$
$$(y(0), \psi) = (y_0, \psi)$$

for all φ, ψ in $C_0^\infty(0, 1)$.

Here

$$a(w, y, \varphi, \psi) = D_1 \int_0^1 \left(\frac{\partial w}{\partial r} - \frac{\partial y}{\partial r}\right)\frac{\partial \varphi}{\partial r}\,\mathrm{d}r + D_2 \int_0^1 \frac{\partial y}{\partial r}\left(\frac{\partial \varphi}{\partial r} + \frac{\partial \psi}{\partial r}\right)\mathrm{d}r + \int_0^1 w[\varphi + B(r)\psi]\,\mathrm{d}r + \int_0^1 [A_0^2\psi - B(r)\psi - \varphi]y(r)\,\mathrm{d}r + \int_0^1 g(w, y)\psi\,\mathrm{d}r.$$

LEMMA. *Suppose $(w(t), y(t))$ is a weak solution of (2.7)–(2.10) on $(0, \tau)$ such that $(w(t), y(t))$ is in K for almost all t. Then there are positive constants α, β and constants C_1, C_2, C_3 such that*

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}[\alpha\|w\|_2^2 + \beta\|y\|_2^2] \leq C_1\|w\|_2^2 + C_2\|y\|_2^2 + C_3. \tag{2.13}$$

Proof: From (2.7)–(2.8) one has

$$\int_0^1 \frac{\partial w}{\partial t} w\,\mathrm{d}r = -D_1 \int_0^1 \left(\frac{\partial w}{\partial r}\right)^2 \mathrm{d}r + (D_1 - D_2)\int_0^1 \frac{\partial y}{\partial r}\frac{\partial w}{\partial r}\,\mathrm{d}r + \int_0^1 [y - w + b(r) + A(r) - A_0]w\,\mathrm{d}r$$

and

$$\int_0^1 \frac{\partial y}{\partial t} y \, \mathrm{d}r = -D_2 \int_0^1 \left(\frac{\partial y}{\partial r}\right)^2 \mathrm{d}r - \int_0^1 [Bw + (B - A_0^2)y + g(y, w) + b(r)]y \, \mathrm{d}r.$$

Thus

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}&[\alpha\|w\|_2^2 + \beta\|y\|_2^2] \\ &= \alpha \int_0^1 \frac{\partial w}{\partial t} w \, \mathrm{d}r + \beta \int_0^1 \frac{\partial y}{\partial t} y \, \mathrm{d}r \\ &= -\alpha D_1 \int_0^1 \left(\frac{\partial w}{\partial r}\right)^2 \mathrm{d}r - \alpha(D_2 - D_1) \int_0^1 \frac{\partial y}{\partial r}\frac{\partial w}{\partial r} \mathrm{d}r - \beta D_2 \int_0^1 \left(\frac{\partial y}{\partial r}\right)^2 \mathrm{d}r \\ &\quad + \int_0^1 \{(\alpha - \beta B)wy - \alpha w^2 - \beta y^2[(B - A_0^2) + (w - y + A_0)^2]\} \, \mathrm{d}r \\ &\quad + \int_0^1 [A(r) - A_0]w \, \mathrm{d}r - \frac{\beta B}{A_0}\int_0^1 (w - y)^2 y \, \mathrm{d}r + \int_0^1 b(r)(w + y) \, \mathrm{d}r.\end{aligned}$$

The first part of the right-hand side may be written as

$$I_1 = -\alpha D_1 \left[\int_0^1 \left(\frac{\partial w}{\partial r} - \tfrac{1}{2}(\gamma - 1)\frac{\partial y}{\partial r}\right)^2 \mathrm{d}r + \left(\frac{\beta\gamma}{\alpha} - \tfrac{1}{4}(\gamma - 1)^2\right)\int_0^1 \left(\frac{\partial y}{\partial r}\right)^2 \mathrm{d}r\right].$$

Here $\gamma = D_2/D_1$. Choose $\alpha > 0$ and β so that

$$\left[\beta - \frac{\alpha}{4\gamma}(\gamma - 1)^2\right] = \frac{\epsilon}{\gamma D_1} > 0. \tag{2.14}$$

Then

$$I_1 \leq -\epsilon \int_0^1 \left(\frac{\partial y}{\partial r}\right)^2 \mathrm{d}r \leq 0.$$

Let

$$I_2 = \int_0^1 \{(\alpha - \beta B)wy - \alpha w^2 - \beta y^2[(B - A_0)^2 + (w - y + A_0)^2 - A_0^2]\} \, \mathrm{d}r.$$

Then

$$I_2 \leq |\alpha - \beta B| \; \|w\|_2\|y\|_2 - \alpha\|w\|_2^2 + \beta(2A_0B - B^2)\|y\|_2^2$$

using Schwarz's inequality

$$\leq (\tfrac{1}{2}|\alpha - \beta B| - \alpha)\|w\|_2^2 + [\beta(2A_0B - B^2) + \tfrac{1}{2}|\alpha - \beta B|]\|y\|_2^2.$$

Similarly one has from Schwarz's inequality that

$$\int_0^1 [A(r) - A_0 + b(r)]w \, \mathrm{d}r \leq \|A(r) - A_0 + b(r)\|_2\|w\|_2$$

$$\int_0^1 b(r)y \, \mathrm{d}r \leq \|b(r)\|_2\|y\|_2$$

and finally since $y(r) \geq -B/A_0$ one has

$$-\frac{\beta B}{A_0}\int_0^1 (w-y)^2 y \,\mathrm{d}r \leq \frac{\beta B^2}{A_0^2}\int_0^1 (w-y)^2 \,\mathrm{d}r \leq \frac{2\beta B^2}{A_0^2}[\|w\|_2^2 + \|y\|_2^2].$$

Adding these inequalities one finds that there are constants k_1, k_2, k_3, k_4 such that

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}[\alpha\|w\|_2^2 + \beta\|y\|_2^2] \leq k_1\|w\|_2^2 + k_2\|y\|_2^2 + k_3\|w\|_2 + k_4\|y\|_2$$

when α, β are chosen to obey (2.14). This implies (2.13) holds.

COROLLARY 1. *Under the above assumptions on w, y, there exist constants K, K_0 and μ such that*

$$\|w(t)\|_2^2 \leq K\,\mathrm{e}^{\mu t} + K_0 \quad \textit{and} \quad \|y(t)\|_2^2 \leq K\,\mathrm{e}^{\mu t} + K_0. \tag{2.15}$$

Proof: Let $u(t) = \alpha\|w(t)\|_2^2 + \beta\|y(t)\|_2^2$ where α, β as in the lemma. Then (2.13) may be written

$$\frac{\mathrm{d}u}{\mathrm{d}t} \leq \mu u(t) + C_3 \quad \text{with} \quad u(0) = \alpha\|w_0\|_2^2 + \beta\|y_0\|_2^2.$$

Thus

$$u(t) \leq \frac{C_3}{\mu}(\mathrm{e}^{\mu t} - 1) + u(0)\,\mathrm{e}^{\mu t}$$

and so (2.15) holds.

COROLLARY 2. *Under the above assumptions on (w, y), there exists a constant c, depending on τ, such that*

$$\int_0^\tau \|w(t)\|_{1,2}^2 \,\mathrm{d}t \leq c \quad \text{and} \quad \int_0^\tau \|y(t)\|_{1,2}^2 \,\mathrm{d}t \leq c.$$

Proof: Returning to the proof of the previous lemma, one sees that instead of (2.13) one could have written

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}[\|w(t)\|_2^2 + \|y(t)\|_2^2] + \epsilon\|y(t)\|_{1,2}^2 \leq C_1\|w\|_2^2 + C_2\|y\|_2^2 + C_3.$$

Integrating this from 0 to τ, one gets

$$\epsilon\int_0^\tau \|y(t)\|_{1,2}^2 \,\mathrm{d}t \leq C_1\int_0^\tau \|w(t)\|_2^2 \,\mathrm{d}t + C_2\int_0^\tau \|y(t)\|_2^2 \,\mathrm{d}t - \tfrac{1}{2}[\|w(\tau)\|_2^2 + \|y(\tau)\|_2^2 - \|w(0)\|_2^2 - \|y(0)\|_2^2] + C_3\tau.$$

Using (2.15) one gets the desired result for y, as $\epsilon > 0$.

Making use of the other term in the expression for I_1 one gets the other estimate.

The two *a priori* bounds given in these corollaries are crucial to proving our main result. One can show by using the Sobolev imbedding theorems and the integral formulation (2.11) of these equations that a weak solution is in fact a classical solution of these equations and thus from Theorem 2.2 one has that if $(w(0), y(0))$ is in K then so is $(w(t), y(t))$ for $0 < t < \tau$ whenever (w, y) is a solution of (2.7)–(2.10) for $0 < t < \tau$. Making use of all these results, one gets the following theorem:

THEOREM 2.3. *Suppose* $X_{\text{in}}(r) \geq 0$ *and* $Y_{\text{in}}(r) \geq 0$, *then in Theorem 2.1,* $T = \infty$.

Proof: If $X_{\text{in}}(r) \geq 0$ and $Y_{\text{in}}(r) \geq 0$ then $(w(0), y(0))$ is in K.

Using the *a priori* bounds given in Corollaries 1 and 2 to the previous lemma one can use the Faedo–Galerkin method (cf. Lions, 1969) to prove there is a weak solution on $[0, \tau]$ for any $\tau > 0$.

This weak solution is a classical solution and thus one has the result.

An immediate consequence of this theorem is the fact that the solutions of (2.7)–(2.10) form a nonlinear semigroup on the set K. That is if $(w(r, t), y(r, t))$ is the solution of (2.7)–(2.10) obeying $w(r, 0) = w_0(r)$, $y(r, 0) = y_0(r)$ and if one defines $T(t)$: $K \to K$ by

$$T(t)(w_0, y_0) = (w(r, t), y(r, t)).$$

Then

$$T(0) = I \quad \text{and} \quad T(t + s) = T(t)T(s) \quad \text{for } t, s \geq 0.$$

The only place in this analysis where we have made essential use of the fact that we are working in a 1-dimensional medium is in the proof that weak solutions are in fact classical solutions. One would expect a similar analysis to hold if one assumed the reactions occurred in a circular region, inside a sphere or in any bounded open set which has a smooth boundary in 2 or 3 dimensions. When one has other nonlinearities (different reaction schemes) one would not expect in general, to get a result such as Theorem 2.2. In such cases, one would have to assume *a priori* that the chemical concentrations X, Y are constrained to be non-negative and then replace (1.2) by a corresponding "variational inequality". Mathematical problems of this type are treated in Lions (1969) Chapter 2.9.

3. Steady State Solutions. A particularly important class of solutions of this system are the non-negative steady state solutions. Such solutions for these equations play a role analogous to the role of critical points in the theory of ordinary differential equations. They are time invariant solutions of the equations and just as for ordinary differential equations one often finds that the system evolves as $t \to \infty$ to such solutions.

The steady state solutions obey the equations obtained from (1.2) upon putting $\partial X/\partial t = 0$ and $\partial Y/\partial t = 0$, viz;

$$\begin{aligned} D_1 \frac{d^2X}{dr^2} - (B+1)X + X^2Y &= -A(r) \\ D_2 \frac{d^2Y}{dr^2} + BX - X^2Y &= 0 \end{aligned} \tag{3.1}$$

and the boundary conditions are

$$X(0) = X(1) = A_0 \qquad Y(0) = Y(1) = B_0/A_0. \tag{3.2}$$

For the remainder of this paper we shall be interested in obtaining rather specific information about the solutions of these equations so we shall assume:

(A) The function $A(r)$ is given by

$$A(r) = A_0 \frac{\cosh[2\alpha(r - \frac{1}{2})]}{\cosh \alpha} \quad \alpha \geq 0 \tag{3.3}$$

and

(B) $$B(r) \equiv B \quad \text{for } 0 \leq r \leq 1. \tag{3.4}$$

Because of assumption (B) we shall write B in place of B_0 henceforth. When A is defined by (3.3) one sees that

(i) $0 < \dfrac{A_0}{\cosh \alpha} \leq A(r) \leq A_0$ for $0 \leq r \leq 1$.

(ii) $A(r)$ is a convex function of r.

(iii) When $\alpha > 0$, $A(r)$ obeys the equation

$$D_A \frac{d^2A}{dr^2} - A = 0$$

with $\alpha = \frac{1}{2}D_A^{-1/2}$ and $A(0) = A(1) = A_0$.

(iv) When $\alpha = 0$, $A(r) \equiv A_0$.

In this section we shall be especially interested in a particular family of solutions of (3.1)–(3.4), namely those which may be connected to the unique solution (X, Y) of the system (3.1)–(3.4) with $B = 0$. We shall show that for all $B > 0$, such solutions obey $X(r) \geq 0$ and $Y(r) \geq 0$.

First we shall prove a general result about non-negative solutions.

THEOREM 3.1. *Suppose* $B > 0$, A *is given by* (3.3) *with* $\alpha > 0$ *and* $(X(r), Y(r))$ *is a non-negative solution of* (3.1)–(3.2). Then

$$X(r) \le A_0 + \frac{D_2 B}{D_1 A_0} + \frac{D_A}{D_1}[A_0 - A(r)]$$

$$Y(r) \le \frac{B}{A_0} + \frac{D_1}{D_2} A_0 + \frac{D_A}{D_2}[A_0 - A(r)].$$

Proof: Let $Z(r) = D_1 X(r) + D_2 Y(r) + D_A A(r)$. Then from the equations and the assumptions of Theorem 3.1 one gets

$$Z'' = X \ge 0 \quad \text{and} \quad Z(0) = Z(1) = (D_1 + D_A)A_0 + D_2 B/A_0.$$

Here, and henceforth, the primes represent differentiation with respect to r. The maximum principle implies

$$Z(r) \le (D_1 + D_A)A_0 + D_2 B/A_0$$

or

$$0 \le D_1 X(r) + D_2 Y(r) \le D_1 A_0 + D_2 B/A_0 + D_A[A_0 - A(r)].$$

Thus

$$X(r) \le A_0 + D_2 B/D_1 A_0 + (D_A/D_1)[A_0 - A(r)].$$

Similarly

$$Y(r) \le \frac{B}{A_0} + \frac{D_1}{D_2} A_0 + \frac{D_A}{D_2}[A_0 - A(r)].$$

COROLLARY. *Suppose* $B \ge 0$, $A(r) \equiv A_0$ *and* $(X(r), Y(r))$ *is a non-negative solution of* (3.1)–(3.2). *Then*

$$\left.\begin{aligned} X(r) &\le A_0 + \frac{A_0}{2D_1} r(1 - r) + \frac{D_2 B}{D_1 A_0} \\ Y(r) &\le \frac{B}{A_0} + \frac{A_0}{2D_2} r(1 - r) + \frac{D_1 A_0}{D_2}. \end{aligned}\right\} \quad \text{for } 0 \le r \le 1$$

Proof: This time take

$$Z(r) = D_1 X(r) + D_2 Y(r) - \frac{A_0}{2} r(1 - r).$$

Continuing just as in the proof of the theorem, one gets the result.

It is worth noting that the function Z introduced in these proofs is always convex on [0, 1].

We would now like to construct some non-negative solutions of (3.1)–(3.4) and to do this one first needs the following lemma.

LEMMA 1. *When* $B = 0$, *there is a unique solution* $(X(r), 0)$ of (3.1)–(3.4) *and* $0 < X(r) \le A_0$ *for* $0 \le r \le 1$.

Proof: When $B = 0$, one has

$$D_2 Y'' - X^2 Y = 0$$

subject to

$$Y(0) = Y(1) = 0.$$

From the maximum principle, the only solution of this is

$$Y(r) = 0.$$

Now

$$D_1 X'' - X = -A(r) \qquad X(0) = X(1) = A_0.$$

This is an inhomogeneous linear equation with a unique solution. Since $0 < A(r) \le A_0$, one gets from the maximum principle that

$$0 < X(r) \le A_0.$$

THEOREM 3.2. *There exists* $\delta > 0$ *such that for* $0 \le B < \delta$, *there is a non-negative solution* (X, Y) *of* (3.1)–(3.4).

Proof: Let

$$x(r) = A_0 - X(r) \qquad y(r) = Y(r) - B/A_0.$$

Then

$$\begin{aligned} D_1 x'' + (B - 1)x - A_0^2 y &= A(r) - A_0 + k(x, y) \\ D_2 y'' + Bx - A_0^2 y &= k(x, y). \end{aligned} \tag{3.5}$$

with

$$x(0) = x(1) = 0 \qquad y(0) = y(1) = 0$$

and

$$k(x, y) = (B/A_0^2)x^2 + xy(x - 2A_0).$$

When $B = 0$, the left-hand side of (3.5) is invertible and so using usual continuation arguments (or the implicit function theorem), (3.5) has a unique solution $(X_B(r), Y_B(r))$ for $0 \le B \le \delta$ while

$$X_B(r) \to X_0(r) \quad \text{and} \quad Y_B(r) \to Y_0(r) \quad \text{in } C[0, 1] \text{ as } B \to 0.$$

Using the maximum principle, one can show these solutions are non-negative (see Appendix 2).

This result may be strengthened somewhat by the following.

THEOREM 3.3. *There exists* $B_1 > 0$ *such that for* $0 < B < B_1$, *there is at most one non-negative solution of* (3.1)–(3.4).

Proof: Suppose the theorem is false. Then there is a sequence $\{B_k\}$ such that B_k converges to 0 and for each k, there are at least 2 different solutions of (3.1)–(3.4). Suppose (X_k, Y_k) and $(\tilde{X}_k, \tilde{Y}_k)$ are such solutions. These solutions obey the *a priori* bounds given in Theorems 3.1 and 3.2, so there is a limit point for each of these sequences in $C^2[0, 1] \times C^2[0, 1]$ (say). Suppose the limit points are (X, Y) and $(\tilde{X}, \tilde{Y})$.

These limit points must both be solutions of (3.1)–(3.4) with $B = 0$. If $X \neq \tilde{X}$ or $Y \neq \tilde{Y}$ on $[0, 1]$, this contradicts the preceding lemma.

If $X = \tilde{X}$ and $Y = \tilde{Y}$, then one has that $B = 0$ is a bifurcation point for the equation (3.1)–(3.4) as in any neighborhood $(X, Y, 0)$ in $C^2[0, 1] \times C^2[0, 1] \times [0, \infty)$ there is more than one solution of (3.1)–(3.4). In the next section, we shall show this is impossible. Thus the theorem holds by contradiction.

Let $\mathscr{S} = \{(X, Y, B): (X, Y)$ is a solution of (3.1)–(3.4) for the corresponding $B, B \geqslant 0\}$. Then

$$\mathscr{S} \subset C^2[0, 1] \times C^2[0, 1] \times [0, \infty).$$

$\mathscr{S}$ may be considered as the set of all solutions of (3.1)–(3.4) for $B \geq 0$, and it is a closed subset of $C^2[0, 1] \times C^2[0, 1] \times [0, \infty)$.

Let $\mathscr{T}$ be a closed, connected subset of $\mathscr{S}$ in $C^2[0, 1] \times C^2[0, 1] \times [0, \infty)$. Then $\mathscr{T}$ will be a "tree" of solutions of (3.1)–(3.4) as it consists of many "branches". Let $\mathscr{T}_0$ be the tree containing $(X_0, Y_0, 0)$.

THEOREM 3.4. *If* (X_B, Y_B, B) *is in* $\mathscr{T}_0$ *then*

$$X_B(r) \geq 0 \quad \text{and} \quad Y_B(r) \geq 0 \quad \text{for } 0 \leq r \leq 1.$$

The proof of this is in the appendix on the maximum principle.

This theorem essentially says that any solution of (3.1)–(3.4) that is connected by branches of solutions to the unique solution at $B = 0$ is non-negative.

When $\alpha = 0$, the functions

$$X_B(r) \equiv A_0 \qquad Y_B(r) \equiv B/A_0 \quad 0 \leq r \leq 1$$

are solutions for all $B \geq 0$.

As we shall see in the next section, there are many branches of new solutions which bifurcate from this "thermodynamic" branch. Theorem 3.4 says that all solutions on these branches (and on any branches obtained by repeated bifurcation from the "thermodynamic" branch) are non-negative. One also sees that when $\alpha = 0$ there are steady state solutions of (3.1)–(3.4) for all $B \geq 0$.

It would be particularly interesting to know if, for this equation, $\mathscr{T}_0 = \mathscr{S}$.

When $\alpha > 0$, one may obtain formal power series solutions of (3.1)–(3.4) in terms of the parameter α. The first few terms of these series often give very good approximations to solutions that have been found numerically.

Let

$$Z(r) = X(r) + (D_2/D_1)Y(r).$$

Then

$$D_1 Z'' - X = -A(r)$$

and

$$Z(0) = Z(1) = A_0 + \frac{D_2 B}{D_1 A_0}.$$

Write

$$A(r) = A_0 + \alpha^2 a(\alpha, r)$$
$$X(r) = A_0 + \alpha^2 x(\alpha, r)$$

and

$$Z(r) = A_0 + \frac{D_2 B}{D_1 A_0} + \alpha^2 z(\alpha, r).$$

Then

$$x(\alpha, 0) = x(\alpha, 1) = z(\alpha, 0) = z(\alpha, 1) = 0$$

and

$$a(\alpha, r) = \frac{A_0}{\alpha^2}\left(\frac{\cosh 2\alpha(r - \frac{1}{2})}{\cosh \alpha} - 1\right) \simeq \frac{-A_0}{2\cosh \alpha}[1 - 4(r - \tfrac{1}{2})^2]$$

for α near 0.

The equations for x, z are

$$D_1 x'' + [(2\gamma^2 - 1)B - \gamma A_0^2 - 1]x + \gamma A_0^2 z = -a(\alpha, r) + \frac{1}{\alpha^2} h(x, z)$$

$$D_1 z'' - x = -a(\alpha, r)$$

where

$$\gamma = \frac{D_1}{D_2} \quad \text{and} \quad h(x, z) = \alpha^4 \gamma x[(z - x)(2A_0 + \gamma\alpha^2 x)] + \frac{\alpha^4 B}{A_0} x^2.$$

If one neglects the terms involving the derivatives, one gets

$$x(\alpha, r) = a(\alpha, r) \tag{3.6}$$

and

$$z(\alpha, r) = \left(1 - \frac{(2\gamma^2 - 1)B}{\gamma A_0^2}\right) a(\alpha, r). \tag{3.7}$$

More generally, if one writes

$$X(r) = \sum_{k=0}^{\infty} \alpha^{2k} X_k(r) \quad \text{and} \quad Z(r) = \sum_{k=0}^{\infty} \alpha^{2k} Z_k(r)$$

and substitutes into the original equation one gets a recursive system of linear equations for the functions (X_k, Z_k), $k \geq 1$. Obviously $X_0(r) \equiv A_0$ and $Z_0(r) \equiv A_0 + D_2B/D_1A_0$, are the first terms in this series.

Finally, one can use the maximum principle to obtain more detailed information about the solutions of (3.1)–(3.4). For example one can easily prove the following result.

THEOREM. *Suppose* (X, Y) *is a solution* of (3.1)–(3.4) *and* $0 \leq X(r) \leq A_0$ *for* $0 \leq r \leq 1$, *then* $Y(r) \geq B/A_0$ *for* $0 \leq r \leq 1$.

4. Linear Stability Analysis. In this section we shall study the stability of some steady state solutions of (3.1)–(3.4). To do this, we shall perform a linear stability analysis of these solutions. One may show that for these equations, linear stability or instability implies the actual stability or instability of the solutions. In particular we shall show that there is a critical value B_c of B such that for $B > B_c$ the uniform steady state solutions (1.3) of (3.1)–(3.4) are unstable. Using the results of this section we will be able to find the new stable steady state solutions of these equations.

The linear stability equations for a solution (X_0, Y_0, B) of the steady state equations are obtained by linearizing the equations for

$$u(r, t) = X(r, t) - X_0(r) \qquad v(r, t) = Y(r, t) - Y_0(r)$$

about $u = v = 0$. The resulting equations give a linear parabolic system and to analyze its asymptotic behavior in time it suffices to find the eigenvalues λ_m and the eigenfunctions (u_m, v_m) of

$$\begin{aligned} D_1 \frac{d^2u}{dr^2} - [(B + 1) - 2X_0(r)Y_0(r)]u + X_0^2(r)v &= \lambda u \\ D_2 \frac{d^2y}{dr^2} + [B - 2X_0(r)Y_0(r)]u - X_0^2(r)v &= \lambda v \end{aligned} \tag{4.1}$$

subject to

$$u(0) = u(1) = v(0) = v(1) = 0. \tag{4.2}$$

When all the eigenvalues λ_m of (4.1)–(4.2) obey

$$\text{Re}\,\lambda_m < 0 \quad m = 1, 2, \ldots$$

then the steady state solution (X_0, Y_0, B) is said to be linearly stable.

If for some m, one has Re $\lambda_m > 0$, then the solution (X_0, Y_0, B) is linearly unstable.

The eigenvalues λ_m and the eigenfunctions (u_m, v_m) of (4.1)–(4.3) must, in general, be calculated numerically. When $\alpha = 0$, and $X_0 = A_0$, $Y_0 = B/A_0$

one can get explicit formulae for the eigenvalues and eigenfunctions. In this case, (4.1) becomes

$$D_1u'' + (B - 1)u + A_0^2v = \lambda u \qquad D_2v'' - Bu - A_0^2v = \lambda v. \tag{4.3}$$

This is a linear system of equations with constant coefficients. Its eigenfunctions must have the form

$$\begin{pmatrix} u_m(r) \\ v_m(r) \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} e^{\nu r} \sin m\pi r.$$

Substituting these in (4.3)–(4.5) one finds $\nu = 0$ and the eigenvalues λ obey the *characteristic equation*

$$\lambda^2 + (\beta_m - \alpha_m)\lambda + A^2B - \alpha_m\beta_m = 0 \tag{4.4}$$

where $\alpha_m = B - 1 - m^2\pi^2D_1$, $\beta_m = A^2 + m^2\pi^2D_2$. (Here and in the rest of this section we shall omit the subscript on A_0).

The solutions of (4.4) are

$$\lambda_m^{\pm} = \tfrac{1}{2}\{\alpha_m - \beta_m \pm \sqrt{[(\alpha_m + \beta_m)^2 - 4A^2B]}\}. \tag{4.5}$$

From these expressions one gets the following results

(i) Re $\lambda_m^{\pm} \to -\infty$ as $m \to +\infty$.

(ii) A real eigenvalue λ_m^{+} has positive real part whenever

$$B > 1 + \frac{D_1}{D_2}A^2 + \frac{A^2}{D_2m^2\pi^2} + D_1m^2\pi^2. \tag{4.6}$$

(iii) The eigenvalues $\lambda_m^{\pm}$ are complex whenever

$(\beta_m + \alpha_m)^2 - 4A^2B < 0$ or $B^2 - 2(A^2 + \delta)B + (A^2 - \delta)^2 < 0$ where $\delta = 1 + m^2\pi^2(D_1 - D_2)$.

This only occurs if $\delta > 0$ and

$$(A - \sqrt{\delta})^2 < B < (A + \sqrt{\delta})^2. \tag{4.7}$$

In particular there are no complex eigenvalues if $D_2 - D_1 \geq 1/\pi^2$.

(iv) A complex eigenvalue λ_m^{+} (or λ_m^{-}) has positive real part provided (4.7) holds and

$$B > 1 + A^2 + m^2\pi^2(D_1 + D_2). \tag{4.8}$$

Combining (4.7) and (4.8) one has that there are such eigenvalues whenever $\delta > 0$ and

$$A^2 + 1 + m^2\pi^2(D_1 + D_2) < B < A^2 + 1 + m^2\pi^2(D_1 - D_2) + 2A\sqrt{[1 + m^2\pi^2(D_1 - D_2)]}.$$

Relation (4.7) may be rewritten as

$$m^4\pi^4(D_2 - D_1)^2 + 2(A^2 + B - 1)(D_2 - D_1)m^2\pi^2 + [(A^2 - B - 1)^2 - 4B] < 0. \quad (4.9)$$

Thus if $D_2 \neq D_1$, there can only be finitely many complex eigenvalues of this system.

However when $D_1 = D_2$, then either all the eigenvalues are complex or else they are all real as the first two terms in relation (4.9) vanish.

From (4.8) one sees that the solution $(A, B/A)$ of (3.1)–(3.4) (in the case where $A(r) \equiv A$) becomes linearly unstable through a real eigenvalue if $B > B_c$ where

$$B_c = \min_{\substack{m \geq 1 \\ m \text{ integer}}} \left[1 + \frac{D_1}{D_2} A^2 + \frac{A^2}{D_2 \pi^2 m^2} + D_1 \pi^2 m^2\right]. \quad (4.10)$$

The expression on the right-hand side of (4.6) is quadratic in m^2. When m is treated as a continuous variable this expression is minimized when

$$m^2 = \mu^2 = \frac{A}{\pi^2 (D_1 D_2)^{1/2}}. \quad (4.11)$$

Also

$$B_c \geq \left[1 + \left(\frac{D_1}{D_2}\right)^{1/2} A\right]^2. \quad (4.12)$$

The critical wave number m_c is the integer m which gives rise to B_c. m_c is either given by (4.11) or it is one of the two integers closest to μ. There could be two critical wave numbers, but this is a singular case as small changes in D_1, D_2 or A will select one of these numbers.

Depending on the values of D_1, D_2 and A, it is also possible that the solution $(A, B/A)$ of (3.1)–(3.4) first becomes unstable through a complex eigenvalue. Suppose $D_1 - D_2 > -1/\pi^2$ and let

$$B_1 = 1 + A^2 + \pi^2(D_1 + D_2)$$

and

$$D_2 < \frac{A}{\pi^2} \sqrt{[1 + \pi^2(D_1 - D_2)]}.$$

Then if $B_1 < B_c$, the first unstable eigenvalues are given by the complex conjugate pair $\lambda_1^{\pm}$.

In particular if $D_1 = D_2 = D$ then the first unstable eigenvalue is complex whenever

$$D < A/\pi^2.$$

To study the bifurcation of solutions of (3.1)–(3.4) from $(A, B/A)$ one needs to know the eigenfunctions corresponding to the eigenvalues with real part zero. If $\lambda_m^\pm = \pm i\omega_m$ where $\omega_m \neq 0$, the new bifurcating solutions are time-periodic solutions of (1.1). We shall make a detailed study of these in a subsequent paper. In this work we shall confine our attention to bifurcating steady state solutions and thus to eigenfunctions corresponding to a zero eigenvalue.

Such an eigenfunction has wave number m provided

$$\alpha_m \beta_m = A^2 B$$

i.e.,

$$m^4 D_1 D_2 - \frac{m^2}{\pi^2}[D_2(B-1) - D_1 A^2] + \frac{A^2}{\pi^4} = 0 \tag{4.13}$$

or

$$B_m = 1 + \frac{D_1}{D_2} A^2 + m^2 D_1 \pi^2 + \frac{A^2}{D_2 m^2 \pi^2}. \tag{4.14}$$

From this one notes that

$$B_m \geq \left[1 + \left(\frac{D_1}{D_2}\right)^{1/2} A\right]^2$$

so $B = 0$ can never be a bifurcation point. This substantiates the claim in the proof of Theorem 3.4.

The eigenvalue 0 is a simple eigenvalue of this system provided there do not exist two positive integers m_1, m_2 such that (4.13) may be written

$$D_1 D_2 (m^2 - m_1^2)(m^2 - m_2^2) = 0.$$

When m_1 is an integer solution of (4.12) this condition is equivalent to the condition that

$$\nu = \frac{1}{\pi^2}\left(\frac{B-1}{D_1} - \frac{A^2}{D_2}\right) - m_1^2$$

is not a square.

When $\lambda = 0$ is a simple eigenvalue of the system, the corresponding normalized eigenvector is

$$\begin{pmatrix} u_m(r) \\ v_m(r) \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin m\pi r \tag{4.15}$$

where

$$c_1^2 + c_2^2 = 2 \quad \text{and} \quad (D_1 m^2 \pi^2 - B_m + 1)c_1 - A^2 c_2 = 0.$$

Thus $c_1 = \sqrt{2}/\sqrt{(1 + \delta_m^2)}$ and $c_2 = \sqrt{2}\delta_m/\sqrt{(1 + \delta_m^2)}$ where

$$\delta_m = \frac{c_2}{c_1} = \frac{D_1 m^2 \pi^2 + 1 - B_m}{A^2}$$

If $m = m_c$ is the critical wave number and is approximated by (4.11) and B_m is approximated by (4.12) one sees that

$$\frac{c_2}{c_1} \simeq -\frac{1}{A}\left(\frac{D_1}{D_2}\right)^{1/2}\left[1 + A\left(\frac{D_1}{D_2}\right)^{1/2}\right] < 0.$$

One often writes (4.3) symbolically as

$$L_B \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix} \tag{4.16}$$

where L_B is a densely defined, closed linear operator on $L^2(0, 1) \times L^2(0, 1)$.

The adjoint L_B^* of L_B is the closure of the operator defined by

$$L_B^*: C_0^2(0, 1) \times C_0^2(0, 1) \to L^2(0, 1) \times L^2(0, 1)$$

where

$$L_B^* \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} D_1 u'' + (B - 1)u - Bv \\ D_2 v'' + A^2 u - A^2 v \end{pmatrix}$$

and $C_0^2(0, 1)$ is the set of functions which are twice continuously differentiable on (0, 1) and which obey

$$u(0) = u(1) = 0.$$

The eigenvalues of L_B^* are the same as those of L_B and if 0 is an eigenvalue of L_B, then the eigenfunction corresponding to the eigenvalue 0 of L_B^* is given by

$$\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} \sin m\pi r$$

where

$$d_1^2 + d_2^2 = 2 \quad \text{and} \quad -(D_2 m^2 \pi^2 + A^2) d_2 + A^2 d_1 = 0$$

$$\text{Thus } d_1 = \epsilon_m \frac{\sqrt{2}}{\sqrt{(1 + \epsilon_m^2)}} \qquad d_2 = \frac{\sqrt{2}}{\sqrt{(1 + \epsilon_m^2)}} \tag{4.17}$$

and

$$\epsilon_m = 1 + \frac{D_2 \pi^2}{A^2} m^2.$$

Finally one should note that the shape of the critical mode (4.15) depends crucially on the boundary conditions. If instead of prescribing the concentrations at the boundary, one prescribes zero fluxes then one would have

$$\begin{pmatrix} x(r) \\ y(r) \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \cos m\pi r.$$

Thus the bifurcating steady state solution would be qualitatively quite different; there is a macroscopic gradient across the system (Babloyantz and Hiernaux, 1975).

5. Bifurcation of Dissipative Structures. In the last section we showed that there is a critical value B_c of B with the property that when $B > B_c$, the homogeneous solution $(A, B/A)$ of (3.1)–(3.2) is linearly unstable. In this section we shall construct some other steady state solutions of the equations, some of which are stable for various ranges of B. These new solutions are not homogeneous, but instead have a number of well-defined maxima and minima. They arise mathematically as new branches of solutions of the steady state equations. They have been called dissipative structures as they can only occur in open systems operating far from thermodynamic equilibrium.

To construct these dissipative structures we shall use bifurcation theory. For a review of the subject see Stakgold (1971) or Sattinger (1973). We shall restrict our calculations in this section to the case where

$$A(r) \equiv A_0.$$

When $\alpha \neq 0$, [i.e., $A(r) \not\equiv A_0$] some interesting new phenomena arise, such as natural boundaries for the dissipative structure. These will be treated in Section 7.

Even in this analysis, one has a very surprising phenomena. Namely one gets qualitatively different results depending on whether the critical wave number m_c is even or odd.

To find these solutions one uses the steady state analogs of (2.3). These are

$$\begin{aligned} D_1 \frac{d^2x}{dr^2} + (B - 1)x + A_0^2 y &= -h(x, y) \\ D_2 \frac{d^2y}{dr^2} - Bx - A_0^2 y &= h(x, y) \end{aligned} \tag{5.1}$$

$$x(0) = x(1) = y(0) = y(1) = 0. \tag{5.2}$$

Note that from Theorem 3.1, if (x, y) is any solution of this system and if $B > 0$, then

$$X(r) = A_0 + x(r) \qquad Y(r) = B/A_0 + y(r) \tag{5.3}$$

is a positive solution of (3.1)–(3.3).

Equations (5.1)–(5.2) may be written

$$L_B \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -h(x, y) \\ h(x, y) \end{pmatrix} \tag{5.4}$$

where L_B is the linear operator defined in (4.16) and h is given by (2.4).

When 0 is not an eigenvalue of L_B, then L_B is invertible and (5.4) is equivalent to the nonlinear integral equation

$$\begin{aligned}\begin{pmatrix} x(r) \\ y(r) \end{pmatrix} &= \int_0^1 \begin{pmatrix} G_{11}(B, r, s) & G_{12}(B, r, s) \\ G_{21}(B, r, s) & G_{22}(B, r, s) \end{pmatrix} \begin{pmatrix} -h[x(s), y(s)] \\ h[x(s), y(s)] \end{pmatrix} ds \\ &= \int_0^1 \begin{pmatrix} [G_{12}(B, r, s) - G_{11}(B, r, s)]h[x(s), y(s)] \\ [G_{22}(B, r, s) - G_{21}(B, r, s)]h[x(s), y(s)] \end{pmatrix} ds. \end{aligned} \tag{5.5}$$

Here we are using vector notation and

$$G(B, r, s) = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}$$

is the matrix Green's function of L_B. From the theory of ordinary differential equations, the operator $G_B\colon C(0, 1) \times C(0, 1) \to C(0, 1) \times C(0, 1)$ defined by

$$G_B \begin{pmatrix} u \\ v \end{pmatrix} (r) = \int_0^1 \begin{pmatrix} G_{11}(B, r, s) & G_{12}(B, r, s) \\ G_{21}(B, r, s) & G_{22}(B, r, s) \end{pmatrix} \begin{pmatrix} u(s) \\ v(s) \end{pmatrix} ds$$

is a compact linear operator. It depends continuously (in fact analytically) on B for $B_m < B < B_{m+1}$ where m is a positive integer and B_m is given by (4.14), $B_0 = 0$.

The functions

$$x(r) \equiv 0, \qquad y(r) \equiv 0$$

are solutions of (5.4) for all values of B.

From a basic theorem in bifurcation, new branches of steady-state solutions can bifurcate from the solution (0, 0) only when

$$B = B_m \quad \text{for some integer } m \geq 1.$$

This is just a necessary condition, it is not a sufficient condition. To see whether there is bifurcation, one usually tries to calculate the new bifurcating solution.

We shall use a method similar to that of Sattinger (1973).

In this method one assumes both the solution and the parameter B have a power series expansion in a new variable ϵ and the method may be justified in a manner similar to his theorem (3.4.1).

The calculation will be done for B close to any one of the possible bifurcation values B_m, given by (4.14), and we will assume the corresponding zero eigenvalue is simple. However, we shall be particularly interested in the first bifurcating solution, in which case, $m = m_c$ is the critical number, B is near its critical B_c and m_c, B_c can be approximated by (4.11)–(4.12).

To calculate these bifurcating solutions one writes

$$\begin{pmatrix} x(r) \\ y(r) \end{pmatrix} = \epsilon \begin{pmatrix} x_0(r) \\ y_0(r) \end{pmatrix} + \epsilon^2 \begin{pmatrix} x_1(r) \\ y_1(r) \end{pmatrix} + \epsilon^3 \begin{pmatrix} x_2(r) \\ y_2(r) \end{pmatrix} + \cdots \tag{5.6}$$

and

$$B - B_m = \epsilon\gamma_1 + \epsilon^2\gamma_2 + \cdots. \tag{5.7}$$

Substitute these expressions in (5.1) which may be rewritten as

$$L_{B_m}\begin{pmatrix} x \\ y \end{pmatrix} + (B - B_m)\begin{pmatrix} x \\ -x \end{pmatrix} = \begin{pmatrix} -h(x, y) \\ h(x, y) \end{pmatrix}. \tag{5.8}$$

Upon identifying terms with equal powers of ϵ, one gets the system of equations

$$L_{B_m}\begin{pmatrix} x_k \\ y_k \end{pmatrix} = \begin{pmatrix} -a_k(r) \\ a_k(r) \end{pmatrix} \quad 0 \le k < \infty \tag{5.9}$$

with

$$x_k(0) = x_k(1) = y_k(0) = y_k(1) = 0. \tag{5.10}$$

Here $a_k(r)$ is an expression involving the parameters in the equation, γ_1, $\gamma_2, \ldots, \gamma_k$ and $x_i(r)$ and $y_i(r)$ for $0 \le i \le k - 1$. The first few expressions for the a_k are

$$a_0(r) = 0$$

$$a_1(r) = \gamma_1 x_0 + (B_m/A_0^2)x_0^2 + 2A_0 x_0 y_0$$

$$a_2(r) = \gamma_2 x_0 + \left(\gamma_1 + \frac{2B_m}{A_0^2}x_0 + 2A_0 y_0\right)x_1 + 2A_0 x_0 y_1 + \gamma_1 x_0^2/A_0 + x_0^2 y_0.$$

Thus

$$\begin{pmatrix} x_0(r) \\ y_0(r) \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin m\pi r \tag{5.11}$$

where this is the normalized zero eigenvector of L_{B_m} given by (4.15).

Since L_{B_m} has 0 as a simple eigenvalue, (5.9) has a solution if and only if, the functions $a_k(r)$ obey a solvability condition. This condition determines the coefficients $\gamma_1, \gamma_2, \ldots, \gamma_n$ and is given by the Fredholm alternative. For this problem it is

$$\int_0^1 a_k(r)(d_1 - d_2)\sin m\pi r \, dr = 0.$$

Here d_1 and d_2 are given by (4.17). Since d_1 can never equal d_2, this may be written

$$\int_0^1 a_k(r)\sin m\pi r \, dr = 0. \tag{5.12}$$

The solutions of the system of (5.9) have very different properties depending on whether m is even or odd, so we shall treat these cases separately. In the following analysis we shall only calculate the first few terms in (5.6), as these already give quite good approximations to the solutions obtained numerically.

5a. *m is even.* When m is even and one uses the expression (5.11), in the compatibility equation (5.12), one finds

$$\gamma_1 = 0.$$

(x_1, y_1) are given by the solutions of (5.9)–(5.10) with $k = 1$ and

$$a_1(r) = \left(\frac{B_m}{A} c_1 + 2Ac_2\right) c_1 \sin^2 m\pi r. \tag{5.13}$$

Here, and in the rest of this section we'll drop the subscript from A_0.

To solve these equations, assume that (x_1, y_1) have a Fourier series expansion

$$\begin{pmatrix} x_1(r) \\ y_1(r) \end{pmatrix} = \sum_{l=1}^{\infty} \begin{pmatrix} p_l \\ q_l \end{pmatrix} \sin l\pi r. \tag{5.14}$$

Substituting this in (5.9) one gets that

$$\begin{pmatrix} -D_1 l^2\pi^2 + B_m - 1 & A^2 \\ -B_m & -(A^2 + D_2 l^2 \pi^2) \end{pmatrix} \begin{pmatrix} p_l \\ q_l \end{pmatrix} = \begin{pmatrix} -b_l \\ b_l \end{pmatrix} \tag{5.15}$$

where $b_l = 2\int_0^1 a_1(r) \sin l\pi r \, dr$, $1 \le l < \infty$.

Using the expression (5.13) for a_1, one sees that

$$b_l = \begin{cases} 0 & \text{if } l \text{ is even} \\ \dfrac{-8\alpha m^2}{\pi(l^2 - 4m^2)l} & \text{if } l \text{ is odd} \end{cases}$$

where

$$\alpha = \left(\frac{B_m}{A} c_1 + 2Ac_2\right) c_1.$$

When l is odd, (5.15) has the unique solution

$$\begin{pmatrix} p_l \\ q_l \end{pmatrix} = \frac{b_l}{\Delta_l} \begin{pmatrix} D_2 l^2 \pi^2 \\ -(1 + D_1 l^2 \pi^2) \end{pmatrix} \tag{5.16}$$

where $\Delta_l = D_1 D_2 l^4 \pi^4 + [(1 - B_m)D_2 + D_1 A^2] l^2 \pi^2 + A^2$.

When l is even, one has

$$p_l = q_l = 0. \tag{5.17}$$

These expressions can be substituted back in (5.14) to get the expressions for x_1, y_1.

When $m \simeq \mu$ and $B_m = B_c$, these expressions may be simplified using (4.11) and (4.12). In this case one gets

$$x_1(r) = \frac{-8\mu^2 c_1^2}{D_1 \pi^3} \left[\frac{2(D_1(\mu\pi)^2 + 1) - B_c}{A}\right] \times \sum_{l \text{ odd}} \frac{l}{l^2 - 4\mu^2} \times \frac{\sin l\pi r}{(l^2 - \mu^2)^2} \tag{5.18}$$

together with a similar expression for $y_1(r)$.

Using these expressions for (x_1, y_1), one may now find γ_2 from (5.12) with $k = 2$. This can be written

$$\gamma_2 \int_0^1 x_0(r) \sin m\pi r \, dr = -2A \int_0^1 (x_0 y_1 + y_0 x_1) \sin m\pi r \, dr - \frac{2B_m}{A} \int_0^1 x_0 x_1 \sin m\pi r \, dr - \int_0^1 x_0^2 y_0 \sin m\pi r \, dr.$$

Substituting (5.11), (5.14) and (5.16) into this equation one sees that

$$\frac{\gamma_2 c_1}{2} = -\tfrac{3}{8} c_1^2 c_2 - 2\left(\frac{B_m c_1}{A^2} + A c_2\right) \sum_{l \text{ odd}} \frac{l p_l}{\pi(l^2 - 4m^2)} - 2A c_1 \sum_{l \text{ odd}} \frac{l q_l}{\pi(l^2 - 4m^2)}.$$

The infinite series appearing here may be summed using the calculus of residues. The calculations are shown in Appendix 1 and one gets

$$\begin{aligned}\frac{\gamma_2}{c_1^2} &= +\frac{3}{4}\frac{(B_m - 1 - D_1 m^2\pi^2)}{A^2} + \frac{2(D_1 m^2 \pi^2 + 1) - B_m}{A} \\ &\quad \times \left\{\frac{3}{2A} - \frac{10}{9D_1(m^2\pi^2)A}\left[1 + \tfrac{8}{5}D_1 m^2\pi^2 + \frac{D_1 m^2 \pi^2 + 1 - B_c}{A}\right]\right\} \\ &= \varphi(m, A, B_m, D_1).\end{aligned}$$

When $m = m_c = \mu$, $B_m = B_c$, and one has (4.11) and (4.12), one finds

$$\begin{aligned}\frac{\gamma^2}{c_1^2} &= \frac{3}{4A}\left(\frac{D_1}{D_2}\right)^{1/2}\left[1 + A\left(\frac{D_1}{D_2}\right)^{1/2}\right] + \frac{1}{A^2}\left(1 - \frac{A^2 D_1}{D_2}\right) \\ &\quad \times \left\{\frac{3}{2A} + 10\pi\left(\frac{D_2}{D_1}\right)^{1/2}\left[\frac{1}{A}\left(\frac{D_1}{D_2}\right)^{1/2} + \frac{D_1}{D_2} - \frac{1}{A} - \frac{8}{5}\left(\frac{D_1}{D_2}\right)^{1/2}\right]\right\} = f\left(A, \frac{D_1}{D_2}\right).\end{aligned}$$

The expression $(D_1/D_2)^{1/2} f(A, D_1/D_2)$ is a cubic in $1/A$ and is quadratic in $(D_1/D_2)^{1/2}$ and may be either positive, negative or zero.

Returning to (5.7) one sees that

$$B - B_c \simeq \epsilon^2 \gamma_2 + \cdots$$

near $B = B_c$, so one sees that when $\gamma_2 > 0$ one has

$$\epsilon \simeq \pm \left(\frac{B - B_c}{\gamma_2}\right)^{1/2} \quad \text{for } B > B_c$$

while if $\gamma_2 < 0$ one has

$$\epsilon \simeq \pm \left(\frac{B_c - B}{\gamma_2}\right)^{1/2} \quad \text{and} \quad B < B_c.$$

The bifurcating steady state solutions near $B = B_c$ are approximated by

$$x(r) = \pm(B - B_c)^{1/2} \times \frac{1}{f^{1/2}(A, D_1/D_2)} \sin m_c\pi r + \frac{(B - B_c)}{f(A, D_1/D_2)} \times \frac{8m_c^2}{D_1 A \pi^3}$$

$$\times [B_c - 2(1 + D_1 m_c^2\pi^2)] \times \sum_{l \text{ odd}} \frac{l}{(l^2 - m_c)^2} \times \frac{\sin l\pi r}{l^2 - 4m_c^2} \tag{5.19}$$

when $\gamma_2 > 0$, $B > B_c$, together with a similar expression for y.

If $\gamma_2 < 0$ one has that (5.18) holds for $B < B_c$, where one replaces the factors

$$\left(\frac{B - B_c}{f^{1/2}(A, D_1/D_2)}\right)^{1/2} \quad \text{by} \quad \left(\frac{B_c - B}{-f(A, D_1/D_2)}\right)^{1/2}.$$

When $\gamma_2 > 0$, the new bifurcating solutions are stable when $B > B_c$. However, when $\gamma_2 < 0$, they are not stable. The bifurcation diagrams for this system may be depicted as below, Figure 1 illustrates the situation when $\gamma_2 > 0$, Figure 2 when $\gamma_2 < 0$.

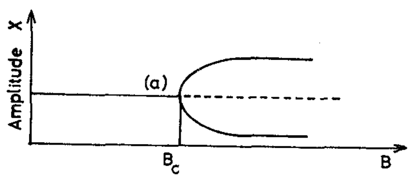

Figure 1

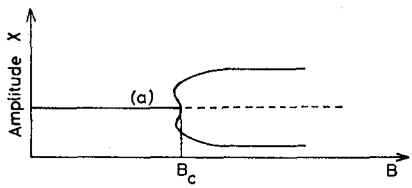

Figure 2

When $\gamma_2 = 0$, one has to continue the calculations still further. However it is a singular case and small changes in either A or D_1/D_2 will bring one into one of the regimes depicted in Figures 1 and 2.

5b. *m is odd.* In this case, the compatibility condition (5.12) implies that

$$\gamma_1 = \frac{-8c_1}{3m\pi}\left[\frac{B_m}{A} + 2A\left(\frac{c_2}{c_1}\right)\right].$$

In particular, when $m = m_c$ is odd one gets

$$\begin{aligned}\frac{\gamma_1}{c_1} &= \frac{-8}{3m_c\pi}\frac{[2(D_1 m_c^2\pi^2 + 1) - B_c]}{A} = g(m_c, A, B_c, D_1) \\ &\simeq \frac{8}{3}\frac{(D_1 D_2)^{1/4}}{A^{3/2}}\left(A^2\frac{D_1}{D_2} - 1\right).\end{aligned} \tag{5.20}$$

(x_1, y_1) can now be determined from (5.9) using

$$a_1(r) = \gamma_1 c_1 \sin m\pi r + \alpha \sin^2 m\pi r$$

where γ_1 as above and $\alpha = [(B_m/A)c_1 + 2Ac_2]c_1$ as before.

Assume a Fourier series expansion (5.14) for x_1 and y_1, then one gets the system of equations (5.15). This time

$$b_l = \begin{cases} 0 & \text{if } l \text{ is even} \\ \dfrac{\alpha l}{\pi(l^2 - 4m^2)} & \text{if } l \text{ is odd, } l \neq m \\ \dfrac{\gamma_1 c_1}{2} - \dfrac{\alpha}{3\pi m} & \text{when } l = m. \end{cases}$$

The solutions (p_l, q_l) are given by (5.16) and (5.17) except when $l = m$. In that case

$$\begin{pmatrix} p_m \\ q_m \end{pmatrix} = \frac{\left(\dfrac{\gamma_1 c_1}{2} - \dfrac{\alpha}{3m\pi}\right)}{A^2(c_1 + c_2) + D_1 m^2 \pi^2 c_1} \times \begin{pmatrix} c_2 \\ -c_1 \end{pmatrix}.$$

Consequently one gets a solution for x_1, y_1 which is almost identical to that obtained when m is even.

Now one finds γ_2 in a manner similar to that used when m is even. However, since $\gamma_1 \neq 0$, there are 2 extra terms and one finds after a calculation that

$$\begin{aligned} \frac{\gamma_2}{c_1^2} = \frac{3}{4}\frac{B_m - 1 - D_1 m^2\pi^2}{A^2} + \frac{2(D_1 m^2 \pi^2 + 1) - B_c}{A} \\ \times \left\{\frac{3}{2A} + \frac{(B_c - 1 - D_1 m^2 \pi^2)}{A^2}\left(\frac{128}{D_1 \pi^7}\right)(m\pi)^4 S_1(m)\right. \\ \left. - \frac{128}{D_1 A \pi^3}[S_1(m) + D_1 \pi^2 S_2(m)]\right\} - \frac{4}{3m\pi A}\frac{\gamma_1}{c_1} = h(m, A, B_c, D_1) \end{aligned}$$

where S_1 and S_2 are the series defined in Appendix 1.

Subsituting this and (5.20) into (5.7) one gets

$$B - B_m = \epsilon c_1 g + \epsilon^2 c_1^2 h. \tag{5.21}$$

When $m = m_c \simeq \mu$ and $B_m = B_c$, one sees that the least value of B for which (5.21) is well defined is

$$\hat{B} = B_c - \frac{g^2}{4h} \quad \text{when } h > 0. \tag{5.22}$$

In this case, one also gets from (5.21) that near the bifurcation point

$$\epsilon c_1 \simeq \frac{B - B_c}{g} - \frac{2(B - B_c)^2 h}{g^3} + 0[(B - B_c)^3]$$

Substituting this back in (5.1) for $x(r)$ one has

$$x(r) = \left(\frac{B - B_c}{g} - \frac{2h}{g^2}(B - B_c)^2\right)\sin m_c\pi r$$
$$- \frac{8(m_c^2\pi^2)}{D_1A\pi^5} \times \frac{(B - B_c)^2}{g^3} \sum_{\substack{l\ \mathrm{odd} \\ l \neq m_c}} \frac{l}{(l^2 - m_c^2)^2} \times \frac{1}{l^2 - 4m_c^2} \sin l\pi\, r. \qquad (5.23)$$

Again there is a similar expression for $y(r)$.

In this case one sees that the bifurcating solution is defined for B on both sides of B_c. The new bifurcating solution is stable on the supercritical branch where $B > B_c$ and unstable on the subcritical branch where $B < B_c$. From Theorem 3.4, one knows that there is a minimum value of B for which there are 2 distinct solutions and consequently the new branch can only be defined for $B \geq B_{\min} > 0$. It appears that $\hat{B}$ given by (5.20) is a good approximation to $B_{\min}$.

The bifurcation diagram for this system can be depicted as in Figure 3.

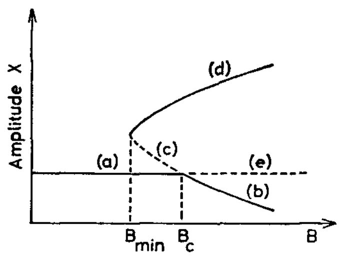

Figure 3

The branches (a), (b) and (d) are stable, while (c) and (e) are unstable. When $B > B_c$ and there are 2 stable steady-state solutions, the system tends asymptotically as $t \to \infty$ to one or other of these solutions depending on the initial conditions. This is a phenomenon which is very similar to hysteresis.

The computer simulation, reported in the paper of Herschkowitz-Kaufman (1975), also obtained these two branches of solution and the hysteresis effect.

One can formally approximate the solutions on the branch (d), by taking the other solution to (5.21) rather than the one used previously. That is,

$$\epsilon c_1 = -\frac{g}{h} - \frac{(B - B_c)}{g} + 0[(B - B_c)^2].$$

Substituting this in (5.6) one gets

$$x(r) = -\left(\frac{g}{h} + \frac{B - B_c}{g}\right)\sin m_c\pi r - \left[\left(\frac{g}{h}\right)^2 + \frac{2(B - B_c)}{h}\right]\frac{8m_c^2}{D_1A\pi^3}$$
$$\times \sum_{\substack{l\ \mathrm{odd} \\ l \neq m_c}} \frac{l}{(l^2 - m_c^2)^2} \times \frac{1}{l^2 - 4m_c^2} \cdot \sin l\pi r + 0[(B - B_c)^2]. \qquad (5.24)$$

6. Qualitative Properties of Dissipative Structures. The new bifurcating solutions obtained in the last section have many interesting qualitative features, some of which will be discussed below.

6a. *m_c is even.* (1) The new solutions given by (5.19) have a *critical exponent* of $\frac{1}{2}$ and are *degenerate.* This is a striking example of a *symmetry breaking* transition at the bifurcation point.

(2) The infinite series in (5.19) introduces *subharmonic terms* which only vanish under very special conditions. These terms are a nonlinear effect and they introduce *spatial asymmetry* into the solutions. A typical comparison of $\epsilon x_0(r)$ and $x(r)$ is given in Figure 4.

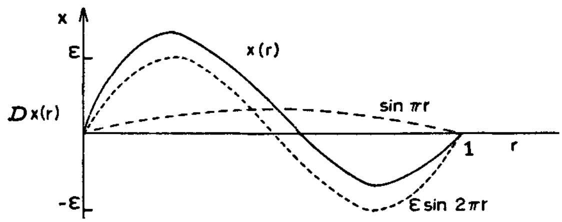

Figure 4

(3) The expression (5.17) indicates that the new solutions may be considered as a superposition of the critical mode (proportional to $\sin m_c \pi r$) and a distortion. The dominant contributions to the distortion are given by terms proportional to $\sin l\pi r$, where l is an odd integer near μ or 2μ.

(4) The total amount of the constituent X in the system is not conserved in the transition to the dissipative structure. To see this one evaluates

$$\bar{x} = \int_0^1 x(r)\,\mathrm{d}r = \frac{B - B_c}{f(A, D_1/D_2)} \times \frac{16m_c^2}{D_1 A \pi^4} \times [B_c - 2(D_1 m_c^2 \pi^2 + 1)]$$

$$\times \sum_{l\,\mathrm{odd}} \frac{1}{(l^2 - m_c^2)^2} \times \frac{1}{(l^2 - 4m_c^2)}.$$

This infinite series may be summed using the method in Appendix 1 and one has that

$$\sum_{l\,\mathrm{odd}} \frac{1}{(l^2 - \mu^2)^2} \times \frac{1}{l^2 - 4\mu^2} = \frac{-\pi^2}{12\mu^4}.$$

Using (4.11) and (4.12) this can be simplified to

$$\bar{x} = \frac{(B - B_c)}{f(A, D_1/D_2)} \times \frac{4}{3A^2}\left(\frac{D_2}{D_1}\right)^{1/2}\left(1 - \frac{A^2 D_1}{D_2}\right).$$

(5) The contribution to $\bar{x}$ comes from the terms proportional to $(B - B_c)$. Thus $\bar{x}$ is an approximate invariant, as it doesn't depend on terms proportional to $(B - B_c)^{1/2}$.

The distortion is a function with mean $\bar{x}$ and when $\bar{x} > 0$ one sees it tends to raise the value of $x(r)$ above that given by the dominant term. When $\bar{x} < 0$ it tends to lower the values of $x(r)$. Figure 4 depicts a case where $\bar{x} > 0$.

6b. m_c *is odd.* (1) This time the solutions (5.23) or (5.24) only exhibit symmetry-breaking for $B > B_c$ as there is only one branch crossing the critical point. Instead one has an effect similar to hysteresis near the bifurcation point. When $B < B_c$, there are also two dissipative structures, one of which (that on branch (d) of Figure 3) requires an abrupt transition from the uniform solution. The other subcritical dissipative structure is unstable for B close to B_c.

(2) The expression (5.23) shows that, in this case, the new solution may be considered as a superposition of the critical mode (proportional to $\sin m_c\pi r$) and a distortion. This distortion is proportional to $(B - B_c)^2$ and introduces spatial asymmetry to the solutions.

In (5.24), this spatial asymmetry occurs in the leading terms, and does not disappear when $B = B_c$.

(3) Again, in this case, the total amount of the constituent X is not conserved in the transition to the dissipative structure. From (5.23) one sees that

$$\bar{x} = \int_0^1 x(r)\,\mathrm{d}r = \frac{2}{g(m_c\pi)}(B - B_c) + 0[(B - B_c)^2].$$

Or, using (4.11), (4.12)

$$\bar{x} = -\tfrac{3}{4}A(B - B_c) \times \left(1 - \frac{A^2 D_1}{D_2}\right)^{-1}. \tag{6.1}$$

Similarly,

$$\bar{y} \simeq \tfrac{3}{4}(B - B_c)\left(\frac{D_1}{D_2}\right)^{1/2}\left[1 + A^2\left(\frac{D_1}{D_2}\right)^{1/2}\right]\left(1 - A^2\frac{D_1}{D_2}\right)^{-1}. \tag{6.2}$$

Thus $\bar{x}$ is not conserved even in the dominant order, contrary to the case where m_c is even.

If one uses (5.24) one gets

$$\bar{x} = -\frac{2g}{hm_c\pi} - \left(\frac{g}{h}\right)^2 \frac{16m_c^2}{D_1A\pi^4} \sum_{\substack{l\ \mathrm{odd} \\ l \neq m_c}} \frac{1}{(l^2 - m_c^2)} \times \frac{1}{l^2 - 4m_c^2} + 0[(B - B_c)].$$

6c. $m \neq m_c$. When m is not equal to the critical wave number m_c, there will be bifurcation of a new branch from the uniform solution at $B = B_m$, at least when 0 is a simple eigenvalue of L_{B_m}. These new solutions will be similar to those bifurcating from $B = B_c$, which have been described above. When m is even, the new branches will be degenerate and have a critical exponent of $\frac{1}{2}$, while if m is odd, the new branch will be similar to those described in 6b.

Unfortunately we do not know in what regions, if any, these new branches are stable.

When B is much greater than B_c, there will be many possible dissipative structures, some of which will be stable to small perturbations and others which won't be. In her computer simulation Herschkowitz-Kaufman found values of B for which there were a number of different stable solutions arising from different branches. The situation may be depicted by Figure 5.

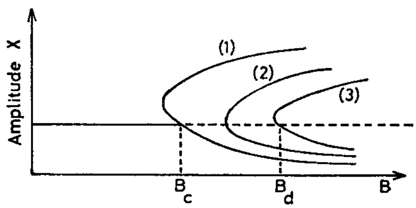

Figure 5

In this figure branch (1) bifurcates when $B = B_c$, but branches (2) and (3) bifurcate when $B > B_c$. One sees that when $B > B_d$, there are seven possible solutions of the equations.

6d. *Entropy production.* The entropy production of the system is also affected by the transition to dissipative structures. To study this we introduce small inverse reaction rates, k in the scheme (1.1).

The total entropy production is

$$P = \int_0^1 \left[(A - kX) \ln \frac{A}{kX} + (BX - kYD) \ln \frac{BX}{kYD} + (X^2Y - kY^3) \ln \frac{Y}{kX} \right.$$
$$\left. + (X - kE) \ln \frac{X}{kE} + \frac{D_1}{X}\left(\frac{\partial X}{\partial r}\right)^2 + \frac{D_2}{Y}\left(\frac{\partial Y}{\partial r}\right)^2 \right] dr. \tag{6.3}$$

We are interested in this for k small, so upon keeping the terms of 0(1) and 0(ln k) but not of 0(k), one gets, using (1.2),

$$P = \int_0^1 \left[A \ln A - BX \ln \frac{B}{D} - X \ln E \right] dr + D_1 \left(\ln X \frac{\partial X}{\partial r} \right)_0^1 +$$
$$D_2 \left(\ln Y \frac{\partial Y}{\partial r} \right)_0^1 - 2(B + 1) \ln k(A + \bar{x}) + D_1 \ln X \left(\frac{\partial X}{\partial r} \right)_0^1 . \tag{6.4}$$

As an example, we shall calculate this expression to $0(B - B_c)$ in the case where m is odd. From (5.23) one obtains after subtracting the entropy production at the uniform steady state

$$\Delta P = P - P_0 = \left\{B \ln \frac{B}{D} - \ln E - 2(B+1)\ln k\right\}\bar{x} - A\left(\frac{D_1}{D_2}\right)^{1/2}\bar{x}\ln Ak - A\left(\frac{D_2}{D_1}\right)^{1/2}\bar{y}\ln\frac{B}{A}. \tag{6.5}$$

When $\bar{x} \neq 0$ and $\bar{y} \neq 0$, the dominant terms in this expression are

$$\Delta P \simeq -\left[2(B+1) + A\left(\frac{D_1}{D_2}\right)^{1/2}\right]\bar{x}\ln k. \tag{6.6}$$

For $k < 1$, this term has the same sign as $\bar{x}$. When $(A^2 D_1)/D_2 > 1$, ΔP will be enhanced on the supercritical dissipative structure, and diminished on the (unstable) subcritical branch. From (5.23) and (6.1) one sees that the enhancement of ΔP will be larger for larger B and critical wave number m_c.

It is also interesting to compare the differences in the entropy production per unit mass between the uniform steady state and the dissipative structure. The dominant term in (6.3) may be written as

$$P \simeq -\ln k[A + X^2 Y + (B+1)X]. \tag{6.7}$$

Let M_0, M be the total mass at the uniform state and at the dissipative structure. We want to compute:

$$\Delta\left(\frac{P}{M}\right) = \frac{P_0 + \Delta P}{M_0 + \Delta M} - \frac{P_0}{M_0} \simeq \frac{1}{M_0}\left(\Delta P - P_0\frac{\Delta M}{M_0}\right) \quad \text{for small } \Delta P, \Delta M.$$

We have just calculated ΔP in (6.7). From (6.1), (6.2) one gets

$$\Delta M = \bar{x} + \bar{y} = \tfrac{3}{4}(B - B_c)\left(1 - \frac{A^2 D_1}{D_2}\right) \times \left\{A\left(\frac{D_1}{D_2}\right) + \left(\frac{D_1}{D_2}\right)^{1/2} - A\right\}.$$

However from (6.7)

$$P_0 \simeq -2\ln k(A + AB).$$

Thus

$$\Delta\left(\frac{P}{M}\right) \simeq -\ln k\left\{2(B_c+1)\bar{x} + A\left(\frac{D_1}{D_2}\right)^{1/2}\bar{x} - \frac{2A^2(1+B_c)}{A^2+B_c}(\bar{x}+\bar{y})\right\}$$
$$= -\bar{x}\ln k\left\{2(B_c+1) + A\left(\frac{D_1}{D_2}\right)^{1/2} - 2A^2\left(\frac{1+B_c}{A^2+B_c}\right)\left(1 - \frac{1}{A}\left(\frac{D_1}{D_2}\right)^{1/2} - \frac{D_1}{D_2}\right)\right\}.$$

Remembering that B_c varies as A^2, one sees that $\Delta(P/M)$ is positive for A large and negative for A small. When A is large, one sees from (1.1) that the production mechanism for X is very fast and occurs on a different time scale to the other chemical transformation. This agrees with Prigogine *et al.*, (1972) and Prigogine and Lefever (1974) who pointed out that the occurrence of fast pathways always tends to enhance the rate of dissipation per unit mass. The entropy production itself [see (6.6)] will also increase sharply as $A \to \infty$.

Similar conclusions apply for m_c even. The difference is that in this case both ΔP and $\Delta(P/M)$ will vanish in the dominant degree $[0(B - B_c)^{1/2}]$ and one has to continue the calculation to $0(B - B_c)$.

6e. *Dependence on length.* Hitherto we have normalized the length of the interval to be 1. When (1.2) are solved on the interval $0 \leq r \leq L$, the length L may be treated as another parameter in the system.

The analysis of the case of arbitrary length can be deduced from the preceding analysis by making the change of variables

$$s = r/L.$$

If the boundary conditions were

$$X(0, t) = X(L, t) = A_0$$
$$Y(0, t) = Y(L, t) = B_0/A_0$$

then under this change of variables one gets the boundary conditions (1.4), while (1.2) becomes

$$\frac{\partial X}{\partial t} = \frac{D_1}{L^2}\frac{\partial^2 X}{\partial s^2} - (B + 1)X + X^2Y + A$$
$$\frac{\partial Y}{\partial t} = \frac{D_2}{L^2}\frac{\partial^2 X}{\partial s^2} + BX - X^2Y.$$

Thus changing L may be viewed as changing the diffusion coefficients in our problem. All the preceding results hold provided one substitutes D_1/L^2 and D_2/L^2 for D_1 and D_2. One sees that μ [from (4.11)] goes up as L is increased but that B_c is approximately constant. Similarly, the expressions obtained in Section 5 for the bifurcating steady state solutions can be transformed to give the corresponding solutions on $0 \leq r \leq L$. The qualitative nature of these analyses do not change as one varies L but the specific values at which certain transitions occur often (but not always) involve the length (Hanson, 1974; Babloyantz and Hiernaux, 1975).

7. Localized Spatial Structures. The dissipative structures described in the last two sections arose under the assumption that A was uniformly distributed throughout the system. In this section we shall extend some of the previous calculations to the case where A has an inhomogeneous distribution, given by (3.3) for $\alpha > 0$. As will be seen, this "spatial dispersion" of A will result in the localization of the dissipative structures within natural boundaries.

We shall assume that $A(r)$ is defined by

$$A(r) = A_0 \frac{\cosh [2\alpha(r - \frac{1}{2})]}{\cosh \alpha} \quad \alpha > 0. \tag{3.3}$$

Then one can find approximations to the solutions on the thermodynamic branch as described at the end of Section 3. Let (X_0, Y_0) be such a solution pair. We are interested in studying the form of the solutions bifurcating from (X_0, Y_0) when $\lambda = 0$ is an eigenvalue of the linear stability equations. To do this, one considers (4.1)–(4.2) with $\lambda = 0$.

Adding the two equations in (4.1) one gets

$$D_1 u'' + D_2 v'' - u = 0.$$

Let

$$z = D_1 u + D_2 v,$$

then (4.1) may be written as the single fourth order equation

$$D_1 D_2 z'''' + [(2X_0 Y_0 - B - 1)D_2 - D_1 X_0^2]z'' + X_0^2 z = 0. \tag{7.1}$$

Assume this equation has a solution of the form

$$z(r) = e^{\varphi(r)} \tag{7.2}$$

where $\varphi(r)$ is a rapidly varying function of r.

Neglecting all derivatives of φ except the first (in a manner similar to the WKB approximation) one obtains

$$D_1 D_2 (\varphi')^4 + [(2X_0 Y_0 - B - 1)D_2 - D_1 X_0^2]\varphi'^2 + X_0^2 = 0. \tag{7.3}$$

The solution of this equation is

$$\varphi'(r)^2 = + \frac{1}{2D_1}\left[1 + \frac{D_1}{D_2} X_0^2 - F(r)\right] \pm \frac{1}{2D_1} \sqrt{\{[F(r) - B_+(r)][F(r) - B_-(r)]\}} \tag{7.4}$$

where

$$F(r) = 2X_0(r)Y_0(r) - B \qquad B_\pm(r) = \left[X_0(r)\left(\frac{D_1}{D_2}\right)^{1/2} \pm 1\right]^2.$$

From (7.3) and (7.4), one observes that one can never have

$$\varphi'(r)^2 = 0$$

as if this were the case then $[X_0^2(r)]/(D_1 D_2) = 0$ which is impossible. However $\varphi'(r)$ can change from real to complex values when the right-hand side of (7.4) changes from real to complex values. In fact one sees from (7.4) that $\varphi'(r)$ is real only when

$$F(r) \leq 1 + \frac{D_1}{D_2} X_0^2(r) \tag{7.5}$$

and

$$F(r) \geq B_+(r) \quad \text{or} \quad F(r) \leq B_-(r). \tag{7.6}$$

For this problem, we shall see that these conditions hold in certain regions of space and are violated elsewhere. The boundaries between the two types of behavior will be called the turning points of the equation. At a turning point

$$F(r) = B_+(r) \quad \text{or} \quad F(r) = B_-(r). \tag{7.7}$$

On one side of a turning point the solutions $z(r)$ will be monotonic [and $\varphi'(r)$ will be real] while on the other side $z(r)$ will be oscillatory [and $\varphi'(r)$ will be complex].

This condition for a turning point in this problem is somewhat different to the definition for the second order equation

$$z'' + f(r)z = 0. \tag{7.8}$$

For (7.8) a turning point must obey

$$\varphi'(r) = 0 \tag{7.9}$$

which, as we have seen, is not the case for our problem.

When $F(r) > B_+(r)$, one observes that (7.5) is contradicted, so that one cannot get a turning point in this manner, and one only finds delocalized structures.

If $F(r) \leq B_-(r)$ then (7.5) automatically holds. The turning points are thus given by the equation

$$2X_0(r)Y_0(r) - B = \left[X_0(r)\left(\frac{D_1}{D_2}\right)^2 - 1\right]^2. \tag{7.10}$$

Using our approximations (3.6) and (3.7) for X_0, Y_0, this becomes

$$r^2 - r + \beta = 0$$

where

$$\beta = \frac{1}{\alpha^2\lambda} - \frac{B}{\alpha^2(\lambda - 1)^2\lambda} \quad \text{and} \quad \lambda = A_0(D_1/D_2)^{1/2}.$$

The roots of this are given by

$$r_{\pm} = \tfrac{1}{2} \pm \tfrac{1}{2}\sqrt{(1 - 4\beta)}.$$

When $0 \leq \beta < \frac{1}{4}$ one sees that $0 < r_- < r_+ < 1$, and r_-, r_+ are symmetrically situated about $r = \frac{1}{2}$. When $0 \leq r < r_-$ or $r_+ < r \leq 1$, $z(r)$ will be monotonic, but in the middle $r_- < r < r_+$ it will be oscillatory.

As β tends to 0, one sees that these turning points are pushed to the boundaries $r = 0$ and $r = 1$. In terms of B, this requires

$$B < B_b = \left[A_0 \left(\frac{D_1}{D_2}\right)^{1/2} - 1\right]^2.$$

The size of the dissipative structure is approximately

$$2\beta = \frac{2}{\alpha^2\lambda}\left[1 - \frac{B}{(\lambda - 1)^2}\right] \tag{7.11}$$

and this is a decreasing function of λ for large λ.

To find the approximate form of $z(r)$ near the turning points, one has to approximate $\varphi'(r)$ near those points. Using only the first terms in the Taylor series expansions about r_-, one finds

$$\begin{aligned} 2D_1\varphi'(r)^2 \simeq &- \Big\{F(r_-) + F'(r_-)(r - r_-) - 1 \\ &- \frac{D_1}{D_2}[X_0^2(r_-) + 2X_0(r_-)X_0'(r_-)(r - r_-)]\Big\} \\ &\pm i\sqrt{\{[F(r_-) - B_+(r_-)]|r_+ - r_-|\}}\cdot\frac{(r - r_-)^{1/2}}{\alpha}(\lambda - 1)\lambda^{1/2}. \end{aligned}$$

Keeping only the highest order terms, one gets

$$\begin{aligned} \sqrt{(2D_1)}\varphi'(r) &= \pm\Big\{\Big[1 + \frac{D_1}{D_2}X_0^2(r_-) - F(r_-)\Big]^{1/2} \\ &\qquad \pm \frac{i\lambda^{1/2}(\lambda - 1)(r - r_-)^{1/2}}{2\mathscr{A}(r_-)\alpha}\sqrt{([F(r_-) - B_+(r_-)]|r_+ - r_-|)}\Big\} \\ &= \pm[\mathscr{A}(r_-) \pm i\mathscr{B}(r_-)(r - r_-)^{1/2}] \end{aligned}$$

where $\mathscr{A}(r)^2 = -F(r) + 1 + (D_1/D_2)X_0^2(r)$.

Thus

$$z(r) \propto \exp\left[\pm(2D_1)^{-1/2}\mathscr{A}(r_-)r + \frac{2i}{3}(2D_1)^{-1/2}\mathscr{B}(r_-)(r - r_-)^{3/2}\right]$$

and this is non-sinusoidal.

However, near $r = \frac{1}{2}$, one gets a very different form for the solution. Using (3.6) as an approximation to $X_0(r)$, one gets

$$B_{\pm}(\tfrac{1}{2}) \simeq B_{\pm}(0) - \frac{\alpha^2}{8}\lambda.$$

Thus

$$\begin{aligned} 2D_1\varphi'(r)^2 &= \mathscr{A}(\tfrac{1}{2})^2 \pm i|B - B_+(\tfrac{1}{2})|^{1/2}|B - B_-(\tfrac{1}{2})|^{1/2} + 0[(r - \tfrac{1}{2})^2] \\ &= \rho\, e^{\pm i\theta} + 0[(r - \tfrac{1}{2})^2] \end{aligned}$$

near $r = \frac{1}{2}$.

The corresponding expression for $z(r)$ is

$$z(r) \propto \exp\left[\pm\left(\frac{\rho}{2D_1}\right)^{1/2}(r - \tfrac{1}{2})\cos\frac{\theta}{2}\right]\exp\left[\pm i\left(\frac{\rho}{2D_1}\right)^{1/2}(r - \tfrac{1}{2})\sin\frac{\theta}{2}\right]$$

and this is approximately sinusoidal. The approximate wavelength near $r = \frac{1}{2}$ is

$$\frac{1}{2\pi}\left(\frac{\rho}{2D_1}\right)^{-1/2}\frac{1}{\sin\theta/2}.$$

When $B_+(r)$ and $B_-(r)$ vary considerably on [0, 1] and $\varphi'(r)$ is complex then the complex part of $\varphi'(r)$ also varies considerably. As a result, the corresponding oscillatory solution does not have a uniform wavelength. The successive maxima and minima are at differing distances from one another. Near the turning points given by (7.10) the oscillatory solution has a long wavelength. This is often sufficiently large that the oscillations appear negligible and so the exact boundaries of the dissipative structure are hard to identify. This we believe is the explanation of why the computer simulation reported in the paper by Herschkowitz-Kaufman obtains solutions with highly oscillatory regions which are always smaller than those predicted by (7.11).

Finally it is worth noting that when

$$B \geq B_b = \left[A\left(\frac{D_1}{D_2}\right)^{1/2} - 1\right]^2$$

the solution (7.2) becomes oscillatory near the boundary and the dissipative structure is no longer localized to the interior of the interval. This is obtained directly from (7.4) by noting that at the boundary

$$X_0 = A, \quad Y_0 = B/A, \quad F = B \quad \text{and} \quad B_{\pm} = \left[A\left(\frac{D_1}{D_2}\right)^{1/2} \pm 1\right]^2.$$

Again in this case the distances between successive maxima and minima vary considerably and sometimes the solution does not appear to be oscillatory near the boundary.

These equations have a wealth of detailed structure and these calculations provide only a rough indication of the nature of some of the phenomena encountered.

8. Concluding Remarks. This paper has been devoted to the analysis of the steady state solutions of a system of nonlinear parabolic equations which describe a chemical system undergoing reactions and diffusion. Although the analysis has been performed for a very particular system, one would expect similar results for other reaction schemes.

The main results include the proof of the existence of non-negative solutions of these equations for all positive time and the construction of new steady state solutions of these equations using bifurcation theory. These new steady states have many interesting properties. They show the possibility of symmetry breaking transitions, of bistable behavior and of hysteresis effects, while the type of solution depends on the symmetry of the critical mode. Also the transition to the new steady states may be accompanied by an enhancement of the dissipation per unit mass in the system.

These results provide a first answer to the question of the role of diffusion in nonlinear chemical systems. One sees that one can obtain a great variety of spatial organization and pattern formation when one is away from thermodynamic equilibrium. Most importantly, the introduction of diffusion provides a mechanism for obtaining spontaneously a self-organizing process in a previously homogeneous medium.

For certain values of the parameters, one may also obtain wave-like solutions of these equations. These waves may be either standing waves or propagating waves and some results about them will be described in a forthcoming paper.

Finally there are many interesting questions about these systems that still are unanswered, especially those concerning the behavior of this system when one is far from the first bifurcation point of this system.

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APPENDIX I

SUMMATION OF THE SERIES IN SECTION 5

We would like to evaluate the expressions

$$S_1 = \sum_{l \text{ odd}} \frac{1}{(l^2 - m^2)^2} \frac{1}{(l^2 - 4m^2)^2} \tag{A1}$$

and

$$S_2 = \sum_{l \text{ odd}} \frac{l^2}{(l^2 - m^2)^2} \frac{1}{(l^2 - 4m^2)^2} \tag{A2}$$

where m is even.

Consider the meromorphic function

$$f(z) = \frac{1}{[(2z+1)^2 - m^2]^2} \times \frac{1}{[(2z+1)^2 - 4m^2]^2}.$$

The function has double poles at $z = \frac{1}{2}(-1 \pm m)$ and at $z = \frac{1}{2}(-1 \pm 2m)$. Also,

$$\lim zf(z) = 0.$$

From the calculus of residues, one has the well-known formula, for $\delta > 0$

$$\begin{aligned} 0 &= \int_{-\infty+i\delta}^{\infty+i\delta} \pi f(z) \cot \pi z \, dz \\ &= 2\pi i \left\{ \sum_{l=-\infty}^{\infty} f(l) + \pi \times [\text{residues of } f(z) \cot \pi z \text{ at poles of } f(z)]. \right\} \end{aligned} \tag{A3}$$

The residues a_i at the double poles z_i, $i = 1, 2, 3, 4$, are

$$a_1 = a_2 = \frac{-\pi}{144m^6}, \qquad a_3 = a_4 = \frac{-\pi}{576m^6}.$$

Substituting this in (A3) and using the symmetry in l one finds that for m even

$$S_1 = \frac{5\pi^2}{576m^6}.$$

Similarly if one uses

$$g(z) = \frac{(2z+1)^2}{[(2z+1)^2 - m^2]^2[(2z+1)^2 - 4m^2]^2}$$

one has that when m is even,

$$S_2 = \frac{\pi^2}{72m^4}.$$

APPENDIX II

THE MAXIMUM PRINCIPLE

Throughout this paper, we have used various forms of the maximum principle to obtain information about the solutions of our equations. In this appendix, we shall give explicit statements of the theorems we have used and complete the details of the proofs depending on the maximum principle.

The simplest form of the maximum principle is a statement about convexity. If u is a C^2-function on an interval $[a, b]$ obeying

$$\frac{d^2u}{dr^2} \geq 0$$

then

$$u(r) \leq \max[u(a), u(b)].$$

This is all that was required to get the upper bounds in Theorem 3.1.

A more general form of the maximum principle is the following

THEOREM B1. *Suppose u is continuous on $[a, b]$ and of class C^2 on (a, b) and that g and h are continuous on $[a, b]$, with $h(r) \leq 0$, for $a \leq r \leq b$.* If

$$u''(r) + g(r)u'(r) + h(r)u(r) \geq 0 \quad \text{for } a < r < b$$

then

$$u(r) \leq \max [0, u(a), u(b)].$$

If

$$u''(r) + g(r)u'(r) + h(r)u(r) \leq 0 \quad \text{for } a < r < b$$

then

$$u(r) \geq \min [0, u(a), u(b)].$$

This theorem is a direct consequence of Theorem 3, Chapter 1 of Protter and Weinberger (1967).

To prove Lemma 1 in Section 3, we first use both parts of this theorem to get $Y(r) \leq 0$ and $Y(r) \geq 0$ and thus

$$Y(r) \equiv 0 \quad \text{on } [0, 1].$$

From the equation for X, one sees that

$$X(r) \geq \min (0, A_0) = 0.$$

If $X(\tilde{r}) = 0$ for some $0 < \tilde{r} < 1$, then $X''(\tilde{r}) \geq 0$ (as it must be a local minimum) and so, from the equation

$$D_1 X''(\tilde{r}) = -A(\tilde{r}).$$

But this is impossible as the left-hand side is non-negative and $-A(r) < 0$ for $0 < r < 1$, so $X(\tilde{r}) \neq 0$. Thus one has the strict inequality $X(r) > 0$.

To get the upper bound, let $u(r) = X(r) - A_0$. Then

$$D_1 u'' - u = A_0 - A(r) \geq 0$$
$$u(0) = u(1) = 0.$$

From the first part of the maximum principle, one gets

$$u(r) \leq 0 \quad \text{or} \quad X(r) \leq A_0.$$

Similarly Lemma 2 in Section 3 depends on a direct application of the second part of the maximum principle.

Our other applications of the maximum principle were to elliptic and parabolic systems. Firstly we shall give an appropriate form for semilinear parabolic systems. We shall only treat the case of one space variable but it is easy to generalize the results to an arbitrary number of space variables.

We shall be interested in forms of the maximum principle which apply to semilinear parabolic systems of the form

$$\frac{\partial u_i}{\partial t} = a_i(r, t) \frac{\partial^2 u_i}{\partial r^2} + b_i(r, t) \frac{\partial u_i}{\partial r} + c_i(r, t, u_1, \ldots, u_k) \quad 1 \leq i \leq k. \tag{B1}$$

Here we assume $0 < r < 1$, $0 < t < T$, that a_i, b_i and c_i are continuous functions of their variables, and that

$$a_i(r, t) \geq \delta > 0 \quad \text{for all } 1 \leq i \leq k,\ 0 < r < 1,\ 0 < t < T.$$

We are not using a summation convention here; such systems are called weakly coupled as in the i^{th} equation, the functions u_j, for $j \neq i$, enter only through the lowest order terms.

Assume that

$$u_i(r, 0) = u_{0i}(r) \tag{B2}$$

is given and that

$$u_i(0, t) = \alpha_i(t) \quad \text{and} \quad u_i(1, t) = \beta_i(t) \tag{B3}$$

are also prescribed. Assume also that

$$c_i(r, t, u_1, \ldots, u_k) = \sum_{j=1}^{k} c_{ij}(r, t, u_1, \ldots, u_k) u_j + c_i(r, t, 0, 0, \ldots, 0). \tag{B4}$$

THEOREM B2. *Suppose* $u\colon [0, 1] \times [0, T) \to \mathbb{R}^k$ *is a classical solution of* (B1)–(B4). If

(i) $u_{0i}(r) \geq 0$ for $1 \leq i \leq k$ and $0 \leq r \leq 1$,
(ii) $\alpha_i(t) \geq 0$, $\beta_i(t) \geq 0$ for $1 \leq i \leq k$ and $0 \leq t < T$,
(iii) $c_{ii}(r, t, u_1, \ldots, u_k) \leq 0$ for $1 \leq i \leq k$ and all r, t, u,
(iv) $c_{ij}(r, t, u_1, \ldots, u_k) \geq 0$ whenever $i \neq j$ and all r, t, u and
(v) $c_i(r, t, 0, \ldots, 0) \geq 0$ for all i, r, t

then $u_i(r, t) \geq 0$ for $1 \leq i \leq k$, $0 \leq r \leq 1$ and $0 \leq t < T$.

Proof: Let L_i be the parabolic operator defined by

$$L_i v = a_i(r, t)\,\frac{\partial^2 v}{\partial r^2} + b_i(r, t)\,\frac{\partial v}{\partial r} - \frac{\partial v}{\partial t}.$$

From (B1) and (v) one sees that

$$L_i u_i + c_i(r, t, u_1, \ldots, u_k) - c_i(r, t, 0, \ldots, 0) \leq 0$$

or

$$L_i u_i + \sum_{j=1}^{k} c_{ij}(r, t, u_1, \ldots, u_k) u_j \leq 0.$$

Applying Theorem 13, Chapter 3 of Protter and Weinberger (1967) to this expression one gets that

$$-u_i(r, t) \leq 0 \quad \text{for all } i,\ r,\ t.$$

Thus one has the theorem.

In the application of this result to our system, one has $k = 2$, $b_i(r, t) = 0$ and $a_i(r, t) = D_i$. Also

$$c_1(r, t, X, Y) = A(r) - [B(r) + 1]X + X^2 Y$$
$$c_2(r, t, X, Y) = B(r)X - X^2 Y$$
$$\alpha_1(t) = \beta_1(t) = B_0/A_0 \geq 0 \quad \text{and} \quad \alpha_2(t) = \beta_2(t) = A_0 > 0.$$

This system obeys all the requirements of the above theorem and so Theorem 2.2 holds.

Next one would like to have analogous maximum principles for weakly coupled semi-linear elliptic systems. To get such results one should first look at weakly coupled linear elliptic systems. When one has only one space variable these may be written

$$a_i(r)\,\frac{d^2 u_i}{dr^2} + b_i(r)\,\frac{du_i}{dr} + \sum_{j=1}^{k} c_{ij}(r) u_j = d_i(r) \quad 0 < r < 1. \tag{B6}$$

Here a_i, b_i, d_i and c_{ij} are assumed to be continuous on $[0, 1]$ and $a_i(r) \geq \delta > 0$ for $0 \leq r \leq 1$.

If one merely assumes, as in the previous two theorems, that $d_i(r) \geq 0$ and $c_{ii}(r) \leq 0$ for $1 \leq i \leq k$ and $c_{ij}(r) \geq 0$ for $i \neq j$, one need not always get a maximum principle. For example, consider the system

$$u_1'' - u_1 + \alpha u_2 = \tfrac{1}{2} \quad \text{for } 0 < r < 1$$
$$u_2 = 1$$

subject to the boundary conditions

$$u_1(0) = u_1(1) = 0 \quad \text{and} \quad u_2(0) = \tfrac{1}{2} \quad u_2(1) = 1.$$

The solutions of this system are given by

$$u_2(r) = \tfrac{1}{2}(1 + r^2) \quad \text{and} \quad u_2'' - u_1 = \tfrac{1}{2}(1 - \alpha) - \frac{\alpha r^2}{2}.$$

When $\alpha = 0$, a maximum principle holds, but when $\alpha \geq 1$, one has that $u_1(r) \geq 0$ and a minimum principle holds for u_1.

However, one does have some results when the functions $u_i(r)$ are constrained to be nonpositive on the boundary, and certain spectral properties hold. Such results are proved using homotopy methods and here we shall use similar methods to prove Theorem 3.4.

First one should note that if $X_B(r) \geq 0$ for $0 \leq r \leq 1$ then from Theorem B1 and from the equation

$$D_2 Y'' - X^2 Y = -BX$$

and the boundary conditions for Y, one gets $Y_B(r) \geq 0$.

Thus for Theorem 3 to hold, it suffices to prove the following.

THEOREM B3. *If* (X, Y, B) *is in* $\mathscr{T}_0$, *then* $X(r) \geq 0$ *for* $0 \leq r \leq 1$.

Proof: If (X, Y, B) is in $\mathscr{T}_0$, then there is a continuous mapping $\mathrm{X}: [0, B] \to C^2(0, 1)$ such that for each $0 \leq b \leq B$, $\mathrm{X}(b)$ is the X-component of a solution of (3.1)–(3.4) and $\mathrm{X}(0) = X_0$, $\mathrm{X}(B) = X$.

Let

$$m(b) = \inf_{0 \leq r \leq 1} x_b(r).$$

Then from Lemma 1, $m(0) > 0$, and since X is continuous, $m(b)$ is a continuous function of b.

Let $b_0 = \inf \{b: m(b) < 0\}$. Then $m(b_0) = 0$ and when $B = b_0$, there is a solution $\mathrm{X}(b_0) = \tilde{X}$ of (3.1)–(3.4) and a point $\tilde{r}$ in (0, 1) such that

$$\tilde{X}(\tilde{r}) = 0 \quad \text{and} \quad \tilde{X}''(\tilde{r}) \geq 0 \quad (\text{as } \tilde{X} \text{ attains its minimum at } \tilde{r}).$$

But from (3.1)

$$D_1 \tilde{X}''(\tilde{r}) = -A(\tilde{r}).$$

Since $A(r) > 0$ for all $0 \leq r \leq 1$, this is impossible and so there is no such b_0. Thus the theorem is proven.

In fact this proof shows that if (X, Y, B) is in $\mathscr{T}_0$, then $X(r) > 0$ for $0 \leq r \leq 1$.

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