A FREE BOUNDARY PROBLEM MODELLING ZONING IN ROCKS

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Abstract

Oscillatory zoning in rocks can be explained by a kinetic mathematical model of crystal growth. In this model, zoning is an autonomously occurring phenomenon resulting from the interaction of crystal growth dynamics and diffusion of solutes within the solution. Here the rates of crystal formation have a positive feedback dependency such that these rates depend on the composition of the crystal surface.

A moving free boundary problem is presented describing the growth of two essential crystal end-members that are formed from two solutes on a solid-solute interface. The simplest possible case is presented in which there are two first order crystal formation reactions, and all the variation of concentration is confined to one solute. Bifurcation analysis is used as a criteria for the local existence of oscillatory zoning. Under certain physical conditions, we can show, using rigourous analysis, that planar constant composition front solutions lose their stability to oscillatory solutions through a Hopf bifurcation when important parameter values exceed some critical value. The analysis is very sensitive to the precise stoichiometry of the crystal formation reactions and to the initial conditions of the state.

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Contents

Chapter 1

Introduction

Oscillatory zoning is observed in many naturally occurring crystals. With no externally imposed periodicities on the state, this zoning can be explained as an autonomously occurring phenomenon resulting from the interaction of crystal growth dynamics and diffusion of solutes within the melt [22]. For example, naturally occurring plagioclase feldspar frequently exhibits oscillatory zoning between two end-member crystals: anorthite, $CaAl_2Si_2O_8$, and albite, $NaAlSi_3O_8$. In particular, quantitative results have already been obtained on certain parameters that control the oscillatory behaviour in plagioclase feldspar [16].

Any mathematical model describing crystal growth from melts should incorporate the following qualitative ideas from [22]. First, for oscillation to occur we require a potential feedback loop in the chemical kinetics of crystal growth, i.e., a surface rich in, say, crystal A, should favour construction of A-member units over the construction of any other unit due to steric or energetic considerations. This will be achieved, as we shall see in Chapter 2, by requiring the reaction rates for the formation of crystals (which are determined by the stoichiometry of the crystal reactions) to depend on, not only the concentration

of solutes, but also on the composition of the crystal surface. Secondly, any oscillation patterns should result without the intervention of any externally imposed periodicities on the state (e.g. pressure or temperature). Zoning should be explained by the diffusion of solutes from the melts along with the associated chemical kinetics involved in the formation of crystals on the interface.

With the above ideas in mind, the simplest possible mathematical model that allows for the possibility of oscillatory zoning will be presented. We shall show analytically that zoning is achieved under certain reasonable physical conditions. In this thesis we present a moving free boundary problem describing the growth of two crystalline end-members, c_A and c_B, that are formed from two solutes, c_1 and c_2, on a solid-solute interface. Our analysis is very sensitive to the stoichiometry of the crystal formation reactions. We shall consider the simplest mathematical stoichiometry for the formation of two crystals which are represented by the two following first order reactions

$$c_1 \xrightarrow{k_A} c_A$$
$$c_2 \xrightarrow{k_B} c_B.$$

We assume that we are far from chemical equilibrium (irreversible reactions) since we are interested in the initial growth of the crystal. To simplify the analysis, all the variation in concentration will be confined to the solute c_1. This may be achieved by choosing the diffusion constant of the other species c_2 to be much larger then that of species c_1 ($D_2 \gg D_1$). Also, the rate constant of the solute with the large diffusion constant is chosen to be a constant, i.e., $k_B =$ constant. With these simplifications, the qualitative ideas above for oscillation still carry through. Lastly, the simplest form for the rate constant k_A will be chosen to incorporate the positive feedback dependency on the crystal growth. One must note that in real applications, there are multi-melt species and

multi-crystal end-member species present. The stoichiometry is much more complicated and the correct rate laws must be determined experimentally. However we start with the simpler case above, and show analytically that, even here, oscillation does indeed occur under certain physical conditions.

The thesis outline is as follows. In Chapter 2 the mathematical model is presented along with the relevant physical description for zoning. Two models will be presented based on a parameter ε, which represents the order of the thickness of the "rough" solid-solute interface. With a sharp interface ($\varepsilon = 0$) we have the *nonequilibrium fractionation surface model*, and with a rough interface ($\varepsilon > 0$) we have the *dynamic fractionation surface model* [22]. Throughout the rest of the thesis we shall concentrate only on the second model above (the stability result of Chapter 4 and the Hopf bifurcation of Chapter 5 are proven for the dynamic fractionation surface model). However, Chapter 6 will include numerical simulations for both models. At the end of Chapter 2, planar constant composition front solutions will be explicitly computed (this is possible from the choice $D_2 \gg D_1$). These special solutions correspond to homogeneous rocks with no zoning. These shall serve as our basis solutions for linearization in Chapter 4. In Chapter 3, we prove the existence of a classical solution with the desired positivity of the concentration. In Chapter 4, the question of stability of the constant composition front solutions is examined. The problem is posed as a bifurcation problem in an abstract evolution space. The necessary condition for a Hopf bifurcation is obtained, namely, that the spectrum of the linearized operator contains a pair of complex eigenvalues that cross the imaginary axis as an important parameter value exceeds some critical value while the rest of the spectrum has negative real values. The *principle of linearized stability* will be proved in this chapter. Below the critical value of the bifurcation value, the stability of the linearized solution will imply the stability

of the full nonlinear system if the initial conditions are chosen sufficiently close to the constant composition solution. In Chapter 5, the existence of a Hopf bifurcation shall be proved; the ideas of Crandall and Rabinowitz [5] and Frankel and Roytburd [7] will be employed. In Chapter 6, numerical simulations are presented which suggest that the resulting periodic orbits are stable above the critical bifurcation value. In Chapter 7, we conclude with a discussion of the results. Appendix A contains the modified van der Pol's equation which motivates the choice of the specific point about which to do our linearization and also serves to suggest a bifurcation parameter. Even though our problem is fundamentally different since we have time delays introduced through diffusion, the modified van der Pol's equation, nevertheless, serves as a guide for our local analysis. Appendix B contains definitions and basic results for the norms involving fractional powers of the linearized operator of Chapter 4. These norms are required to obtain the desired Sobolev estimates for the stability proof in Chapter 4 (Theorem 4.9). Finally, Appendix C contains regularity results for the linearized problem.

Chapter 2

The Model

In this chapter we describe more fully the growth of a rock consisting of two crystal end-members from a diffusion-kinetic process involving two solutes. These rocks are formed from the cooling of molten lava. As the lava solidifies, the solutes react chemically on a solid-solute interface to form dark and light crystals. It is the relative periodic distribution of these crystals that gives rise to the characteristic oscillatory zoning observed in rocks such as plagioclase feldspar. For this two species diffusion-kinetic model, we first state the basic equations that are involved using conservation and chemical kinetic principles. Then we present two surface models that involve the thickness of the attachment interface. Both of these models involve a positive feedback mechanism in the growth of the crystals. In Figure 2.1, the interface grows to the right at geological rates leaving the trace pattern observed in this typical cross section of plagioclase feldspar. Zoning occurs between two end-member crystals, anorthite, $CaAl_2Si_2O_8$ and albite, $NaAlSi_3O_8$. Planar growth, which initially started at the left (the core of the rock) and grew into the melt, is observed. Each x-position represents a point in the history of the growth of this rock, where at one time, a crystal surface interface seperated the rock from the melt.

The end result depicts growth from the core to the rim of the plagioclase grain.

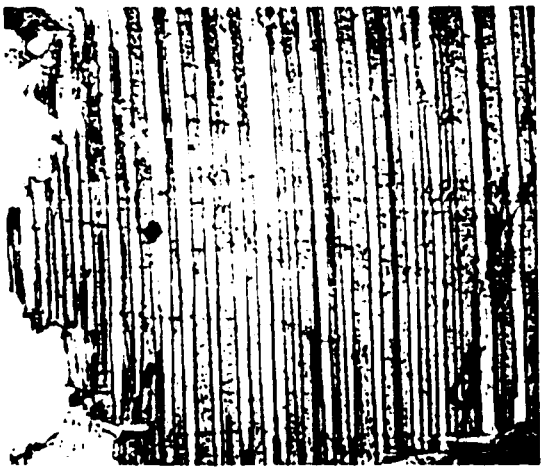

Figure 2.1 : Cross section of a sample of plagioclase feldspar.

2.1 Preliminary Analysis of the Diffusion-Kinetic Model

We model crystal growth as a moving free boundary problem with a planar front moving in the x direction. At the front, the two crystals are forming and are attaching to the solid. Let $c_1(x,t)$ and $c_2(x,t)$ be the concentrations of the relevant solutes. Denote the position of the moving planar boundary by $R(t)$. We seek solutions of $c_1(x,t)$, $c_2(x,t)$, and $R(t)$ subject to the following diffusion equation along with the following nonlinear boundary conditions

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} \qquad i = 1,2 \quad x > R(t) \tag{2.1}$$

$$\frac{dR}{dt} = v(c) \qquad x = R(t) \tag{2.2}$$

$$D_i \frac{\partial c_i}{\partial x} = I_i(c) - v(c)c_i \qquad x = R(t) \tag{2.3}$$

$$c_i \rightarrow c_{i\infty} \qquad x \rightarrow \infty \tag{2.4}$$

where

c represents both c_1 and c_2,

D_i is the diffusion constant of species i,

$v(c)$ is the velocity of the front,

$c_{i,\infty}$ is the ambient concentration of species i far from the front, and

$I_i(c)$ is the incorporation rate of species i.

The term on the left hand side of Equation (2.3) represents the flux, which describes the net transport of material by diffusion. The flux is defined to be the net amount of solute that diffuses through the planar front per unit area, per unit time in the x-direction. Empirically, one finds that the flux is directly proportional to the concentration gradient. This is known as Fick's first law,

$$\text{flux} = +D\frac{\partial c}{\partial x}.$$

Note the sign convention, positive flux corresponds to solute diffusing *into* the planar front from the right side of $x = R(t)$. Let us examine Equation (2.3) more closely. Rewriting this equation we have

$$I_i(c) = D_i\frac{\partial c_i}{\partial x} + v(c)c_i.$$

The incorporation rate $I_i(c)$ of a solute is simply the rate at which this solute enters into the interface. With a stationary front ($v(c) = 0$), the incorporation rate is simply the flux. If there is no concentration gradient ($\partial c/\partial x = 0$), the incorporation rate is the rate at which the solute is transversed by the moving front. Thus, there are two ways the solute enters the interface; one is a diffusion process represented by Fick's law, the other simply by the movement of the planar front.

From chemical kinetics we can get an explicit form for $I_i(c)$. We may also think of the incorporation rate, $I_i(c)$, as the rate at which the solute c_i is

consumed in the formation of crystals on the solid-solute interface. One may write a generalized reaction for this as

$$\begin{aligned} \tilde{a}c_1 + \tilde{b}c_2 &\xrightarrow{k_A} c_A \\ \tilde{a}c_1 + \tilde{b}c_2 &\xleftarrow{k_{-A}} c_A \\ \tilde{d}c_1 + \tilde{e}c_2 &\xrightarrow{k_B} c_B \\ \tilde{d}c_1 + \tilde{e}c_2 &\xleftarrow{k_{-B}} c_B \end{aligned} \tag{2.5}$$

where k_A, k_B, k_{-A}, and k_{-B} are rate "constants" that depend on the mole fractions of c_A and c_B. Typically, these terms only depend on the temperature. However, as we shall discuss later in this chapter, their dependency on the mole fraction (i.e., the slight affinity of a crystal to attach to a like member) is what allows for the possibility of oscillatory zoning. The positive integers $\tilde{a}$, $\tilde{b}$, $\tilde{d}$, and $\tilde{e}$ determine the stoichiometry of the chemical reactions. The stability analysis is very sensitive to the stoichiometry of (2.5); in particular, different stoichiometry will give different dispersion relations. We assume that we are far from equilibrium, i.e., k_{-A} and k_{-B} are negligible. This corresponds to the amount of c_A and c_B present to be small compared to c_1 and c_2, a situation encountered during the initial growth of the rock. Thus, consider the following reactions

$$\tilde{a}c_1 + \tilde{b}c_2 \xrightarrow{k_A} c_A$$

$$\tilde{d}c_1 + \tilde{e}c_2 \xrightarrow{k_B} c_B.$$

Mathematically, the simplest proposed mechanism for the formation of c_A and c_B is

$$\begin{aligned} c_1 &\xrightarrow{k_A} c_A \quad (\tilde{a} = 1, \tilde{b} = 0) \\ c_2 &\xrightarrow{k_B} c_B \quad (\tilde{d} = 1, \tilde{e} = 0). \end{aligned} \tag{2.6}$$

A *proposed mechanism* is simply a combination of elementary reaction steps. An *elementary reaction step* is the single step in a chemical reaction which

describes the actual event. Now we are interested in writing down reaction rates for the solutes and crystals. From chemical kinetics, one empirically finds that the reaction rate of a species is proportional to the product of the concentration of the reactants involved from the proposed mechanism. For instance, if the reaction

$$mX + nY \xrightarrow{k} P$$

is an elementary reaction, the reaction rate for P is $k[X]^m[Y]^n$ (square brackets denote concentration). Similarly, for X it is $mk[X]^m[Y]^n$. Obviously, the later rate is m times faster since for every P that is formed, m X's are consumed. So, for (2.6) the incorporation rates for c_1 and c_2 are

$$\begin{aligned} I_1(c) &= k_A c_1 \qquad (I_1(c) = \tilde{a}k_A c_1^{\tilde{a}} c_2^{\tilde{b}} + \tilde{d}k_B c_1^{\tilde{d}} c_2^{\tilde{e}}) \\ I_2(c) &= k_B c_2 \qquad (I_2(c) = \tilde{b}k_A c_1^{\tilde{a}} c_2^{\tilde{b}} + \tilde{e}k_B c_1^{\tilde{d}} c_2^{\tilde{e}}). \end{aligned}$$

Also we may write down reaction rates for c_A and c_B as

$$\begin{aligned} A &= k_A c_1 \qquad (A = k_A c_1^{\tilde{a}} c_2^{\tilde{b}}) \\ B &= k_B c_2 \qquad (B = k_B c_1^{\tilde{d}} c_2^{\tilde{e}}) \end{aligned}$$

where A and B are reaction rates for c_A and c_B. Thus, $A = I_1(c)$ and $B = I_2(c)$ for the simplest of all mechanisms (2.6).

2.2 The Nonequilibrium and Dynamic Fractionation Surface Models

As described by Ortoleva [22], an explanation for zoning results from a potential feedback loop in the chemical kinetics of crystal growth. We give a brief description below. First we may assume that $v(c) > 0$ since we are far from chemical equilibrium. Hence, at any given time we may express the mole

fraction of the crystals as a ratio of reaction rates. Thus, we may write the mole fraction of c_A as

$$f = \frac{A}{A+B}, \text{ on } x = R(t). \tag{2.7}$$

We refer to this as the **nonequilibrium fractionation relation**. The mole fraction of c_B is simply then $(1-f)$. Now if we assume that the right hand side of Equation (2.7) depends not only on c_1 and c_2 but also on the mole fraction f of c_A, it can give a nonlinear relation in f. This can allow for multiple solutions of f for a given value of c_1 and c_2. To see this analytically, substitute $A = k_A(f)c_1$ and $B = k_B(f)c_2$ into (2.7) yielding

$$f = \frac{k_A(f)c_1}{k_A(f)c_1 + k_B(f)c_2} = \frac{K(f)\frac{c_1}{c_2}}{K(f)\frac{c_1}{c_2} + 1}$$

where $K(f) = k_A(f)/k_B(f)$ is the ratio of the reaction rate constants. Solving for c_1/c_2 gives

$$\frac{c_1}{c_2} = \frac{f}{K(f)(1-f)}. \tag{2.8}$$

When $f = 0$, $c_1 = 0$ and as f approaches 1, c_1/c_2 approaches infinity. For multiple solutions, we require that a local maximum and minimum must be present (i.e., $\frac{d(c_1/c_2)}{df} = 0$). Differentiating (2.8) with respect to f gives

$$\frac{d}{df}\left(\frac{c_1}{c_2}\right) = \frac{K(f) - K'(f)f(1-f)}{K^2(f)(1-f)^2}. \tag{2.9}$$

For the numerator to equal zero, we require that $K'(f) > 0$ (i.e. $K(f)$ must be an increasing function of f). Since $K(f) = k_A(f)/k_B(f)$, this equivalently means that $k_A(f)$ is an increasing function of the mole fraction f of c_A and that $k_B(f)$ is an increasing function of the mole fraction $(1-f)$ of c_B. Thus, for any hope of oscillatory zoning, there must be a positive feedback dependency of the rate constants on the composition of the crystal surface. A possible plot for (2.8) is shown in Figure 2.2. This plot allows for multiple values of f for a

given c_1/c_2. Inverting this plot gives Figure 2.3. Here there are two branches present, the lower branch is rich in c_B whereas the upper branch is rich in c_A.

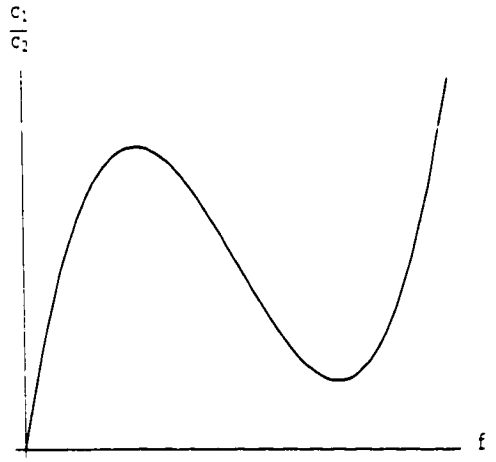

Figure 2.2 : Possible plot of c_1/c_2 vs. f.

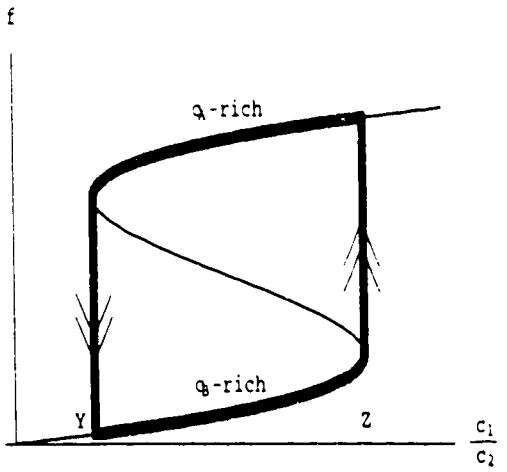

Figure 2.3 : Possible plot of f vs. c_1/c_2.

Now we give a physical argument for the requirement of the positive dependency of $K(f)$ on f. Consider the solid-solute interface where c_A and c_B are forming and attaching to the crystal surface. In this interface, c_1, c_2, c_A, and c_B are present. When the surface is rich in one crystal, there are steric factors that will favour further formation of this crystal over the other. Thus

c_A growth is favoured by c_A-rich surfaces and similarly for c_B. These physical considerations are captured by the positive dependency of $k_A(f)$ and $k_B(f)$ on the composition of the surface. Suppose the crystal surface is initially rich in c_A. Since $k_A(f)$ is an increasing function of f, one expects that c_A will attach to the surface first over c_B since its formation is favoured, i.e., the rich c_A surface has an affinity for itself. This corresponds to the top branch of Figure 2.3. However, c_1 is consumed at a faster rate than the rate it enters this interface. Thus, as the rock grows, c_1 decreases in the interface and the mole fraction f decreases. During this time, c_2 will begin to build up as the interface advances through the solute. As c_1/c_2 drops below Y, the mole fraction f then drops down to the lower branch. Now we are in a rich c_2 environment, and c_B starts to attach to the surface. Since $k_B(f)$ is an increasing function of $(1-f)$ (the mole fraction of c_B), c_B starts to attach to the surface and similarly has an affinity for itself. Similarly, more c_2 is used up in the formation of c_B than enters the interface. Thus, the mole fraction of c_B decreases (f increases) as depicted on the lower branch of Figure 2.3. Now c_1 begins to build up and as we pass Z, most of the c_2 is depleted and the mole fraction will jump up to the rich c_A upper branch completing one cycle.

Now we shall attempt to determine the mathematical form for $K(f)$ which captures the ideas above. Since $K(f)$ is an increasing function of f, we may start with the simple function

$$K(f) = a + bf$$

where a and b are constants. The term a means that there is always some attachment site on the crystal surface. This term is important because no matter how rich the surface is in one crystal, there are still attachment sites for the other crystal. Note, in our physical argument this idea is needed as

the system jumps between branches from the nonequilibrium fractionation equation. The power of f corresponds to the number of enhancement sites; c_A will attach more readily if a single crystal of A is alreday present. The above function does not allow for multiple values of f. Substituting this expression into (2.9) and setting it equal to zero gives the complex values $f = \pm i\sqrt{a/b}$ which are inadmissible. Next we try

$$K(f) = a + bf^2$$

where we have two enhancement sites; c_A will attach more readily provided two crystals of A are already present. This form will give us multiple values for f. Depending on the ratio b/a of the ratio of the reaction-rate constants $K(f)$, we can have two possible plots (see Figure 2.4). Substituting $K(f)$ into (2.9) we can find a critical value, $(b/a)_0$, where the local minimum and local maximum begin to appear. Below this critical value, there are no local extrema, whereas above this critical value there is a local minimum and local maximum (see Figure 2.4).

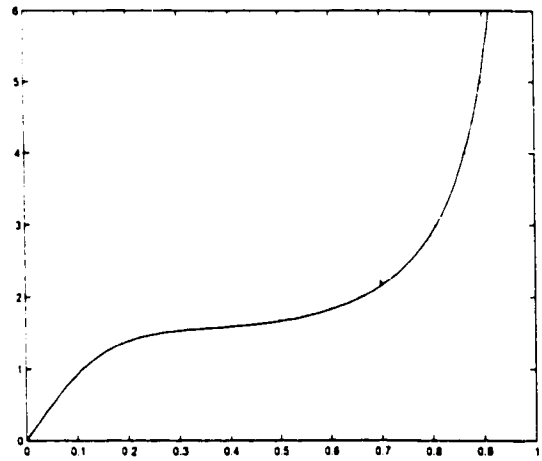

Figure 2.4a : Plot of c_1/c_2 vs. f for $b/a < (b/a)_0$.

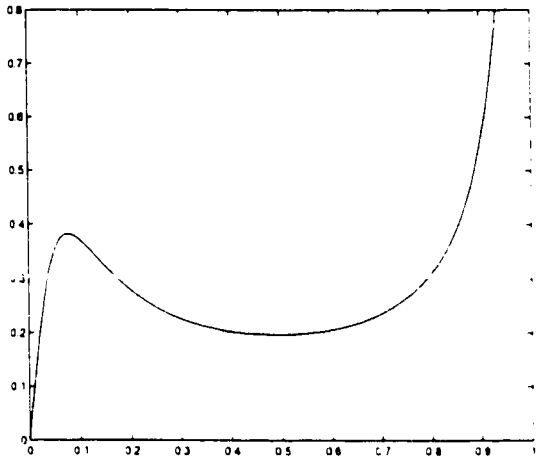

Figure 2.4b : Plot of c_1/c_2 vs. f for $b/a > (b/a)_0$.

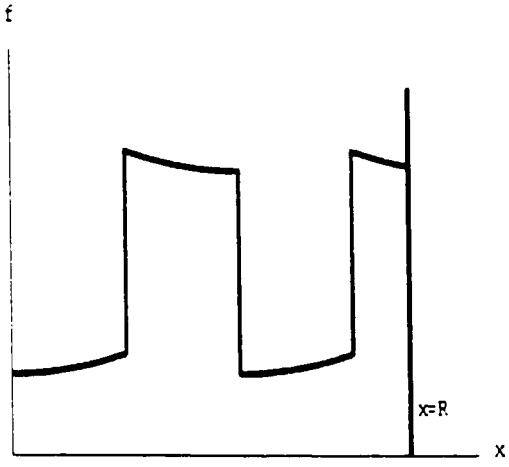

Figure 2.5 : Zoning profiles.

In analogy to the modified van der Pol's equation (see Appendix A), we shall carry out all our local stability analysis near the inflection point. Our bifurcation parameter will be b/a and we speculate that a Hopf bifurcation will occur in the vicinity of the critical value. It will be displaced from $(b/a)_0$ by the interaction of this oscillatory mechanism with the time delays introduced by diffusion (from Equation (2.1)).

Equation (2.7) results in discontinuous oscillatory zoning profiles since there is an abrupt change in f between branches in the plot of c_1/c_2 vs. f;

see Figure 2.5, a plot of f vs. $R(t)$ representing zoning profiles. To smooth out these discontinuities an improved model is introduced by the following expression for f on the front,

$$\frac{\varepsilon}{\dot{R}(t)}\frac{df}{dt} = -f + \frac{A}{A+B}.$$

Here ε is the **statistical coherence length** and it represents the order of the surface roughness amplitude. Its length is much smaller than the characteristic length associated with macroscopic zoning, yet it is large enough to capture all the microscopic rough interface where c_A and c_B are forming and attaching to the crystal surface. For a derivation of this equation above see Ortoleva [22]. When $\varepsilon = 0$ we obtain our original expression for the mole fraction of c_A. We shall refer to this $\varepsilon = 0$ model as the **nonequilibrium fractionation surface model** (nonequilibrium since we are far from chemical equilibrium). When $\varepsilon > 0$ we refer to this as the **dynamic fractionation model**. Note the correct sign of ε is positive; in the graph of c_1/c_2 vs. f, the flow must move in horizontally inward to the curve $f = A/(A+B)$ in order to get a limit cycle (this is in analogy to the modified van der Pol's equation (see Figure A.1)).

Finally, for Equation (2.2) we impose the boundary condition

$$\rho v(c) = A + B, \quad x = R(t)$$

where ρ is the density of the rock. This is a mass balance equation. The total number of crystals deposited on the surface of the interface per area, per unit time is $\rho\dot{R}(t)$. This is balanced by the rate of production of both crystals

which is simply $A + B$. Thus, in summary, our model is

$$\left.\begin{aligned}
\frac{\partial c_i}{\partial t} &= D_i \frac{\partial^2 c_i}{\partial x^2} \qquad i = 1,2 \qquad x > R(t) \\
\rho \frac{dR}{dt} &= A + B \qquad\qquad\qquad x = R(t) \\
D_i \frac{\partial c_i}{\partial x} &= I_i(c) - \dot{R}(t) c_i \qquad x = R(t) \\
\frac{\varepsilon}{R} \frac{df}{dt} &= -f + \frac{A}{A+B} \qquad x = R(t) \\
c_i &\to c_{i\infty} \qquad\qquad\qquad x \to \infty
\end{aligned}\right\} \tag{2.10}$$

where

$$\begin{aligned}
I_1 &= A &&= k_A(f) c_1 \\
I_2 &= B &&= k_B(f) c_2 \\
K(f) &= \frac{k_A(f)}{k_B(f)} &&= a + bf^2.
\end{aligned}$$

System (2.10) describes the growth of a rock consisting of two crystals that are formed from two solutes. The analysis is very sensitive to the stoichiometry of the crystal formation reactions. Our explicit expressions for I_1, I_2, A, and B above represent the simplest case, which is a set of first order reactions. Our form for $K(f)$ is the simplest that will allow for the possibility of oscillatory zoning since it allows for two branches to be present in the graph of f vs. c_1/c_2. Note, there are no externally imposed periodicities on this system; zoning is explained as an autonomous phenomenon through the interaction of the diffusion process in the melt with the chemical kinetics associated with the crystal formation reactions on the interface. To simplify the analysis even further a rescaled version will be used that encompasses the essential features above. First, assume that $D_2 \gg D_1$. From the first and third equations of System (2.10) we obtain, formally,

$$c_{2xx} = \frac{1}{D_2} c_{2t} \overset{D_2 \to \infty}{\longrightarrow} 0$$

$$c_{2x} = \frac{1}{D_2}[I_2(c) - v(c)c_2] \overset{D_2 \to \infty}{\longrightarrow} 0.$$

Thus, $c_2(x,t)$ approaches a constant in this asymptotic limit. Physically, this means that $c_2(x,t)$ diffuses into the solid-solute interface at a much faster rate than $c_1(x,t)$ and this corresponds to $c_2(x,t)$ being constant throughout the solute. With $c_2(x,t) \equiv c_{2\infty}$, the partial differential equation is identically satisfied. Another simplification is to take $k_B(f)$ to be a *constant*,

$$k_B(f) = k_b.$$

This, with our previous assumption ($D_2 \gg D_1$), will still capture all the essential features required for oscillatory zoning as described earlier in this chapter. We may replace c_1/c_2 by $c_1/c_{2\infty}$ in Figures 2.2 and 2.3 since $D_2 \gg D_1$. Since k_B is a constant, c_B no longer has an affinity for itself. All the variation is within c_1 if we let $k_A(f) = a_1 + b_1 f^2$. Species A still has an affinity for itself on the crystal surface and this can allow for oscillatory behaviour. To simplify further, take $D_1 = 1$ by rescaling distance with some typical length scale L and time with L^2/D_1. Finally, $c_{2\infty}$ may be scaled out by introducing the new variables: $\tilde{c} = c_1/c_{2\infty}$, $c_\infty = c_{1\infty}/c_{2\infty}$, $\tilde{\rho} = \rho/c_{2\infty}$, $\tilde{A} = k_A(f)\tilde{c}$, $\tilde{B} = k_b$, $\tilde{f} = f$. After dropping the tildes, the rescaled version is

$$\left.\begin{aligned}
\frac{\partial c}{\partial t} &= \frac{\partial^2 c}{\partial x^2} && x > R(t) \\
\rho\frac{dR}{dt} &= k_b K(f)c + k_b && x = R(t) \\
\frac{\partial c}{\partial x} &= k_b K(f)c - \dot{R}(t)c && x = R(t) \\
\frac{\varepsilon}{\dot{R}}\frac{df}{dt} &= -f + \frac{K(f)c}{K(f)c+1} && x = R(t) \\
c &\to c_\infty && x \to \infty
\end{aligned}\right\} \qquad (2.11)$$

where

$$K(f) = \frac{k_A(f)}{k_b} = a + bf^2.$$

2.3 The Planar Constant Composition Front

In this section we look for constant composition front solutions (i.e., solutions where the mole fraction f is a constant on the planar front). Physically, this corresponds to a homogeneous grey rock with no zoning. A preliminary analysis of the dispersion relation has already been done in the author's Master's dissertation [28]. In a suitable parameter space, there exist a pair of complex conjugate eigenvalues that cross the imaginary axis as b/a increases past a critical value $(b/a)_{cr}$. This suggests the presence of a Hopf bifurcation. In Chapter 4, the stability of the constant composition front is examined using bifurcation theory. We shall see that below the critical value, $b/a < (b/a)_{cr}$, these solutions are stable, whereas above the critical value they are unstable. In Chapter 5, we shall prove that a Hopf bifurcation does indeed take place. Chapter 6 indicates that these constant composition front solutions lose stability to periodic orbits.

The constant composition front solution is obtained by substituting travelling wave solutions of the form

$$\begin{aligned} c(x,t) &= \bar{c}(x-\bar{v}t) \\ v(t) &= \bar{v} \end{aligned}$$

into System (2.11) where $\bar{v}$ represents the constant velocity of the front. This yields the constant composition front solution,

$$\begin{aligned} \bar{c}(x-\bar{v}t) &= c_\infty + Ae^{-\bar{v}(x-\bar{v}t)} \\ \bar{v} &= k_b \\ \bar{f} &= \frac{c_\infty}{c_\infty + 1} \end{aligned}$$

where

$$\begin{aligned} A &= \frac{c_\infty}{K(\bar{f})} - c_\infty \\ K(\bar{f}) &= a + b\bar{f}^2. \end{aligned}$$

These nontrivial solutions are present if and only if

$$\rho = c_\infty + 1.$$

We remark that choosing $D_2 \gg D_1$ in the previous section has allowed us to explicitly compute a unique travelling wave solution. Otherwise, an infinite number of travelling wave solutions would exist if D_1 and D_2 are of the same order of magnitude.

Chapter 3

Classical Results

In this chapter we establish the existence of a classical solution to the free boundary problem. A maximum principle argument is then used to show that these solutions are positive. We follow the ideas of Friedman [10], where an equivalent integral representation is formulated involving Green's functions for the heat equation. These integrals are evaluated on the unknown free boundary $R(t)$. Our case is similar to Frankel and Roytburd [8], where the integral equation is written in terms of the Dirichlet condition, whereas, in Friedman's case, an integral equation involving the Neumann condition was formulated.

Consider the free boundary problem (2.11)

$$
\begin{aligned}
c_t &= c_{xx} && x > R(t),\ t > 0 && (3.1)\\
\dot{R} &= \frac{k_b}{\rho}\left(K(f)c + 1\right) && x = R(t),\ t > 0 && (3.2)\\
c_x &= B(c, f) && x = R(t),\ t > 0 && (3.3)\\
\dot{f} &= \frac{k_b}{\rho\varepsilon}\left[-f\left(K(f)c + 1\right) + K(f)c\right] && x = R(t),\ t > 0 && (3.4)
\end{aligned}
$$

where

$$B(c, f) = k_b K(f)c - \dot{R}c$$

along with initial data

$$\begin{aligned} c(x,0) &= c_0(x) \\ f(0) &= f_0 \\ R(0) &= 0. \end{aligned}$$

We require that

A1. $c_0(x)$ is continuously differentiable with $\lim_{x\to\infty} c_0(x) = c_\infty > 0$.

A2. The following compatibility condition is satisfied

$$v(0) = \frac{k_b}{\rho}\left(K(f_0)c_0(0) + 1\right)$$

where $v(t) = \dot{R}(t)$.

The condition A2 will ensure that $c(x,t)$ is a continuous solution at $t = 0$. This will allow us to employ the maximum principle in the proof of Theorem 3.3 to show that $c(x,t)$ is positive.

We begin by pointing out some preliminary properties of the boundary conditions (3.2)-(3.3). There is a linear relation between $v(t)$ and $K(f)c(R(t),t)$: the graph of v versus Kc is a line with slope k_b/ρ and intercept k_b/ρ (see Figure 3.1). For positive solutions c we shall require that $v > k_b/\rho$. Recall from Section 2.2, that the rate constant for crystal B was taken to be a constant, $k_B(f) = k_b$. Thus crystal B will attach at a constant rate, and consequently there will be a minimum velocity for crystal growth as long as the concentration c is positive. The second boundary condition, (3.3), may be written in terms of f and v,

$$c_x(R(t),t) = -\frac{\rho}{k_b K(f(t))}v(t)^2 + \left(\frac{1}{K(f(t))} + \rho\right)v(t) - k_b.$$

For a fixed time t, this is a parabola opening downward with roots $k_b K(f)$ and k_b/ρ (see Figure 3.2). Figures 3.1-3.2 will be used in the proof of Theorem 3.3

presented in Section 3.3. The case $K(f) < 1/\rho$ is more desirable since complex eigenvalues were found in this range for the linearized stability analysis in the author's Master's dissertation [28]. The scaled density and rate constant are $\rho = 1 + c_{1\infty}/c_{2\infty}$ and $K(f) = k_A(f)/k_b = (a_1 + b_1 f^2)/k_b$ respectively. They imply that $K < 1$, or alternatively that the travelling wave velocity k_b is sufficiently large. With a higher velocity there will be a build up of solute on the moving front and this may allow for the possibility of oscillatory zoning.

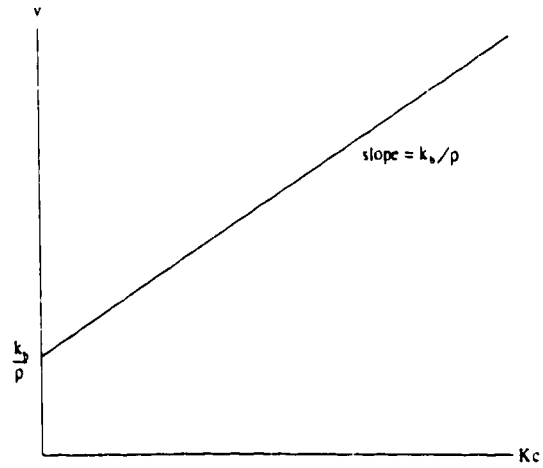

Figure 3.1 : Plot of v vs. Kc.

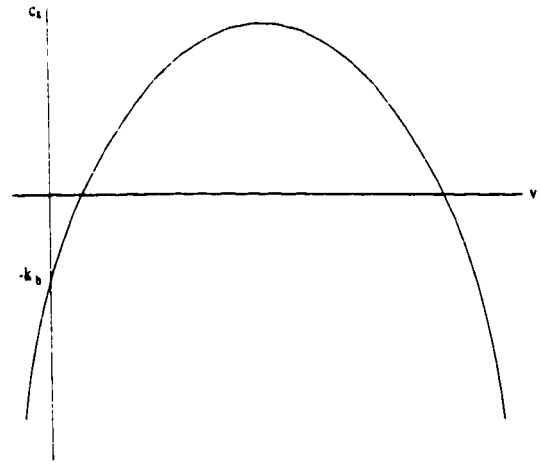

Figure 3.2 : Plot of c_x vs. v. The roots are k_b/ρ and $k_b K(f)$.

The functions $c(x,t), f(t), R(t)$ form a *classical solution* to the Equations (3.1)-(3.4), with the above prescribed initial data, if for all $t < \sigma$ $(0 < \sigma \leq \infty)$

(i) c_{xx}, c_t are continuous for $x > R(t), 0 < t < \sigma$.

(ii) c, c_x are continuous for $x \geq R(t), 0 < t < \sigma$.

(iii) c is continuous for $0 \leq t < \sigma$.

(iv) $R(t), f(t)$ are continuously differentiable for $0 \leq t < \sigma$.

(v) Equations (3.1)-(3.4) are satisfied.

3.1 The Integral Representation

The fundamental solution to the heat equation is

$$G(x,t;\xi,\tau) = \frac{1}{\sqrt{4\pi(t-\tau)}} \exp\left\{-\frac{(x-\xi)^2}{4(t-\tau)}\right\}.$$

Suppose $c(x,t), R(t), f(t)$ is a classical solution, then integrating Green's identity

$$(Gc_\xi - G_\xi c)_\xi - (cG)_\tau = 0$$

over the domain $R(\tau) < \xi < \infty, 0 < \tau < t$ gives

$$\begin{aligned} c(x,t) &= -\int_0^t G(x,t;R(\tau),\tau)\left[B(\tau) + \dot{R}(\tau)c(R(\tau),\tau)\right] d\tau \\ &\quad + \int_0^t G_\xi(x,t;R(\tau),\tau)c(R(\tau),\tau)\, d\tau \\ &\quad + \int_0^\infty G(x,t;\xi,0)c_0(\xi)\, d\xi. \end{aligned} \tag{3.5}$$

where

$$B(\tau) = B(c(R(\tau),\tau), f(\tau)).$$

Since we assume that we have a classical solution, we may choose time σ, sufficiently small such that $R(t)$ satisfies a Lipschitz condition. Thus we assume

the a priori estimate $|G_\xi(R(t),t;R(\tau),\tau)| \le C|t-\tau|^{-1/2}$. Passing to the limit $x \to R(t)^+$ in Equation (3.5) and using the boundary conditions gives the following integral equation

$$\begin{aligned} c(R(t),t) &= -\int_0^t G(R(t),t;R(\tau),\tau)k_b K(f(\tau))c(R(\tau),\tau)\,d\tau \\ &\quad + \int_0^t G_\xi(R(t),t;R(\tau),\tau)c(R(\tau),\tau)\,d\tau \\ &\quad + \int_0^\infty G(R(t),t;\xi,0)c_0(\xi)\,d\xi. \end{aligned} \tag{3.6}$$

This is a coupled system along with

$$f(t) = f(0) + \frac{k_b}{\rho\varepsilon}\int_0^t \left[-f\,(K(f)c+1) + K(f)c\right]\,d\tau \tag{3.7}$$

$$R(t) = R(0) + \frac{k_b}{\rho}\int_0^t (K(f)c+1)\,d\tau. \tag{3.8}$$

These two equations are obtained from integrating Equations (3.4) and (3.2) with respect to time. Thus if $c(x,t), R(t), f(t)$ is a classical solution to the free boundary problem then $c(R(t),t), f(t)$ solves the integral equations (3.6)-(3.7) respectively, where $R(t)$ is given by (3.8).

Suppose conversely, for some $\sigma > 0$ $(0 \le t < \sigma)$ that $c(R(t),t), f(t)$ is a continuous solution of (3.6)-(3.7) with $R(t)$ defined by (3.8). Now we shall establish the equivalence of these integral equations to the original free boundary problem. The integral equation (3.5) defines a solution to the heat equation. Equation (3.4) is trivially satisfied. Also $c(x,t) \overset{x\to R(t)^+}{\longrightarrow} c(R(t),t)$ since $c(R(t),t)$ is a solution to the integral equation (3.6) which was defined by this limit. We need to verify Equation (3.3),

$$\lim_{x\to R(t)^+} c_x(x,t) = B(c(R(t),t),f(t)) = B(t).$$

Integrating Green's identity and subtracting (3.5) yields

$$\int_0^t G(x,t;R(\tau),\tau)\left[c_\xi(R(\tau),\tau) - B(\tau)\right]\,d\tau = 0.$$

Differentiating with respect to x and using the following jump condition from Friedman [10].

Lemma 3.1 *Let $\rho(t)$ $(0 \le t \le \sigma)$ be any continuous function and let $R(t)$ $(0 \le t \le \sigma)$ satisfy a Lipschitz condition. Then for any $t \in (0, \sigma]$*

$$\lim_{x \to R(t)^+} \frac{\partial}{\partial x} \int_0^\tau \rho(\tau) G(x, t; R(\tau), \tau)\, d\tau = \tfrac{1}{2}\rho(t) + \int_0^t \rho(\tau) \left[G_x(x, t; R(\tau), \tau)\right]_{x=R(t)}\, d\tau$$

gives

$$\tfrac{1}{2}\left[c_x(R(t), t) - B(t)\right] + \int_0^t G_x(R(t), t; R(\tau), \tau)\left[c_x(R(\tau), \tau) - B(\tau)\right] d\tau = 0.$$

The bound $|G_x(R(t), t; R(\tau), \tau)| < C|t - \tau|^{-1/2}$ implies that the above equation is a contraction mapping for sufficiently small t. Thus

$$c_x(R(t), t) - B(t) = 0,$$

and the equivalence between the free boundary problem (3.1)-(3.4) and the integral equations (3.5)-(3.8) is complete.

3.2 Local Existence and Uniqueness

In this section we prove that a unique solution exists for the integral representation for small times $0 \le t < \sigma$, i.e., where σ is sufficiently small. This will involve showing that the integral equations are contraction mappings on a suitable Banach space. Let C_σ denote the Banach space of continuous functions $v(t)$ defined on $0 \le t \le \sigma$ with the uniform norm

$$\|v\| = \sup_{0 \le t \le \sigma} |v(t)|.$$

Let the ball of radius M be defined by

$$C_{\sigma,M} = \{v \in C_\sigma : \|v\| \leq M\}.$$

Consider the following nonlinear transformation defined on the cartesian product,

$$T : C_{\sigma,M} \times C_{\sigma,M} \to C_\sigma \times C_\sigma$$

$$T\begin{pmatrix} c \\ f \end{pmatrix} = \begin{pmatrix} T_1(c,f) \\ T_2(c,f) \end{pmatrix}$$

where $T_1(c,f)$ and $T_2(c,f)$ are the right hand sides of Equations (3.6)-(3.7) respectively. Clearly $C_\sigma \times C_\sigma$ is a Banach space with

$$\left\| \begin{pmatrix} c \\ f \end{pmatrix} \right\| = \|c\| + \|f\|.$$

We need to show that

(1) $T : C_{\sigma,M} \times C_{\sigma,M} \to C_{\sigma,M} \times C_{\sigma,M}$, and

(2) T is a contraction mapping.

Then the Banach contraction principle gives the existence of a unique point $(c^*, f^*) \in C_{\sigma,M} \times C_{\sigma,M}$ such that

$$\begin{pmatrix} c^* \\ f^* \end{pmatrix} = T\begin{pmatrix} c^* \\ f^* \end{pmatrix}.$$

(1) $T : C_{\sigma,M} \times C_{\sigma,M} \to C_{\sigma,M} \times C_{\sigma,M}$

Note that

$$|G(x,t;\xi,\tau)| \leq \frac{C}{|t-\tau|^{1/2}}.$$

The Lipschitz condition for the position of the free boundary, locally in time

$$\begin{aligned} |R(t) - R(\tau)| &= \frac{k_b}{\rho} \left| \int_\tau^t (Kc + 1)\, d\xi \right| \\ &\leq \frac{k_b}{\rho} \left[(a + bM^2)M + 1 \right] |t - \tau| = M^*|t - \tau| \end{aligned}$$

gives the estimate

$$|G_\xi(R(t),t;R(\tau),\tau)| \le C\frac{M^*}{|t-\tau|^{1/2}}.$$

Let $T_1(c,f) = I_1 + I_2 + I_3$ where I_i denotes the three integrals of the right hand side of Equation (3.6), then we have

$$\begin{aligned}
|I_1| &\le k_b\Big|\int_0^t GKc\,d\tau\Big| \le C_1\left[(a+bM^2)M\right]\Big|\int_0^t G\,d\tau\Big| \\
&\le C_1\left[(a+bM^2)M\right]\sqrt{t} \\
|I_2| &\le \tfrac{1}{2}\Big|\int_0^t \frac{R(t)-R(\tau)}{t-\tau}Gc\,d\tau\Big| \le C_2MM^*\sqrt{t} \\
|I_3| &\le \Big|C\int_0^\infty c_0(\xi)t^{-1/2}e^{-(R(t)-\xi)^2/4t}\,d\xi\Big| \le \|c_0\|_\infty
\end{aligned}$$

where $\|\cdot\|_\infty$ denotes the L^∞ norm. Hence,

$$\|T_1(c,f)\| \le C_1\left[(a+bM^2)M\right]\sqrt{\sigma} + C_2MM^*\sqrt{\sigma} + \|c_0\|_\infty .$$

The estimate for $T_2(c,f)$ is

$$\begin{aligned}
\|T_2(c,f)\| &= \left\|f(0) + \frac{k_b}{\rho\varepsilon}\int_0^t\left[-f(Kc+1)+Kc\right]d\tau\right\| \\
&\le |f_0| + \tfrac{k_b}{\rho\varepsilon}M\left[(a+bM^2)M+1+(a+bM^2)\right]\sigma \\
&\le |f_0| + \tfrac{1}{\varepsilon}MM^*\sigma + \tfrac{k_b}{\rho\varepsilon}M(a+bM^2)\sigma.
\end{aligned}$$

Thus, if we take $\sigma < 1$,

$$\begin{aligned}
\left\|T\begin{pmatrix} c \\ f \end{pmatrix}\right\| \le\ & \left[C_1(a+bM^2)M + C_2MM^*\right. \\
& \left. + \tfrac{1}{\varepsilon}MM^* + \tfrac{k_b}{\rho\varepsilon}M(a+bM^2)\right]\sqrt{\sigma} \\
& + \|c_0\|_\infty + |f_0|.
\end{aligned}$$

Take $M = \|c_0\|_\infty + |f_0| + 1$, then if,

$$\sqrt{\sigma} \le \frac{1}{C_1(a+bM^2)M + C_2MM^* + \frac{1}{\varepsilon}MM^* + \frac{k_b}{\rho\varepsilon}M(a+bM^2)}$$

we have

$$\left\| T \begin{pmatrix} c \\ f \end{pmatrix} \right\| \leq M.$$

Thus T maps $C_{\sigma,M} \times C_{\sigma,M}$ into itself.

(2) T is a contraction mapping.

Let $\phi = T_2(c, f)$ and $\phi' = T_2(c', f')$, then

$$\phi - \phi' = \frac{k_b}{\rho\varepsilon} \int_0^t \left[(Kc - K'c') + (f' - f) + (K'f'c' - Kfc) \right] d\tau.$$

Using the triangle inequality we have the following bound

$$\begin{aligned} \|cf - c'f'\| &= \|cf - cf' + cf' - c'f'\| \\ &\leq M \|f - f'\| + M \|c - c'\|. \end{aligned}$$

Similarly,

$$\begin{aligned} \|cf^2 - c'f'^2\| &\leq 2M^2 \|f - f'\| + M^2 \|c - c'\| \\ \|cf^3 - c'f'^3\| &\leq 3M^3 \|f - f'\| + M^3 \|c - c'\|. \end{aligned}$$

Thus

$$\|T_2(c, f) - T_2(c', f')\| \leq A_1 \|c - c'\| + A_2 \|f - f'\|.$$

Letting $\varphi = T_1(c, f), \varphi' = T_1(c', f')$ we obtain

$$\begin{aligned} \varphi - \varphi' &= k_b \left\{ - \int_0^t G(R(t), t; R(\tau), \tau) K c \, d\tau \right. \\ &\quad \left. + \int_0^t G(R'(t), t; R'(\tau), \tau) K' c' \, d\tau \right\} \\ &\quad + \left\{ \int_0^t G_\xi(R(t), t; R(\tau), \tau) c \, d\tau - \int_0^t G_\xi(R'(t), t; R'(\tau), \tau) c' \, d\tau \right\} \\ &\quad + \left\{ \int_0^\infty G(R(t), t; \xi, 0) c_0(\xi) \, d\xi - \int_0^\infty G(R'(t), t; \xi, 0) c_0(\xi) \, d\xi \right\} \\ &= B_1 + B_2 + B_3. \end{aligned}$$

For the estimates B_i, we follow Frankel and Roytburd [8]. Using the mean value theorem twice, we obtain the following identity

$$\begin{aligned}
|\Delta G| &\equiv |G(R(t),t;R(\tau),\tau) - G(R'(t),t;R'(\tau),\tau)| \\
&= |G(R(t)-R(\tau),t-\tau;0,0) - G(R'(t)-R'(\tau),t-\tau;0,0)| \\
&= |G_x(\tilde{R},t-\tau;0,0)||R(t)-R(\tau)-(R'(t)-R'(\tau))| \\
&= \left|\frac{\tilde{R}G(\tilde{R},t-\tau;0,0)}{2(t-\tau)}\right||R(t)-R(\tau)-(R'(t)-R'(\tau))| \\
&= |\frac{\tilde{R}}{2}G(\tilde{R},t-\tau;0,0)|\left|\frac{R(t)-R(\tau)-(R'(t)-R'(\tau))}{t-\tau}\right| \\
&= \frac{1}{2}\left|\frac{dR(\tilde{\tau})}{dt}-\frac{dR'(\tilde{\tau})}{dt}\right||\tilde{R}G(\tilde{R},t-\tau;0,0)|
\end{aligned}$$

where $\tau < \tilde{\tau} < t$ and $\tilde{R}$ is strictly between $R(t)-R(\tau)$ and $R'(t)-R'(\tau)$. Since

$$\begin{aligned}
\left\|\frac{dR(\tilde{\tau})}{dt}-\frac{dR'(\tilde{\tau})}{dt}\right\| &= \frac{k_b}{\rho}\|Kc-K'c'\| \\
&\le L(\|c-c'\|+\|f-f'\|)
\end{aligned}$$

and

$$|\tilde{R}| \le \max\{|R(t)-R(\tau)|,|R'(t)-R'(\tau)|\} \le M^*|t-\tau|$$

we have

$$\begin{aligned}
|\Delta G| &\le \tfrac{1}{2}L(\|c-c'\|+\|f-f'\|)M^*|t-\tau|\frac{C}{|t-\tau|^{1/2}} \\
&\le K_1(\|c-c'\|+\|f-f'\|)|t-\tau|^{1/2}.
\end{aligned}$$

Similarly

$$\begin{aligned}
|\Delta\frac{\partial G}{\partial \xi}| &\equiv |G_\xi(R(t),t;R(\tau),\tau) - G_\xi(R'(t),t;R'(\tau),\tau)| \\
&\le K_2(\|c-c'\|+\|f-f'\|)|t-\tau|^{-1/2}.
\end{aligned}$$

Now we can make the following estimates for B_1 and B_2:

$$\begin{aligned} |B_1| &= k_b \left| \int_0^t \Delta G K c \, d\tau - \int_0^t G(R'(t), t; R'(\tau), \tau) \left[K'c' - Kc \right] d\tau \right| \\ &\leq K_3 \left(\|c - c'\| + \|f - f'\| \right) t^{1/2} t + K_4 \left(\|c - c'\| + \|f - f'\| \right) t^{1/2} \\ &\leq \left(K_3 t^{3/2} + K_4 t^{1/2} \right) \left(\|c - c'\| + \|f - f'\| \right) \end{aligned}$$

$$\begin{aligned} |B_2| &= \left| \int_0^t \Delta \frac{\partial G}{\partial \xi} c \, d\tau - \int_0^t \frac{\partial G'}{\partial \xi} (c' - c) \, d\tau \right| \\ &\leq K_5 \left(\|c - c'\| + \|f - f'\| \right) t^{1/2} + K_6 \|c - c'\| t^{1/2}. \end{aligned}$$

For the last estimate B_3, we define

$$\begin{aligned} \delta G &\equiv G(R(t), t; \xi, 0) - G(R'(t), t; \xi, 0) \\ &= G(R(t) - \xi, t; 0, 0) - G(R'(t) - \xi, t; 0, 0). \end{aligned}$$

We now subdivide the spatial coordinate, suppose $0 < R'(t) < R(t)$. Then

$$\begin{aligned} B_3 &= \int_0^{R'(t)} \delta G c_0(\xi) \, d\xi + \int_{R'(t)}^{R(t)} \delta G c_0(\xi) \, d\xi + \int_{R(t)}^{\infty} \delta G c_0(\xi) \, d\xi \\ &= B_{31} + B_{32} + B_{33}. \end{aligned}$$

By the mean value theorem

$$\begin{aligned} \delta G &= G_x(\tilde{R} - \xi, t; 0, 0) \left[R(t) - R'(t) \right] \\ &= -\frac{R(t) - R'(t)}{2t} (\tilde{R} - \xi) G(\tilde{R} - \xi, t; 0, 0), \end{aligned}$$

where $R'(t) < \tilde{R}(t, \xi) < R(t)$. For the first and last integral, we use the estimate

$$\begin{aligned} (\tilde{R} - \xi) G(\tilde{R} - \xi, t; 0, 0) &= (4\pi t)^{-1/2} (\tilde{R} - \xi) e^{-(\tilde{R} - \xi)^2 / 4t} \\ &= (4\pi t)^{-1/2} \frac{\tilde{R} - \xi}{\sqrt{8\pi t}} e^{-(\tilde{R} - \xi)^2 / 8t} \sqrt{8\pi t} e^{-(\tilde{R} - \xi)^2 / 8t} \\ &\leq C G(\tilde{R} - \xi, 2t; 0, 0) t^{1/2}. \end{aligned}$$

For the first integral we have $0 < \xi < R' < \tilde{R} < R$, thus

$$G(\tilde{R} - \xi, 2t; 0, 0) \leq G(R'(t) - \xi, 2t; 0, 0).$$

Similarly, for the third integral we use

$$G(\hat{R} - \xi, 2t; 0, 0) \leq G(R(t) - \xi, 2t; 0, 0).$$

Thus

$$\begin{aligned} |B_{33}| &\leq C \left| \frac{R(t) - R'(t)}{t} \right| t^{1/2} \int_{R(t)}^{\infty} G(R - \xi, 2t; 0, 0) |c_0(\xi)| \, d\xi \\ &\leq C \left(\|c - c'\| + \|f - f'\| \right) t^{1/2} \|c_0\|_\infty \end{aligned}$$

and

$$|B_{31}| \leq C \left(\|c - c'\| + \|f - f'\| \right) t^{1/2} \|c_0\|_\infty .$$

The second estimate is

$$\begin{aligned} |B_{32}| &\leq 2|R(t) - R'(t)| \sup G \, \|c_0\|_\infty \\ &\leq C \left(\|c - c'\| + \|f - f'\| \right) t t^{-1/2} \|c_0\|_\infty \\ &\leq C \left(\|c - c'\| + \|f - f'\| \right) \|c_0\|_\infty t^{1/2}. \end{aligned}$$

The above three estimates give

$$|B_3| \leq K_7 \left(\|c - c'\| + \|f - f'\| \right) \|c_0\|_\infty t^{1/2}.$$

Note that this estimate holds also for $R'(t) < 0 < R(t)$ and $R'(t) < R(t) < 0$.

Combining all the estimates above yields

$$\left\| T \begin{pmatrix} c \\ f \end{pmatrix} - T \begin{pmatrix} c' \\ f' \end{pmatrix} \right\| = \|T_1(c, f) - T_1(c', f')\| + \|T_2(c, f) - T_2(c', f')\|$$

$$
\begin{aligned}
&\leq \left\{K_3 t^{3/2} + (K_4 + K_5 + K_6 + K_7 \|c_0\|_\infty)\, t^{1/2}\right\} \\
&\quad \times (\|c - c'\| + \|f - f'\|) \\
&\quad + A_1 \|c - c'\|\, t + A_2 \|f - f'\|\, t \\
&\leq \left(K_8 \sigma^{3/2} + K_9 \sigma^{1/2} + K_{10} \sigma\right) (\|c - c'\| + \|f - f'\|) \\
&\leq (K_8 + K_9 + K_{10})\, \sigma^{1/2} (\|c - c'\| + \|f - f'\|)
\end{aligned}
$$

provided $\sigma < 1$. Now if we also choose σ such that

$$(K_8 + K_9 + K_{10})\, \sigma^{1/2} < 1,$$

then T is a contraction mapping on $B_{\sigma,M} \times B_{\sigma,M}$.

Theorem 3.2 *There exists a $\sigma > 0$ such that the free boundary problem (3.1)-(3.4) with continuously differentiable data $c_0(x)$ satisfying A1 and the compatibility condition A2, has a unique classical solution for $0 < t < \sigma$.*

Proof: This follows from the results of Sections 3.1 and 3.2. Note that any solution, regardless if it is bounded by M or not, must coincide with the above solution to the integral equation in their common interval of existence. See Friedman [10] for more details. □

3.3 Positive Solutions

In this section we prove that the concentration and mole fraction are positive. Recall that for positive concentration solutions, there will be a minimum free boundary velocity, k_b/ρ, corresponding to the constant rate of attachment of crystal B (see Chapter 2). The following argument is similar to Roytburd and Frankel's [8]; we shall comment on the differences at the end of the proof.

Theorem 3.3 *Suppose there exists a classical solution* $c(x,t), f(t), R(t)$ *for* $0 \le t < \sigma$ *and that the initial data* $c_0(x)$ *and* $f_0 \in (0,1)$ *are nonnegative with* $c_0(x) > 0$. *Suppose that* $1/\rho < K_{\min} = a$ *or* $K_{\max} = a + b < 1/\rho$. *If (A1) and (A2) hold then*

$$0 \le c(x,t),$$

$$\frac{k_b}{\rho} \le v(t),$$

$$0 \le f(t) < 1.$$

Moreover, if $K(f) < 1/\rho$ *then* $c_x(R(t),t) < 0$. *If we assume, in addition to A1 and A2,*

$$A3. \qquad c_{0x}(0) = B(c_0(0), f_0)$$

then

$$c_x(x,t) \le \max[c_{0x}(x), c_x(R(t),t)].$$

Proof: By the continuity of c and since $c_0(0) > 0$, we have $c(R(t),t) > 0$ for sufficiently small times. From Equation (3.2), we have

$$v(t) > \frac{k_b}{\rho} \Leftrightarrow c(R(t),t) > 0.$$

Define

$$T^* = \sup\{t : v(t) > \frac{k_b}{\rho} \text{ for } 0 < t < \sigma\} \quad \text{and}$$

$$D_{T^*} = \{(x,t) : x > R(t), 0 < t < T^*\}.$$

By the maximum principle, $c(x,t) \ge 0$ in D_{T^*}. Now we prove that σ cannot be larger than T^*. Let $T^* < \sigma$, then $v(T^*) = k_b/\rho$ and $c(R(T^*), T^*) = 0$. We need to use the boundary condition involving c_x in order to get a contradiction. As suggested by Figure 3.2, this boundary condition has roots at

$$v(t) = \frac{k_b}{\rho}, v(t) = k_b K(f).$$

In the interval $[0, T^*]$, $f(t)$ is bounded in $[0, 1)$ (see the end of the proof). Suppose $K_{\max} = a+b < 1/\rho$. Then $K(f(T^*)) < 1/\rho$. At $t = T^*$, $c_x(R(T^*), T^*) = 0$, and so we choose a time arbitrarily smaller,

$$T' = T^* - \delta$$

such that $K(f(T')) < 1/\rho$, i.e., $K(f) < 1/\rho$ for $t \in [T', T^*]$. In the interval $[0, T']$, $v > k_b/\rho$ and c will attain a positive minimum at some time $T'' \in [0, T']$,

$$c_x(R(T''), T'') \geq 0.$$

We can always choose δ sufficiently small such that the minimum of c is on the boundary $x = R(t)$ as opposed on $t = 0$ since $c_0(x) > 0$. But from the boundary condition (3.3)

$$\begin{aligned} c_x(R(T''), T'') &= (k_b K(f) - v)\, c \\ &< \left(\frac{k_b}{\rho} - v\right) c \\ &< 0. \end{aligned}$$

This gives a contradiction, thus c must be positive. Similarly, if $K_{\min} = a > 1/\rho$ then $K(f(T^*)) > 1/\rho$. We choose a time arbitrarily larger than T^*, $T' = T^* + \delta$, to obtain a contradiction. In this case, we assume that c attains negative values in $[T^*, T']$. Thus there exists a time $T'' \in [T^*, T']$ where c attains a negative minimum,

$$c_x(R(T''), T'') \geq 0.$$

Again from the boundary condition (3.3)

$$\begin{aligned} c_x(R(T''),T'') &= (k_b K(f) - v)\, c \\ &= (v - k_b K(f))\,|c| \\ &< k_b \left(\frac{1}{\rho} - K(f)\right)|c| \\ &< 0 \end{aligned}$$

we obtain the desired contradiction.

Note that $c \geq 0$ implies that $f \geq 0$. From the differential equation involving f, the horizontal component of the vector field of the phase plane $(f(t), c(R(t),t))$ points towards the nullcline $\dot{f} = 0$. This nullcline is given by the curve $f = Kc/(Kc+1) = (v - k_b/\rho)/v$, which has positive f values in $[0,1]$ for positive $c(R(t),t)$. Since $c(R(t),t) \geq 0, f_0 > 0$, the trajectories of $(f(t), c(R(t),t))$ will lie in the positive quadrant.

The estimate for c_x follows immediately from the maximum principle and condition A3. Note that $u = c_x$ satisfies the heat equation with the boundary condition $u(R(t),t) = c_x(R(t),t)$. We also have $u(x,t) \xrightarrow{t\to 0} c_{0x}(x)$ for $x > 0$ and at $x = 0$ by A3. Thus u is continuous at $t = 0$ and $x = R(t)$, and then by the maximum principle we obtain the desired estimate. Note that $c_x(R(t),t)$ has a maximum value since $K(f)$ is bounded between $K_{\min} = K(0) = a$ and $K_{\max} = K(1) = a + b$ (see Figure 3.2). □

This proof differs from Frankel and Roytburd [8] in the following way; in our case we had not only $c(R(T^*),T^*) = 0$ but also $c_x(R(T^*),T^*) = 0$. Thus it was necessary to obtain a contradiction at a time close to T^*.

Remark 3.4 *The condition $K(f) < 1/\rho$ gives $c_x(R(t),t) < 0$. This is a condition that we required in order to obtain oscillatory solutions for the linearized problem. The linearized stability analysis was performed about the constant*

composition front (the travelling wave solution). Selecting a suitable parameter space, the spectrum of the linearized problem consists of a pair of complex conjugate roots that cross the imaginary axis as the parameter is varied. Physically, the condition $K(f) < 1/\rho$, means that the concentration at the boundary is greater than the surrounding medium. Here the travelling wave velocity k_b was sufficiently large to allow the solute to accumulate on the moving boundary.

Since f is bounded between 0 and 1, the solution curve $(c(R(t),t), v(t))$ must lie between the lines given in Figure 3.3. The bottom line has slope $k_b K_{\min}/\rho$ whereas the upper line has slope $k_b K_{\max}/\rho$, where $K_{\min} = K(0) = a$, $K_{\max} = K(1) = a + b$. Similarly, for the case $k_b/\rho > k_b K_{\max}$, the graph of $c_x(R(t),t)$ versus v must lie in the region $v > k_b/\rho$ and between the two parabolas of Figure 3.4. The other cases may be similarly plotted.

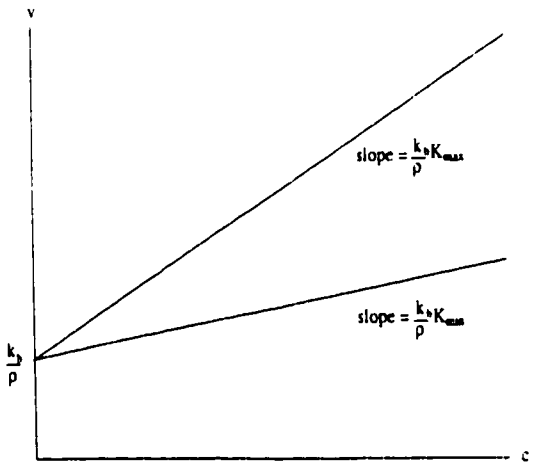

Figure 3.3 : Plot of v vs. c. The trajectory $(c(R(t),t), v(t))$ must lie between these two lines.

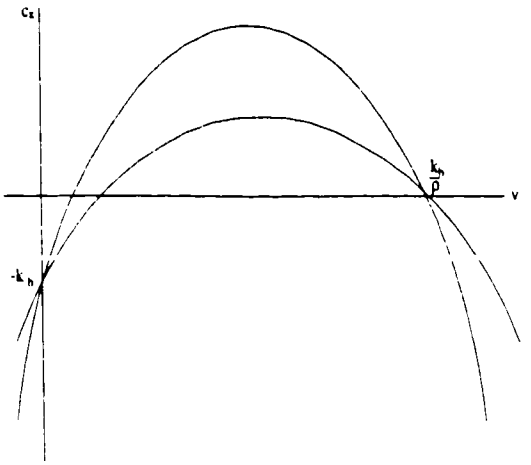

Figure 3.4 : Plot of c_x vs. v when $k_b K_{\max} < k_b/\rho$. In this case $(v, c_x(R(t), t))$ lies in the region between the parabolas and $v > k_b/\rho$.

3.4 Comments on Global Existence

From Equation (3.8), the position $R(t)$ may be written in two parts,

$$R(t) - R(\tau) = \frac{k_b}{\rho}(t - \tau) + \frac{k_b}{\rho}\int_\tau^t K(f(s))c(R(s), s)\,ds = T_1 + T_2$$

where the first part has a Lipschitz constant of k_b/ρ while the second part contains an integrand depending on f and $c(R(t), t)$. For each individual term there are methods to establish global existence. For the Lipschitz term by itself ($T_2 = 0$), one may use the procedure used to prove (3.6), integrating time from $t_0 - \delta$ to t instead of from 0 to t. See Friedman [10] for more details. For similar terms of the second type, Baillon, Bertsch, Chadam, Ortoleva, and Peletier [2] have proven global existence for small initial conditions.

For both terms, the two methods above cannot be used simultaneously. However, in Chapter 4, a global result is established for small initial data and for a certain parameter space (see Theorem 4.9). The drawback here, as opposed to the methods above, is that the parameter space must lie in the stable range, i.e., where the planar constant composition front is stable.

Chapter 4

Bifurcation Methods

In this chapter we shall formulate our original problem as a bifurcation problem. We shall examine the stability of the steady state solution obtained in Section 2.3 as a bifurcation parameter is varied. Note that in Chapter 3 we have the existence of a general classical solution provided that the initial data is sufficiently smooth.. However, this does not provide any information about the stability of our base solution as the parameter space varies, and consequently, we address this issue through the modern approach of bifurcation theory. The partial differential equation along with the ordinary differential equation involving the mole fraction can be written as an abstract nonlinear evolution system (the precise correspondence will be detailed in Sections 4.1.2 and 4.2),

$$\begin{pmatrix} u \\ f \end{pmatrix}_t = L(\mu)\begin{pmatrix} u \\ f \end{pmatrix} + \begin{pmatrix} N(u,f,\mu) \\ n(u,f,\mu) \end{pmatrix}$$

where

μ is the bifurcation parameter,

$L(\mu)$ is the linearized operator about the steady state solution,

u is the perturbation from the concentration base solution,

f is the perturbation from the mole fraction base solution, and

N and n are the nonlinear operators such that

$$N(0,0,\mu) = N_u(0,0,\mu) = N_f(0,0,\mu) = 0$$
$$n(0,0,\mu) = n_u(0,0,\mu) = n_f(0,0,\mu) = 0.$$

The nonstandard feature here is the coupling of the ordinary equation with the partial differential equation. Such systems, even where u and f can be decoupled may have a subtle effect on the spectrum; i.e., if

$$L(\mu) = \begin{pmatrix} L_1(\mu) & 0 \\ 0 & l_2(\mu) \end{pmatrix}$$

one may have $\sigma(L) \neq \sigma(L_1)$ where σ denotes the spectrum of a given linear operator (see Appendix B).

In this formulation our partial differential equation appears as an ordinary differential equation in a suitable Banach space, B, which will be specified in the next section. We are interested in the following initial value problem

$$\begin{pmatrix} u \\ f \end{pmatrix}_t = L(\mu)\begin{pmatrix} u \\ f \end{pmatrix} + \begin{pmatrix} N(u,f,\mu) \\ n(u,f,\mu) \end{pmatrix}$$
$$\begin{pmatrix} u(0) \\ f(0) \end{pmatrix} = \begin{pmatrix} u_0 \\ f_0 \end{pmatrix}$$

where we identify $u(\cdot) = u(\cdot,t)$ as an element of the Banach space, and $f(\cdot)$ as an element of the (non-negative) real line $\mathbf{R}$ where both of these variables are parameterized by time t. The initial data (u_0, f_0) is an element of the cartesian product $B \times \mathbf{R}$. The linearized problem will be solved using semigroup

theory. We shall follow the philosophy of Henry [18], and Hale and Meyer [14], where methods from ordinary differential equations are generalized. First the state space will be decomposed into subspaces invariant with respect to linearization, and then exponential bounds will be established for the solution to the linearized equation. These bounds will be used in the nonlinear analysis. A generalization of the variation of constants formula is then required to tackle the full nonlinear problem. Stability will be established for small initial data and for μ below some critical value by employing a contraction mapping principle.

4.1 Linearized Problem

In Chapter 2, a constant composition front solution was found. Linearizing about this solution will give us the necessary conditions for a Hopf bifurcation (see [28]). We now perform some preliminary transformations. The following change of coordinates will translate the moving interface to the origin,

$$\begin{aligned} x' &= x - R(t) \\ t' &= t. \end{aligned}$$

Now we make the following perturbations about the planar solutions,

$$\begin{aligned} c(x,t) &= c_1(x,t) + \bar{c}(x), \\ f(t) &= f_1(t) + \bar{f}, \\ v(t) &= v_1(t) + \bar{v}. \end{aligned}$$

Dropping the primes and the subscripts, the transformed system is

$$\left.\begin{aligned} c_t &= c_{xx} + (v(t) + k_b)c_x - k_b A v(t) e^{-k_b x} && x > 0 \\ v(t) &= \frac{k_b}{\rho}\left(k(f)(\bar{c} + c) - c_\infty\right) && x = 0 \\ c_x &= k_b k(f)(\bar{c} + c) - v(t)(\bar{c} + c) - k_b c - k_b c_\infty && x = 0 \\ \dot{f} &= \frac{k_b}{\rho\varepsilon}\left[-\bar{f} - f + k(f)(\bar{c} + c)(1 - \bar{f} - f)\right] && x = 0 \\ c &\to 0 && x \to \infty \end{aligned}\right\} \tag{4.1}$$

where

$$k(f) = a + b\bar{f}^2 + 2b\bar{f}f + bf^2. \tag{4.2}$$

The travelling wave solution is now $(c, v, f) = (0, 0, 0)$. Note that the boundary conditions are evaluated at $x = 0$ as opposed to the moving boundary. This is done at the expense of boundary terms appearing in the partial differential equation. Linearizing the system about $(0, 0, 0)$ gives

$$\left.\begin{aligned} c_t &= c_{xx} + k_b c_x - k_b A v(t) e^{-k_b x} && x > 0 \\ v(t) &= \frac{k_b}{\rho}\left(k(0)c + k'(0)\bar{c}f\right) && x = 0 \\ c_x &= k_b\left(k(0) - 1\right)c + k_b k'(0)\bar{c}f - \bar{c}v && x = 0 \\ \dot{f} &= \frac{k_b}{\rho\varepsilon}\left[\left(-\rho + k'(0)\bar{c}(1 - \bar{f})\right)f \right. && x = 0 \\ &\quad \left. + k(0)(1 - \bar{f})c\right] \\ c &\to 0 && x \to \infty. \end{aligned}\right\} \tag{4.3}$$

Next we consider the parameter space $(\varepsilon, c_\infty, k_b, a, b)$. The value of the density shall henceforth be fixed at $\rho = 1 + c_\infty$. (Recall that this is the condition for nontrivial travelling wave solutions). From our discussion in Chapter 2, we choose $\mu = b/a$ as our bifurcation parameter. Recall that this quantity is a measure of the affinity of like crystals to attach to the moving interface. The

other quantities, $\varepsilon, c_\infty, k_b$, and a will be held constant as μ is varied. Under certain values of the parameter space (specific values will be given in Chapter 6) one can show that the spectrum $\sigma(L)$ of the linearized problem lies within the region

$$(\mathrm{Im}(\lambda))^2 \leq -k_0^2 \mathrm{Re}(\lambda) \quad (\lambda \in \mathbf{C})$$

along with a pair of eigenvalues that cross the imaginary axis as μ varies. These calculations have been done in the author's Masters dissertation [28]. This is the standard formulation of the Hopf bifurcation except for the addition of zero to the spectrum. This latter problem, as we shall see, is easily remedied by employing Sattinger's idea [25]; the continuous spectrum may be shifted by the introduction of weights. We shall now summarize in the next subsection the results in terms of an eigenvalue problem.

4.1.1 The Linearized Eigenvalue Problem and its Spectrum

We shall now set up our evolution equation for the linearized operator along with the appropriate evolution phase space. Substituting

$$\begin{aligned} c(x,t) &= e^{\lambda t} c(x) \\ f(t) &= e^{\lambda t} f(0) \end{aligned}$$

into our linearized system

$$\begin{pmatrix} c \\ f \end{pmatrix}_t = L \begin{pmatrix} c \\ f \end{pmatrix}$$

yields the eigenvalue problem

$$L \begin{pmatrix} c(x) \\ f(0) \end{pmatrix} = \lambda \begin{pmatrix} c(x) \\ f(0) \end{pmatrix} \tag{4.4}$$

where L is the linearized operator obtained from the first and fourth equations of System (4.3) with domain

$$D(L) = \left\{(c, f) \in H^2((0,\infty)) \times \mathbf{R} : c_x = k_b\,(k(0) - 1)\,c + k_b k'(0)\bar{c}f - \bar{c}v\right\}.$$

The space $H^2((0,\infty))$ is the Sobolev space of functions which together with their first and second distributional derivatives are elements of $L^2((0,\infty))$. The definition of L incorporates the above Neumann condition, whereas, the Dirichlet boundary condition

$$v(t) = \frac{k_b}{\rho}\left(k(0)c + k'(0)\bar{c}f\right)$$

serves as our definition of the velocity. Thus c and f are regarded as the unknowns. The underlying evolution space is the Banach space $B = L^2((0,\infty)) \times \mathbf{R}$ with norm

$$\left\| \begin{pmatrix} c \\ f \end{pmatrix} \right\| = \|c\| + |f|$$

where $\|\cdot\|$ on the right hand side denotes the L^2 norm. Our space is a Hilbert space with the inner product

$$\left\langle \begin{pmatrix} c_1 \\ f_1 \end{pmatrix}, \begin{pmatrix} c_2 \\ f_2 \end{pmatrix} \right\rangle = \int_0^\infty c_1 \bar{c}_2\,dx + f_1 f_2.$$

The eigenvalue problem (4.4) can then be explicitly written as

$$\begin{pmatrix} \partial_{xx} + k_b\partial_x - \lambda & -\frac{k_b^2 A}{\rho}k'(0)\bar{c}e^{-k_b x} \\ 0 & \alpha_1 - \lambda \end{pmatrix} \begin{pmatrix} c(x) \\ f(0) \end{pmatrix} + \begin{pmatrix} -\frac{k_b^2 A}{\rho}k(0)e^{-k_b x} \\ \alpha_2 \end{pmatrix} c(0) = 0 \tag{4.5}$$

where

$$\alpha_1 = \frac{k_b}{\varepsilon\rho}\left(-\rho + k'(0)\bar{c}(1 - \bar{f})\right)$$

$$\alpha_2 = \frac{k_b}{\varepsilon\rho}k(0)(1 - \bar{f}).$$

The resulting differential equation is easily solved, giving the following solution

$$\begin{aligned} \phi(x) &= A_+(\lambda) f_0 e^{\left(-k_b+\sqrt{k_b^2+4\lambda}\right)\frac{x}{2}} + A_-(\lambda) f_0 e^{\left(-k_b-\sqrt{k_b^2+4\lambda}\right)\frac{x}{2}} \\ &\quad - \frac{k_b A}{\lambda} M(\lambda) e^{-k_b x} f_0 \\ f(0) &= f_0 \end{aligned} \tag{4.6}$$

where f_0 is an arbitrary constant. The ordinary differential equation involving f, and the remaining boundary conditions, reduce to

$$\begin{aligned} \phi(0) &= H(\lambda) f_0 \\ v(0) &= M(\lambda) f_0 \\ \phi_x(0) &= N(\lambda) f_0 \end{aligned}$$

where

$$\begin{aligned} H(\lambda) &= \frac{\lambda - \alpha_1}{\alpha_2} \\ M(\lambda) &= \frac{\varepsilon\lambda + k_b}{1 - \bar{f}} \\ N(\lambda) &= \frac{\varepsilon\lambda(k(0)\rho - \rho - c_\infty) + k(0)k_b\rho - k_b(\rho + c_\infty) + k_b k'(0)\bar{c}(1-\bar{f})}{k(0)(1-\bar{f})} \\ A_+(\lambda) &= \frac{\lambda N(\lambda) - k_b^2 A M(\lambda) - R(\lambda)\left(\lambda H(\lambda) + k_b A M(\lambda)\right)}{\lambda\sqrt{k_b^2 + 4\lambda}} \\ A_-(\lambda) &= H(\lambda) + \frac{k_b A}{\lambda} M(\lambda) - A_+(\lambda) \\ R(\lambda) &= \frac{1}{2}\left(-k_b - \sqrt{k_b^2 + 4\lambda}\right). \end{aligned}$$

A is given in Section 2.3 and $k(f)$ is given by Equation (4.2). The dependency on the bifurcation parameter μ appears explicitly only in these two terms. For $\lambda = 0$ and $\lambda = -k_b^2/4$ there are slight modifications to the terms $A_+(\lambda)$ and $A_-(\lambda)$ (due to division by zero) which we shall omit.

The first two terms of Equation (4.6) are linearly independent solutions while the third term is the particular solution to the eigenvalue equation. These two linearly independent solutions are

$$\phi_{\pm}(x) = e^{\left(-k_b \pm \sqrt{k_b^2+4\lambda}\right)\frac{x}{2}}.$$

Bounded solutions involving linear combinations of these two solutions correspond to the continuous spectrum $\sigma_C(L)$ of the linear operator in $L^2((0,\infty)) \times \mathbf{R}$,

$$-k_b^2 \mathrm{Re}(\lambda) \geq (\mathrm{Im}(\lambda))^2 .$$

Actually this condition comes from nonzero $A_+(\lambda)$ (i.e., when $\phi_+(x)$ is present). The solution $\phi_-(x)$ is always a decaying solution

$$\phi_-(x) \overset{x\to\infty}{\longrightarrow} 0.$$

A pair of eigenvalues $\lambda_\pm$ is determined by imposing the boundary conditions on this decaying solution, i.e., set $A_+(\lambda) = 0$. As discussed in the previous section, in the appropriate parameter space, these eigenvalues will cross the imaginary axis as the bifurcation value μ increases over a suitable interval I containing the critical value μ_{cr}, i.e.,

$$\begin{aligned} \lambda_\pm(\mu) &= \alpha(\mu) \pm i\beta(\mu) \qquad \text{where } \beta(\mu) \neq 0 \text{ for } \mu \in I \\ \lambda_\pm(\mu_{cr}) &= \pm i\beta(\mu_{cr}) \\ \frac{d}{d\mu}\mathrm{Re}\,\lambda(\mu)\Big|_{\mu=\mu_{cr}} &> 0 \end{aligned}$$

The eigenvectors associated with the eigenvalues $\lambda_\pm$ are

$$e_\pm = \begin{pmatrix} \psi_\pm \\ 1 \end{pmatrix}$$

where

$$\begin{aligned}\psi_{\pm}(x) &= A_{-}(\lambda_{\pm})\phi_{-}(x,\lambda_{\pm}) - \frac{k_b A}{\lambda_{\pm}} M(\lambda_{\pm}) e^{-k_b x} \\ &= A_{-}(\lambda_{\pm}) e^{-\frac{k_b}{2}x} e^{-r(\lambda_{\pm})x} - \frac{k_b A}{\lambda_{\pm}} M(\lambda_{\pm}) e^{-k_b x} \\ r(\lambda) &= \sqrt{\tfrac{k_b^2}{4} + \lambda}.\end{aligned}$$

Remark 4.1 *Looking at Equation (4.5) one might expect that $\lambda = \alpha_1$ belongs to the spectrum. This is only so if $\alpha_1 < 0$, since the boundary conditions dictate that λ must lie within the parabolic region $-k_b^2 \mathrm{Re}(\lambda) \geq (\mathrm{Im}(\lambda))^2$. This case corresponds to the initial concentration $c(x)$ satisfying $c(0) = 0$.*

A regular Hopf bifurcation cannot take place, since $0 \in \sigma(L)$. Using Sattinger's idea [25], we introduce the weight $W(x) = \exp(k_b x/2)$. We now consider the linear operator L as a transformation on the weighted Banach space

$$B_W = \left\{(c, f) : Wc \in L^2((0,\infty)),\ f \in \mathbf{R}\right\}.$$

Now we shall assume that the initial data decays exponentially and that the linearized solution decays exponentially,

$$\begin{pmatrix} c(x,0) \\ f(0) \end{pmatrix} = \begin{pmatrix} c_0(x) \\ f_0 \end{pmatrix} \in B_W$$

$$\begin{pmatrix} c(\cdot,t) \\ f_0 \end{pmatrix} \in B_W.$$

There is an isomorphism between B_W and B. We make the following transformation

$$u(x,t) = e^{\frac{k_b}{2}x} c(x,t).$$

This will shift the continuous spectrum; the parabola enclosing the region $-k_b^2 \mathrm{Re}(\lambda) \geq (\mathrm{Im}(\lambda))^2$ collapses to the ray

$$\left\{\lambda : \mathrm{Im}(\lambda) = 0, \mathrm{Re}(\lambda) \leq -\frac{k_b^2}{4}\right\}.$$

In this weighted space the first component of the eigenfunctions still belongs to L^2,

$$\begin{aligned} e^{k_b\frac{x}{2}}\psi_\pm &\in L^2((0,\infty)) \quad \text{or} \\ \begin{pmatrix} e^{k_b\frac{x}{2}}\psi_\pm \\ 1 \end{pmatrix} &\in B \end{aligned}$$

since $\mathrm{Re}\,(r(\lambda_\pm)) > 0$. With the above transformation we may again consider the space $B = L^2 \times \mathbf{R}$. With this transformation our full system becomes

$$\begin{aligned} u_t &= u_{xx} + vu_x - \frac{k_b}{4}(2v + k_b)\,u - k_b A v e^{-k_b\frac{x}{2}} && x > 0 \\ v &= \frac{k_b}{\rho}\left(k(f)(\bar{c} + u) - c_\infty\right) && x = 0 \\ u_x &= k_b k(f)(\bar{c} + u) - v(\bar{c} + u) - k_b c_\infty - \frac{k_b}{2}u && x = 0 \\ \dot{f} &= \frac{k_b}{\rho\varepsilon}\left[-\bar{f} - f + k(f)(\bar{c} + u)(1 - \bar{f} - f)\right] && x = 0 \\ u &\to 0 && x \to \infty \end{aligned}$$

along with the linearized system

$$\begin{aligned} u_t &= u_{xx} - \frac{k_b^2}{4}u - k_b A v e^{-k_b\frac{x}{2}} && x > 0 \\ v &= \frac{k_b}{\rho}\left(k(0)u + k'(0)\bar{c}f\right) && x = 0 \\ u_x &= \left(k_b k(0) - \frac{k_b}{2}\right)u + k_b k'(0)\bar{c}f - \bar{c}v && x = 0 \\ \dot{f} &= \frac{k_b}{\rho\varepsilon}\left[k(0)(1 - \bar{f})u - \left(\rho - k'(0)\bar{c}(1 - \bar{f})\right)f\right] && x = 0 \\ u &\to 0 && x \to \infty. \end{aligned}$$

As before, we write the linearized system as

$$\begin{pmatrix} u \\ f \end{pmatrix}_t = L \begin{pmatrix} u \\ f \end{pmatrix}$$

where

$$D(L) = \left\{ (c, f) \in H^2((0,\infty)) \times \mathbf{R} : u_x = \left(k_b k(0) - \frac{k_b}{2} \right) u + k_b k'(0) \bar{c} f - \bar{c} v \right\}.$$

The Dirichlet condition continues to serve as our definition for the velocity v.

Finally, in order to simplify $D(L)$, we shall perform one more transformation. The mole fraction $f(t)$ can be eliminated from the Neumann condition through the substitution

$$w(x,t) = u(x,t) + \Omega \epsilon^{-\frac{k_b}{2} x} f(t)$$

where

$$\Omega = \frac{k'(0)\bar{c}}{k(0)}.$$

Our nonlinear system becomes

$$\left.\begin{array}{rcll} w_t &=& w_{xx} + v w_x - \dfrac{k_b}{4}(2v + k_b)\, w & x > 0 \\ & & + \Omega \epsilon^{-\frac{k_b}{2} x}(\dot{f} + k_b v f) - k_b A v \epsilon^{-\frac{k_b}{2} x} & \\ v &=& \dfrac{k_b}{\rho}\left(k(f)(\bar{c} + w - \Omega f) - c_\infty\right) & x = 0 \\ w_x &=& k_b k(f)(\bar{c} + w - \Omega f) - v(\bar{c} + w - \Omega f) & x = 0 \\ & & - k_b c_\infty - \dfrac{k_b}{2} w & \\ \dot{f} &=& \dfrac{k_b}{\rho \bar{c}}\left(-\bar{f} - f + k(f)(\bar{c} + w - \Omega f)(1 - \bar{f} - f)\right) & x = 0 \\ w &\to& 0 & x \to \infty \end{array}\right\} \quad (4.7)$$

and our linearized system becomes

$$
\begin{aligned}
w_t &= w_{xx} - \frac{k_b^2}{4} w + \Omega \dot{f} e^{-\frac{k_b}{2}x} - k_b A v e^{-\frac{k_b}{2}x} && x > 0 \\
v &= \frac{k_b}{\rho} k(0) w && x = 0 \\
w_x &= \alpha w && x = 0 \\
\dot{f} &= \frac{k_b}{\rho \varepsilon} \left[k(0)(1 - \bar{f}) w - \rho f \right] && x = 0 \\
w &\to 0 && x \to \infty
\end{aligned}
$$

where

$$
\alpha = k_b k(0) - \frac{k_b}{2} - \frac{k_b}{\rho} c_\infty . \tag{4.8}
$$

We write the above system as

$$
\begin{aligned}
\begin{pmatrix} w \\ f \end{pmatrix}_t &= L \begin{pmatrix} w \\ f \end{pmatrix} \\
&= L_0 \begin{pmatrix} w \\ f \end{pmatrix} + L_B \begin{pmatrix} w \\ f \end{pmatrix} \\
&= \begin{pmatrix} \Delta - \frac{k_b^2}{4} & 0 \\ 0 & b_1 \end{pmatrix} \begin{pmatrix} w \\ f \end{pmatrix} + \begin{pmatrix} B_2(x) & B_1(x) \\ b_2 & 0 \end{pmatrix} \begin{pmatrix} w(0) \\ f \end{pmatrix}
\end{aligned} \tag{4.9}
$$

where

$$
\begin{aligned}
D(L) &= \{(w, f) \in H^2((0, \infty)) \times \mathbf{R} : w_x = \alpha w\} \\
\Delta &= \frac{\partial^2}{\partial^2 x} \\
B_1(x) &= -\left(\frac{k_b k'(0) \bar{c}}{k(0) \varepsilon} \right) e^{-\frac{k_b}{2}x} = B_1 e^{-\frac{k_b}{2}x} \\
B_2(x) &= \left(\frac{k_b k'(0) \bar{c}}{\rho^2 \varepsilon} - \frac{k_b^2 k(0) A}{\rho} \right) e^{-\frac{k_b}{2}x} = B_2 e^{-\frac{k_b}{2}x} \\
b_1 &= -\frac{k_b}{\varepsilon}
\end{aligned}
$$

$$b_2 = \frac{k_b k(0)}{\rho^2 \varepsilon}.$$

The linear system above is subdivided into two parts, the second term contains all the coupled terms along with the boundary term $w(0,t)$ while the first term has no coupled terms. We define the *principal part* of L by

$$L_P = \begin{pmatrix} \Delta & 0 \\ 0 & b_1 \end{pmatrix}.$$

The operator L_0 differs from L_P only by the presence of the term $k_b^2/4$. Both these operators contain the highest order spatial derivative of w. When developing the L^2 bounds of Section 4.1.3 and the regularity results of Appendix C, we shall follow the theme below. First the desired result will be obtained for L_P, and then proved for all of L via the variation of parameters formula. Along with the variation of parameters formula, the results of Appendix B will also serve in deriving the L^2 estimates. In this appendix, equivalent Sobolev norms involving fractional powers between L_P and L are developed.

Note that the eigenvectors corresponding to the linear operator L above are

$$\begin{pmatrix} e^{\frac{k_b}{2}x}\psi_{\pm}(x) + \Omega e^{-\frac{k_b}{2}x} \\ 1 \end{pmatrix} \in B = L^2((0,\infty)) \times \mathbf{R}.$$

We close this section with a proposition that summarizes the results of this section.

Proposition 4.2 *The linear operator L defined by (4.9), considered as an evolution operator defined on $B = L^2((0,\infty)) \times \mathbf{R}$ has the following spectrum $\sigma(L)$:*

1. A continuous spectrum $\sigma_C(L) = (-\infty, -\frac{k_b^2}{4}]$.

2. A pair of complex eigenvalues $\sigma_P(L) = \{\lambda_\pm(\mu)\}$, *that cross the imaginary axis as* μ *varies over a suitable interval* I. *The associated eigenfunctions are*

$$\epsilon_\pm = \begin{pmatrix} \varphi_\pm \\ 1 \end{pmatrix}$$

where

$$\varphi_\pm(x) = A_-(\lambda_\pm)e^{-r(\lambda_\pm)x} + e^{-\frac{k_b}{2}x}\left(\frac{k'(0)\bar{c}}{k(0)} - \frac{k_b A}{\lambda_\pm}M(\lambda_\pm)\right)$$

and

$$r(\lambda) = \sqrt{\frac{k_b^2}{4} + \lambda}.$$

4.1.2 Linearized Stability

Now we shall establish existence and uniqueness to the Cauchy problem for the linear evolution operator and then state a stability result. The *abstract Cauchy problem* for L with initial conditions (w_0, f_0) consists of solving the initial value problem

$$\begin{pmatrix} w \\ f \end{pmatrix}_t = L\begin{pmatrix} w \\ f \end{pmatrix}$$

$$\begin{pmatrix} w(0) \\ f(0) \end{pmatrix} = \begin{pmatrix} w_0 \\ f_0 \end{pmatrix}$$

where

$$(w_0, f_0) \in D(L) \subset L^2 \times \mathbf{R},$$

such that $(w(t), f(t))$ are continuous functions for $t \geq 0$, continuously differentiable for $t > 0$, and $(w(t), f(t)) \in D(L)$ for $t > 0$. A standard theorem from semigroup theory ([18],[23],[30]) will be employed. In order to use this theorem we must look at projections off the eigenmanifold. First we state this standard theorem,

Theorem 4.3 *Assume*

(i) A is a closed densely defined linear operator on a Banach space B.

(ii) The resolvent of A, $\rho(A)$, contains the sector

$$S(\omega, \phi) = \{\lambda : |\arg(\lambda - \omega)| < \pi - \phi, \ \lambda \neq \omega\}$$

for some real ω and $\phi \in (0, \frac{\pi}{2})$.

(iii) For some $C > 0$,

$$\left\|(\lambda I - A)^{-1}\right\| \leq \frac{C(\omega, \phi)}{|\lambda - \omega|} \qquad \text{for all } \lambda \in S(\omega, \phi).$$

Then A is the infinitesimal generator of an analytic semigroup $T(t)$. Moreover, $w(t) = T(t)w_0$ is a solution to the Cauchy problem where $w_0 \in D(A)$.

For our system L is obviously densely defined since functions in $H^2((0,\infty))$ with the flux condition $w_x(0) = \alpha w(0)$ are dense in $L^2((0,\infty))$. Since $0 \in \rho(L)$ then L^{-1} is continuous. This implies that L^{-1} is closed and consequently L is closed. Part (ii) is satisfied for any $\phi \in (0, \frac{\pi}{2})$ and $\omega \in (-\frac{k_b^2}{4}, 0)$ except for the pair of eigenvalues (see Figure 4.1). We thus must exclude the imaginary eigenvalues by projection operators. Part (iii) will follow from estimates involving one-sided Green's functions.

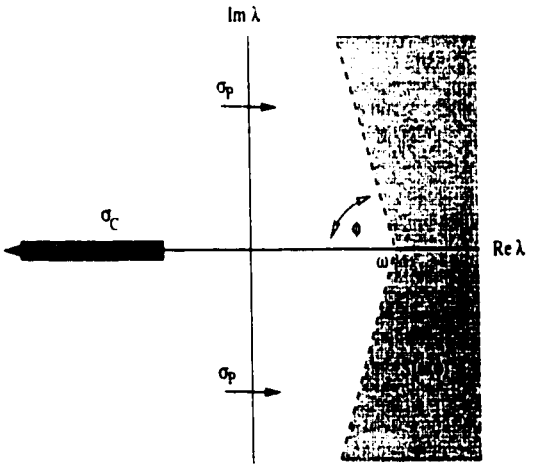

Figure 4.1 : The Spectrum of L and the sector $S(\omega, \phi)$.

Theorem 4.4 *The linear operator L defined in (4.9) is*

(1) closed and densely defined, and

(2) the resolvent operator of L satisfies the estimate

$$\left\| (\lambda I - L)^{-1} \begin{pmatrix} w \\ f \end{pmatrix} \right\| \leq \frac{C(\omega, \phi)}{|\lambda - \omega|} \left\| \begin{pmatrix} w \\ f \end{pmatrix} \right\|$$

for any $\omega \in (0, \infty), \phi \in (0, \frac{\pi}{2})$ in the sector $S(\omega, \phi)$.

Thus L is the infinitesimal generator of an analytic semigroup e^{Lt} and

$$\begin{pmatrix} w \\ f \end{pmatrix} = e^{Lt} \begin{pmatrix} w_0 \\ f_0 \end{pmatrix}$$

is the solution to the Cauchy problem with initial data $(w_0, f_0) \in D(L)$.

Proof: Part (1) was proven above. For the asymptotic estimate we shall look at the resolvent equation away from the poles. The resolvent equation is

$$(L - \lambda I) \begin{pmatrix} w \\ f \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}$$

where $(F_1, F_2) \in L^2 \times \mathbf{R}$. From System (4.9), this equation is explicitly

$$\begin{aligned} w_{xx} - \frac{k_b^2}{4} w + \epsilon^{-\frac{k_b}{2}x} [B_1 f + B_2 w(0)] - \lambda w &= F_1 \\ b_1 f + b_2 w(0) - \lambda f &= F_2 \end{aligned}$$

where the second component is easily solved,

$$f = \frac{F_2 - b_2 w(0)}{b_1 - \lambda}.$$

Note that $b_1 = -k_b/\varepsilon$ so that $b_1 \in \sigma_C(L)$ if ε is small enough. Thus we do not have division by zero for f since $\lambda \in \rho(L)$. The first component will involve boundary valued Green's functions. The homogeneous solution of the above equation (with $F_1 = 0$) is

$$w_h(x) = w_0 e^{-r(\lambda)x} + \left(e^{-\frac{k_2}{2}x} - e^{-r(\lambda)x} \right) \left(\frac{B_1 f + B_2 w(0)}{\lambda} \right)$$

where

$$r(\lambda) = \sqrt{\frac{k_b^2}{4} + \lambda}.$$

The Green's function associated with the boundary condition $w(0) = w(\infty) = 0$ is

$$g(x,s) = \begin{cases} \dfrac{1}{2r(\lambda)} e^{-r(\lambda)x} \left(e^{-r(\lambda)s} - e^{r(\lambda)s} \right) & 0 < s < x \\ \dfrac{1}{2r(\lambda)} e^{-r(\lambda)s} \left(e^{-r(\lambda)x} - e^{r(\lambda)x} \right) & x < s < \infty \end{cases}$$

giving the solution to the inhomogeneous problem

$$w(x) = w_h(x) + \int_0^\infty g(x,s) F_1(s)\, ds.$$

To determine $w(0)$ we impose the boundary condition $w_x(0) = \alpha w(0)$. This gives

$$w_0 = \frac{1}{d} \left[\left(r(\lambda) - \frac{k_b}{2} \right) \frac{b_1 \alpha F_2}{\lambda(\lambda - b_1)} + \int_0^\infty e^{-r(\lambda)s} F_1(s)\, ds \right]$$

where

$$d = -\alpha - r(\lambda) + \frac{2r(\lambda) - k_b}{2\lambda} \left[\frac{b_2 \alpha \lambda}{\lambda - b_1} - \frac{k_b^2 A k(0)}{\rho} \right].$$

One may verify that $d = 0$ precisely at the poles $\lambda_\pm$. For any $\omega \in (0, \infty), \phi \in (0, \frac{\pi}{2})$, the sector $S(\omega, \phi)$ avoids the poles. Thus there exists a positive δ such that $|d|^{-1} < \delta^{-1}$ for $\lambda \in S(\omega, \phi)$. The integral operator defined by

$$Gk(x) = \int_0^\infty g(x,s) k(s)\, ds$$

satisfies the L^2 estimate

$$\|Gk\| \leq \frac{C \|k\|}{|r(\lambda)|^2} \qquad \text{for } \lambda \in S(\omega, \phi).$$

This result is due to Naimark [21]. Using this estimate along with the estimate

$$\left\| e^{-r(\lambda)x} \right\| = \frac{1}{\sqrt{2 \mathrm{Re}\, r(\lambda)}} \leq \frac{C}{|r(\lambda)|^{\frac{1}{2}}}$$

gives the desired estimate away from the poles, namely,

$$\left\| \begin{pmatrix} w \\ f \end{pmatrix} \right\| = \|w\| + |f| \leq \frac{C\,(\|F_1\| + |F_2|)}{|r(\lambda)|^2} = \frac{C}{|r(\lambda)|^2} \left\| \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} \right\|$$

$$\leq \frac{C}{|\lambda - \omega|} \left\| \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} \right\|.$$

Note that $\mathrm{Re}\, r(\lambda) > 0$ for $\lambda \in S(\omega, \phi)$. □

This establishes that the linearized problem has as its solution an analytic semigroup.

Our next result is a stability theorem for the linearized operator. This is obtained through invariant subspaces and exponential bounds from semigroup theory. First some preliminary definitions are given.

Definition 4.5 *Let L be a linear operator defined on a Banach space B, with range also in B. Denote the spectrum of L by $\sigma(L)$. A subset $\tilde{\sigma}$ of the extended spectrum $\sigma_e(L) = \sigma(L) \cup \{\infty\}$ is a* **spectral set** *if $\tilde{\sigma}$ and $\sigma_e(L) \setminus \sigma$ are both closed in the extended complex plane $\mathbf{C} \cup \{\infty\}$.*

Definition 4.6 *The linear operator S in a Banach space B is a* **sectorial operator** *if it is a closed densely defined operator such that:*

1) the resolvent set $\rho(S)$ contains the sector

$$\Sigma_{\omega,\phi} = \{\lambda : \phi \leq |\arg(\lambda - \omega)| \leq \pi,\ \lambda \neq \omega\}$$

for some $\phi \in (0, \frac{\pi}{2})$ and some real ω, and

2) satisfies the following estimate

$$\left\|(\lambda I - S)^{-1}\right\| \leq \frac{M}{|\lambda - \omega|} \quad \textit{for all } \lambda \in \Sigma_{\omega,\phi}.$$

Note that according to this definition the operator $-L$ is sectorial.

Theorem 4.7 *Let σ_1 be the bounded spectral set corresponding to the eigenvalues $\lambda_\pm$. Let $\sigma_2 = \sigma(L) \setminus \sigma_1$ (i.e., $\sigma_1 = \sigma_P(L)$, $\sigma_2 = \sigma_C(L)$). Let E_1 and E_2 be the continuous projections associated with these spectral sets, and let $B_i = E_i(B)$ $i = 1, 2$. Then*

1. $B = B_1 \dotplus B_2$, the subspaces B_i are invariant under L. If L_i is the restriction of L to B_i, then

$$L_1 : B_1 \to B_1 \text{ is bounded and } \sigma(L_1) = \sigma_1$$
$$-L_2 \text{ is sectorial with } D(L_2) = D(L) \cap B_2 \text{ and } \sigma(L_2) = \sigma_2.$$

2. The following estimates exist

$$\left.\begin{aligned} \left\| e^{L_2 t} \right\| &\leq C(\omega) e^{-\omega t} \\ \left\| L_2 e^{L_2 t} \right\| &\leq C(\omega) t^{-1} e^{-\omega t} \end{aligned}\right\} \quad \text{for all } 0 < \omega < \frac{k_b^2}{4}.$$

3. For a given value of the bifurcation parameter μ,

$$\left\| e^{L_1 t} \right\| \leq C e^{\beta t} \quad \text{where } \beta = \operatorname{Re} \lambda_\pm(\mu).$$

Thus when $\mu < \mu_{cr}$ we have stability for the solution operator e^{Lt},

$$\left\| e^{Lt} \right\| \leq C e^{\beta t}.$$

Proof: For the proof of part 1, see Dunford and Schwartz [6] or Taylor [29]. This involves an operational calculus, where Cauchy integrals are used to define continuous projection operators associated with the spectral sets. Parts 2 and 3 follow from Theorem 1.5.3 from Henry [18]. For completeness we state this proof. The operator $A = -L$ is sectorial. Let $\tilde{\sigma}_1 = \{-\lambda_\pm\}$ and $\tilde{\sigma}_2 = \sigma(A) \setminus \tilde{\sigma}_1 = \{[k_b^2/4, \infty)\}$. By part 1, we have the projection operators A_i $(i = 1, 2)$ on the invariant subspaces $X_i = A_i(B)$. Suppose $x \in X_2$, $\|x\| \leq 1$, and $\lambda \notin \sigma(A)$, then $\left\| (\lambda I - A_2)^{-1} x \right\| = \left\| (\lambda I - A)^{-1} x \right\| \leq C |\lambda|^{-1}$ for $|\lambda| > R$ and for $|\arg \lambda| > \phi$ for some $R > 0$ and $\phi \in (0, \frac{\pi}{2})$. Since $\operatorname{Re} \sigma(A_2) > \omega$

for $\omega \in (0, \frac{k_b^2}{4})$, then $\left\|(\lambda I - A_2)^{-1}\right\| \leq |C\lambda - \omega|^{-1}$ for $|\arg(\lambda - \omega)| > \phi'$ for some $\phi' \in (0, \frac{\pi}{2})$. Thus the operator A_2 is sectorial, and the estimates for $e^{-A_2 t} = e^{L_2 t}$ follow since the real part of the spectrum of A_2 is strictly positive. The estimate for $e^{L_1 t}$ follows since L_1 is a bounded operator (see [18],[23]). □

4.1.3 L^2 Bounds for the Linearized Operator

First L^2 bounds for the principal linear system are developed and then we pass to the full linear system by the variation of parameters formula. These estimates are required when we pass to the nonlinear system of the next section. By the variation of parameters formula, there will be convolution terms involving nonlinear terms and the analytic semigroup generated by L. We follow Frankel and Roytburd's [7] treatment. The first proposition follows immediately from their work since for the principal linear system L_P, w and f are a decoupled set of differential equations.

Proposition 4.8 *Suppose $(w(t), f(t))$ is the linearized solution with initial conditions $w_0 \in H^1((0,\infty))$, $f_0 \in (0,1)$. Then $(w(t), f(t))$ is continuous for $x \geq 0$, $t \geq 0$. If $\mu < \mu_{cr}$ then*

$$\left.\begin{array}{r} \|w\| \\ |f| \end{array}\right\} \leq C \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\| e^{-\delta t}$$

$$\left.\begin{array}{r} \|w_x\| \\ |w(0,t)| \end{array}\right\} \leq C \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\|_1 e^{-\delta t}$$

where

$$\left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\|_1 = \|w_0\|_{H^1} + |f_0| = \|w_0\| + \|w_{0x}\| + |f_0|.$$

Proof: By Sobolev's lemma, we may identify w_0 with a continuous function. Continuity then follows from the proof of Theorem C.1. The solution to the

principal linear solution is (see Appendix C)

$$w(x,t) = \begin{cases} \alpha F(x,t) + F_x(x,t) & \alpha \geq 0 \\ -2\alpha\Phi(-\alpha^2)e^{\alpha x}e^{\alpha^2 t} + \alpha F(x,t) + F_x(x,t) & \alpha < 0 \end{cases}$$

$$f(t) = f_0 e^{b_1 t}$$

where $F(x,t)$ is the solution to the heat equation on the line with odd data

$$\tilde{F}_0(x) = \begin{cases} F_0(x) & x \geq 0 \\ -F_0(-x) & x < 0 \end{cases}$$

and where

$$F_0(x) = \int_0^x e^{-\alpha(x-s)} U_0(s)\, ds.$$

Recall that α is given by Equation (4.8). As in Appendix C, the initial data is decomposed as follows. If $\alpha < 0$ let

$$u_0(x) = -2\alpha\Phi(-\alpha^2)e^{\alpha x} + U_0(x).$$

For $\alpha \geq 0$ we shall identify U_0 with w_0, thus we write

$$w_0(x) = \begin{cases} U_0(x) & \alpha \geq 0 \\ -2\alpha\Phi(-\alpha^2)e^{\alpha x} + U_0(x) & \alpha < 0 \end{cases}$$

where for $\alpha < 0$

$$\Phi(-\alpha^2) = \int_0^\infty w_0(x)e^{\alpha x}\, dx$$

$$\int_0^\infty U_0(x)e^{\alpha x}\, dx = 0.$$

Now we shall give the L^2 estimates. Let e^{Lt} be the solution operator to the full linearized problem. If $\mu < \mu_{cr}$ then by Theorem 4.7

$$\left\| \begin{pmatrix} w \\ f \end{pmatrix} \right\| = \left\| e^{Lt} \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\| \leq Ce^{-\delta t} \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\|$$

where $\delta > 0$ is determined from the linearization. The estimate for w_x is more involved and consists of two parts. We need to fix $T > 0$ and establish L^2 estimates for the principal linear system in the fixed time interval $0 \le t \le T$. By the ordinary Fourier transform, we obtain for $\alpha < 0$, the following estimate

$$\begin{aligned}
\|F_0\|^2 &= \left\| -\int_x^\infty e^{-\alpha(x-s)} U_0(s)\, ds \right\|^2 \\
&= \left\| -\int_x^\infty e^{-\alpha(x-s)} \int_{-\infty}^\infty \hat{U}_0(p) e^{ips}\, dp\, ds \right\|^2 \\
&= \left\| \int_{-\infty}^\infty \frac{\hat{U}_0(p)}{\alpha + ip} e^{ipx}\, dp \right\|^2 \\
&= \left\| \int_{-\infty}^\infty \frac{|\hat{U}_0(p)|^2}{|\alpha + ip|^2}\, dp \right\|^2 \\
&\le \frac{1}{\alpha^2} \|U_0\|^2 \\
&\le C \|w_0\|^2 .
\end{aligned}$$

One can show that the same estimate also holds for $\alpha > 0$. Thus

$$\begin{aligned}
|\Phi(-\alpha^2)| &\le C \|w_0\| \\
\|F_0'\| &= \|U_0 - \alpha F_0\| \le C \|w_0\| .
\end{aligned}$$

The L^2 estimates of w_x follow from the L^2 estimates of F and F_x. For a fixed time interval $0 \le t \le T$, the first term of $w(x,t)$ and its spatial derivative are bounded by $C \|w_0\|$ for $\alpha < 0$. We require estimates for the term

$$\begin{aligned}
\tilde{w}(x,t) &= \alpha F(x,t) + F_x(x,t) \\
&= \alpha \Gamma(\tilde{F}_0) + \frac{\partial}{\partial x} \Gamma(\tilde{F}_0) \\
&= \Gamma(\alpha \tilde{F}_0 + \tilde{F}_0')
\end{aligned}$$

where Γ is the solution operator of the heat equation on the line. Note that

$$\begin{aligned}
\|\tilde{w}\| &= \left\| \Gamma(\alpha \tilde{F}_0 + \tilde{F}_0') \right\| \\
&\le C \left(\left\| \alpha \tilde{F}_0 \right\| + \left\| \tilde{F}_0' \right\| \right) .
\end{aligned}$$

For $w_0 \in H^1$,

$$\|w_x\| \leq C \|w_0\|_1$$

since w_x involves $\tilde{F}_0'$ and $\tilde{F}_0''$. This same estimate holds for the full linearized problem via the variation of parameters formula. For $t > T$ the proof is based on semigroup theory. The estimates below use the norms that were developed in Appendix B; they involve fractional powers of the operators L_P and L. The estimate for w_{xx} is

$$\begin{aligned}
\|w_{xx}\| &= \|-\Delta w\| \leq C \|w\|_{2,-\Delta} = C \|(-\Delta + m) w\| \\
&\leq C \left\| \begin{pmatrix} -\Delta + m & 0 \\ 0 & b_1 + m \end{pmatrix} \begin{pmatrix} w \\ f \end{pmatrix} \right\| = C \left\| (-L_P + m) \begin{pmatrix} w \\ f \end{pmatrix} \right\| \\
&\leq C \left\| (-L + d) \begin{pmatrix} w \\ f \end{pmatrix} \right\| \\
&\leq C \left\| L \begin{pmatrix} w \\ f \end{pmatrix} \right\| + Cd \left\| \begin{pmatrix} w \\ f \end{pmatrix} \right\| \\
&\leq C \left\| L e^{Lt} \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\| + C e^{-\delta t} \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\| \\
&\leq (CT^{-1} e^{-\delta t} + C e^{-\delta t}) \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\| \\
&\leq C e^{-\delta t} \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\|.
\end{aligned}$$

The estimate for w_x is

$$\begin{aligned}
\|w_x\|^2 &= \int_0^\infty |w_x|^2 \, dx = w_x \bar{w}|_0^\infty - \int_0^\infty w_{xx} \bar{w} \, dx \\
&= -\alpha \, |w(0)|^2 - (-\Delta w, w) \\
&\leq |\alpha| \, \|w\|_{2,-\Delta}^2 + \|\Delta w\| \, \|w\| \quad \text{(by Sobolev's ineq.)} \\
&\leq Ce^{-2\delta t} \left\| \begin{pmatrix} w_0 \\ f_0 \end{pmatrix} \right\|^2 .
\end{aligned}$$

Combining this last estimate with the estimate for $0 \leq t \leq T$ gives the desired result. Finally, the estimate for $w(0,t)$ follows from Sobolev's inequality. □

4.2 The Nonlinear Problem

The main result of this section is the existence and uniqueness of a solution to the full nonlinear problem. The *principle of linearized stability* holds here, where linearized stability implies nonlinear stability. In particular, we shall see that for sufficiently small initial data, the solution to the nonlinear problem is stable below the threshold bifurcation value μ_{cr}. First we formally write an integral representation of the nonlinear system via the variation of parameters formula. Then we prove that this is a contraction mapping, and hence that a unique solution exists. The L^2 estimates for the linearized system developed from the previous section are crucial for our analysis.

The nonlinear system (4.7) may be transformed such that the mole fraction f may be eliminated from the Neumann condition just as in the linearized system (4.9). This may be done by the substitution

$$u(x,t) = w(x,t) - U_1(x) \left[w_x(0,t) - \alpha w(0,t) \right]$$

where

$$U_1(x) = xe^{-\frac{k_b}{2}x}.$$

Our system is then in the form

$$\begin{pmatrix} u \\ f \end{pmatrix}_t = Q(\mu)\begin{pmatrix} u \\ f \end{pmatrix} = L(\mu)\begin{pmatrix} u \\ f \end{pmatrix} + \begin{pmatrix} N(u,f,\mu) \\ n(u,f,\mu) \end{pmatrix}$$

where N and n contain all the nonlinear terms of u and f, and μ is the bifurcation parameter. The domain of Q becomes

$$D(Q) = \left\{(u,f) \in H^2 \times \mathbf{R} : u_x(0) = \alpha u(0)\right\}.$$

With this transformation the operator L remains the same; it is the same as in System (4.9). As in our linear analysis, we subdivide the operator L, as a sum consisting of a decoupled operator L_0, along with a coupled operator L_B. By the variation of parameters formula, we obtain, formally, the following integral equation

$$\begin{aligned} \begin{pmatrix} u \\ f \end{pmatrix} &= \epsilon^{L_0 t}\begin{pmatrix} u_0 \\ f_0 \end{pmatrix} + \int_0^t \epsilon^{L_0(t-s)} L_B \begin{pmatrix} u(s) \\ f(s) \end{pmatrix} ds \\ &\quad + \int_0^t \epsilon^{L_0(t-s)} \begin{pmatrix} N(s) \\ n(s) \end{pmatrix} ds \end{aligned} \tag{4.10}$$

where

$$\epsilon^{L_0 t} = \begin{pmatrix} \epsilon^{-\frac{k_b^2}{4}t} G(t) & 0 \\ 0 & e^{b_1 t} \end{pmatrix} = \begin{pmatrix} H(t) & 0 \\ 0 & \epsilon^{b_1 t} \end{pmatrix}.$$

The operator $G(t)$ solves the heat equation for $x > 0$ with the boundary condition $u_x(0) = \alpha u(0)$.

We shall write Equation (4.10) explicitly in terms of our old system (4.7) where the boundary conditions are of the form

$$\begin{aligned} v &= V(f(t), u(0,t)) \\ w_x &= W(f(t), u(0,t)) \\ f_t &= F(f(t), u(0,t)) \end{aligned}$$

with V, W, F the corresponding right hand sides of System (4.7). We denote the linearized terms by V_L, W_L, F_L (i.e., the associated linear boundary terms of System (4.9)). Note that $W_L = \alpha u(0,t)$. The nonlinear terms that appear on the boundary, are of the form

$$\begin{aligned} V - V_L &: f^2, f^3, fu, f^2u \\ W - W_L &: f^2, f^3, f^4, fu, f^2u, f^3u, f^2u^2 \\ F - F_L &: f^2, f^3, f^4, fu, f^2u, f^3u. \end{aligned}$$

The integral equation is explicitly,

$$\begin{aligned} u(t) &= H(t)u_0 + \int_0^t H(t-s)e^{-\frac{k_b}{2}x}\left[B_1 f(s) + B_2 u(0,s)\right] ds \\ &+ H * vu_x - \frac{k_b}{2} H * vu \\ &+ \frac{k'(0)}{k(0)} \bar{c} H * e^{-\frac{k_b}{2}x}\left[(F - F_L) + k_b v f\right] \\ &- k_b A H * e^{-\frac{k_b}{2}x}\left[V - V_L\right] \\ &+ u_1(0)\left[W - \alpha u\right] - u_1(t)\left[W_0 - \alpha u_0\right] - (u_1)_t * \left[W - \alpha u\right] \\ &+ u_2 * v\left[W - \alpha u\right] + u_3 * \left[W - \alpha u\right] \\ f(t) &= f_0 e^{b_1 t} + b_2 \int_0^t e^{b_1(t-s)} u(0,s)\, ds + \int_0^t e^{b_1(t-s)}\left[F - F_L\right](s)\, ds \end{aligned} \tag{4.11}$$

where

$$\begin{aligned} H * f &= \int_0^t H(t-s) f(s)\, ds \\ u_1(t,x) &= H(t) U_1 \\ u_2(t,x) &= H(t)\left(\dot{U}_1 - \tfrac{k_b}{2} U_1\right) \\ u_3(t,x) &= H(t)\left(\ddot{U}_1 - \tfrac{k_b^2}{4} U_1\right). \end{aligned}$$

Integration by parts was used on the term $H * U_1[W - \alpha u]_t$.

The nonlinear stability theorem for the above problem can be stated as follows.

Theorem 4.9 *If $\mu < \mu_{cr}$, then there exists an $\varepsilon > 0$, such that for any*

$$\left\| \begin{pmatrix} u_0 \\ f_0 \end{pmatrix} \right\|_1 = \|u_0\|_{H^1} + |f_0| = \|u_0\| + \|u_{0x}\| + |f_0| < \varepsilon,$$

the integral equation has an unique solution with the following bound

$$\left\| \begin{pmatrix} u(\cdot,t) \\ f(t) \end{pmatrix} \right\|_1 \leq C e^{-\delta t}.$$

Proof: We consider the Banach space

$$X = \left\{ (u,f) : u \in C([0,\infty), L^2) \cap C((0,\infty), H^1), f \in C([0,\infty)) \right\}$$

with the norm

$$\left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_X = \|u\|_X + |f|_X$$

where

$$\|u\|_X = \sup_t \|u(\cdot,t)\|_1 e^{\delta t} < \infty$$

$$|f|_X = \sup_t |f(t)| e^{\delta t} < \infty.$$

We denote the right hand sides of (4.11) by $K_1(u,f)$ and $K_2(u,f)$, so

$$K \begin{pmatrix} u \\ f \end{pmatrix} = \begin{pmatrix} K_1(u,f) \\ K_2(u,f) \end{pmatrix}.$$

The operator K, maps X into X, i.e.,

$$K : X \to X.$$

This follows from the continuity of the linearized solution. Now let

$$\left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_X < r \quad (r < 1),$$

this implies $\|u\|_1 < re^{-\delta t}$ and $|f(t)| < re^{-\delta t}$.

In order to show that K is a contraction mapping we begin by summarizing a series of estimates. First we give some preliminary estimates that are obtained from Proposition 4.8 and Sobolev's inequality,

$$\begin{aligned}
\left\| e^{Lt} \begin{pmatrix} u \\ f \end{pmatrix} \right\|_1 &\leq C \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_1 e^{-\delta t} \\
|u(0,t)| &\leq C \|u\|_1 \leq Cre^{-\delta t} \\
|V_L| &\leq Cre^{-\delta t} \\
|V - V_L| &\leq C|f| \left(|u(0,t)| + |f|\,|u(0,t)| + |f| + |f|^2 \right) \leq Cr^2 e^{-2\delta t}.
\end{aligned}$$

The first nonlinear term of K_1 is $H * vu_x$. We begin with the following estimate: for any $\tilde{u} \in L^2((0,\infty))$ we have

$$\begin{aligned}
\|H(t)\tilde{u}\|_1 &\leq \|H(t)\tilde{u}\| + \|H(t)\tilde{u}_x\| \\
&\leq Ce^{-\delta t} \left\| \begin{pmatrix} \tilde{u} \\ f \end{pmatrix} \right\| + C \left\| (-L+d)^{\frac{1}{2}+\epsilon} e^{Lt} \begin{pmatrix} \tilde{u} \\ f \end{pmatrix} \right\| \\
&\leq Cre^{-2\delta t} + C \left\| e^{Lt} (-L+d)^{\frac{1}{2}+\epsilon} \begin{pmatrix} \tilde{u} \\ f \end{pmatrix} \right\| \\
&\leq Cre^{-2\delta t} + Ct^{-\frac{1}{2}-\epsilon} \left\| \begin{pmatrix} \tilde{u} \\ f \end{pmatrix} \right\|
\end{aligned}$$

which is true for all $t > 0$. With $\varepsilon = 1/4$, and $t > 1$, we obtain

$$\|H(t)\tilde{u}\|_1 = \|H(t-1)H(1)\tilde{u}\|_1 \leq Ce^{-\delta(t-1)} \|H(1)\tilde{u}\|_1 \leq Ce^{-\delta t} 1^{-\frac{3}{4}} \left\| \begin{pmatrix} \tilde{u} \\ f \end{pmatrix} \right\|.$$

Thus,

$$\begin{aligned}
\|H * vu_x\|_1 &\le \left\| \int_0^{t-1} H(t-s) v u_x \, ds \right\|_1 + \left\| \int_{t-1}^{t} H(t-s) v u_x \, ds \right\|_1 \\
&\le C \int_0^{t-1} e^{-\delta(t-s)} \left\| \begin{pmatrix} vu_x \\ vf \end{pmatrix} \right\| ds + C \int_{t-1}^{t} (t-s)^{-\frac{3}{4}} \left\| \begin{pmatrix} vu_x \\ vf \end{pmatrix} \right\| ds \\
&\le C \int_0^{t-1} e^{-\delta(t-s)} r^2 e^{-2\delta s} \, ds + C \int_0^{t-1} (t-s)^{-\frac{3}{4}} r^2 e^{-2\delta s} \, ds \\
&\le C r^2 e^{-\delta t}.
\end{aligned}$$

Similarly, the estimate for the second nonlinear term is

$$\|H * vu\|_1 \le C r e^{-\delta t}.$$

From Proposition (4.8), we have

$$\|u_i\|_1 \le C e^{-\delta t} \quad \text{for } i = 1, 2, 3$$

since $U_1 \in H^1$. Now we outline the estimates that involve u_i:

$$\|u_1 (W_0 - \alpha u_0)\|_1 \le C \|u_1\|_1 r^2 e^{-2\delta \cdot 0} \le C r^2 e^{-\delta t}.$$

$$\|u_1(0)[W - \alpha u]\|_1 \le C r^2 e^{-2\delta t},$$

$$\begin{aligned}
\|u_2 * v[W - \alpha u]\|_1 &= \left\| \int_0^t u_2(x, t-s) v [W - \alpha u] \, ds \right\|_1 \\
&\le \int_0^t \|u_2(x, t-s)\|_1 r^3 e^{-3\delta s} \, ds \\
&\le \int_0^t C e^{-\delta(t-s)} r^3 e^{-3\delta s} \, ds \\
&\le C r^3 e^{-\delta t} \int_0^t e^{-2\delta s} \, ds \\
&\le C r^3 e^{-\delta t},
\end{aligned}$$

and similarly,

$$\|u_3 * [W - \alpha u]\|_1 \le C r^2 e^{-\delta t}.$$

Note that $\|u_{1t}\|_1 \leq Ct^{-3/4}$. This estimate follows from the representation of u_1 involving $\tilde{F}_0(x)$ of Proposition C.1. The norm $\|u_{1t}\|_1$ involves the L^2 integral of δ_x. This gives the following estimate

$$\begin{aligned}
\|(u_1)_t * (W - \alpha u)\|_1 &\leq \left\| \int_0^{t-1} (u_1)_t (t-s) [W - \alpha u](s)\, ds \right\|_1 \\
&\quad + \left\| \int_{t-1}^{t} (u_1)_t (t-s) [W - \alpha u](s)\, ds \right\|_1 \\
&\leq C \int_0^{t-1} \|(u_1)_t\|_1 r^2 \epsilon^{-2\delta s}\, ds + C \int_{t-1}^{t} \|(u_1)_t\|_1 r^2 \epsilon^{-2\delta s}\, ds \\
&\leq Cr^2 \int_0^{t-1} \epsilon^{-\delta(t-s)} \epsilon^{-2\delta s}\, ds + Cr^2 \int_{t-1}^{t} (t-s)^{-\frac{3}{4}} \epsilon^{-2\delta s}\, ds \\
&\leq Cr^2 \epsilon^{-\delta t}.
\end{aligned}$$

The remaining nonlinear terms of K_1 involve the estimates

$$\left.\begin{aligned} |(F - F_L) + k_b v f| \\ |V - V_L| \end{aligned}\right\} \leq r^2 \epsilon^{-2\delta t}.$$

which yield

$$\left.\begin{aligned} \left\| H * \epsilon^{-\frac{k_b}{2} x} [(F - F_L) + k_b v f] \right\|_1 \\ \left\| H * \epsilon^{-\frac{k_b}{2} x} [V - V_L] \right\|_1 \end{aligned}\right\} \leq Cr^2 \epsilon^{-\delta t}.$$

Finally, we estimate the operator $K_2(u, f)$. The largest nonlinear term that appears in the integrand is $r^2 \epsilon^{-2\delta s}$. Thus

$$\begin{aligned}
|K_2(u, f)| &\leq Ce^{-\delta t} + \int_0^t e^{b_1(t-s)} |F - F_L|(s)\, ds \\
&\leq Ce^{-\delta t} + Cr^2 \int_0^t e^{b_1(t-s)} e^{-2\delta s} ds \\
&\leq Ce^{-\delta t} + Cr^2 \epsilon^{-\delta t}.
\end{aligned}$$

Thus we have

$$\begin{aligned} \|K_1(u,f)\|_1 &\leq C \left\| \begin{pmatrix} u_0 \\ f_0 \end{pmatrix} \right\|_1 e^{-\delta t} + Cre^{-\delta t} \\ |K_2(u,f)| &\leq C \left\| \begin{pmatrix} u_0 \\ f_0 \end{pmatrix} \right\|_1 e^{-\delta t} + Cr^2 e^{-\delta t}. \end{aligned}$$

Now let $x = (u, f)$, so that $\|Kx\|_1 \leq C \|x_0\|_1 e^{-\delta t} + Cre^{-\delta t}$, or equivalently,

$$\|Kx\|_X \leq C_1 \|x_0\|_1 + C_2 \|x\|_X .$$

We shall show that K is a contraction mapping using the estimates developed above. We have

$$\|Kx - K\tilde{x}\| \leq C_3 \max\{\|x\|_X , \|\tilde{x}\|_X\} \|x - \tilde{x}\|_X .$$

Using a standard iteration argument, we can find a fixed point if the data is chosen sufficiently small. Define

$$\begin{aligned} x^0 &= 0 \\ x^n &= Kx^{n-1}, \ n \geq 1. \end{aligned}$$

We need to show that $\{x^n\}$ is a Cauchy sequence. From the estimate

$$\|Kx^n - Kx^m\|_X \leq C_3 \max\{\|x^n\|_X , \|x^m\|_X\} \|x^n - x^m\|_X ,$$

we need to show $C_3 \|x^n\|_X$ is less than one for all n. This will require the following estimate

$$\begin{aligned} \|Kx^n\|_X - \|Kx^0\|_X &\leq \|Kx^n - Kx^0\|_X \leq C_3 \|x^n\|_X \|x^n\|_X \\ \|Kx^n\|_X &\leq C_3 \|x^n\|_X^2 + \|Kx^0\|_X \\ &\leq C_3 \|x^n\|_X^2 + C_1 \|x_0\|_1 . \end{aligned}$$

Now we shall show that $C_3 \|x^n\|_X$ is bounded by $\frac{1}{2}$ if we choose our initial condition sufficiently small such that $C_1 C_3 \|x_0\|_1 < \frac{1}{4}$. We give the first two estimates,

$$\begin{aligned}
C_3 \|x^1\|_X &\leq C_3 \|K x^0\|_X \leq C_1 C_3 \|x_0\|_1 < \tfrac{1}{4} \\
C_3 \|x^2\|_X &= C_3 \|K x^1\|_X \leq C_3 C_3 \|x^1\|_X^2 + C_1 C_3 \|x_0\|_1 \\
&\leq (C_3 \|x^1\|_X)^2 + C_1 C_3 \|x_0\|_1 \\
&\leq (C_1 C_3 \|x_0\|_1)^2 + C_1 C_3 \|x_0\|_1 \\
&< \left(\tfrac{1}{4}\right)^2 + \tfrac{1}{4}.
\end{aligned}$$

One can show inductively that

$$C_3 \|x^n\|_X < a_n$$

where

$$\begin{aligned}
a_1 &= \tfrac{1}{4} \\
a_{n+1} &= a_n^2 + a_1 \quad \text{for } n \geq 1.
\end{aligned}$$

This is a monotonically increasing sequence with limit $\frac{1}{2}$, and so consequently, we have

$$\begin{aligned}
\|K x^n - K x^m\|_X &< \tfrac{1}{2} \|x^n - x^m\|_X = \tfrac{1}{2} \|K x^{n-1} - K x^{m-1}\|_X \\
&< \left(\tfrac{1}{2}\right)^{m+1} \|x^{n-m} - x^0\|_X \quad (\text{for } n > m) \\
&< \left(\tfrac{1}{2}\right)^{m+1} \tfrac{1}{2C_3}
\end{aligned}$$

This Cauchy sequence gives the existence of a unique fixed point, i.e.,

$$K \bar{x} = \bar{x}.$$

□

Chapter 5

The Hopf Bifurcation

To rigorously prove the existence of a Hopf bifurcation we shall use the approach of Crandall and Rabinowitz [5]. Our system, written as an abstract evolution equation, is

$$\begin{pmatrix} u \\ f \end{pmatrix}_t = L(\mu) \begin{pmatrix} u \\ f \end{pmatrix} + \begin{pmatrix} N(u, f, \mu) \\ n(u, f, \mu) \end{pmatrix} \tag{5.1}$$

where $L(\mu)$ is the parameter dependent linearized operator. As shown earlier, the operator L has the necessary conditions for a Hopf bifurcation. At the bifurcation value $\mu = \mu_{cr}$, L has two purely imaginary eigenvalues while the rest of the spectrum has negative real part. The formulation in Crandall and Rabinowitz's work [5] is slightly different, namely, their evolution equation is

$$u_t = L_0 u + R(\mu, u)$$

where L_0 is the linearized operator evaluated at the bifurcation value $\mu = \mu_{cr}$. Otherwise our procedure is the same as theirs. We write (5.1) as an equivalent integral equation via the variation of parameters formula. This integral equation is considered on a space of periodic functions. The implicit

function theorem is used to prove that periodic solutions exist. We shall show that a one parameter family of solutions exists for the concentration, mole fraction, bifurcation parameter, and the period.

First we shall review the idea of a bifurcation in a Banach space (see, for example Smoller [27]). Consider the function

$$\begin{aligned} f &: \mathbf{R} \times B_1 \to B_2 \\ f(\mu, x) &= 0 \end{aligned} \tag{5.2}$$

where B_i are Banach spaces. In particular, f could represent a system of differential or integral equations. The solution set is

$$f^{-1}(0) = \{(\mu, x) \in \mathbf{R} \times B_1 : f(\mu, x) = 0\}.$$

Without loss of generality, suppose we have the solution set $x = 0$ for μ in some interval I, i.e.,

$$f(\mu, 0) = 0 \quad \text{for } |\mu - \mu_0| < \delta.$$

We shall denote this solution set by Γ,

$$\Gamma = \{(\mu, x(\mu)) : \mu \in I, x = 0\}.$$

Now let $(\mu_0, 0)$ be an interior point of the curve Γ. We are interested when a neighbourhood of this interior point contains solutions of Equation (5.2) which do not lie on Γ (see Figure 5.1). When this occurs, we say that $(\mu_0, 0)$ is a *bifurcation point* with respect to Γ. Solutions not lying on Γ are called *bifurcating solutions*. In particular, we are interested in the existence of a continuous branch, Γ', emerging from $(\mu_0, 0)$. Obviously the Banach space version of the implicit function theorem fails at this point. In order to prove existence we need to first modify Equation (5.2) in order to use the implicit

function theorem. This is done by dividing out the zero solution; the implicit function theorem may then be used on a certain quotient space of B_1.

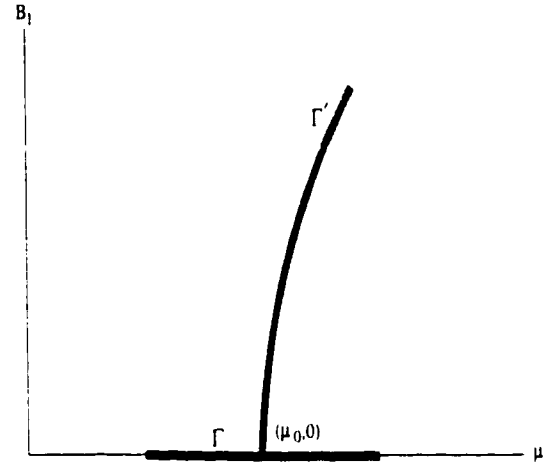

Figure 5.1 : Bifurcation diagram.

There is also a relation between the solution $f^{-1}(0)$ near a bifurcation point and the spectrum of the linearized operator. This becomes apparent when we Taylor expand the function f. If $f \in C^2(U, Y)$ for some neighbourhoods $U \subset B_1, Y \subset B_2$ then

$$f(\mu, u) = L_0 u + (\mu - \mu_0) L_1 u + r(\mu, u) \tag{5.3}$$

where

$$\begin{aligned} L_0 &= D_2 f(\mu_0, 0) \\ L_1 &= D_1 D_2 f(\mu_0, 0) \\ r(\mu, 0) &= 0 \\ D_2 r(\mu_0, 0) &= D_1 D_2 r(\mu_0, 0) = 0. \end{aligned}$$

The operators $D_i f$ above are Frechet derivatives with respect to the i-th variable of the function f.

5.1 Periodic Solutions

The linearized period at $\mu = \mu_{cr}$ is $p_0 = \frac{2\pi i}{\lambda(\mu_{cr})}$. Following the procedure of Crandall and Rabinowitz [5], we introduce the nondimensional period

$$p = \frac{p'}{p_0} = \frac{p_0 + \varepsilon p_1}{p_0}$$

where p' is the perturbation from the linearized period at bifurcation. Note that $p = 1$ gives the linearized period at bifurcation. We also make the substitution $\tau = t/p$, so that the integral equation corresponding to Equation (5.1) becomes

$$\begin{pmatrix} u \\ f \end{pmatrix}(\tau) = e^{p\tau L(\mu)} \begin{pmatrix} u_0 \\ f_0 \end{pmatrix} + p \int_0^\tau e^{p(\tau-\xi)L(\mu)} \begin{pmatrix} N(u(\xi), f(\xi), \mu) \\ n(u(\xi), f(\xi), \mu) \end{pmatrix} d\xi.$$

We seek p_0 periodic solutions to this equation. This corresponds to nontrivial periodic solutions of Equation (5.1) of period p' since $t = p\tau$. Define the integral operator

$$\begin{aligned} \Psi(p, \mu, (u, f))(\tau) &= \begin{pmatrix} u \\ f \end{pmatrix}(\tau) - e^{p\tau L(\mu)} \begin{pmatrix} u_0 \\ f_0 \end{pmatrix} \\ &\quad - p \int_0^\tau e^{p(\tau-\xi)L(\mu)} \begin{pmatrix} N(u(\xi), f(\xi), \mu) \\ n(u(\xi), f(\xi), \mu) \end{pmatrix} d\xi. \end{aligned}$$

Consider the following spaces

$$\begin{aligned} C_\pi &= \{u \in C([0, p_0], H^1) : u(0) = u(p_0)\} \\ c_\pi &= \{f \in C([0, p_0]) : f(0) = f(p_0)\} \\ C_0 &= \{u \in C([0, p_0], H^1) : u(0) = 0\} \\ c_0 &= \{f \in C([0, p_0]) : f(0) = 0\}. \end{aligned}$$

Ψ is then a mapping of a subset of $\mathbf{R} \times \mathbf{R} \times C_\pi \times c_\pi$ for which the mapping makes sense, into $C_0 \times c_0$. That this mapping is as regular as (N, n) is a theorem due to

Henry [18]. Now we take linear combinations of the eigenvectors corresponding to the purely imaginary eigenvalues $\lambda_{\pm}(\mu_{cr})$ from Proposition 4.2 to obtain two real linearly independent solutions, $\xi^{\pm} \in L^2 \times \mathbf{R}$. Define

$$\mathbf{e}_+(\tau) = e^{\tau L(\mu_{cr})}\xi^+$$

where $e^{\tau L(\mu_{cr})}$ is the infinitesimal generator of the linear operator L at $\mu = \mu_{cr}$ (see Theorem 4.7). We define the two dimensional nullspace of $I - e^{L(\mu_{cr})p_0}$, as $M_0 = N(I - e^{L(\mu_{cr})p_0})$ with basis $\{\xi^+, \xi^-\}$. Let M be the following two dimensional subspace of $C_\pi \times c_\pi$,

$$M = \left\{ (u, f) \in C_\pi \times c_\pi : \begin{pmatrix} u \\ f \end{pmatrix} (\tau) = e^{\tau L(\mu_{cr})}\mathbf{x}, \mathbf{x} \in M_0 \right\},$$

and let $Z = C_\pi \times c_\pi \ominus M$, be the complementary subspace of M. Now define the following map

$$Y(s, p, \mu, \mathbf{v}) = \begin{cases} \dfrac{\Psi(p, \mu, s(\mathbf{e}_+ + \mathbf{v}))}{s} & s \neq 0 \\ \Psi_{\mathbf{w}}(p, \mu, 0)(\mathbf{e}_+ + \mathbf{v}) & s = 0 \end{cases}$$

where $\Psi_{\mathbf{w}}(p, \mu, 0)$ is the Frechet derivative of the map $(w, f) \to \Psi(p, \mu, (w, f))$ at the point $(p, \mu, \mathbf{v}) = (1, \mu_{cr}, 0)$. Y is a continuous mapping of one degree less than Ψ, from a neighbourhood of $(0, 1, \mu_{cr}, 0) \in \mathbf{R}^3 \times Z$ into $C_0 \times c_0$. The Frechet derivative of the map $(p, \mu, \mathbf{v}) \to Y(s, p, \mu, \mathbf{v})$ at the point $(0, 1, \mu_{cr}, 0)$ is

$$dY(\hat{p}, \hat{\mu}, \hat{\mathbf{v}}) = Y_{\mathbf{v}}\hat{\mathbf{v}} + Y_p\hat{p} + Y_\mu\hat{\mu}, \tag{5.4}$$

where

$$\begin{aligned} Y_{\mathbf{v}}\hat{\mathbf{v}}(\tau) &= \hat{\mathbf{v}}(\tau) - e^{\tau L(\mu_{cr})}\hat{\mathbf{v}}(0) \\ Y_p(\tau)\hat{p} &= -\tau L(\mu_{cr})e^{\tau L(\mu_{cr})}\mathbf{e}_+(0)\hat{p} \\ Y_\mu(\tau)\hat{\mu} &= -\frac{\partial}{\partial \mu}e^{\tau L(\mu)}\Big|_{\mu=\mu_{cr}} \mathbf{e}_+(0)\hat{\mu}. \end{aligned}$$

We may explicitly write out these Frechet differentials in terms of u and f. If we let $\Psi = (\Psi_1, \Psi_2), \mathbf{e}_+ = (\mathbf{e}_{+1}, \mathbf{e}_{+2}), \mathbf{v} = (v_1, v_2)$, then the Frechet derivative is

$$
\begin{aligned}
dY(\hat{p}, \hat{\mu}, \hat{v}_1, \hat{v}_2) &= \left[\begin{array}{cccc} (Y_1)_p & (Y_1)_\mu & (Y_1)_{v_1} & (Y_1)_{v_2} \\ (Y_2)_p & (Y_2)_\mu & (Y_2)_{v_1} & (Y_2)_{v_2} \end{array} \right]_{(p,\mu,v_1,v_2)=(1,\mu_{cr},0,0)} \left(\begin{array}{c} \hat{p} \\ \hat{\mu} \\ \hat{v}_1 \\ \hat{v}_2 \end{array} \right) \\
&= \left[\begin{array}{cc} (Y_1)_p & (Y_1)_\mu \\ (Y_2)_p & (Y_2)_\mu \end{array} \right] \left(\begin{array}{c} \hat{p} \\ \hat{\mu} \end{array} \right) + \left[\begin{array}{cc} (Y_1)_{v_1} & (Y_1)_{v_2} \\ (Y_2)_{v_1} & (Y_2)_{v_2} \end{array} \right] \left(\begin{array}{c} \hat{v}_1 \\ \hat{v}_2 \end{array} \right)
\end{aligned}
$$

where

$$
\begin{aligned}
(Y_1)_{v_1}\hat{v}_1 &= \hat{v}_1(\tau) - H(\tau)\hat{v}_1(0) - \int_0^\tau H(\tau-\xi)B_{20}e^{-\frac{k_b}{2}x}\hat{v}_1(0,\xi)\,d\xi \\
(Y_1)_{v_2}\hat{v}_2 &= -\int_0^\tau H(\tau-\xi)B_{10}e^{-\frac{k_b}{2}x}\hat{v}_2(\xi)\,d\xi \\
(Y_2)_{v_1}\hat{v}_1 &= -b_{20}\int_0^\tau e^{b_1(\tau-\xi)}\hat{v}_1(0,\xi)\,d\xi \\
(Y_2)_{v_2}\hat{v}_2 &= \hat{v}_2(\tau) - e^{b_1\tau}\hat{v}_2(0) \\
(Y_1)_p\hat{p} &= -l\tau H(\tau)\xi^+\hat{p} - \hat{p}\int_0^\tau H(\tau-s)\left[B_{10}\mathbf{e}_{+2}(s) + B_{20}\mathbf{e}_{+1}(0,s)\right]e^{-\frac{k_b}{2}x}\,ds \\
&\quad - \hat{p}\int_0^\tau (\tau-s)lH(\tau-s)\left[B_{10}\mathbf{e}_{+2}(s) + B_{20}\mathbf{e}_{+1}(0,s)\right]e^{-\frac{k_b}{2}x}\,ds \\
(Y_1)_\mu\hat{\mu} &= \hat{\mu}\int_0^\tau H(\tau-s)\left[\frac{dB_{10}}{d\mu}\mathbf{e}_{+2}(s) + \frac{dB_{20}}{d\mu}\mathbf{e}_{+1}(0,s)\right]e^{-\frac{k_b}{2}x}\,ds \\
(Y_2)_p\hat{p} &= -b_1\tau e^{b_1\tau}\mathbf{e}_{+2}(0)\hat{p} - b_{20}\hat{p}\int_0^\tau (1+b_1(\tau-s))\,e^{b_1(\tau-s)}\mathbf{e}_{+1}(0,s)\,ds \\
(Y_2)_\mu\hat{\mu} &= -\frac{db_{20}}{d\mu}\hat{\mu}\int_0^\tau e^{b_1(\tau-s)}\mathbf{e}_{+1}(0,s)\,ds \\
l &= \Delta - k_b^2/4.
\end{aligned}
$$

Note that B_1, B_2, and b_2 from System (4.9) depend upon μ; B_{10}, B_{20}, and b_{20} denote their values at $\mu = \mu_{cr}$. The second matrix above is precisely $Y_{\mathbf{v}}\hat{\mathbf{v}}$. The

first matrix also agrees with the previous representation. The first representation (5.4) will be used in the following analysis.

Now we would like to use the implicit function theorem to establish the existence of a branch of solutions $(p(s), \mu(s), u(s), f(s))$ where $|s| < \delta$ for some $\delta > 0$. Note that

$$Y(0, 1, \mu_{cr}, 0)(\tau) = \Psi_{\mathbf{w}}(1, \mu_{cr}, 0)\mathbf{e}_+(\tau) = \mathbf{e}_+(\tau) - \epsilon^{\tau L(\mu_{cr})}\mathbf{e}_+(0) = 0.$$

Once dY is shown to be an isomorphism we may use the implicit function theorem to obtain solutions $(s, p(s), \mu(s), \mathbf{v}(s))$ of $Y = 0$ near $(0, 1, \mu_{cr}, 0)$. Setting

$$\begin{pmatrix} u(s) \\ f(s) \end{pmatrix}(\tau) = s\left(\epsilon^{L\tau}\xi^+ + \mathbf{v}(s)(\tau)\right)$$

gives the solution curve $(s, p(s), \mu(s), (u(s), f(s)))$ to $\Psi = 0$. Thus establishing that dY is an isomorphism gives the existence of periodic solutions:

Theorem 5.1 *There exists a $\delta > 0$ and continuous functions $(p(s), \mu(s), (u(s), f(s))) \in (\mathbf{R}, \mathbf{R}, C_\pi \times c_\pi)$ such that*

$$\Psi(p(s), \mu(s), (u(s), f(s))) = 0 \quad \text{for } |s| < \delta$$

with $(p(0), \mu(0), (u(0), f(0))) = (1, \mu_{cr}, (0, 0))$ and $u(s) \neq 0, f(s) \neq 0$ if $0 < |s| < \delta$.

The theorem above will follow from the following Lemma. Part (1) follows from Crandall and Rabinowitz [5] while parts (3) and (4) follow from Frankel and Roytburd [7].

Lemma 5.2 *Let $\Pi = Y_{\mathbf{v}}(1, \mu_{cr}, 0)$ be the mapping from $C_\pi \times c_\pi$ into $C_0 \times c_0$ and let $N(\Pi)$ and $R(\Pi)$ denote the nullspace and range of the operator Π, respectively. Then*

(1) $\mathbf{w} \in R(\Pi)$ *if and only if* $\mathbf{w}(p_0) \in R(I - e^{p_0 L(\mu_{cr})})$.

(2) $N(\Pi) = M$, *so that* $\dim N(\Pi) = 2$.

(3) $R(\Pi)$ *is a closed subspace of* $C_0 \times c_0$ *with* $\operatorname{codim} R(\Pi) = 2$.

(4) Y_p *and* Y_μ *span a two dimensional space which is complementary to* $R(\Pi)$, *i.e.*,

$$\text{if} \quad Y_p(\tau)\hat{p} + Y_\mu(\tau)\hat{\mu} \in R(\Pi), \quad \text{then} \quad \hat{p} = \hat{\mu} = 0.$$

Proof: (1) Suppose $\mathbf{w} \in R(\Pi)$ then $\mathbf{w}(\tau) = \mathbf{v}(\tau) - e^{\tau L(\mu_{cr})}\mathbf{v}(0)$ for some $\mathbf{v} \in C_\pi \times c_\pi$. Then $\mathbf{w}(p_0) = (I - e^{p_0 L(\mu_{cr})})\mathbf{v}(0)$. For the converse, suppose $\mathbf{w}(p_0) = (I - e^{p_0 L(\mu_{cr})})\mathbf{u}_0$. One can verify that $\mathbf{u}(\tau) = \mathbf{w}(\tau) - e^{\tau L(\mu_{cr})}\mathbf{u}_0$ satisfies $\mathbf{u}(\tau) - e^{\tau L(\mu_{cr})}\mathbf{u}(0) = \mathbf{w}(\tau)$ and that $\mathbf{u} \in C_\pi \times c_\pi$. Thus $\mathbf{w} \in R(\Pi)$. Part (2) is obvious. (3) The operator $I - e^{p_0 L(\mu_{cr})}$ is invertible when restricted to $(I - P)(H^1 \times \mathbf{R})$, where P is the projector on the subspace spanned by the eigenvectors $\xi^{\pm}$. Note by Theorem 4.7 we have

$$\left\| e^{\tau L(\mu_{cr})}(I - P) \right\| = \left\| e^{\tau L_2} \right\| \le C(\delta) e^{-\delta\tau} \text{ for } \delta \in (0, \frac{k_b^2}{4}).$$

We also have by Proposition 4.8 for $\mathbf{u} \in (I - P)(H^1 \times \mathbf{R})$

$$\left\| e^{\tau L(\mu_{cr})}\mathbf{u} \right\|_1 \le \left\| L_2^{1/2} e^{\tau L(\mu_{cr})}\mathbf{u} \right\| \le C e^{-\delta\tau} \|\mathbf{u}\|_1$$

where $\|\mathbf{u}\|_1 = \|(u_1, u_2)\|_1 = \|u_1\|_{H^1} + |u_2|$. Using the Neumann series for the operator $(I - e^{p_0 L(\mu_{cr})})^{-1}$,

$$\left\| \sum \left(e^{p_0 L(\mu_{cr})} \right)^n \right\|_1 = \left\| \sum e^{n p_0 L(\mu_{cr})} \right\|_1 \le \frac{C}{1 - e^{-\delta p_0}},$$

we see that $(I - e^{p_0 L(\mu_{cr})})^{-1}$ is bounded and thus that $R(I - e^{p_0 L(\mu_{cr})})$ is closed. Suppose $\tilde{\mathbf{w}}$ belongs to the closure of $R(\Pi)$, then by (1) $\tilde{\mathbf{w}} \in \overline{R(I - e^{p_0 L(\mu_{cr})})}$. Since $R(I - e^{p_0 L(\mu_{cr})})$ is closed, $\tilde{\mathbf{w}}(p_0) \in R(I - e^{p_0 L(\mu_{cr})})$, again by (1), $\tilde{\mathbf{w}} \in R(\Pi)$. (4) By (1), this is equivalent to showing that

$$\text{if} \quad Y_p(p_0)\hat{p} + Y_\mu(p_0)\hat{\mu} \in R(I - e^{p_0 L(\mu_{cr})}) \quad \text{then} \quad \hat{p} = \hat{\mu} = 0.$$

We have

$$\begin{aligned} Y_p(p_0) &= -p_0 L(\mu_{cr}) e^{p_0 L(\mu_{cr})} \mathbf{e}_+(0) = -p_0 L(\mu_{cr}) \mathbf{e}_+(0) = -p_0 \lambda_+(\mu_{cr}) \mathbf{e}_+(0) \\ &= -2\pi i \xi^+ \end{aligned}$$

and

$$\begin{aligned} Y_\mu(p_0) &= -\frac{\partial}{\partial \mu} \left[e^{p_0 L(\mu)} \right]_{\mu=\mu_{cr}} \xi^+(\mu_{cr}) \\ &= -\frac{\partial}{\partial \mu} \left[e^{p_0 L(\mu)} \xi^+(\mu) \right]_{\mu=\mu_{cr}} + e^{p_0 L(\mu_{cr})} \frac{\partial}{\partial \mu} \left[\xi^+(\mu) \right]_{\mu=\mu_{cr}} \\ &= -\frac{\partial}{\partial \mu} \left[e^{p_0 \lambda_+(\mu)} \xi^+(\mu) \right]_{\mu=\mu_{cr}} + e^{p_0 L(\mu_{cr})} \frac{\partial}{\partial \mu} \left[\xi^+(\mu) \right]_{\mu=\mu_{cr}} \\ &= -p_0 e^{p_0 \lambda_+(\mu_{cr})} \frac{\partial}{\partial \mu} \left[\lambda_+(\mu) \right]_{\mu=\mu_{cr}} \xi^+(\mu_{cr}) - e^{p_0 \lambda_+(\mu_{cr})} \frac{\partial}{\partial \mu} \left[\xi^+(\mu) \right]_{\mu=\mu_{cr}} \\ &\quad + e^{p_0 L(\mu_{cr})} \frac{\partial}{\partial \mu} \left[\xi^+(\mu) \right]_{\mu=\mu_{cr}} \\ &= -p_0 \frac{\partial}{\partial \mu} \left[\lambda_+(\mu) \right]_{\mu=\mu_{cr}} \xi^+(\mu_{cr}) - \frac{\partial}{\partial \mu} \left[\xi^+(\mu) \right]_{\mu=\mu_{cr}} \\ &\quad + e^{p_0 L(\mu_{cr})} \frac{\partial}{\partial \mu} \left[\xi^+(\mu) \right]_{\mu=\mu_{cr}}. \end{aligned}$$

To show that $\hat{p} = \hat{\mu} = 0$ we need to look at the adjoint operator L^*. Let $\xi^*_\pm$ denote the adjoint eigenvectors with corresponding eigenvalues $\bar{\lambda}_\pm(\mu_{cr})$. We also have

$$\left(e^{p_0 L^*(\mu_{cr})} - I \right) \xi^*_\pm = 0.$$

The following inner product gives

$$\begin{aligned} \left\langle Y_p(p_0)\hat{p} + Y_\mu(p_0)\hat{\mu}, \xi^*_+ \right\rangle &= \left(-2\pi i \hat{p} - p_0 \tfrac{\partial}{\partial \mu} \left[\lambda_+(\mu) \right]_{\mu=\mu_{cr}} \hat{\mu} \right) \left\langle \xi^+, \xi^*_+ \right\rangle \\ &= 0. \end{aligned}$$

The coefficient for $\hat{\mu}$ contains a nonzero real term while the coefficient for $\hat{p}$ is purely imaginary. Thus the term is zero only if $\hat{p} = \hat{\mu} = 0$. Using similar reasoning as above, one can show that the span of Y_p and Y_μ with real coefficients contains both ξ^+ and $i\xi^+$ and hence is a two dimensional real space. □

Chapter 6

Numerics

6.1 Numerical Algorithm

The numerical algorithm that is used for the free boundary problem is a modified version of that used by Frankel, Roytburd, and Sivashinsky [9]. Their procedure is closely followed, the difference in our case being the addition of the ordinary differential equation involving the mole fraction to the boundary conditions. To obtain zero boundary conditions we take System (4.1) and make the following substitution

$$w(x,t) = u(x,t) - e^{-x}\left[(1+x)u(0,t) + xu_x(0,t)\right].$$

This was done in order to reduce the roundoff error. The transformed system is then

$$\left.\begin{aligned} w_t &= w_{xx} + (v+k_b)w_x + F(x,v,f,\dot{v},\dot{f}) \\ w(0,t) &= 0 \\ w_x(0,t) &= 0 \\ w(\infty,t) &= 0 \\ \dot{f} &= \frac{k_b+v}{\varepsilon}\left(-\bar{f} - f + \frac{\rho(v+k_b)-k_b}{\rho(v+k_b)}\right) \end{aligned}\right\} \qquad (6.1)$$

where

$$\begin{aligned} F &= -k_b A v e^{-k_b x} - \epsilon^{-x}[(1+x)\dot{u}(0,t) + x\dot{u}_x(0,t) \\ &\quad - (x-1-x(v+k_b))u(0,t) - (x-2+(1-x)(v+k_b))u_x(0,t)] \end{aligned}$$

The algorithm is applied to a finite domain $0 \leq x \leq L$, with decay at infinity replaced by $w(L,t) = 0$. Suppose the concentration w_j^k, velocity v^k, and mole fraction f^k are known at the k-th time step. The subscript j denotes the spatial discretization of the concentration. Now we need to evaluate these three quantities at the next time step $k+1$. This is done as follows:

1. A guess for the velocity, $(v^{k+1})_0$, is made.

2. The mole fraction $(f^{k+1})_0$ is computed using $(v^{k+1})_0$ via an explicit scheme from the fifth equation from System (6.1).

3. By steps 1 and 2 we now have an overdetermined system. For the moment we shall neglect the Neumann condition and solve for $(w_j^{k+1})_0$ using the Dirichlet condition (the second equation of (6.1)). The Crank-Nicolson method is used to solve the heat equation.

4. An integrated version of the Neumann condition (the third equation of (6.1)) is computed and then used as a test for the solution.

5. If the desired precision is met, we simply repeat steps 1-4 for the next $k+2$ time step. Otherwise, a new guess for the velocity $(v^{k+1})_1$ is computed using Newton's method for the integrated Neumann condition.

This procedure is identical to Frankel, Roytburd, and Sivashinsky [9] except for step 2, which includes the coupling of the ordinary differential equation to our system. If $\varepsilon = 0$ then f is given explicitly; if not, then a discretization of f is required. As in Frankel, Roytburd, and Sivashinsky's paper [9],

the Neumann condition $w_x(0,t) = 0$, is replaced by an equivalent condition derived as follows. First we integrate the first equation of System (6.1) with respect to x from 0 to infinity,

$$\begin{aligned}\frac{d}{dt}\int_0^\infty w\,dx &= w_x\,|_0^\infty + (v+k_b)w\,|_0^\infty + \int_0^\infty F(x,v,f,\dot{v},\dot{f})\,dx \\ &= \int_0^\infty F(x,v,f,\dot{v},\dot{f})\,dx\end{aligned}$$

Integrating over one time step from t_k to t_{k+1} yields,

$$\left[\int_0^\infty w\,dx\right]_{t=t_k}^{t=t_{k+1}} = \int_{t_k}^{t_{k+1}}\left[\int_0^\infty F(x,v,f,\dot{v},\dot{f})\,dx\right]dt$$

The integrated version of the Neumann condition is defined to be

$$\begin{aligned}R(v^{k+1},f^{k+1};v^k,f^k) &= \left[\int_0^\infty w\,dx\right]_{t=t_k}^{t=t_{k+1}} \\ &\quad - \int_{t_k}^{t_{k+1}}\left[\int_0^\infty F(x,v,f,\dot{v},\dot{f})\,dx\right]dt \qquad (6.2) \\ &= 0\end{aligned}$$

Since f^{k+1} is a function of v^{k+1} and f^k by step 2, we may consider R as a function of v^{k+1},

$$R(v^{k+1};v^k,f^k) = 0.$$

The integrated version (6.2) is used as our check for the guess $(v^{k+1})_0$. If the desired precision is not met, a new velocity $(v^{k+1})_1$ is computed from $R(v^{k+1}) = 0$, via Newton's method.

In order to ensure that L was chosen large enough to simulate decay at infinity, and that the spatial and temporal discretizations Δx, Δt, were chosen sufficiently small, the above algorithm was first used to numerically solve the linearized problem and compare it to the exact solution. In Figures 6.1-6.2 the same set of parameters were used except for the length L. For the first figure where $L = 10$, the numerical and exact solutions begin to diverge as time increases. For the second figure where $L = 100$, the numerical and exact

solutions agree well. For all the figures that follow, the values of L, Δx, and Δt used for the nonlinear system were first tested for the linearized system in order to achieve agreement of the exact and numerical solutions.

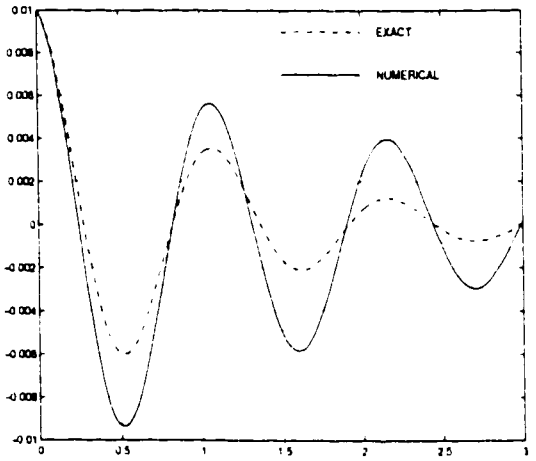

Figure 6.1 : Plot of v vs. t for $L = 10$; $(k_b, c_\infty, a, b, \varepsilon) = (5, 1, .1/5, .5/5, 0)$.

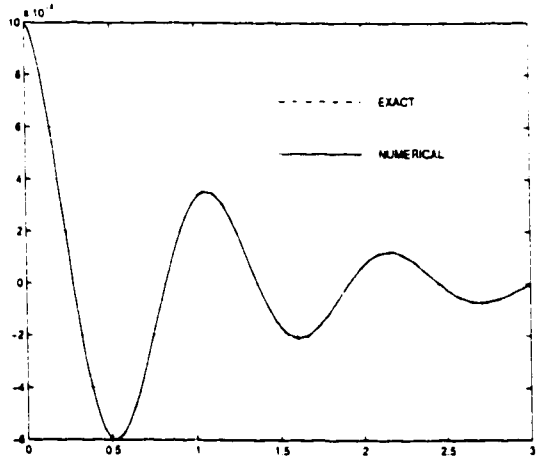

Figure 6.2 : Plot of v vs. t for $L = 100$; $(k_b, c_\infty, a, b, \varepsilon) = (5, 1, .1/5, .5/5, 0)$.

6.2 Numerical Results

The linearization was done about a specific point which was motivated by a modified version of van der Pol's equation (see Appendix A). In this section we shall examine the nonlinear problem as the bifurcation parameter $\mu = b/a$ exceeds some critical value. We expect to see stable limit cycles above the threshold value. Note that in some of the cases we shall examine, the critical value of the bifurcation parameter appears before a local maximum and minimum appear for the nullcline $\dot{f} = 0$ in the graph of the phase portrait of the boundary concentration $c(0,t)$ vs. the mole fraction $f(t)$. This seems reasonable in light of the discussion in Appendix A. Introducing time delays to the modified van der Pol's equation had the effect of decreasing the threshold bifurcation value. In our problem there are time delays present from diffusion.

We shall also examine the effects of varying the parameter ε. Recall that $\varepsilon = 0$ is the nonequilibrium fractionation model, while $\varepsilon > 0$ corresponds to the dynamic fractionation model discussed in Chapter 2. All the threshold bifurcation values have been determined from earlier work ([28]). In the following figures, we shall vary ε and b/a while the other parameters are held fixed. We set $\rho = 2$, $k_b = 5$, $a = 1/50$, $L = 100$, and choose exponentially decaying initial conditions. No noticeable changes are observed in decreasing the spatial and temporal discretizations below $\Delta x = .0125$ and $\Delta t = .001$. In Figure 6.3 finite amplitude periodic solutions appear above the threshold bifurcation value. Below the critical value the zero solution is stable (this solution corresponds to the constant composition front). Similar behaviour appears for $\varepsilon = 0.01$ and $\varepsilon = 0.1$ in Figures 6.4-6.5. For nonzero ε we also plot the phase portrait of the boundary concentration $c(0,t)$ vs. the mole fraction $f(t)$.

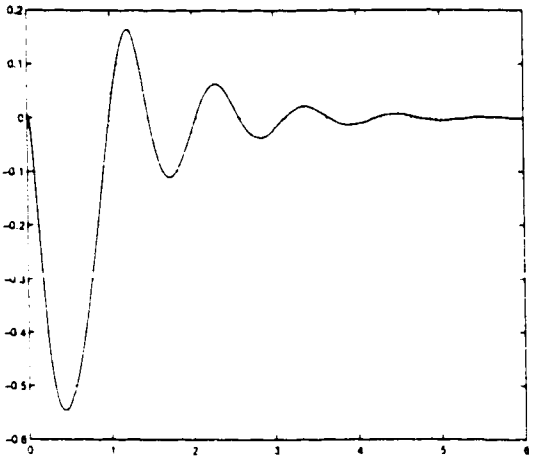

Figure 6.3a : Plot of v vs. t; $\varepsilon = 0, b/a = 5$.

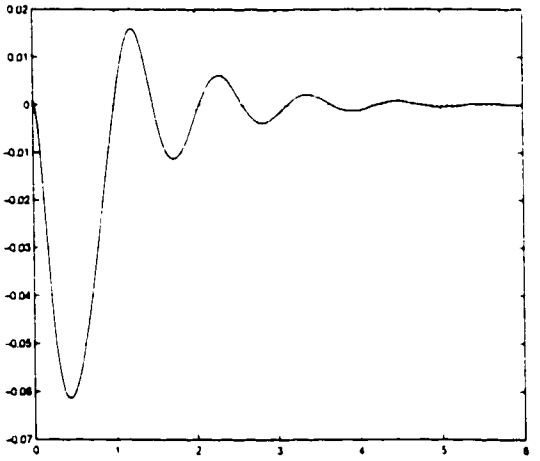

Figure 6.3b : Plot of f vs. t; $\varepsilon = 0, b/a = 5$.

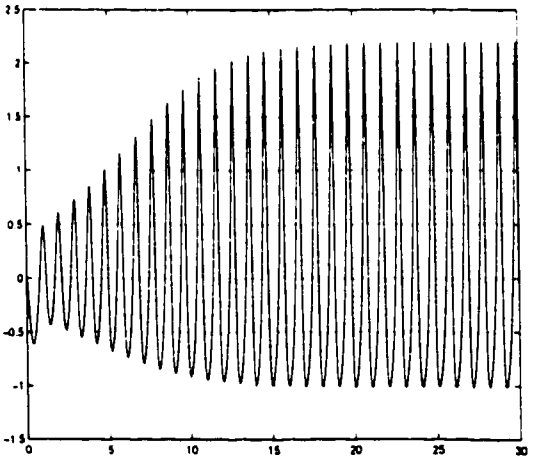

Figure 6.3c : Plot of v vs. t; $\varepsilon = 0, b/a = 6$.

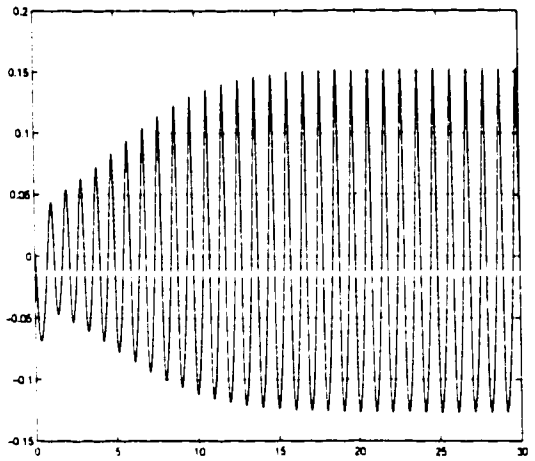

Figure 6.3d : Plot of f vs. t; $\varepsilon = 0, b/a = 6$.

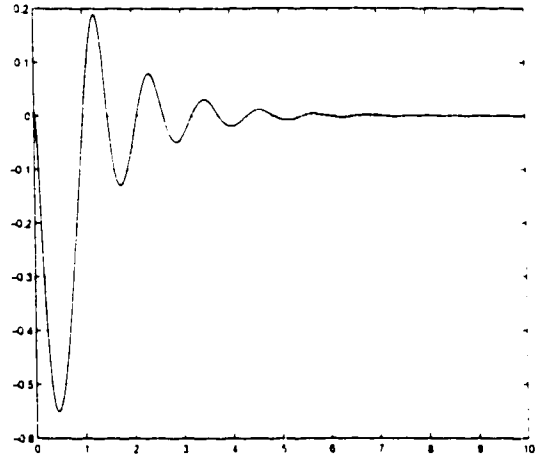

Figure 6.4a : Plot of v vs. t; $\varepsilon = 0.01, b/a = 5$.

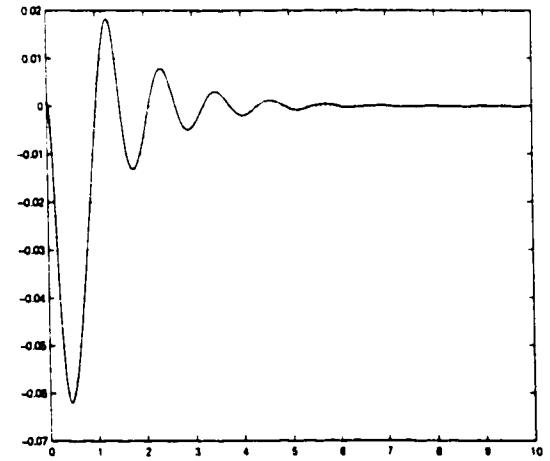

Figure 6.4b : Plot of f vs. t; $\varepsilon = 0.01, b/a = 5$.

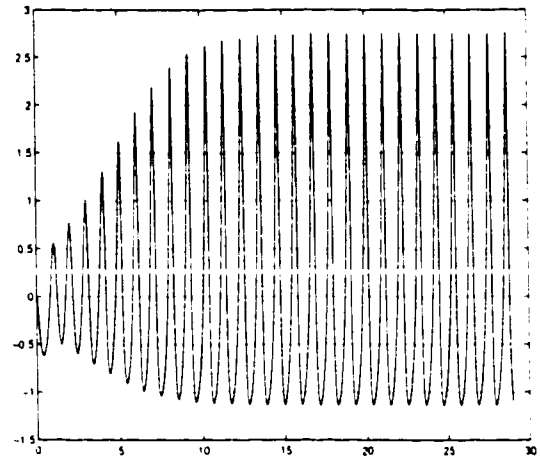

Figure 6.4c : Plot of ι vs. t; $\varepsilon = 0.01, b/a = 6$.

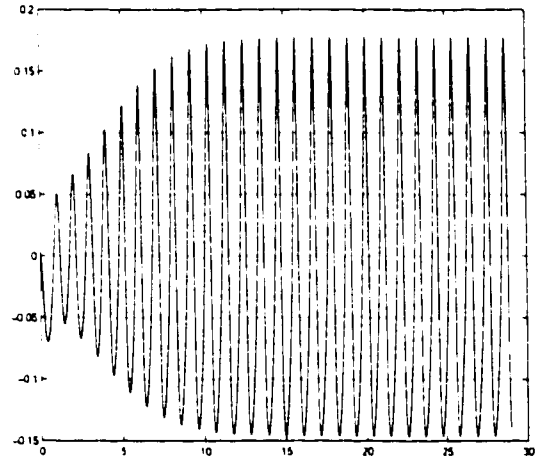

Figure 6.4d : Plot of f vs. t; $\varepsilon = 0.01, b/a = 6$.

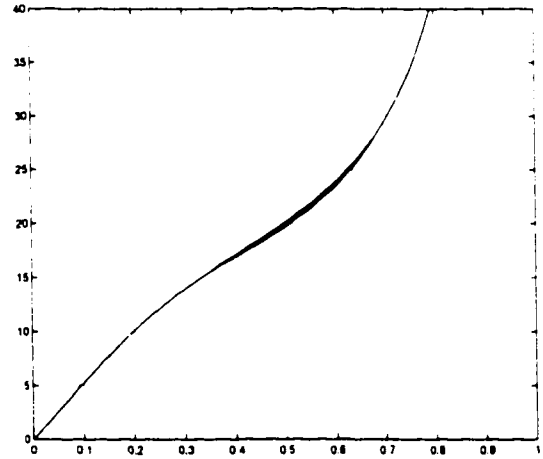

Figure 6.4e : Plot of c vs. f; $\varepsilon = 0.01, b/a = 6$.

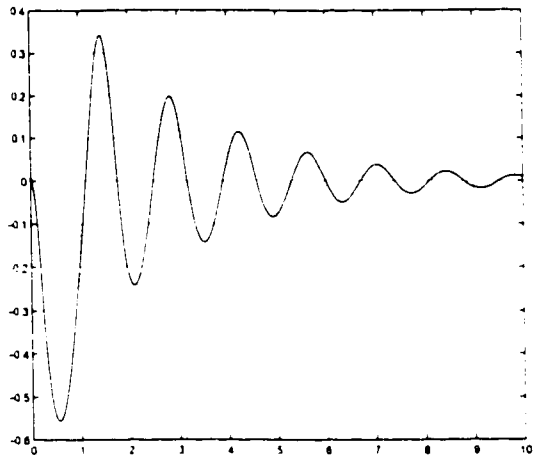

Figure 6.5a : Plot of v vs. t; $\varepsilon = 0.1, b/a = 5$.

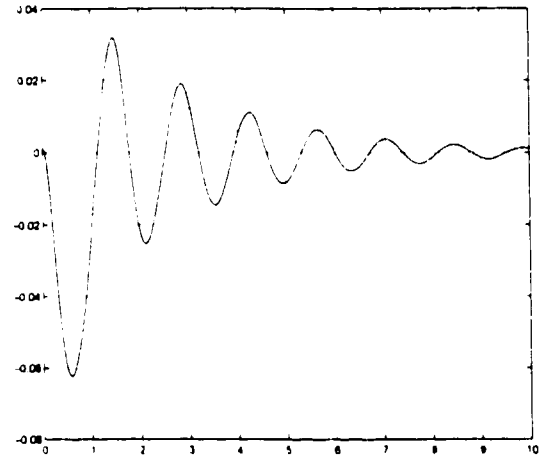

Figure 6.5b : Plot of f vs. t; $\varepsilon = 0.1, b/a = 5$.

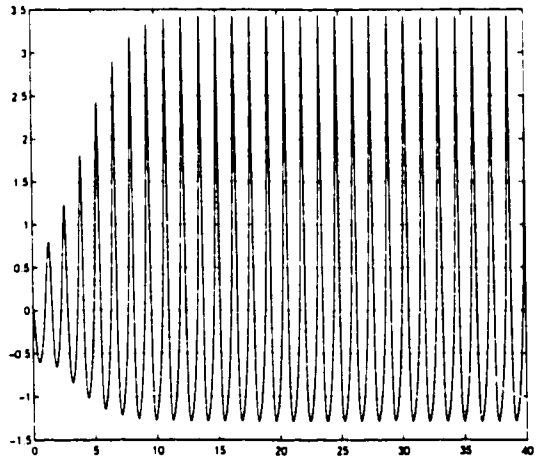

Figure 6.5c : Plot of v vs. t; $\varepsilon = 0.1, b/a = 6$.

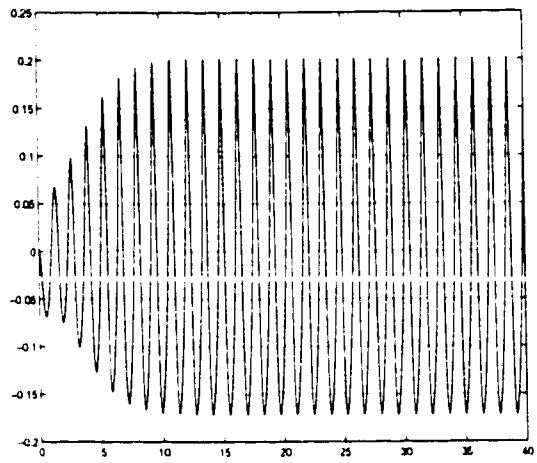

Figure 6.5d : Plot of f vs. t; $\varepsilon = 0.1, b/a = 6$.

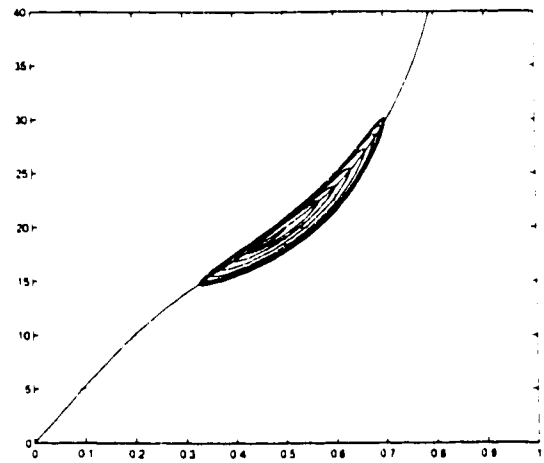

Figure 6.5e : Plot of c vs. f; $\varepsilon = 0.1, b/a = 6$.

Now we shall further increase the bifurcation parameter such that multiple branches appear in the phase portrait of $c(0,t)$ vs. $f(t)$ for the nullcline $\dot{f} = 0$. In Figures 6.6-6.7, the amplitude of the periodic solutions increase as b/a is increased. However, for the case $\varepsilon = 0.1$, as the bifurcation value is further increased, the periodic orbit loses stability to the zero solution (see Figure 6.8). From the linearization one can verify that the real part of the eigenvalues will decrease and once more become negative. One must be careful here with

this observation. This behaviour does not seem to be physically sound. Recall that ε should be small; it represents the microscopic level where the crystals are forming and attaching to the moving front. If ε is too large we are no longer adequately modelling this phenomenon. Thus $\varepsilon = 0.1$ is not sufficiently small to model the attachment front while $\varepsilon = 0.01$ is consistent. As b/a increases, the local maximum and local minimum of the nullcline $\dot{f} = 0$ begin to separate. The horizontal component of the vector field for the differential equation of f is of the order ε^{-1}; this is not large enough in magnitude to maintain an oscillatory solution. The trajectory of $(f(t), c(0,t))$ gets trapped between the local extrema, and decays to zero in an oscillatory fashion (see Figure 6.8). For $\varepsilon = 0.01$ this never occurs since the horizontal component of the vector field is sufficiently large in magnitude.

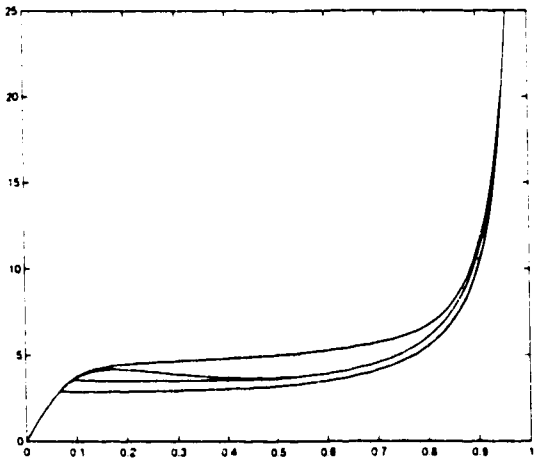

Figure 6.6 : Plot of c vs. f; $\varepsilon = 0.01, b/a = 50$.

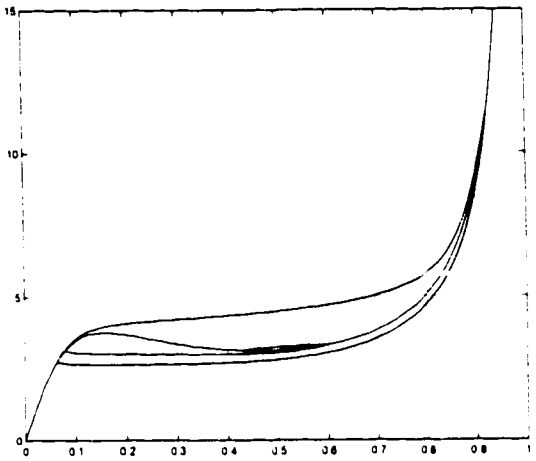

Figure 6.7 : Plot of c vs. f; $\varepsilon = 0.01, b/a = 60$.

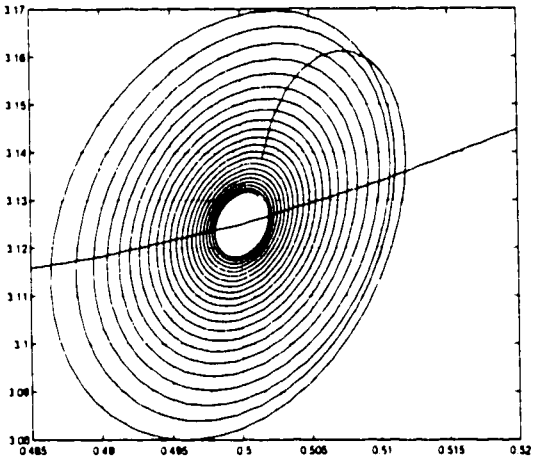

Figure 6.8 : Plot of c vs. f; $\varepsilon = 0.1, b/a = 60$.

Now we examine the effect of initial conditions. In the following analysis, we shall choose initial conditions outside the stable limit cycle of $c(0,t)$ vs. $f(t)$. In Figures 6.9-6.10, the trajectories tend to the limit cycle. Thus the numerics suggest that the periodic orbits are stable in this parameter range.

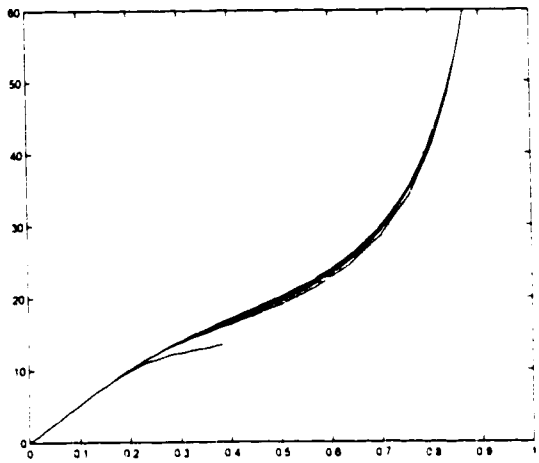

Figure 6.9 : Plot of c vs. f; $\varepsilon = 0.01, b/a = 6$.

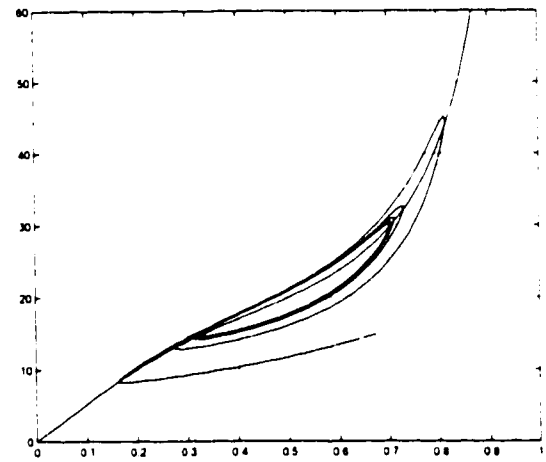

Figure 6.10 : Plot of c vs. f; $\varepsilon = 0.1, b/a = 6$.

Again we stress that all numerical simulations above were first tested on the linearized system where the analytical solution is known. There were other parameter values where there was a discrepancy between the numerical and exact linear solutions. In these cases, even with very small Δx and Δt values, the iteration scheme for the velocity at the next time step failed to converge to a specific value (see step 5 in Section 6.1). Fundamentally, Newton's method failed to converge; the initial guess at the $k+1$ time step $(v^{k+1})_0$, was not

close enough to the exact root of $R(v^{k+1}; v^k) = 0$. Thus for future work, a more robust code will be needed for certain choices of the parameter space.

Chapter 7

Summary and Discussion

In this thesis a free moving boundary model was developed describing the growth of a rock consisting of two crystal end-members. Without any externally imposed periodicities on the state, oscillatory zoning of the solid can be qualitatively explained by the diffusion of solutes in the melt along with the associated chemical kinetics involved for the formation of crystals in the interface. In particular, the dependency of the rate constants on the composition of the advancing crystal surface is essential for oscillatory zoning in the model.

The problem we considered was the simplest possible for this crystal growth free moving boundary model. First we assumed the simplest possible stoichiometry, a set of first order reactions for the formation of crystals on the interface. Next, the simplest possible ratio for the rate constants was chosen that would allow for the possibility of zoning. Also the diffusion constant of one of the solute species was chosen much larger than the other, such that explicit constant composition front solutions could be computed. Lastly, the rate constant of the solute with the large diffusion constant was chosen to be a constant. This allowed all the variation in concentration to be confined to one solute. All these conditions above still allowed for the possibility of oscillatory

zoning in our physical arguments. One must remember that the above is a simplistic model describing crystal growth. In real applications, the correct stoichiometry and rate constants must be determined. Nevertheless, the above model may serve as a starting point for more complicated systems.

Linearization was carried out about the constant composition planar solution. A parameter space was found that gave the necessary conditions for a Hopf bifurcation (a pair of complex conjugate eigenvalues crossing the imaginary axis as the bifurcation value varied). The ratio of the coefficients, b/a of the rate constant $K(f) = a + bf^2$ was chosen as the bifurcation parameter. The term b/a is a measure of the affinity of like crystals to attach to the moving interface. For small b/a, diffusion should dominate and one would expect the constant composition solution (grey homogeneous rock) to be stable. This was indeed found to be true (see Theorem 4.9). To date, complex eigenvalues were found when $c_x(R(0),0) < 0$, i.e., the concentration of solute slightly ahead of the moving front was less. This physically corresponds to an initial build up of solute on the moving front. The condition $c_x < 0$, was satisfied when k_b, the velocity of the constant composition front, was sufficiently large. By picking k_b large enough solute is allowed to accumulate on the interface. Now we were able to vary b/a to obtain complex eigenvalues crossing the imaginary axis. Similar initial conditions have been used in other parabolic systems (i.e., solid combustion problems [7]). With the dynamic fractionation surface model (i.e., the model corresponding to a small finite thickness of the interface), an analogy was considered with a modified version of van der Pol's oscillator. This served to suggest a point about which to do our linearized stability analysis. As mentioned above the necessary conditions for a Hopf bifurcation were observed for large velocities of the planar front as the parameter b/a was increased. This bifurcation did not occur precisely at $b/a = (b/a)_0$, the value

where a local minimum and local maximum appear for the nullcline $\dot{f} = 0$, as predicted by the modified van der Pol's equation, but in the vicinity of this value since there were time delays introduced by the diffusion equation.

The results of Chapter 4 and Chapter 5 apply to the dynamic fractionation surface model. In Chapter 4, the principle of linearized stability was proven. Linearized stability implied nonlinear stability for $b/a < (b/a)_{cr}$ and small initial conditions. In this same theorem, global existence in time was also proven for $b/a < (b/a)_{cr}$. Note that a solution to the integral equation of Theorem 4.9 is in fact a weak type of a solution; the Banach space under consideration contained only one spatial derivative (as opposed to two). Since we have the existence of a unique classical solution, this integral solution must coincide with the classical solution if the initial data are smooth and satisfy the appropriate compatibility conditions (see Chapter 3). The Hopf bifurcation was proven via the Banach space version of the implicit function theorem in the context of an integral equation which was set up in the appropriate periodic spaces (cf. [5],[7]). In Chapter 6, the numerics suggest that the periodic orbits that were proven to exist in the previous chapter, were stable above the critical bifurcation value. The numerical algorithm used was that of [9]. Before analyzing the full nonlinear problem, all simulations were first tested for the linearized system in order to achieve agreement of the numerical solution and the exact solution, which is available here. The parameter space under consideration in this chapter was chosen to meet this criteria. Numerical simulations of the mole fraction and boundary concentration, $(f(t), c(R(t), t))$, tended to a limit cycle when picking initial conditions close to the constant composition front. If initial conditions were chosen outside the limit cycle the numerical trajectories converged to the limit cycle. This suggests that there was a region of attraction surrounding the limit cycle.

Appendix A

Modified van der Pol's Equation

In this Appendix a modified version of van der Pol's equation is examined. In this autonomous dynamical system a bifurcation parameter is present such that as its value increases past a critical value, a stable limit cycle appears. If we linearize about a certain point, we find that this point will lose stability to a limit cycle through a Hopf bifurcation. This appendix serves to suggest a specific point about which to do our linearized stability analysis. It also suggests that our bifurcation parameter should be the ratio b/a of the rate constant, $K(f) = a + bf^2$. Also, essential criteria to develop a finite dimensional approximation to the full partial differential equation shall be stated. A finite dimensional dynamical system may be obtained through a spatial discretization of the free boundary problem.

Consider van der Pol's equation

$$\ddot{x} - \frac{1}{\varepsilon}(1 - x^2)\dot{x} + x = 0 \quad \varepsilon > 0$$

or equivalently, consider the following system of first order ordinary differential

equations

$$\begin{aligned} \dot{x} &= y - \frac{1}{\varepsilon}\left(\frac{x^3}{3} - x\right) \\ \dot{y} &= -x. \end{aligned}$$

Now suppose ε is small. Substituting $y' = \varepsilon y$ and then dropping the primes in the above equations gives

$$\begin{aligned} \dot{x} &= \frac{1}{\varepsilon}\left(y - \left(\frac{x^3}{3} - x\right)\right) \\ \dot{y} &= -\varepsilon x. \end{aligned}$$

For small ε, the change in y is negligible when we are not close to the curve $y = x^3/3 - x$. The family of horizontal lines, $y =$ constant, approximates the flow of the above system away from the curve. When $| y - (x^3/3 - x) | \sim O(\varepsilon^2)$, both $\dot{x}$ and $\dot{y}$ are of the same order, and the flow will follow the curve $y = x^3/3 - x$ except at the critical points $(\pm 1, \mp 2/3)$ where the solutions leave the curve and follow a horizontal line onto another point on the curve. Figure A.1 illustrates these ideas and a stable limit cycle is present (see Guckenheimer and Holmes [11] for more details).

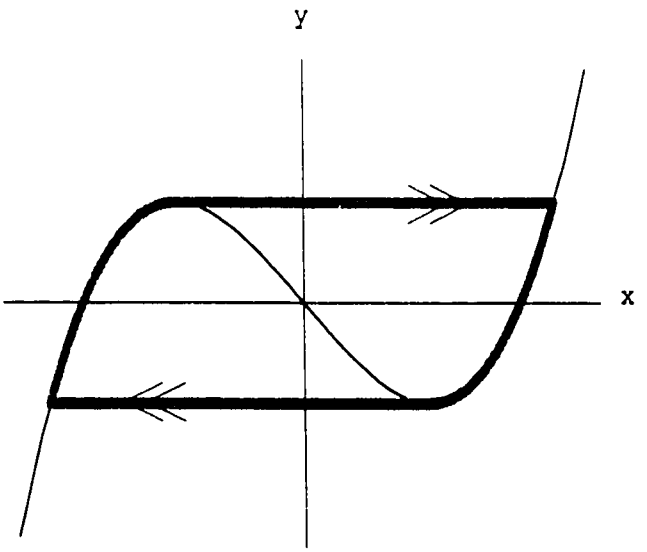

Figure A.1 : Relaxation oscillations.

In our model (see, for example, Equations (3.4) and (3.6)) we have

$$\begin{aligned} \varepsilon \dot{f} &= V(t)\left(-f + \frac{K(f)c}{K(f)c+1}\right) \\ \dot{c} &= \tilde{G}(c,f) + I(t) \end{aligned}$$

where $V(t)$ is the velocity of the moving front, $I(t)$ represents initial conditions, and $\tilde{G}(c,f)$ is an integral representation containing Green's functions of the diffusion equation. There are terms in this integral involving the position of the planar front $R(t)$, which is an unknown. Rescaling time with $t = \sqrt{\varepsilon}t'$, and then substituting in the above system after dropping the primes gives

$$\dot{f} = \frac{V}{\sqrt{\varepsilon}}\left(-f + \frac{K(f)c}{K(f)c+1}\right) \tag{A.1}$$

$$\dot{c} = \sqrt{\varepsilon}\,(G(c,f) + I(t)). \tag{A.2}$$

Our model is similar to the following modified version of van der Pol's equation

$$\dot{x} = \frac{1}{\varepsilon}\left(y - \left(\frac{x^3}{3} - \lambda x\right)\right) \tag{A.3}$$

$$\dot{y} = -\varepsilon x \tag{A.4}$$

where λ is a constant. Let $(b/a)_0$ denote the value of b/a when a local maximum and local minimum appear for the nullcline $\dot{f} = 0$. Note the similarity between $\dot{x}$ and $\dot{f}$; the horizontal components of both of these vector fields move towards the nullclines $\dot{x} = 0$ and $\dot{f} = 0$ respectively. In both cases local extrema appear when $\lambda > 0$ and when $b/a > (b/a)_0$.

Now we shall examine the stability of the critical point $(0,0)$ for the modified van der Pol equation (A.3)-(A.4). Linearizing about $(0,0)$ gives the following eigenvalues:

$$\frac{\lambda \pm \sqrt{\lambda^2 - 4\varepsilon^2}}{2\varepsilon}.$$

For ε fixed ($\varepsilon > 0$), a Hopf bifurcation occurs at the critical value $\lambda_0 = 0$. When $\lambda > 0$, *multiple branches* appear for the nullcline $\dot{x} = 0$ (i.e., one local

maximum and one local minimum appears). As soon as these branches appear, the critical point $(0,0)$ loses its stability to a limit cycle. Time delays (through diffusion in our model (A.1)-(A.2)) and the shape of the "vertical" nullcline (see Figure 2.4 or 6.7 with the vertical nullcline included like Figure A.2) can alter the location of the critical point for Hopf bifurcations.

Let us examine Equations (A.3)-(A.4) in more detail for the effects of time delays and the shape of the "vertical" nullcline. If we replace Equation (A.4) by

$$\dot{y} = -\varepsilon x(t-T) \tag{A.5}$$

where T represents a discrete time delay, the characteristic equation corresponding to Equations (A.3) and (A.5) is then

$$z^2 - \frac{1}{\varepsilon}\lambda z + e^{-zT} = 0.$$

If we substitute $z = r + is$ into the characteristic equation and set $r = 0$ to obtain purely imaginary roots, then

$$\begin{aligned} s^2 &= \cos sT \\ \lambda &= -\varepsilon\frac{\sin sT}{s}. \end{aligned}$$

If we denote the solution to $s^2 = \cos sT$ by $s_0(T)$ for $0 < s_0 < \frac{\pi}{2T}$, then

$$\lambda_0(T) = -\varepsilon\frac{\sin s_0(T)T}{s_0(T)}$$

is our critical bifurcation value. Using a result from Hale [13] (Lemma 6.1, Theorem 6.1), the system above has a Hopf bifurcation at $\lambda = \lambda_0(T)$, and moreover, a nonconstant periodic solution exists for $\lambda > \lambda_0(T)$. Thus, a discrete time delay has the effect of decreasing the original bifurcation value $\lambda_0 = 0$, i.e., a stable periodic orbit appears before the appearance of multiple branches. If one takes a continuous delay of the form

$$\dot{y} = -\varepsilon\int_0^t x(\tau)G(t-\tau)\,d\tau$$

where the delay kernel is exponential, $G(u) = e^{-au}$ $(a > 0)$, one may obtain necessary conditions for a Hopf bifurcation. With this particular choice of the kernel, complex roots of the characteristic equation will cross the real axis at a negative critical value $\lambda_0 < 0$.

Now we shall examine the effect of the particular shape of the nullcline $\dot{y} = 0$. If we replace Equation (A.4) by

$$\dot{y} = -\varepsilon(x + y),$$

the nullcline $\dot{y} = 0$ is the curve $y = -x$. The associated eigenvalues are

$$\frac{\lambda - \varepsilon^2 \pm \sqrt{(\varepsilon^2 - \lambda) + 4\varepsilon^2(\lambda - 1)}}{2\varepsilon}.$$

A Hopf bifurcation will occur at the value $\lambda_0 = \varepsilon^2$ if $\varepsilon < 1$. This has the opposite effect of a time delay. The critical bifurcation value will be increased from zero, i.e., for small values of λ, the equilibrium point $(0, 0)$ is still stable in the presence of multiple branches. In this case, initial points will decay to the origin in an oscillatory fashion (this is due to the eigenvalues above possessing nonzero complex parts).

By analogy with the above analysis for the modified van der Pol's equation, we may develop some intuition about what might happen for our model (A.1)-(A.2). In order to get relaxation oscillations we would require the following to hold:

1. The horizontal component of the vector field should be much greater in magnitude than the vertical component.
2. The point of linearization should lie somewhere between the extrema.
3. The intersection of the nullcline $\dot{c} = 0$ should not have slope close to zero and it should not lie in the boundary layer of $\dot{f} = 0$.
4. The direction of the vector fields must be like Figure A.2.

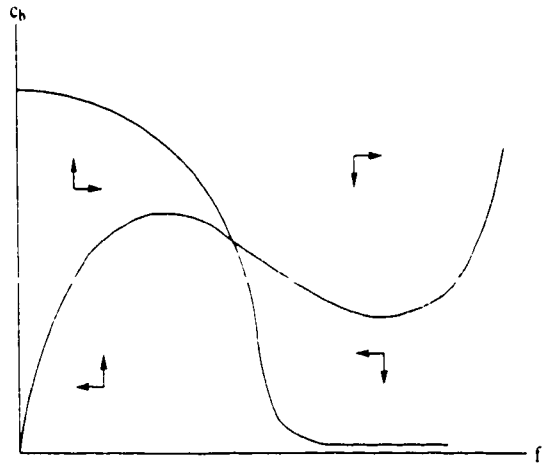

Figure A.2 : Nullclines $\dot{c}_b = 0, \dot{f} = 0$, and possible directions of the vector fields.

For the full system, fine spatial and temporal discretizations were used (see Chapter 6). As one might expect from the discussion above, oscillations may occur before the appearance of multiple branches due to delays from diffusion (e.g., see Figure 6.5e in Chapter 6). In the presence of multiple branches, the point of linearization was chosen to lie between the extrema (e.g., see Figure 6.7). In this case we obtain a similar result to Figure A.2 where the nullclines intersect between the extrema.

Appendix B

Equivalent Sobolev Norms

In this Appendix we shall provide details about equivalent norms that are more convenient in obtaining the L^2 estimate for the first component of our linear system. In particular we shall show that Sobolev norms are equivalent to norms that are defined in terms of fractional powers of operators involved in our analysis. We follow the treatment of Roytburd and Frankel [7] with modifications due to the presence of the mole fraction differential equation.

We begin with some well known facts. First consider the following initial-boundary value problem

$$\left.\begin{array}{rcll} u_t &=& u_{xx} & x > 0,\ t > 0 \\ u_x(0,t) &=& \theta u(0,t) & t > 0 \\ u(x,0) &=& u_0(x) & x \geq 0. \end{array}\right\} \tag{B.1}$$

We define the following linear operator

$$\Delta = \frac{\partial^2}{\partial x^2}$$

with domain

$$D = \left\{ u \in L^2((0,\infty)) : u'' \in L^2,\ u'(0) = \theta u(0) \right\}.$$

This operator is self adjoint with a continuous and point spectrum, $\sigma(\Delta) = \{\lambda \leq 0\} \cup \{\lambda = \theta^2\}$. Consider the following generalization of the Fourier cosine transform and its inversion formula:

for $\theta \geq 0$,

$$\begin{aligned} \Phi(\lambda) &= \int_0^\infty f(x) \left[\cos x\sqrt{\lambda} + \frac{\theta}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\right] dx \\ f(x) &= \frac{1}{\pi} \int_0^\infty \Phi(\lambda) \left[\cos x\sqrt{\lambda} + \frac{\theta}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\right] \frac{\sqrt{\lambda}}{\lambda + \theta^2} d\lambda \end{aligned}$$

and for $\theta < 0$,

$$\Phi(\lambda) = \begin{cases} \displaystyle\int_0^\infty f(x) \left[\cos x\sqrt{\lambda} + \frac{\theta}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\right] dx & \lambda \geq 0 \\ \displaystyle\int_0^\infty f(x) e^{\theta x} dx & \lambda = -\theta^2 \\ 0 & \lambda < 0,\ \lambda \neq -\theta^2 \end{cases}$$

$$f(x) = -2\theta\Phi(-\theta^2)e^{\theta x} + \frac{1}{\pi} \int_0^\infty \Phi(\lambda) \left[\cos x\sqrt{\lambda} + \frac{\theta}{\sqrt{\lambda}} \sin x\sqrt{\lambda}\right] \frac{\sqrt{\lambda}}{\lambda + \theta^2} d\lambda.$$

For a derivation of these formulas see Akheizer and Glazman [1] or Naimark [21]. Note that the generalized Fourier transform of $F(-\Delta)f(x)$ is $F(\lambda)\Phi(\lambda)$ where $F(-\Delta)$ is an operator function of $-\Delta$.

Now consider the principal linear system

$$L_P \begin{pmatrix} u \\ f \end{pmatrix} = \begin{pmatrix} \Delta & 0 \\ 0 & b_1 \end{pmatrix} \begin{pmatrix} u \\ f \end{pmatrix}$$

with domain

$$D_S = \{(u, f) : u \in D,\ f \in \mathbf{R}\}$$

defined in the Hilbert space $L^2 \oplus \mathbf{R}$ with inner product

$$\left\langle \begin{pmatrix} u_1 \\ f_1 \end{pmatrix}, \begin{pmatrix} u_2 \\ f_2 \end{pmatrix} \right\rangle = \int_0^\infty u_1 \bar{u}_2 \, dx + f_1 f_2.$$

This is a decoupled set of differential equations, and thus, the spectral theory of L_P follows from Δ with minor modifications. Note that in general $\sigma(\Delta) \neq \sigma(L_P)$, since we have the addition of the eigenvalue b_1 with the corresponding eigenvector

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

If $b_1 < 0$, then it is embedded in the continuous spectrum. In particular, the continuous spectrum, in this case, is then $\sigma_C(L_P) = (-\infty, b_1) \cup (b_1, 0]$.

Now we shall define norms involving fractional powers of linear operators (see Henry [18], Pazy [23], or Yosida [30]). If A is a sectorial operator (see Definition 4.6) with $\mathrm{Re}\,\sigma(A) > 0$, we define the *negative fractional power* of A,

$$A^{-\alpha} = \frac{1}{\Gamma(\alpha)} \int_0^\infty t^{\alpha-1} e^{-At}\, dt \quad \text{for any } \alpha > 0.$$

Since A is sectorial, $-A$ is the infinitesimal generator of an analytic semigroup e^{-At}. With $\mathrm{Re}\,\sigma(A) > 0$, the operator $A^{-\alpha}$ is a bounded operator which is also 1-1. This allows us to define the *positive fractional powers* in terms of $A^{-\alpha}$,

$$A^{\alpha} = \left(A^{-\alpha}\right)^{-1}.$$

If $\mathrm{Re}\,\sigma(A) > \delta > 0$ we have the following useful estimates

$$\left\| A^{\alpha} e^{-At} \right\| \leq M_\alpha t^{-\alpha} e^{-\delta t} \quad \text{for } \alpha \geq 0 \text{ and } t > 0.$$

For the linear system (B.1), define

$$\|u\|_{s,-\Delta} = \left\| (-\Delta + m)^{\frac{s}{2}}\, u \right\| \quad \text{where } m > \theta^2.$$

With this choice of m, the spectrum of $-\Delta + m$ has positive real values. Since this operator is sectorial the above fractional powers are well defined. Using the

transforms above along with Plancheral's theorem gives the following Sobolev type inequalities

$$\sup |u^{(k)}(x)| \leq C \|u\|_{s,-\Delta} \quad \text{if } s > k + \frac{1}{2} \text{ and } u \in D.$$

Now we examine the full linear system (4.9) along with the principal linear system. First we choose $m > \max\{\theta^2, b_1\}$ so that $-L_P + m$ has positive spectrum. Similarly, we can find a positive d such that $\sigma(-L + d)$ has positive real values. Recall that $\sigma(-L)$ consists of $\{\lambda \geq \frac{k^2 b}{4}\}$ along with a pair of eigenvalues $\{-\lambda_{\pm}(\mu)\}$ that vary with μ. In analogy to the norms $\|\cdot\|_{s,-\Delta}$ we define

$$\begin{aligned}
\left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L_P} &= \left\| (-L_P + m)^{\frac{s}{2}} \begin{pmatrix} u \\ f \end{pmatrix} \right\| \\
&= \left\| (-\Delta + m)^{\frac{s}{2}} u \right\| + (m - b_1)^{\frac{s}{2}} |f| \\
\left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L} &= \left\| (-L + d)^{\frac{s}{2}} \begin{pmatrix} u \\ f \end{pmatrix} \right\|
\end{aligned}$$

where both $-L_P + m$ and $-L + d$ have the same domain $D_S = D \dotplus \mathbf{R}$. Now we state our main result.

Proposition B.1 *The Sobolev scales defined above in terms of fractional powers are equivalent;*

$$C_1 \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L_P} \leq \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L} \leq C_2 \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L_P} \quad \textit{for } 0 \leq s \leq 2.$$

Thus,

$$\sup |u^k(x)| \leq C \max \left\{ \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L_P}, \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|_{s,-L} \right\} \quad \textit{for } k + \frac{1}{2} < s \leq 2.$$

Proof: This theorem follows directly from Theorem 1.4.8 from Henry [18]. We state his theorem: Let A_1 and A_2 be sectorial operators with the same domain such that their spectra have positive real part, $\mathrm{Re}\,\sigma(A_i) > 0$, $i = 1, 2$. Assume $(A_1 - A_2) A_1^{-\alpha}$ is a bounded operator for some $\alpha < 1$. Then the norms

$$\|x\|_{\beta,j} = \left\| A_j^{\beta} x \right\| \quad j = 1, 2$$

are equivalent for $0 \leq \beta \leq 1$.

Now for our problem, we let $A_1 = -L_P + m$, $A_2 = -L + d$, and set

$$\begin{pmatrix} w \\ g \end{pmatrix} = A_1^{-\alpha} \begin{pmatrix} u \\ f \end{pmatrix}.$$

The proposition follows from the estimate

$$\begin{aligned}
\left\| (A_1 - A_2) A_1^{-\alpha} \begin{pmatrix} u \\ f \end{pmatrix} \right\| &= \left\| \left(m - d - \tfrac{k_b^2}{4} \right) w + B_1(x) g - B_2(x) w(0) \right\| \\
&\quad + |(m-d) g + \alpha_1 w(0)| \\
&\leq \left| m - d - \tfrac{k_b^2}{4} \right| \|w\| + C\,|w(0)| + C\,|g| \\
&\leq C\,\|w\| + C\,\|w\|_{2\alpha,-\Delta} + C\,|g| \\
&= C\,\|w\| + C\left\| (-\Delta + m)^{\frac{2\alpha}{2}} w \right\| + C\,|g| \\
&\leq C\,(\|w\| + |g|) + C\,\|(-\Delta + m)^{\alpha} w\| \\
&\quad + C\,(b_1 + m)^{\alpha}\,|g| \\
&\leq C\left\| A_1^{-\alpha} \right\| \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\| + C \left\| A_1^{\alpha} \begin{pmatrix} w \\ g \end{pmatrix} \right\| \\
&\leq C \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\| + C \left\| A_1^{\alpha} A_1^{-\alpha} \begin{pmatrix} u \\ f \end{pmatrix} \right\|
\end{aligned}$$

$$\leq C \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|.$$

In the second inequality we use Sobolev's inequality with $k = 0$ and $s = 2\alpha$. We choose $\alpha \in \left(\frac{1}{4}, 1\right)$ in order to use both Sobolev's inequality and Henry's theorem. In the fifth inequality,

$$\|w\| + |g| = \left\| \begin{pmatrix} w \\ g \end{pmatrix} \right\| \leq \left\| A_1^{-\alpha} \right\| \left\| \begin{pmatrix} u \\ f \end{pmatrix} \right\|$$

and the relation

$$A_1^{\alpha} = \begin{pmatrix} -\Delta + m & 0 \\ 0 & b_1 + m \end{pmatrix}^{\alpha} = \begin{pmatrix} (-\Delta + m)^{\alpha} & 0 \\ 0 & (b_1 + m)^{\alpha} \end{pmatrix}$$

were used. The sixth inequality follows from semigroup theory, namely, negative fractional powers of sectorial operators with positive real spectra are bounded. □

Appendix C

Regularity of the Linearized Solution

Now we turn to the solution of (B.1). A solution to (B.1) may be found using the spectral decomposition of the operator $-\Delta$. If $\theta < 0$ the initial data may be decomposed as follows (see Appendix B)

$$u_0(x) = -2\theta\Phi(-\theta^2)e^{\theta x} + U_0(x).$$

For $\theta \geq 0$ we shall identify U_0 with u_0, thus we write

$$u_0(x) = \begin{cases} U_0(x) & \theta \geq 0 \\ -2\theta\Phi(-\theta^2)e^{\theta x} + U_0(x) & \theta < 0 \end{cases}$$

where for $\theta < 0$

$$\begin{aligned} \Phi(-\theta^2) &= \int_0^\infty w_0(x)e^{\theta x}\,dx \\ \int_0^\infty U_0(x)e^{\theta x}\,dx &= 0. \end{aligned}$$

The solution is

$$u(x,t) = \begin{cases} \theta F(x,t) + F_x(x,t) & \theta \geq 0 \\ -2\theta\Phi(-\theta^2)e^{\theta x}e^{\theta^2 t} + \theta F(x,t) + F_x(x,t) & \theta < 0 \end{cases}$$

where

$$\begin{aligned} F(x,t) &= \frac{1}{\sqrt{4\pi t}}\int_0^\infty \left[e^{-\frac{(x-\xi)^2}{4t}} - e^{-\frac{(x+\xi)^2}{4t}}\right] F_0(\xi)\,d\xi \\ F_0(x) &= \int_0^x e^{-\theta(x-s)}U_0(s)\,ds. \end{aligned}$$

We assume that the initial data $u_0(x)$ has uniformly bounded derivatives up to order two and that $u_0 \in C^2([0,\infty))$. The function F is obtained by Green's functions on the half axis $x > 0$ with zero Dirichlet boundary conditions. See Frankel and Roytburd [7] for a derivation of these results. Thus, for the principal linear system L_P, the solution is simply

$$\left.\begin{aligned} u(x,t) &= \begin{cases} \theta F(x,t) + F_x(x,t) & \theta \geq 0 \\ -2\theta\Phi(-\theta^2)e^{\theta x}e^{\theta^2 t} + \theta F(x,t) + F_x(x,t) & \theta < 0 \end{cases} \\ f(t) &= f_0 e^{b_1 t}. \end{aligned}\right\} \quad (C.1)$$

From Chapter 3 we have the existence of a classical solution. With smooth initial conditions, this classical solution coincides with the solution generated by the semigroup e^{Lt} from Chapter 4. Now we shall state a regularity theorem for the linearized system. The proof is basically that of Frankel and Roytburd [7] with slight modifications which we highlight.

Proposition C.1 *Let $(w(x,t), f(t))$ be a solution to the full linearized system with initial condition $f_0 \in (0,1)$ and $w_0 \in C^2_B([0,\infty))$ (w_0 is bounded along with its derivatives). Then*

1. $w(x,t)$ is continuous for $x \geq 0,\ t \geq 0$.

2. $w_x,\ w_{xx},\ w_t$ are continuous for $x \geq 0,\ t \geq 0,\ (x,t) \neq (0,0)$.

3.

$$\left.\begin{aligned} |w_x| &\leq C \\ |w_{xx}| &\leq \frac{C}{\sqrt{t}} \\ |w_t| &\leq \frac{C}{\sqrt{t}} \end{aligned}\right\} \quad x \geq 0,\ 0 < t \leq T,\ (x,t) \neq (0,0).$$

4. $f \in C^1([0,\infty)) \cap C^2((0,\infty))$.

Proof: These estimates are first proved for the solution to the principal linear system (C.1) and then for the full linear system by the variation of parameters formula. It is desirable to work first with L_P since u and f satisfy a decoupled set of differential equations. The initial data $F_0(x)$ has the odd extension

$$\tilde{F}_0(x) = \begin{cases} F_0(x) & x > 0 \\ -F_0(-x) & x < 0, \end{cases}$$

so that $F(x,t)$ can also be written equivalently as

$$F(x,t) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \tilde{F}_0(\xi) e^{-\frac{(x-\xi)^2}{4t}} d\xi.$$

Thus $F(x,t)$ is the restriction on the half axis $x > 0$, to the solution of the initial value problem

$$\begin{aligned} U_t &= U_{xx} \qquad x \in \mathbf{R},\ t > 0 \\ U(x,0) &= \tilde{F}_0(x) \qquad x \in \mathbf{R}. \end{aligned}$$

If $\tilde{F}_0$ has uniformly bounded derivatives of order up to s then $F(x,t)$ is of class C^s for $t \geq 0$ and all x (see F. John [19]). Note that since $u_0 \in C^2_B$, $\tilde{F}_0 \in C^3((-\infty,\infty))$ except at $x = 0$. By (C.1) the estimates for u follow from that of $F(x,t)$ and its derivatives, but the behaviour of these derivatives follow from the initial data $\tilde{F}_0$. Thus the solution u will depend on the continuity of $\tilde{F}_0$ and $\tilde{F}_0'$. At $x = 0$ both of these functions are continuous, and thus u is continuous for $x \geq 0$ and $t \geq 0$. For u_x the terms $\tilde{F}_0'$ and $\tilde{F}_0''$ appear. The function $\tilde{F}_0''$ has a jump at $x = 0$, and initial conditions in the form of Heaviside functions have bounded solutions. For u_{xx} and u_t, the term $\tilde{F}_0'''$ gives an initial condition in the form of a delta function, and the corresponding solution will be bounded by $Ct^{-1/2}$, i.e., there will be a term in the solution of u_{xx} and u_t

containing the term

$$\frac{1}{\sqrt{4\pi t}}\int_{-\infty}^{\infty}\delta(\xi)e^{-\frac{(x-\xi)^2}{4t}}\,d\xi \le \frac{C}{\sqrt{t}}.$$

Finally, $f \in C^{\infty}([0,\infty))$ and $|f| \le C$ since the solution is $f = f_0 e^{b_1 t}$ with $b_1 < 0$.

The full linear problem (4.9) is

$$\begin{aligned} w_t &= w_{xx} - \tfrac{1}{4}k_b^2 w + \epsilon^{-\frac{k_b}{2}x}\left[B_1 f + B_2 w(0,t)\right] \\ f_t &= b_1 f + b_2 w(0,t) \\ w_x(0,t) &= \alpha w(0,t). \end{aligned}$$

We may subdivide the linear system into two parts, where the second part contains all the coupled terms along with the boundary term $w(0,t)$.

$$\begin{aligned} \begin{pmatrix} w \\ f \end{pmatrix}_t &= \begin{pmatrix} \Delta - \frac{k_b^2}{4} & 0 \\ 0 & b_1 \end{pmatrix}\begin{pmatrix} w \\ f \end{pmatrix} + \begin{pmatrix} B_2\epsilon^{-\frac{k_b}{2}x} & B_1\epsilon^{-\frac{k_b}{2}x} \\ b_2 & 0 \end{pmatrix}\begin{pmatrix} w(0) \\ f \end{pmatrix} \\ &= L_0\begin{pmatrix} w \\ f \end{pmatrix} + L_B\begin{pmatrix} w \\ f \end{pmatrix}. \end{aligned}$$

The first term differs from the principal linear operator L_P only by the presence of the term $k_b^2/4$. The change of variables

$$\begin{pmatrix} \tilde{w} \\ \tilde{f} \end{pmatrix} = \epsilon^{\frac{k_b^2}{4}t}\begin{pmatrix} w \\ f \end{pmatrix}$$

will eliminate this term and allow us to use the previous results from L_P. The solution operator of L_P is then

$$e^{L_P t} = \begin{pmatrix} G(t) & 0 \\ 0 & e^{b_1 t} \end{pmatrix}$$

where $G(t)$ is the solution operator to (B.1). Thus the solution to

$$\begin{pmatrix} w \\ f \end{pmatrix}_t = L_0 \begin{pmatrix} w \\ f \end{pmatrix}$$

is

$$e^{L_0 t} = \begin{pmatrix} e^{-\frac{k_1^2}{4}t} G(t) & 0 \\ 0 & e^{b_1 t} \end{pmatrix} = \begin{pmatrix} H(t) & 0 \\ 0 & e^{b_1 t} \end{pmatrix}.$$

For the full linearized system, the variation of constants formula gives

$$w(x,t) = \varphi_0(x,t) + \int_0^t \varphi_1(x, t-s)\left[B_2 w(0,s) + B_1 f(s)\right] ds \qquad (C.2)$$

$$f(t) = f_0 e^{b_1 t} + b_2 \int_0^t e^{b_1(t-s)} w(0,s)\, ds \qquad (C.3)$$

where

$$\varphi_0(x,t) = H(t)u_0$$
$$\varphi_1(x,t) = H(t)e^{-\frac{k_1}{2}x}.$$

The solution operators φ_0 and φ_1 are continuous by the results from the principal linear system. Formally substituting f into w and changing the limits of integration gives

$$\begin{aligned} w(x,t) = {} & \varphi_0(x,t) + \int_0^t \varphi_1(x, t-\tau)\left[B_2 w(0,\tau) + B_1 f_0 e^{b_1 \tau}\right] d\tau \\ & + B_1 b_2 \int_0^t \left(\int_s^t \varphi_1(x, t-\tau) e^{b_1 \tau}\, d\tau \right) e^{-b_1 s} w(0,s)\, ds. \end{aligned}$$

Formally, we let $x = 0$, and obtain the following integral equation

$$\begin{aligned} w(0,t) = {} & \varphi_0(0,t) + \int_0^t \varphi_1(0, t-\tau) B_1 f_0 e^{b_1 \tau}\, d\tau \\ & + \int_0^t w(0,\tau) \Big[B_2 \varphi_1(0, t-\tau) \\ & \quad + B_1 b_2 e^{-b_1 \tau} \left(\int_\tau^t \varphi_1(0, t-s) e^{b_1 s}\, ds \right) \Big] d\tau. \end{aligned}$$

It can be shown that this a Volterra equation and thus a unique solution exists, $w(0,t) \in C([0,T])$. We define $w(x,t)$ by Equation (C.2) and f given

by Equation (C.3) is well defined since w is continuous. Since the limit

$$\lim_{x \to 0^+} w(x,t) = w(0,t)$$

exists, we see that $w(x,t)$ from (C.2) solves the integral equation and is continuous for $x > 0$ and $t \geq 0$.

Now we shall examine the regularity of the derivatives of $w(x,t)$, with

$$\begin{aligned} w_t &= \frac{\partial \varphi_0}{\partial t} + \varphi_1(x,0)\left[B_1 f(t) + B_2 w(0,t)\right] \\ &\quad + \int_0^t \frac{\partial \varphi_1}{\partial t}(x, t-s)\left[B_1 f(s) + B_2 w(0,s)\right] ds. \end{aligned}$$

Note that

$$\left| \frac{\partial \varphi_i}{\partial t}(x,t) \right| \leq \frac{C}{\sqrt{t}},$$

i.e., we have an integrable singularity at $t = 0$ and the regularity of w_t is determined from $(\varphi_0)_t$, thus

$$|w_t| \leq \frac{C}{\sqrt{t}}.$$

The spatial derivatives are

$$\begin{aligned} w_x &= \frac{\partial \varphi_0}{\partial x} + \int_0^t \frac{\partial \varphi_1}{\partial x}(x, t-s)\left[B_1 f(s) + B_2 w(0,s)\right] ds \\ w_{xx} &= \frac{\partial^2 \varphi_0}{\partial x^2} + \int_0^t \frac{\partial^2 \varphi_1}{\partial x^2}(x, t-s)\left[B_1 f(s) + B_2 w(0,s)\right] ds. \end{aligned}$$

The bounds for w_x and w_{xx} follow from the bounds of $(\varphi_0)_x$ and $(\varphi_0)_{xx}$.

Finally, the second term of f contains $w(0,t)$ in its integrand. Thus $f \in C^2((0,\infty)) \cap C([0,\infty))$ since w_t is not continuous at $(0,0)$. □

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