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A HYDRODYNAMIC STABILITY ANALYSIS OF SOME
PROPOSED MODEL EQUATIONS FOR BIOFLUIDS

by

James M. Hutfilz

A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF

Doctor of Philosophy

Thesis Director's Signature:

Houston, Texas

April 1976
To My Father
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CHAPTER 1

INTRODUCTION

The prediction of the response of a fluid which has been subjected to a perturbation superposed on a basic steady state is an interesting and challenging problem in fluid mechanics. This area of fluid mechanics, often called hydrodynamic stability analysis, is of great importance in any attempt to understand the mechanics of fluid motion and the corresponding transfer of heat and/or mass.

The classical approach to hydrodynamic stability analysis is known as linear stability analysis. In this method of analysis terms of second or higher order in the perturbation of the steady state are neglected. This process yields linear partial differential equations describing the system mathematically. These equations are then solved to determine the behavior of the perturbation as time proceeds. If the perturbation decays with time, the system is said to be stable with respect to that perturbation. Two well known and readable references in this area are the books by Chandrasekhar (7) and Lin (51).

Another approach to hydrodynamic stability is to do a non-linear stability analysis. In this case the terms
quadratic in the perturbation are not neglected so that the resulting system of governing equations is non-linear. Much of the work done in this area has been done by Stuart and his co-workers. One of the first papers in the area was by Meksyn and Stuart (54) in which they treated plane Poiseuille flow. The non-linear method of analysis was more completely outlined by Stuart (90,91) and Watson (104,105). At this time the basic physical principles behind the analysis and a good mathematical foundation for it were laid down. A later paper by Reynolds and Potter (71) contributed a procedure through which the non-linear partial differential equations could be reduced to a sequence of linear ordinary differential equations. The book by Eckhaus (18) provides an introduction to the general area of non-linear stability theory.

A third method of analysis is often referred to as the energy method of stability analysis. This method is in effect an application of Liapunov's second or direct method and is not always a true energy method. The method was initially introduced by Reynolds (70) and Orr (58). The basic idea is to analyze the "energy" of the perturbation. If the energy decreases with time, the system is said to be stable. Interest in using the method was reawakened by Serrin (81) and Joseph (41). The nature of the process used often causes the results from this method to be somewhat conservative.

One of the effects which can cause a physical system
to be unstable is the presence of a density gradient in a gravity field. One of the simplest problems in this area is the Bénard problem. The physical situation in this problem consists of a horizontal layer of fluid which is heated from below. The effect of temperature on the density of the fluid causes the bottom to be less dense than the top. As the temperature difference between these regions is increased beyond a critical value, the layer of fluid becomes unstable. The instability in this problem sets in as steady cellular convection. The gradient of temperature is included in a dimensionless number called the Rayleigh number. This number along with the Prandtl number determines the behavior of the system.

This problem has been analyzed using both a theoretical approach and an experimental one. Linear stability theory has been used to predict the behavior of this problem. Chandrasekhar (7) presents a good summary of the problem and its development up until about 1960. He also considers the effects of rotation and/or a magnetic field on the system. The review book by Turner (95) treats this problem and others related to the general field of buoyancy effects. In addition very many articles have been published in recent years dealing with the problem.

A great deal of work has been done in the past ten years in an attempt to model the Bénard problem more effectively. The mathematical description of the problem is
relatively simple, and thus it is a very popular one in the literature. Very many permutations of the basic problem have been done, and a few of them are discussed below.

In the basic problem of a fluid heated from below, the heat source is assumed to be constant with no internal generation of heat. The addition of a non-constant source of heat on the bottom plate has been studied theoretically by Davey (12) and Driessche (17) and experimentally by Schetz and Eichhorn (80). Driessche also included the possibility of internal heat generation within the system. This problem of a spatially distributed internal heat source was also studied by Watson (103), Thirlby (93), Roberts (73), and Sparrow, et al. (84). Gershuni and co-workers (31) also considered the internal heat source problem with the additional complication of inclination away from horizontal geometry. An interesting analog of the varying heat source case was done by Gresko and Sani (34). They considered gravity modulation by periodic shaking of the fluid.

Another related problem is the consideration of an additional effect on density in the form of a solute gradient. This problem has classically been called that of thermohaline convection because of its original application in oceanography. A more proper name is thermosolutal convection, however the names are often used interchangeably. In the Bénard problem the convection is steady (or stationary)
at its onset. In the thermohaline problem the initial convection can be oscillatory. The solute gradient can arise from several sources.

One of the favorite problems for analysis has been the initiation of a solute gradient due to the Soret effect. This is simply a diffusional flux established by the presence of the temperature gradient, or thermally induced diffusion. The corresponding effect of temperature gradient established because of the presence of a solute gradient (du Four effect) is quite small, and little has been done with this problem.

The Soret effect problem has been studied both theoretically and experimentally by many workers. The onset initially of oscillatory convection has been observed experimentally (Platten and Chavepeyer (64), Caldwell (6), and Hurle and Jakeman (37)). Linear stability theory predicts that this type of convection is possible (Veronis (99), Platten and Chavepeyer (64), Schechter, Prigogine, and Hamm (77)). Stationary convection is also possible depending on the physical parameters used. The oscillatory instability becomes steady as the convection grows to finite amplitude. This fact has been observed experimentally by the same authors as above. The use of non-linear stability theory also predicts an identical result (same theoretical authors). A very interesting result for the Soret problem has been predicted by Schechter, et al. (77) and Velarde and
Schechter (98). This is that convective instabilities can occur in this problem even for a fluid heated from above. They predict that this result may account for some of the difficulties which have been encountered in the measurement of Soret coefficients (relating the strength of the thermal diffusion). Qualitative experimental evidence for the existence of this effect has been mentioned by Whitaker and Pigford (106).

The problem of a solute gradient present because of a concentration difference between boundaries behaves similarly to the Soret problem. The conditions for stationary or oscillatory convection in this case have been found using linear stability theory by Nield (56), Baines and Gill (1), and Straus (89). Sani (76) found that finite amplitude oscillatory convective states are theoretically possible for this problem. Experimentally, Shirtcliffe (83) and Turner (96) observed the establishment of steady finite cellular convection.

Several other complicating effects introduced into the Bénard or thermohaline convection problems have also been studied. An interesting problem is that of the effect of surface tension on the stability of a fluid layer. If one (or both) of the boundaries is a free surface, then interfacial tension may play a role in the system. The initiation of instability caused by variations in interfacial surface tension is known as the Marangoni effect. This
problem was treated by Pearson (62), Sternling and Scriven (87,88), Cabelli (5), Palmer (60,61), and McConaghy and Finlayson (53). Cabelli and Palmer also included the effect of the Biot number (surface convection) on their systems, and Palmer considered the presence of surface elasticity.

The addition of chemical reaction into the system contributes an entirely new dimension to the problem. The field of multicomponent chemically reactive systems is an active area of research. One approach which has been used in describing the thermochemistry of these systems incorporates the concepts of entropy, equilibrium, and stability. Using these techniques the phenomenological form for constitutive relations can be derived, and conditions for the stability of equilibrium states can be found. This is not a hydrodynamics approach, but rather it has its origins in thermodynamics and continuum mechanics. Much of the work in this area has been done by Coleman (8,9) and Bowen (4). The book by de Groot and Mazur (14) is a good reference in this general field. A related but somewhat different approach in this same area has been used by Prigogine (65,66).

The stability of reacting systems subjected to the effect of gravity has also been studied using a hydrodynamic approach. The behavior of a fluid undergoing a dissociation reaction was the subject of research done by Frisch and co-workers (25,26,27,28,29) and by Wankat (102). The first set of authors used linear stability theory for the majority
of their results and non-linear stability theory for a few problems. The latter author used both linear stability theory and the energy method to obtain his results.

An interesting application of the analysis of chemically reactive systems is discussed by Wollkind and Segel (108). The system they consider is a problem in metallurgy. In this problem the freezing of a dilute binary alloy is studied using non-linear stability analysis. The shape of the moving surface between the liquid and solid phases is investigated. Convection in the liquid is neglected in their analysis. Farhadieh and Tankin (19) are currently doing some work on a related problem. They are looking at the problem of the freezing of sea water. In their work they are experimentally analyzing the interaction of convection currents in the fluid with the solid-liquid interface.

A splendid example of a complex chemically reactive system is a biological cell. The role of diffusion and reaction in the communication and transport within a cell and from one cell to another is an interesting and challenging problem. The relation of these processes to the concept of the origin of life is an interesting problem in science as well as in philosophy.

Prigogine and Nicolis (67) provide an interesting discussion of the entropy inequality as it relates to natural order and the chemical origin of life. These same
authors also discuss the possibility of differentiation in a chemical system through the presence of instabilities arising from the dissipative mechanisms of reaction and diffusion (68). Some pioneering work in the area of chemical reaction and diffusion as applied to interaction in biological systems was done by Turing (94). He proposed the presence of "morphogens" in living cells which may cause the differentiation of cells as an organism develops. These chemical substances were assumed to be transported from cell to cell by diffusion. This particular idea was extended to more complex situations by Othmer and Scriven (59) and Gmitro and Scriven (33).

The work mentioned in the preceding paragraph provides for communication and transport between cells via the processes of reaction and diffusion. They neglect the effect of protoplasmic movement within a cell. This movement within a cell, and possibly from cell to cell, is known as protoplasmic streaming. It is a very important characteristic of biological systems.

The phenomenon of protoplasmic streaming is an interesting and unsolved problem in the field of biological science. The protoplasm of a living cell (plant or animal) is observed to circulate within the cell. In some cases the circulation is a steady flow around the interior of the cell (Donaldson (15) and Jahn (40)), while in other cells there exists a rhythmic reversal of the flow within the cell.
(Kamiya and Seifriz (42) and Tyree (97)). The mechanisms for these motions remain unknown. These problems are therefore active areas for research in biology, fluid mechanics, or biochemistry.

Quite a volume of work has been done in attempting to measure the "motive" or driving force for this streaming motion (Kamiya and Kuroda (43), Tazawa (92), and Donaldson (16)). The mechanisms behind the motion were not the subject of these articles, but rather they were interested in the magnitude of the force required to stop the flow. In this way the force behind the motion could be approximated. A further discussion of the methods used to do this is beyond the scope of this thesis.

Several models have been set forth in an attempt to explain the mechanism behind the streaming in a cell. One of these models is called the contraction-hydraulic model. In this system the contractions of regions of cell membrane in a direction perpendicular to the flow are assumed to cause the streaming. This model was discussed by Jahn, Rinaldi, and Brown (39) and by Jahn (40). A similar model is discussed by Donaldson (15). Here the contractile elements are tangential to the flow. The cyclic contraction and relaxation of these elements causes the motion. A third unrelated model proposed by Rashevsky (69) and discussed by Jahn (40) explains the flow by means of a diffusion-drag mechanism. In this model the interaction of the large
protein solute molecules with the remainder of the protoplasm causes the streaming. A fairly good summary of several proposed mechanisms is given in the review article by Wolpert (109).

Some other models which have been proposed are due to Finlayson and Scriven (21). Their models incorporate a coupling of concentration and temperature gradients in the stress tensor describing the fluid. There is a coupling between these gradients and the mechanical motion of the protoplasm. An "active stress" term in the stress tensor accounts for this coupling. Their models consist of this active stress term added to the stress tensor for an incompressible Newtonian fluid.

An interesting characteristic of biochemical reactions is that the reaction rate is often bounded by zero and first order kinetics. The existence of these bounds is caused by the phenomenon of saturation in enzymatic reactions. If the reaction $S \overset{E}{\rightarrow} P$ is considered, where $S$ is the reactant (substrate), $E$ is an enzyme (catalyst), and $P$ is the product of the reaction; the reaction rate shows interesting behavior. If the concentration of the substrate is low, the reaction rate is first order with respect to the substrate. For high concentration of the substrate, the reaction is zero order with respect to the substrate.

A possible mechanism which can account for this behavior was proposed by Michaelis and Menton (see for example
Lehninger (50)). Their model involves the formation of an intermediate enzyme-substrate complex (ES).

\[ S + E \xrightarrow{k_1}{k_2} ES \]

\[ ES \xrightarrow{k_3}{k_4} E + P \]

If the concentration of the complex ES is assumed constant, and the rate constant \( k_4 \) is small; the rate of formation of P is given by

\[
\frac{d[P]}{dt} = k_3[S][E]/\left( \frac{k_2+k_3}{k_1} + [S] \right).
\]

In this equation the square brackets indicate the concentration of a component. This simple model does display the observed dependence on the concentration of the substrate S.

The subject of this thesis is one of the models proposed by Finlayson and Scriven. The behavior of this model in the field equations of fluid mechanics is analyzed using the non-linear stability analysis of Reynolds and Potter (71). The temperature and concentration gradients in the active stress term arise from the presence of chemical reaction in the system combined with the effect of diffusion. Both zero and first order reaction kinetics are used. Various boundary conditions are used for velocity,
temperature, and concentration. The initial state is assumed to be quiescent for all problems. For one particular case of the active stress problem, the energy method is used to analyze the system.

The effect of a gravity field on the active stress problem is also analyzed using non-linear stability theory. Setting the active stress term equal to zero yields the problem of a chemically reactive incompressible Newtonian fluid under the influence of buoyancy. This problem is discussed in brief, and some comments on the possibility of oscillatory convective states are made.

The main purpose of this research is therefore to determine whether the active stress mechanism can cause circulatory flows (stationary or oscillatory) in a fluid system. The driving forces for this convection are the gradients of temperature and concentration which appear in the active stress portion of the stress tensor.
CHAPTER 2

PHYSICAL PROBLEM

Section 2.1. The Constitutive Model

The constitutive model used in this work was one proposed by Finlayson and Scriven (21). The stress tensor in their models is that of an incompressible Newtonian fluid with an added "active stress" term. This can be written as:

\[
T = -pI + 2\mu D + T_a; \quad D = \frac{1}{2}[\nabla y^2(\nabla y)^T]
\]  \hspace{1cm} 2.1.1

where \(T_a\) is the active stress tensor. The form of this tensor is such that it represents a coupling of concentration and temperature gradients (or two concentration gradients). Two of the specific models proposed were:

\[
T_a = k_e \cdot (\nabla c_1 \times \nabla c_2) \quad \text{(Antisymmetric)} \hspace{1cm} 2.1.2
\]

and

\[
T_a = h[\nabla c_1 \nabla c_2 + \nabla c_2 \nabla c_1 - \frac{2}{3} I (\nabla c_1 \cdot \nabla c_2)] \hspace{1cm} 2.1.3
\]

In these models \(h\) (or \(k\)) is an active stress coefficient which gives the importance of the active stress term in the
constitutive relation. If \( h = 0 \) (or \( k = 0 \)), then the fluid is simply an incompressible Newtonian fluid. The first of the above models was the subject of some work done by Lin and McIntire (52). The second is the model used in this work.

Some restrictions on the form of the constitutive equations proposed were dealt with in the paper by Finlayson and Scriven. This paper details the development quite well and a repeat of the process will not be given here. One of the main considerations in their treatment is the "Curie Principle." They argue that the principle is often misquoted and does not prohibit the dependence of a second order tensor on a vector in a non-isotropic medium. For the case of a linear isotropic medium, however, the possibility of the above dependence does disappear.

The use of a Newtonian based fluid to represent the behavior of cellular protoplasm may be a rather naive approximation. The presence of macromolecules in the protoplasm (enzymes and proteins) in many cases causes the fluid to show visco-elastic properties. The Newtonian concept does provide a good starting point for investigation however, since in this way concentration can be focused on the effect of the active stress term in the constitutive relation.

Section 2.2. The Physical Situation

The physical situation considered was that of
parallel plates infinite in the x and z directions and separated by a distance L in the y direction (Figure 1). This geometry should yield the main interesting results with minimum complication of the equations due to reference frame considerations. In rectangular Cartesian co-ordinates the contravariant and covariant forms of the stress tensor are identical. Use of this geometry therefore allows the selection of either form. Had any other geometry been used, this would not have been possible since the forms are not the same.

The fluid between the plates is assumed to be of a homogeneous nature. A homogeneous chemical reaction in the fluid is also considered. The homogeneity of the fluid is perhaps an unrealistic assumption in dealing with biological systems, since cell bodies such as mitochondria, vacuoles, and nucleii are present in a living cell. This homogeneity, however, does allow comparison of the results with more conventional convection problems. Also, the protoplasm of a cell when considered by itself is reasonably homogeneous when viewed on a macroscopic level.

One other aspect of the physical problem is the use of the Boussinesq approximation (3,7). This deals with the variation in physical properties due to temperature changes. For most parameters this variation is small due to the small value of the thermal coefficient of volumetric expansion. One effect cannot be neglected, however. This is the
change in density $\rho$ in the buoyancy term of the equation of motion. In order to take this effect into account, a linear dependence on temperature is used;

$$\rho = \rho_0[1-\alpha_T(T-T_0)]$$

where $\alpha_T$ is the coefficient of thermal volume expansion and $\rho_0$ is the density at some reference temperature $T_0$.

By a similar argument, the effects of varying concentration on the physical properties can be considered. The only contribution is again considered to arise from the density in the buoyancy term. The resulting form of the density approximation is thus:

$$\rho = \rho_0[1-\alpha_T(T-T_0) - \bar{s}\alpha_c(c-c_0)]$$

Here $\alpha_c$ is the coefficient of volume expansion due to concentration effects and the parameter $\bar{s}$ defines the concentration effect on density. $\bar{s}$ has the value of $+1$ when the density decreases with increasing concentration and the value of $-1$ when density increases with concentration.

One temperature effect which is neglected, but which could be a non-negligible effect, is that of the temperature dependence of the chemical reaction rate. If the usual Arrhenius type of dependence is assumed, then the temperature effect could be quite large. One obvious way to circumvent this particular problem would be to consider
FIGURE 1. THE PHYSICAL SITUATION
isothermal situations. This eliminates some cases of potential interest, however. Another method would be to choose some average temperature in the reaction rate expression. This possibility will be discussed in more detail later.

Section 2.3. The Governing Equations

The system as described in the previous section is defined by the following equations. In these equations heat and mass transfer through diffusion and chemical reaction are considered.

Constitutive equation:

\[ T = -p + 2\mu \dot{\epsilon} + T_a \]  \hspace{1cm} (2.1.1)

Equation of motion:

\[ \frac{\partial v}{\partial t} + v \cdot \nabla v = -\frac{\nabla p}{\rho_0} + \nabla \nabla^2 v + \frac{v \cdot T_a}{\rho_0} + \frac{\rho}{\rho_0} g \] \hspace{1cm} (2.3.1)

Mass transfer equation:

\[ \frac{\partial c}{\partial t} + v \cdot \nabla c = D_2 \nabla^2 c + R_2 \] \hspace{1cm} (2.3.2)

Heat transfer equation

\[ \frac{\partial \xi}{\partial t} + v \cdot \nabla \xi = D_1 \nabla^2 \xi + R_1 \] \hspace{1cm} (2.3.3)

Equation of continuity: \[ v \cdot v = 0 \] \hspace{1cm} (2.3.4)
The quantities $D_1$ and $D_2$ are the thermal and mass diffusivities respectively. $R_1$ and $R_2$ are the heat and mass source or sink terms respectively. In actuality $\xi$ could be a second concentration instead of the temperature. For the rest of the work it will be considered to be temperature, however. The term $T_a$ is the active stress portion of the stress tensor which was discussed in Section 2.1.

The above equations were non-dimensionalized using the following form of dimensionless variables. For the moment the body force term will be dropped in order to focus attention on the active stress contribution to the convection. In some of the numerical work in this paper this term was included as can be seen in Chapter 7.

\[
\bar{v} = vL/v \quad \bar{c} = c/c_0 \quad S_c = v/D_2
\]

\[
\bar{t} = t\nu/L^2 \quad \bar{x} = x/L \quad S = c_0\xi_0 h/\nu^2 \quad 2.3.5
\]

\[
\bar{\xi} = \xi/\xi_0 \quad Pr = v/D_1
\]

This choice of dimensionless variables makes the velocity a vectorial Reynolds number. The Reynolds number does not appear explicitly, but it does appear as this dimensionless velocity. The parameter $S$ is the active stress number for the system.

The equations become in dimensionless form (dropping the bars representing non-dimensionality):
\[ \frac{\partial V}{\partial t} + v \cdot \nabla v + \nabla p - v^2 v - SV \cdot \nabla T_a = 0 \]  \hspace{1cm} 2.3.6

\[ \text{Sc} \left( \frac{\partial c}{\partial t} + v \cdot \nabla c \right) - v^2 c - \xi_2 |R_2| L^2 / D_2 c_0 = 0 \]  \hspace{1cm} 2.3.7

\[ \text{Pr} \left( \frac{\partial \xi}{\partial t} + v \cdot \nabla \xi \right) - v^2 \xi - \xi_1 |R_1| L^2 / D_1 \xi_0 = 0 \]  \hspace{1cm} 2.3.8

At this time the centerline between the planes is made to correspond to \( y = 0 \), so that the surfaces are \( y = 1/2 \) and \( y = -1/2 \). \( \xi_1 \) and \( \xi_2 \) are equal to \( +1 \) and represent the source (+) or sink (-) behavior of the \( R_1 \) and \( R_2 \) terms. The form of \( R_1 \) and \( R_2 \) depends on the reaction kinetics and will now be discussed.

The case of no reaction with buoyancy corresponds to the situation encountered in the Rayleigh-Jeffreys or thermohaline convection problem. In this case \( R_1 \) and \( R_2 \) are equal to zero (no internal sources) and the quantity \( c_0 \) (\( \xi_0 \)) is chosen as some characteristic concentration (temperature) difference; for example the difference in value between the two bounding surfaces.

\[
\begin{align*}
  y = 1/2 & \quad \underline{c = c_2} \\
  y = 0 & \quad \underline{c_0 = c_1 - c_2} \\
  y = -1/2 & \quad \underline{c = c_1}
\end{align*}
\]
For this case the variable $c$ ($\xi$) is modified in the following manner: $\bar{c} = (c-c_2)/(c_1-c_2)$. The steady state solutions corresponding to equations (2.3.7) and (2.3.8) are then:

$$\bar{c} = \left( \frac{1}{2} - y \right) \quad 2.3.9$$

$$\bar{\xi} = \left( \frac{1}{2} - y \right) \quad 2.3.10$$

Two different types of reaction kinetics were studied, zero and first order reactions. The non-dimensionalizing variables in these cases are different since a characteristic gradient may not exist. For simplicity the case of constant, equal values on the boundaries will be discussed. The extension to other boundary conditions is very straightforward.

\[ \begin{array}{c}
1/2 \quad \frac{c=c_1}{c=c_1} \\
y = 0 \quad \cdots \cdots \cdots \cdots \cdots \cdots \\
-1/2 \quad \frac{c=c_1}{c=c_1}
\end{array} \]

**Zeroth order reaction**

$$|R_2| = k, \quad |R_1| = kQ, \quad Q = \frac{|\Delta H|}{\rho c_p}$$

With these expressions the values of $c_0$ and $\xi_0$ are:
\[ c_0 = \frac{kL^2}{D_2}, \quad \xi_0 = \frac{kQL^2}{D_1} \]

Redefining \(c\) and \(\xi\) to be,

\[ \tilde{c} = \frac{(c-c_1)}{c_0}, \quad \tilde{\xi} = \frac{(\xi-\xi_1)}{\xi_0} \]

the resulting steady states are:

\[ \tilde{c} = \frac{\xi_2}{2} \left( \frac{1}{4} - y^2 \right) \]

\[ \tilde{\xi} = \frac{\xi_1}{2} \left( \frac{1}{4} - y^2 \right) \]

**First order reaction**

\[ |R_2| = k'c \quad |R_1| = k'cQ \]

The values of \(c_0\) and \(\xi_0\) become (\(c_1\) is the non-dimensional surface concentration):

\[ c_0 = \frac{k_c L^2}{D_2} \quad \xi_0 = \frac{k_c L^2 Q}{D_1} \]

Redefining \(\xi\) as:

\[ \tilde{\xi} = \frac{(\xi-\xi_1)}{\xi_0} \]

the resulting steady states are:
\[ \lambda_1 = \lambda_2 = 1 \]

\[ c = \frac{\cos(y)}{\cos(0.5)} \quad 2.3.13 \]

\[ \tilde{\xi} = \frac{\cos(y)}{\cos(0.5)} - 1 \quad 2.3.14 \]

\[ \lambda_2 = \lambda_1 = -1 \]

\[ c = \frac{\cosh(y)}{\cosh(0.5)} \quad 2.3.15 \]

\[ \tilde{\xi} = \frac{\cosh(y)}{\cosh(0.5)} - 1 \quad 2.3.16 \]

The corresponding active stress numbers for the above two reacting cases are:

\[ S_{0th}^{th} = \frac{k' L^4 Qh}{\rho v^2 D_1 D_2} ; \quad S_{1st}^{1st} = \frac{k' c_1 L^4 Qh}{\rho v^2 D_1 D_2} \quad 2.3.17, 2.3.18 \]

For the problem of a non-constant temperature the active stress number can be evaluated at some average temperature in the interval. The non-dimensionalizing concentration and temperature are also a function of temperature. An average temperature could also be used in these expressions. This is one assumption which is not exceedingly good, however to use a non-linear or non-constant reaction rate would grossly complicate the analysis. The argument can
always be made that the two functions \( c \) and \( \xi \) are both concentrations, thus eliminating the problem.

Section 2.4. Boundary Conditions

There are many different surface effects which could be of interest for the present problem. The phenomena of surface tension effects, heat or mass exchange with the surroundings, heterogeneous reaction at the surface, and an elastically compliant wall are all problems which could have significance in the biological active stress problem. In addition to these conditions, several kinematic conditions could be of interest, for example fixed walls, free surfaces, or fixed surfaces with a prescribed shape.

The problems mentioned in the previous paragraph represent a very sizable number of possibilities. A complete analysis of all of them would be a monumental task. For this reason a few sets of conditions were analyzed. Since in this work it was desired to focus attention on the active stress effect itself, relatively simple boundary conditions were used.

Most of the work was done using two rigid walls with a no slip condition at the boundary. The mathematical expression for this situation is simply:

\[
\mathbf{v} = 0 \quad \text{at} \quad y = \pm 1/2
\]

2.4.1

The flat free surface condition yields the following
mathematical boundary conditions

\[ T_{xy} = T_{zy} = 0 \quad \text{and} \quad v_y = 0 \quad \text{(2.4.2)} \]

The stress components contain the active stress term with coupled temperature and concentration gradients. Therefore in order to say anything more about this condition, it is necessary to know the temperature and concentration boundary conditions.

Several temperature and concentration situations were considered. The one most commonly used was constant and equal conditions on each wall

\[ \xi = \xi_1 \quad \text{and} \quad c = c_1 \quad \text{at} \quad y = \pm \frac{1}{2} \quad \text{(2.4.3)} \]

For a few cases the condition of zero flux at the upper plane was used

\[ \frac{\partial \xi}{\partial y} = 0 \quad \text{and} \quad \frac{\partial c}{\partial y} = 0 \quad \text{at} \quad y = \frac{1}{2} \quad \text{(2.4.4)} \]

One last set which was used was that of constant but unequal conditions at the bounding surfaces

\[ \xi = \xi_1 \quad \text{and} \quad c = c_1 \quad \text{at} \quad y = -\frac{1}{2} \]

\[ \xi = \xi_2 \quad \text{and} \quad c = c_2 \quad \text{at} \quad y = \frac{1}{2} \quad \text{(2.4.5)} \]

\[ \xi_1 \neq \xi_2, \quad c \neq c_2 \]
In light of these conditions for concentration and temperature, the free surface conditions can now be evaluated. The zero stress boundary conditions are for a flat free surface:

\[
T_{xy} = \mu \left[ \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right] + h \left[ \frac{\partial c}{\partial x} \frac{\partial \xi}{\partial y} + \frac{\partial \xi}{\partial x} \frac{\partial c}{\partial y} \right] = 0
\]

2.4.6

\[
T_{zy} = \mu \left[ \frac{\partial v_z}{\partial y} + \frac{\partial v_y}{\partial z} \right] + h \left[ \frac{\partial c}{\partial z} \frac{\partial \xi}{\partial y} + \frac{\partial \xi}{\partial z} \frac{\partial c}{\partial y} \right] = 0
\]

The constant temperature and concentration conditions imply that the terms \( \frac{\partial c}{\partial x}, \frac{\partial \xi}{\partial x}, \frac{\partial c}{\partial z}, \frac{\partial \xi}{\partial z} \) are all equal to zero. The zero flux conditions give that the terms \( \frac{\partial \xi}{\partial y}, \frac{\partial c}{\partial y} \) are equal to zero. These circumstances eliminate the active stress portion of the tangential stress at the boundary. The final conditions then are

\[
T_{xy} = \mu \left[ \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right]
\]

2.4.7

\[
T_{zy} = \mu \left[ \frac{\partial v_z}{\partial y} + \frac{\partial v_y}{\partial z} \right]
\]

The fact that the y-component of the velocity field is zero implies that \( \frac{\partial v_y}{\partial x} = \frac{\partial v_y}{\partial z} = 0 \), and the conditions become

\[
\frac{\partial v_x}{\partial y} = \frac{\partial v_z}{\partial y} = 0
\]

2.4.8
The equation of continuity is differentiated with respect to $y$, and the above expressions are used to yield the condition

$$\frac{\partial^2 v}{\partial y^2} = 0$$

at the free surface.
CHAPTER 3

LINEAR STABILITY THEORY

Section 3.1. Linear Theory

The linear theory of hydrodynamic stability is used to predict the onset of instability via the growth of infinitesimal disturbances in laminar flow. The conditions given by the theory are thus sufficient conditions for instability or necessary conditions for stability. The theory has been used for a wide variety of problems in fluid mechanics and rheology. A number of these problems are elucidated by Chandrasekhar (7). Lin (51) has also treated, in somewhat less detail, several problems using linear theory.

The first step in linear stability theory is to expand each independent variable for the system of interest in terms of a steady (time independent) basic component \( s(x) \) and a time dependent perturbation \( s'(x,t) \). These expansions are then substituted into the governing equations. The resulting system is linearized by neglecting terms of second or higher order in the perturbation quantities and their derivatives. The equations for the basic motion are then subtracted out, giving a linear system of partial differential equations which can be solved for the perturbation.
This linear system of equations has time independent coefficients allowing for an exponential solution in time \(\exp(\sigma t)\). The behavior of the disturbances in time is then determined by the nature of the coefficient \(\sigma\) which becomes an eigenvalue in the differential equations. The real part of \(\sigma\) dictates whether or not the disturbances grow or decay with time. The imaginary portion of \(\sigma\) indicates a perturbation of either stationary or oscillatory nature. The three possibilities for the real part are discussed below.

1. \(\sigma_r < 0\) The disturbance decays with time and no instability develops.

2. \(\sigma_r = 0\) This is called the marginal or neutral condition. The disturbance is of constant amplitude and is either stationary \((\sigma_i = 0)\) or oscillatory \((\sigma_i \neq 0\), overstability).

3. \(\sigma_r > 0\) Instabilities develop as the disturbance grows in time.

In connection with the above cases the "Principle of the Exchange of Stabilities" (7) has been defined. It is: if \(\sigma_r\) is non-negative, and \(\sigma_i = 0\); then the principle is said to hold. This situation is characterized by stationary marginal states. The principle is often misinterpreted as implying that \(\sigma\) must be real. In fact this circumstance is a subset of the actual principle.
The above time dependence must be analyzed for all possible infinitesimal disturbances. The treatment of arbitrary disturbances is in practice quite an ambitious task. The usual technique is to assume disturbances of a spatially periodic (or modal) nature. Then the mode which gives the lowest value of some particular system parameter (for example Rayleigh number) for the case $\sigma_r = 0$ is said to be the critical mode. The corresponding parameter is the critical parameter. After making the assumption of infinite plates, the use of spatially periodic disturbances is not very limiting. Most disturbances can be built up by a superposition of periodic modes. Only discontinuous disturbances cannot be approximated in this manner. In a physical system most (if not all) disturbances will be of a continuous nature.

Figure 2 shows the type of result obtained by the application of linear theory to the problem of a fluid layer uniformly heated from below (the Bénard problem). In this figure the results give sufficient conditions for instability. The area below the curve, although labeled as stable in the figure, may or may not exhibit unstable behavior. Another method of analysis, for example non-linear or energy, must be used to comment about this region of the curve. The equations governing this system are called the Boussinesq equations.
Figure 2. Neutral Curve for the Benard Problem

Rayleigh Number (10^-2) vs Wave Number

- Unstable
- Critical Point
- Stable
Section 3.2. Application of Linear Stability Theory

This section outlines the derivation of the linear equations for the system given in Chapter 2. A complete reduction to an ordinary differential system by introduction of spatially periodic functions will not be done, since the linear system is the first series of equations in the nonlinear analysis. The derivation for this analysis is outlined in the next chapter.

The governing equations once again are simply equations 2.3.1-2.3.4. They are repeated here for completeness.

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = - \frac{\gamma p}{\rho_0} + \nu \nabla^2 u + \nu \cdot \nabla \frac{T_a}{\rho_0} + \frac{\rho}{\rho_0} g \tag{2.3.1}
\]

\[
\frac{\partial c}{\partial t} + u \cdot \nabla c = D_2 \nabla^2 c + R_2 \tag{2.3.2}
\]

\[
\frac{\partial \xi}{\partial t} + u \cdot \nabla \xi = D_1 \nabla^2 \xi + R_1 \tag{2.3.3}
\]

\[\nabla \cdot u = 0 \tag{2.3.4}\]

Following the procedure outlined previously the expansions;

\[
u^*(x,t) = \nu(x) + u'(x,t) \quad T^*_a(x,t) = T_a(x) + T'_a(x,t) \tag{3.2.1}
\]

\[
\xi^*(x,t) = \xi(x) + \xi'(x,t) \quad R^*_1(x,t) = R_1(x) + R'_1(x,t)
\]

\[
c^*(x,t) = c(x) + c'(x,t) \quad p^*(x,t) = p(x) + p'(x,t)
\]
are put into equations 2.3.1-2.3.4. The resulting equations are, after linearization and subtraction of the steady state solutions:

\[
\frac{3u'}{3t} + u' \cdot \nabla u + u \cdot \nabla u' = - \frac{\nabla p'}{\rho_0} + \nu \nabla^2 u' \\
+ \frac{\nabla}{\rho_0} \cdot T_a' - g(\alpha_T c' + \sigma \cdot c c') \tag{3.2.2}
\]

\[
T_a' = h(\nabla' c' c' + \nabla c' c' - \frac{2}{3} \frac{1}{\kappa}(\nabla' c' \cdot \nabla c') + \nabla c' \nabla c') \\
+ \nabla' c' c' - \frac{2}{3} \frac{1}{\kappa}(\nabla c \cdot \nabla c')] \\
= T_a(c', \xi) + T_a(c, \xi') \tag{3.2.3}
\]

\[
\frac{3\xi'}{3t} + u' \cdot \nabla \xi + u \cdot \nabla \xi' = D_1 \nabla^2 \xi' + R_1' \tag{3.2.4}
\]

\[
\frac{3c'}{3t} + u' \cdot \nabla c + u \cdot \nabla c' = D_2 \nabla^2 c' + R_2 \tag{3.2.5}
\]

\[
\nabla \cdot u' = 0 \tag{3.2.6}
\]

For the present problem the quiescent initial state dictates that:

\[
u = 0, \quad \nabla u = 0
\]

Making use of this fact the final linearized equations become:
\[
\frac{\partial u'}{\partial t} = -\frac{\nu p'}{\rho_0} + \nu \nabla^2 u' + \frac{\nu}{\rho_0} \cdot T_a(c', \xi) + \frac{\nu}{\rho_0} \cdot T_a(c, \xi') - g(a_T \xi' + \alpha_c c') \quad 3.2.7
\]

\[
\frac{\partial \xi'}{\partial t} + u' \cdot \nabla \xi = D_1 \nabla^2 \xi' + R_1' \quad 3.2.8
\]

\[
\frac{\partial c'}{\partial t} + u' \cdot \nabla c = D_2 \nabla^2 c' + R_2' \quad 3.2.9
\]

\[
\nabla \cdot u' = 0 \quad 3.2.10
\]

These are the equations which determine the behavior of the system to infinitesimal disturbances.
CHAPTER 4

NON-LINEAR THEORY

Section 4.1. Introduction

As previously mentioned, the linear theory of hydrodynamic stability predicts the onset of instability due to the action of infinitesimal disturbances. The time dependence of these disturbances is such that they grow exponentially with time and will eventually attain finite amplitude. Because of the linearizing assumptions, linear stability is not rigorously applicable when this process occurs. The neglected terms (non-linear in the disturbances) become important in analyzing the system behavior. For periodic finite amplitude disturbances, linear theory does not account for three basic processes (90,91):

(1) The distortion of the mean motion.
(2) The generation of higher harmonics of the fundamental mode.
(3) The distortion of the y-dependence of the fundamental mode.

Any consideration of finite amplitude disturbances
should take these effects into account. Examples of this application are the prediction of the laminar-turbulent transition in fluid flows and the cellular convection patterns caused by buoyancy, surface tension, or other related effects. The problem dealt with in this work is of the latter category.

There have been several mathematical formalisms developed in order to treat systematically problems in non-linear stability. Two of these methods are those of Eckhaus (18) and Stuart (90,91). The method of Stuart, as extended by Reynolds and Potter (71), was used in this work and will be discussed in detail later. The methods of Eckhaus are (a) series expansions in terms of the eigenfunctions of the linear problem and (b) asymptotic expansions in terms of suitably defined small parameters. These methods are described in the above reference and used by Pekeris and Skholler (63) to treat plane Poiseuille flow and by Wollkind and Segel (108) to treat a problem in metallurgy.

In all of the non-linear methods the time derivative of the disturbance is the main factor of interest. The time dependence can be considered to be contained in the disturbance amplitude \( A \). With this format, the following equation is the heart of non-linear stability theory:

\[
\frac{dA}{dt} = a_0A + a_1A^2 + a_2A^3 + \ldots = a_{n-1}A^n
\]

\[ n = 1, 2, \ldots \infty \] 4.1.1
Landau and Lifschitz (46) consider this form of the equation in dealing with the onset of turbulence. They remark that in time averaging of the derivative the terms on the right hand side which involve even powers of \(A\) vanish, since they contain a periodic factor. In actuality these terms do not vanish but yield higher order odd power contributions which are assumed to be included in the corresponding terms in the expansion.

The resulting differential equation for the amplitude is:

\[
\frac{dA}{dt} = a_0 A + a_2 A^3 + \ldots = a_{2n-2} A^{2n-1}
\]

\[n = 1, 2, \ldots \infty \quad 4.1.2\]

The above equation truncated after one term is the form governing linear theory. Consideration of the second term gives the first order non-linear contribution to the disturbance. The solution of the differential equation involving these first two terms is:

\[
A^2 = A_0^2 e^{2a_0 t} / \{1 + \frac{A_0^2}{A_\infty^2} (e^{2a_0 t} - 1)\}
\]

\[4.1.3\]

In this expression \(A_0\) is the initial amplitude of the disturbance at \(t = 0\); and \(A_\infty^2\) is the quantity defined by:

\(A_\infty^2 = -a_0 / a_2\). Looking at the differential equation, it is
obvious that if $a_0$ and $a_2$ have the same sign, then the linear and the first non-linear effects merely reinforce each other. There are thus two cases of interest in this analysis:

Case (1) $a_0 < 0$ and $a_2 > 0$

Case (2) $a_0 > 0$ and $a_2 < 0$

For the first case, the disturbances are stable in the infinitesimal sense. However, the first non-linear contribution is destabilizing. The quantity $A_\infty$ thus becomes a critical amplitude $A_C$. If the initial amplitude $A_0$ is less than $A_C$, the disturbances will decay. If it is greater than $A_C$, the disturbances will grow with time. Since the finite amplitude effects show the possibility of a growing disturbance when linear theory predicts decay, this situation is called that of "subcritical instabilities" and is illustrated in the phase plane diagram of Figure 3. It should be remarked that as these subcritical instabilities grow, it becomes necessary to consider more non-linear terms in the expansion.

Case 2 is the opposite of Case 1. Here the linear theory predicts instability, while the non-linear contribution is stabilizing. In this situation the quantity $A_\infty$ is an equilibrium amplitude $A_\infty$. This corresponds to the existence of a constant amplitude disturbance as time goes to
FIGURE 3. THE AMPLITUDE PHASE PLANE
infinity. This situation can be considered to be the establishment of a secondary steady state away from the initial steady state configuration. For this reason Case 2 is described as that of "supercritical equilibrium." The phase plane diagram of Figure 3 shows this condition also.

For the present problem, the latter case of supercritical equilibrium is of primary interest. This secondary equilibrium is not really an equilibrium flow in the usual sense, but rather it is a second steady state. In order to differentiate from the initial steady state situation, it will be referred to as an equilibrium state in the remainder of this paper. The Bénard problem provides a good example of this equilibrium flow represented by steady cellular convection. With the addition of complicating forces, for example a solute gradient, subcritical instabilities can also be found for these convective problems (76). The results found for the active stress problem will be discussed in Chapter 7.

Section 4.2. Non-Linear Analysis

The non-linear method used here is the one outlined by Reynolds and Potter (71). Their method is an extension and clarification of the development of Stuart (90,91) and Watson (104,105). The method is basically a series of mathematical substitutions made in order to reduce a non-linear
problem to a sequence of linear ones. These linear problems can then be solved and their solutions combined to give the result of non-linear stability theory.

The equations to be analyzed are 2.3.6-2.3.8 and 2.3.4. These equations are in non-dimensional form and contain no body force term. The equations developed for a first order reaction will be considered here. The zero order case yields the same equations with two fewer terms. With this in mind, the system of equations is:

\[
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + \mathbf{v} \cdot \mathbf{p} - \nabla \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \cdot \frac{\partial \mathbf{T}}{\partial \mathbf{a}} = 0
\]

4.2.1

\[
\text{Sc} \left( \frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c \right) - \nabla^2 c - \kappa_2 c = 0
\]

4.2.2

\[
\text{Pr} \left( \frac{\partial \xi}{\partial t} + \mathbf{v} \cdot \nabla \xi \right) - \nabla^2 \xi - \kappa_1 c = 0
\]

4.2.3

\[
\nabla \cdot \mathbf{v} = 0
\]

4.2.4

The first step in the analysis is to make the change of variables:

\[
\theta = \alpha x + \beta z + \omega t \quad A = A(t)
\]

\[
\omega = \omega(A) \quad y = y
\]

4.2.5

Spatially, this change of variables corresponds to what would be done in linear theory. The method is an application of the "method of two times." In a three dimensional
system, the number of independent variables is reduced from four \((x, y, z, t)\) to three \((x, y, A)\). This transformation is equivalent to Squire's transformation in linear theory (71,85).

When this change of variables is made, the equation of continuity (4.2.4) suggests the introduction of a stream function \(\psi\).

\[
\frac{\partial (\alpha v_x + \beta v_z)}{\partial \theta} + \frac{\partial v_y}{\partial y} = 0
\]

\[
\frac{\partial \psi}{\partial y} = \alpha v_x + \beta v_z, \quad \frac{\partial \psi}{\partial \theta} = -v_y \tag{4.2.6}
\]

The above stream function satisfies the equation of continuity identically, and as a result this equation is no longer carried in the set of governing equations. The pressure term in the equation of motion is eliminated by cross-differentiation with respect to \(\theta\) and \(y\), multiplication of the \(y\) equation by \(\kappa^2 = \alpha^2 + \beta^2\), and subtraction of this equation from the \(\theta\) equation. This process reduces the equation of motion to a single fourth order differential equation. The heat and mass equations remain second order.

The equations 4.2.1-4.2.3 thus become after the above manipulations:
\[
\begin{align*}
\frac{dA}{dt} &\cdot \frac{\partial \xi}{\partial A} + \left( \omega + \frac{dA}{dt} \cdot t \frac{d\omega}{dA} + \frac{\partial \psi}{\partial y} \right) \frac{\partial \xi}{\partial \theta} - \frac{\partial \psi}{\partial \theta} \frac{\partial \xi}{\partial y} \\
&\quad - \kappa^2 \frac{\partial^2 \xi}{\partial \theta^2} - \frac{\partial^2 \xi}{\partial y^2} - \dot{S} \left( \frac{\partial^2 \xi}{\partial y^2} - \kappa^2 \frac{\partial^2 \xi}{\partial \theta^2} \right) \left( \kappa^2 \left[ \frac{\partial c}{\partial \theta} \frac{\partial \xi}{\partial y} + \frac{\partial \xi}{\partial \theta} \frac{\partial c}{\partial y} \right] \right) + 2\kappa^2 \frac{\partial^2 \xi}{\partial \theta \partial y} \left[ \frac{\partial c}{\partial \theta} \frac{\partial \xi}{\partial \theta} - \frac{\partial c}{\partial y} \frac{\partial \xi}{\partial y} \right] = 0 \\
\zeta &= \frac{\partial^2 \psi}{\partial y^2} + \kappa^2 \frac{\partial^2 \psi}{\partial \theta^2} \\
\Pr \left[ \frac{\partial \xi}{\partial A} \frac{dA}{dt} \right] + \left[ \omega + \frac{d\omega}{dA} \right] \frac{dA}{dt} + \frac{\partial \psi}{\partial y} \right] \frac{\partial \xi}{\partial \theta} - \frac{\partial \psi}{\partial \theta} \frac{\partial \xi}{\partial y} \\
&\quad - \kappa^2 \frac{\partial^2 \xi}{\partial \theta^2} - \frac{\partial^2 \xi}{\partial y^2} - \lambda_1 c = 0 \\
\Sc \left[ \frac{\partial c}{\partial A} \frac{dA}{dt} \right] + \left[ \omega + \frac{d\omega}{dA} + \frac{dA}{dt} + \frac{\partial \psi}{\partial y} \right] \frac{\partial c}{\partial \theta} - \frac{\partial \psi}{\partial \theta} \frac{\partial c}{\partial y} \\
&\quad - \kappa^2 \frac{\partial^2 c}{\partial \theta^2} - \frac{\partial^2 c}{\partial y^2} - \lambda_2 c = 0 \\
4.2.7
\end{align*}
\]

The stream function, temperature, and concentration are all expanded in terms of a Fourier series in \( \theta \) and a power series in \( A \). The Fourier series is equivalent to expanding these quantities in terms of their harmonic components and corresponds to what is done in linear theory. The power series in \( A \) is suggested by considering the ways
in which the various harmonics interact (Reynolds and Potter).

\[ \psi(A, y, \theta) = \Lambda^{n}(\phi^{(k;n)}(y)e^{ik\theta}} \]

\[ + \tilde{\phi}^{(k;n)}(y)e^{-ik\theta}) \] \hspace{1cm} 4.2.10

\[ \xi(A, y, \theta) = \Lambda^{n}(\beta^{(k;n)}(y)e^{ik\theta}} \]

\[ + \tilde{\beta}^{(k;n)}(y)e^{-ik\theta}) \] \hspace{1cm} 4.2.11

\[ c(A, y, \theta) = \Lambda^{n}(\Omega^{(k;n)}(y)e^{ik\theta}} \]

\[ + \tilde{\Omega}^{(k;n)}(y)e^{-ik\theta}) \] \hspace{1cm} 4.2.12

The summation convention used by Reynolds and Potter is adopted here. Summation is over all possible integer values of repeated superscripts or powers. Through the use of punctuation, limits can be placed on the starting values of an index.

\[ (n) \quad n \geq 0 \]

\[ [n] \quad n \geq 1 \quad [n;m] = \rightarrow 0 < n \leq m \rightarrow 1 \]

\[ \{n\} \quad n \geq 2 \]

\[ n; m \quad n \leq m \]

When equations 4.2.10-4.2.12 are substituted into equations 4.2.7-4.2.9 there remain two terms which must still
be evaluated. These are:

\[
\frac{dA}{dt} \quad \text{and} \quad \omega + \frac{d\omega}{dA} t \frac{dA}{dt}
\]

The first of these terms was discussed earlier in this chapter. A power series is used of the form:

\[
\frac{dA}{dt} = a(0)A^1 + a(2)A^3 + a(4)A^5 + \ldots = a(2n-2)A^{2n-1}
\]

\[n = 1, 2, \ldots \infty\]

The second term above is expanded in a similar manner:

\[
\omega + \frac{d\omega}{dA} t \frac{dA}{dt} = b(0) + b(2)A^2 + \ldots = b(2n-2)A^{2n-2}
\]

\[n = 1, 2, \ldots \infty\]

These two expansions are now put into the equations, and terms with the same power and the same harmonic are equated. The resulting equations are:

\[
ma^{(n-m)}z^{(k;m)} + b^{(n;m)}ikz^{(k;m)} + \frac{1}{1+\delta_k^m}(D\phi^{(k-j;n-m)}[ijz^{(j;m)}])
\]

\[
+ D\phi^{(j;n-m)}[i(k+j)z^{(k+j;m)}] + D\phi^{(k+j;n-m)}[-ij\phi^{(j;m)}]
\]

\[- [i(k-j)\phi^{(k-j;n-m)}] D\phi^{(j;m)} + [i_j\phi^{(j;n-m)}]
\]

\[
D\phi^{(k+j;m)} - [i(k+j)\phi^{(k+j;n-m)}] D\phi^{(j;m)} - (D^2-k^2\phi^2)z^{(k;n)}
\]
\[-\frac{S}{1+\delta_{\kappa\Omega}}(\kappa^2(D^2+\kappa^2))(i(k-j)\Omega(k-j;n-m)D_B(j;m)+i(k+j)\Omega(k+j;n-m)D_B(k+j;m)\]

\[+i(k+j)\Omega(k+j;n-m)D_B(j;m)i\bar{j}\bar{\Omega}(j;n-m)D_B(k+j;m)\]

\[+i(k-j)\beta(k-j;m)D_B(j;n-m)+i(k+j)\beta(k+j;m)\bar{D}_B(j;n-m)\]

\[+ij\bar{\beta}(j;m)\bar{D}_B(k+j;n-m)+2ikD(\kappa^4[-(k-j)j\Omega(k-j;n-m)\]

\[\bar{\beta}(j;m)\bar{j}(k+j)\bar{\Omega}(j;n-m)\beta(k+j;m)+j\bar{\Omega}(k+j;n-m)\]

\[\bar{\beta}(j;m)\bar{j}(k+j)\bar{\Omega}(j;n-m)\beta(k+j;m)+j\bar{\Omega}(k+j;n-m)\]

\[\bar{\beta}(j;m)\bar{j}(k+j)\bar{\Omega}(j;n-m)\beta(k+j;m)+j\bar{\Omega}(k+j;n-m)\]

\[D_B(k+j;m)+\bar{D}_B(k+j;n-m)\bar{D}_B(j;m)]) = 0 \quad 4.2.13\]

\[D = \frac{d}{dy}; \quad \delta_{\kappa\Omega} = 0, k \neq 0; \quad z(k;n) = (D^2-k^2\kappa^2)\phi(k;n)\]

\[P_{\beta\alpha}(n-m)\beta(k;m)+b(n-m)ik\beta(k;m)+\frac{1}{1+\delta_{\kappa\Omega}}[ij\beta(j;m)\]

\[D_\phi(k-j;n-m)+i(k+j)\beta(k+j;m)\bar{D}_\phi(j;n-m)-ij\bar{\beta}(j;m)\]

\[D_\phi(k+j;n-m)-i(k-j)\phi(k-j;n-m)D_B(j;m)+ij\]

\[\phi(j;n-m)D_B(k+j;m)-i(k+j)\phi(k+j;n-m)\bar{D}_B(j;m)]\]

\[-(D^2-k^2\kappa^2)\beta(k;n) - \Omega(k;n) = 0 \quad 4.2.14\]

\[S_{\beta\alpha}(n-m)\Omega(k;m)+b(n-m)ik\Omega(k;m)+\frac{1}{1+\delta_{\kappa\Omega}}[ij\Omega(j;m)D_\phi(k-j;n-m)\]
\[ + i(k+j)\Omega^{(k+j; m)} D\phi_{(j; n-m)} - ij\Omega^{(j; m)} D\phi^{(k+j; n-m)} \]
\[ - i(k-j)\phi^{(k-j; n-m)} D\Omega^{(j; m)} + ij\phi^{(j; n-m)} D\Omega^{(k+j; m)} \]
\[ - i(k+j)\phi^{(k+j; n-m)} D\Omega^{(j; m)} ] - (D^2 - k^2 \kappa^2) \Omega^{(k; n)} \]
\[ - k^2 \Omega^{(k; n)} = 0 \]

Terms involving \( \phi^{(k; n)} \) are now factored out making use of the fact that \( \phi^{(0; 0)} = 0 \) (quiescent initial conditions). The terms \( \phi^{(0; 0)} \) and \( \Omega^{(0; 0)} \) are left in this form for the moment. Equations 4.2.13-4.2.15 can be written as:

\[ L_{kn} \phi^{[k; n]} - \frac{S}{1+\delta} k_{ko} \Omega^{[k; n]} + Q_{kn} \beta^{[k; n]} \]
\[ = -c^{[n-1]} G_{\delta_k l} H_{kn} + \frac{S}{1+\delta} R_{kn} \]

\[ E_{kn} \beta^{[k; n]} 2ikPrD\phi^{(0; 0)} \phi^{[k; n]} - k \Omega^{[k; n]} = \]
\[ -c^{[n-1]} \beta^{(1; 1)} \delta_{kl} Y_{kn} \]

\[ M_{kn} \Omega^{[k; n]} 2ikScD\phi^{(0; 0)} \phi^{[k; n]} = \]
\[ -c^{[n-1]} \Omega^{(1; 1)} \delta_{kl} W_{kn} \]

\[ c^{[n-1]} = a^{[n-1]} + ib^{[n-1]} \]
\[ L_{kn} = [(na^{(0)} + ikb^{(0)}) (D^2 - k^2_\kappa^2) - (D^2 - k^2_\kappa^2)^2] \]

\[ P_{kn} = 2i\kappa^2 [(D^2 + k^2_\kappa^2) D_\beta (0; 0) - 2D(D_\beta (0; 0) D)] \]

\[ Q_{kn} = 2i\kappa^2 [(D^2 + k^2_\kappa^2) D_\Omega (0; 0) - 2D(D_\Omega (0; 0) D)] \]

\[ G = (D^2 - \kappa^2)^{\phi} (1; 1) \]

\[ H_{kn} = -(ma^{[n-m]} + ikb^{[n-m]}) (D^2 - k^2_\kappa^2)^{\phi} [k; m] + F_{kn} / (1 + \delta_{kn}) \]

\[ F_{kn} = -D_{\phi}^{[k-j; n-m]} i_j (D^2 - j^2_\kappa^2)^{\phi} [j; m] \]

\[ + D_{\phi}^{[k+j, n-m]} (-i j) [D^2 - j^2_\kappa^2] \cdot \phi [j; m] + D^{\phi} [j; n-m] (i (k+j)) \]

\[ (D^2 - (k+j)^2_\kappa^2)^{\phi} [k+j; m] - i (k-j) \phi [k-j; n-m] D (D^2 - j^2_\kappa^2) \phi [j; m] \]

\[ + D [D^2 - (k+j)^2_\kappa^2] \phi [k+j; m] \cdot [i j \phi [j; n-m]] \]

\[ - D (D^2 - j^2_\kappa^2) \phi [j; m] \cdot [i (k+j) \phi [k-j; n-m]] \}

\[ R_{kn} = \kappa^2 [(D^2 + k^2_\kappa^2) [i (k-j) \Omega [k-j; n-m]] D_\beta [j; m] \]

\[ + i (k+j) \Omega [k+j; n-m] D_\beta [j; m] - i j \phi [j; n-m] D_\beta [k+j; m] \]

\[ + i (k-j) \beta [k-j; m] D_\Omega [j; n-m] + i (k+j) \beta [k+j; m] D_\Omega [j; n-m] \]

\[ - i j \beta [j; m] D_\Omega [k+j; n-m] + 2i \kappa^2 D [-(k-j) j \Omega [k-j; n-m] \]
\[ \begin{align*}
\beta[j;m] + i(k+j)\tilde{\omega}[j;n-m] \beta[k+j;m] + (k+j) j \tilde{\omega}[k+j;n-m] \\
\tilde{\beta}[j;m] - 2ikD[D\tilde{\phi}[k-j;n-m]D\beta[j;m] + D\tilde{\phi}[j;n-m] \\
D\beta[k+j;m] + D\tilde{\phi}[k+j;n-m]D\tilde{\beta}[j;m] \} \\
E_{kn} = \{ Pr(\omega[n^0] + ikb[0]) - (D^2 - k^2 \kappa^2) \} \\
Y_{kn} = - Pr(\omega[n-m] + ikb[n-m]) \beta[k;m] - \frac{Pr}{1 + \delta_{k0}}(ij\beta[j;m] \\
D\phi[k-j;n-m] + i(k+j)\beta[k+j;m]D\phi[j;n-m] - ij\beta[j;m] \\
D\phi[k+j;n-m] - i(k-j)\phi[k-j;n-m]D\phi[j;m] + ij\phi[j;n-m] \\
D\beta[k+j;m] - i(k+j)\phi[k+j;n-m]D\tilde{\phi}[j;m] \} \\
M_{kn} = \{ Sc(\omega[n^0] + ikb[0]) - (D^2 - k^2 \kappa^2) - 2\zeta \} \\
W_{kn} = - Sc(\omega[n-m] + ikb[n-m]) \tilde{\omega}[k;m] - \frac{Sc}{1 + \delta_{k0}}(ij\tilde{\omega}[j;m] \\
D\phi[k-j;n-m] + i(k+j)\tilde{\omega}[k+j;m]D\phi[j;n-m] - ij\tilde{\omega}[j;m] \\
D\phi[k+j;n-m] - i(k-j)\phi[k-j;n-m]D\phi[j;m] + ij\phi[j;n-m] \\
D\tilde{\phi}[k+j;m] - i(k+j)\phi[k+j;n-m]D\tilde{\phi}[j;m] \} \\
The preceding systems of equations represent a
series of sequentially solvable equations. The first problem is the case n=1, k=1. This is just the linear stability theory case. Solution of this eigenvalue problem will give the neutral curve of linear theory. The next non-zero eigenfunctions (see Reynolds and Potter) are the (0;2) and (2;2) modes. The equations for these functions are inhomogeneous with a right hand side dependent on the linear solution. All three of these eigenfunctions are associated with the linear eigenvalue $c^{(0)}$. Knowledge of these three eigenfunctions, along with the adjoint function from the system of interest, enables one to solve for the next eigenvalue $c^{(2)}$ (see next section) and its associated eigenfunctions. In theory the process, which is outlined in the flow chart in Figure 4, could be continued indefinitely. In practice it is difficult numerically to go beyond the evaluation of the second eigenvalue due to the inaccuracies involved in this type of computation. In this work the evaluation ceased after finding $c^{(2)}$.

Since the linear result is of interest by itself, the linear equations are presented below. These equations are obtained by setting $n = k = 1$ in the system 4.2.16-4.2.18. The same result could have been obtained by direct application of linear theory as outlined in Chapter 3.
FIGURE 4. THE EIGENVALUE AND EIGENFUNCTION CASCADE
\[
\begin{bmatrix}
  c(0)(D^2-\kappa^2) & 2Si\kappa^2[Dn(0;0)(D^2-\kappa^2)] & 2Si\kappa^2[D\eta(0;0)(D^2-\kappa^2)] \\
  -(D^2-\kappa^2)^2 & -D^3\eta(0;0) & -D^3\eta(0;0) \\
  -2iPrD\eta(0;0) & Prc(0)-(D^2-\kappa^2) & -\lambda_1 \\
  -2iScD\eta(0;0) & 0 & Sc(0)-(D^2-\kappa^2)-\lambda_2 \\
\end{bmatrix} = A
\]

A\Phi = 0; \quad \Phi = (\phi^{(1;1)}, \beta^{(1;1)}, \eta^{(1;1)})^T \quad 4.2.20

The functions \( \beta^{(0;0)} \) and \( \eta^{(0;0)} \) depend on the reaction kinetics and boundary conditions under investigation. They are related to the steady state solutions by:

\[
\beta^{(0;0)} = \frac{1}{2} \xi_{ss}
\]

\[
\eta^{(0;0)} = \frac{1}{2} c_{ss}
\]

In addition, when considering a zero order reaction, the numbers \( \lambda_1 \) and \( \lambda_2 \) in the above matrix are both equal to zero. This follows from the assumption of no perturbation in the zeroth order reaction rate.

If the boundary conditions being studied are symmetric, then the system can be separated into two different modes. These modes are characterized by the following behavior:
The nature of the remaining functions can be determined using the above fact. The relation turns out to be:

**Mode 1**

\[ \phi(1;1) \text{ even} \]
\[ \beta(1;1) \text{ odd} \]
\[ \Omega(1;1) \text{ odd} \]

**Mode 2**

\[ \phi(1;1) \text{ odd} \]
\[ \beta(1;1) \text{ even} \]
\[ \Omega(1;1) \text{ even} \]

\[ \phi(k;n) \text{ even} \quad \phi(k;n) \text{ odd} \]
\[ \beta(k;n) \text{ odd} \quad n = \text{odd} \quad \beta(k;n) \text{ even} \quad n = \text{even} \]
\[ \Omega(k;n) \text{ odd} \quad \Omega(k;n) \text{ even} \]

\[ \phi(k;n) \text{ odd} \quad \phi(k;n) \text{ even} \]
\[ \beta(k;n) \text{ even} \quad n = \text{odd} \quad \beta(k;n) \text{ odd} \quad n = \text{even} \]
\[ \Omega(k;n) \text{ even} \quad \Omega(k;n) \text{ odd} \]
The linear system of equations for the problem of a chemically reactive fluid under the influence of gravity with no active stress is also of interest. This system is given by

\[
\begin{pmatrix}
  c^{(0)} (D^2 - \kappa^2) & Gr_1 i\kappa^2 & Gr_2 i\kappa^2 \\
  -(D^2 - \kappa^2)^2 & & \\
  -2iPrD\beta^{(0;0)} & Pr_c^{(0)} - (D^2 - \kappa^2) & -\lambda_1 \\
  -2iScD\Omega^{(0;0)} & 0 & Sc_c^{(0)} - (D^2 - \kappa^2) - \lambda_2 \\
\end{pmatrix}
\begin{pmatrix}
  \phi^{(1;1)} \\
  \beta^{(1;1)} \\
  \Omega^{(1;1)}
\end{pmatrix}
= 0
\]

\[A'\phi = 0 \quad 4.2.21\]

In the above system the fluid is an incompressible Newtonian fluid.

For the case of no reaction, the functions \(D\beta^{(0;0)}\) and \(D\Omega^{(0;0)}\) are even, and the solutions to the above system can be separated into two modes once again. In this case one mode is where \(\phi^{(1;1)}\), \(\beta^{(1;1)}\) and \(\Omega^{(1;1)}\) are all even functions, and the other is when these eigenfunctions are all odd. If a reaction is present in the system the operators are such that this separation cannot be done.

The linear system for the problem of active stress with buoyancy can be found easily by combination of the two systems given by equations 4.2.20 and 4.2.21. The operators
representing the active stress term ($A_{12}$ and $A_{13}$) and the gravity body force term ($A'_{12}$ and $A'_{13}$) are simply added together. The other operators in the matrix $A$ remain the same.

Section 4.3. Evaluation of $c^{(n)}$

The evaluation of the non-linear eigenvalues $c^{(n)}$ ($n \geq 2$) is done by application of some of the results of the theory of adjoints in differential equations. The details of this theory can be found in any good book on applied mathematics (Friedman (24)) or differential equations (Stakgold (86) or Ince (38)). The theorem stated below is from Stakgold, however comparable theorems can be found elsewhere.

Consider a system of $N$ linear inhomogeneous ordinary differential equations satisfying homogeneous boundary conditions:

(1) \[ L\phi = q \quad \text{L is } N \times N \text{ differential operator} \]
\[ \{B_{x} \phi_{m} = 0\} \text{ at } y_1 \text{ or } y_2 \quad q \text{ is } n\text{-dimensional vector function of } y \]

Suppose now that the adjoint operators to $L$ and $B_{x}$ can be defined as:

(2) \[ L = \phi^{*} = 0 \]
\[ \{B_{x}^{*} \phi^{*} = 0\} \text{ at } y_1 \text{ or } y_2 \]
The homogeneous analog to problem (1) is:

(3) \[ Lu = 0 \]
\[ \{ B \alpha_m u_m = 0 \} \text{ at } y_1 \text{ or } y_2 \]

The following theorem gives a relation between the adjoint function, \( \phi^*(y) \), and the inhomogeneous part of (1), \( q(y) \).

Theorem: (a) If (3) has only the trivial solution \( u(x) = 0 \) in \( y_1 < y < y_2 \), then (2) has only the trivial solution, and (1) has one and only one solution.

(b) If (3) has nontrivial solutions, (2) will have non-trivial solutions [usually different from those of (3)], and (1) has no solution unless the "consistency condition"

\[
\int_{y_1}^{y_2} q(y)\phi^*(y) \, dy = 0
\]

is satisfied for every function \( \phi^*(y) \) which is a solution of (3).

The consistency condition states that the adjoint solution is orthogonal to the inhomogeneous part of (1). In N-space this condition can be written as:

\[
\int_{y_1}^{y_2} \sum_{i=1}^{N} q_i(y)\phi_i^*(y) \, dy = < f, \phi^* > = < \phi^*, f > = 0
\]

If the function \( q \) is now considered to be \( \lambda f - g \), where \( \lambda \) is a scalar constant; the above theorem gives a condition on \( \lambda \). It is assumed here that the eigensolution to (3) exists. With this assumption, (2) has nontrivial solutions
and the following can be written:

\[ \langle \lambda f - g, \phi^* \rangle = \langle \lambda f, \phi^* \rangle - \langle g, \phi^* \rangle = 0 \]

or

\[ \lambda \langle \phi^*, f \rangle - \langle \phi^*, g \rangle = 0 \]

and

\[ \lambda = \frac{\langle \phi^*, g \rangle}{\langle \phi^*, f \rangle} = \int_{y_1}^{y_2} \sum_{i=1}^{N} \phi_i^* g_i \, dy \int_{y_1}^{y_2} \sum_{i=1}^{N} \phi_i^* f_i \, dy \]

This gives a way to find the "eigenvalues" \( \lambda \) for the problem.

For the active stress problem described in the previous section, the adjoint function \( \phi^* \) to be used is the result from the adjoint equation for the linear system (\( n = k = 1 \)). The reason for this is as follows. The adjoint operators for the systems of higher order (\( n = 3, \ n = 5, \ldots \)) differ from the operator for the linear system by a factor of \( n \) multiplying \( a^{(0)} \). Except for the case \( a^{(0)} = 0 \), it is thus unlikely that these problems will possess nontrivial solutions. In order for nontrivial solutions to exist, the eigenvalues \( c_1^{(0)} = a^{(0)} + ib^{(0)} \) and \( c_2^{(0)} = na^{(0)} + ib^{(0)} \) would both have to be eigenvalues of the linear problem (since an operator and its adjoint have the same eigenvalues). This would be quite a rare case, made even rarer by the fact that the main eigenvalue of interest, \( c_1^{(0)} \), is the eigenvalue of smallest magnitude (or the one which has a vanishing real part).
Using the above discussion it is now possible to construct a way to find the higher eigenvalues $c^{(n)}$. For the case $a^{(0)} = 0$, it is completely rigorous to use the linear adjoint function in equation (4.3.1). When $a^{(0)} \neq 0$, in general the value of $c^{(n)}$ could be selected arbitrarily (no nontrivial solution to the corresponding adjoint problem). In order to maintain continuity through the point $a^{(0)} = 0$, equation (4.3.1) is still used when $a^{(0)} \neq 0$. Thus the linear adjoint function, which does exist, is the one used at all times to determine the $c^{(n)} (n \geq 2)$.

The problem of finding $c^{(2)}$, for example, reduces to evaluating the following integrals:

$$
c^{(2)} = \int_{y_1}^{y_2} \sum_{i=1}^{3} \phi_i^* g_i \, dy / \int_{y_1}^{y_2} \sum_{i=1}^{3} \phi_i^* f_i \, dy \quad 4.3.2
$$

The functions $g$ and $f$ are in this case given by:

$$
g_1 = H_{13} + SR_{13} \quad f_1 = (D^2 - \kappa^2) \phi^{(1;1)}
$$

$$
g_2 = Y_{13} \quad f_2 = \beta^{(1;1)} \quad 4.3.3
$$

$$
g_3 = W_{13} \quad f_3 = \omega^{(1;1)}
$$

The linear adjoint equation for the active stress problem can be written in matrix form as:
\[
\begin{bmatrix}
    c^{(0)}(D^2 - \kappa) - (D^2 - \kappa^2)^2 & -2iPrD\beta^{(0;0)} & -2iScD\alpha^{(0;0)} \\
    2Si\kappa^2[D\omega^{(0;0)}(D^2 - \kappa^2)] & Pr\tau^{(0)} & -(D^2 - \kappa^2) \\
    -2D^2\omega^{(0;0)D} & 0 & 0 \\
    2Si\kappa^2[D\beta^{(0;0)}(D^2 - \kappa^2)] & -\varepsilon_1 & Sc\tau^{(0)} \\
    -2D^2\beta^{(0;0)D} & -(D^2 - \kappa^2) - \varepsilon_2 & 0 
\end{bmatrix}
\begin{bmatrix}
    \phi_1^* \\
    \phi_2^* \\
    \phi_3^* 
\end{bmatrix} = 0
\]
CHAPTER 5

ENERGY METHOD

Section 5.1. Introduction

The energy method of stability analysis provides results which give sufficient conditions for stability or necessary conditions for instability. Therefore, this method is truly stability analysis, while linear analysis may be called instability analysis. The procedure is really a form of Liapunov's second or direct method applied to continuous systems. Liapunov analysis is very common in control theory and a general discussion is really out of place here. The books by LaSalle and Lefschetz (48) and Hahn (36) provide a good background in Liapunov stability by the direct method.

The heart of the energy method is to form a positive definite function by suitable manipulation of the governing equations. The time derivative behavior of this expression is then determined. Conditions under which this derivative is less than zero provide the bounds for stability. The real beauty of the method is that it does not require, "a priori," the dropping of terms non-linear in the perturbation of the flow.

In considering flow situations with no heat or mass
transfer the above positive definite function is chosen to
be the kinetic energy of the disturbance. Because of this
fact the method is in reality an "energy method" for these
types of flows. For problems with heat and mass transfer
the selection of corresponding positive definite functions
parallels the use of kinetic energy for simple flow prob-
lems. The functions used in this case are not true ener-
gies, but they are valid forms for Liapunov functionals.
Nonetheless, the concept of an energy does apply still in a
gross sense, and the name is often retained.

One advantage of the method is its relative ease of
implementation. The results do have a tendency to be on the
conservative side, but they still provide some interesting
solutions. For the Bénard problem, in fact, Joseph (41) has
shown that the energy results give the same bounding value
as linear theory. This means that the critical value from
linear theory is now a necessary and sufficient condition for
stability.

Section 5.2. Derivation of the Energy Equations

In this section the energy equations are derived for
one specific problem treated by the linear theory. This is
the problem of a zero order reaction with active stress and
no buoyancy. The boundary conditions are no slip and con-
stant temperature and concentration at the walls. The deri-
vation follows that outlined by Serrin (81) and Joseph (41).
The equations governing the above system are:

\[
\frac{\partial \mathbf{u}}{\partial t} = \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho_0} + \nu \nabla^2 \mathbf{u} + \nabla \cdot T_a / \rho_0
\]  

5.2.1

\[
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{v} = D_1 \nabla^2 \mathbf{v} + R_1
\]  

5.2.2

\[
\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D_2 \nabla^2 c + R_2
\]  

5.2.3

\[
\nabla \cdot \mathbf{u} = 0
\]  

5.2.4

These equations are assumed to be satisfied by a disturbed set of variables \( u^* \), \( \xi^* \), and \( c^* \) in addition to the original solution variables \( u \), \( \xi \), and \( c \). These variables are put into the above equations, and the original equations subtracted from the disturbed equations.

When the following terms are introduced (representing the perturbations themselves):

\[
\mathbf{v} = u^* - u, \quad T = \xi^* - \xi, \quad e = c^* - c, \quad \bar{\mathbf{v}}_a = T^* - T_a
\]

and \( \pi = p^* - p \)

5.2.5

the equations become,

\[
\frac{\partial \mathbf{v}}{\partial t} + u^* \cdot \nabla \mathbf{v} + \mathbf{v} \cdot \nabla u^* + \frac{\nabla p^*}{\rho_0} - \nu \nabla^2 \mathbf{v} - \frac{1}{\rho_0} \nabla \cdot \bar{\mathbf{v}}_a = 0
\]  

5.2.6

\[
\bar{T}_a = T_a(e, T) + T_a(e, \xi) + T_a(c, T)
\]  

5.2.7
\frac{\partial T}{\partial t} + \mathbf{u}^* \cdot \nabla T + \mathbf{v} \cdot \nabla \xi - D_1 \nabla^2 T = 0 \hspace{1cm} 5.2.8

\frac{\partial e}{\partial t} + \mathbf{u}^* \cdot \nabla e + \mathbf{v} \cdot \nabla e - D_2 \nabla^2 e = 0 \hspace{1cm} 5.2.9

\mathbf{v} \cdot \nabla = 0 \hspace{1cm} 5.2.10

In the above equations the source terms \( R_1 \) and \( R_2 \) are considered to be physical constants; and when the subtraction is made, they cancel out. Since the system under consideration is a zero order reaction (uniform volumetric source), this assumption is a good one. Equations 5.2.6 - 5.2.10 represent the equations governing the perturbations \( \mathbf{v} \), \( T \), and \( e \).

The scalar products of 5.2.6 with \( \mathbf{v} \), 5.2.8 with \( T \), and 5.2.9 with \( e \) are now formed, yielding the following:

\( \frac{\partial \left( \frac{v^2}{2} \right)}{\partial t} + \mathbf{u} \cdot \nabla \left( \frac{v^2}{2} \right) = \mathbf{v} \cdot D \cdot \nabla \nabla : \nabla \mathbf{v} \)

\( - \frac{\tau a}{\rho_0} : \nabla \mathbf{v} + \mathbf{v} \cdot (\mathbf{v} \nabla \left( \frac{v^2}{2} \right)) - \mathbf{v} \cdot \frac{\mathbf{p}}{\rho_0} \)

\( - \mathbf{v} \left( \frac{v^2}{2} \right) + \mathbf{v} \cdot \frac{\tau_a}{\rho_0} \) \hspace{1cm} 5.2.11

\( \frac{\partial \left( \frac{T^2}{2} \right)}{\partial t} + \mathbf{u} \cdot \nabla \left( \frac{T^2}{2} \right) = -T \mathbf{v} \cdot \nabla \xi - D_1 \nabla^2 T \cdot \nabla T \)

\( + \mathbf{v} \cdot (D_1 T \nabla T) - \mathbf{v} \left( \frac{T^2}{2} \right) \) \hspace{1cm} 5.2.12
\[ \frac{\partial}{\partial t} \left( \frac{e^2}{2} \right) + u \cdot \nabla \left( \frac{e^2}{2} \right) = -e \nabla \cdot \mathbf{c} - D_2 \nabla \cdot \nabla \epsilon \]

\[ + \nabla \cdot (D_2 \nabla \epsilon - \nabla \left( \frac{e^2}{2} \right)) \]  

5.2.13

In the above equations these relations have been used:

\[ \mathbb{D} = \frac{1}{2}(\nabla u + (\nabla u)^T) \quad \text{and} \quad \nabla \cdot (\nabla \cdot \mathbf{A}) = \nabla \cdot (\nabla \cdot \mathbf{A}^T) - \mathbf{A}^T : \nabla \nabla \]

Equations 5.2.11-5.2.13 are now integrated over the volume V making use of the Reynolds Transport Theorem, the Divergence Theorem, and the definitions:

\[ K = \int_V \frac{1}{2} v^2 \, dV \]  

5.2.14

\[ \theta = \int_V \frac{1}{2} T^2 \, dV \]  

5.2.15

\[ \psi = \int_V \frac{1}{2} e^2 \, dV \]  

5.2.16

The resulting system of equations is:

\[ \frac{dK}{dt} = -\int_V (\nabla \cdot \mathbf{D} \cdot \nabla + \nabla \cdot \nabla \cdot \nabla \cdot \nabla) + \frac{\tau a}{\rho_0} : \nabla \nabla \] 

\[ + \int_S (\nabla \left( \frac{e^2}{2} \right) \] 

\[ - \frac{\tau}{\rho_0} - \nabla \left( \frac{e^2}{2} \right) + \frac{\tau}{\rho_0} \cdot \mathbf{n} \cdot \mathbf{dS} \]  

5.2.17
\[ \frac{d\theta}{dt} = -\int_V (T_v \cdot \nabla \xi + D_1 vT \cdot \nabla T) dV \]
\[ + \int_S (D_1 T vT \cdot \nabla \left( \frac{T^2}{2} \right)) \cdot ndS \quad 5.2.18 \]

\[ \frac{\psi}{dt} = -\int_V (e_v \cdot \nabla c + D_2 e \cdot \nabla e) dV \]
\[ + \int_S (D_2 e_v \cdot \nabla \left( \frac{e^2}{2} \right)) \cdot ndS \quad 5.2.19 \]

If the assumption of spatially periodic variables in the infinite directions is combined with the boundary conditions given earlier, the surface integrals in the equations 5.2.17-5.2.19 vanish (see for example Joseph (41)).

The three preceding equations are still in dimensional form. These equations are non-dimensionalized using the following set of variables.

\[ \bar{v} = \frac{vL}{\nu} \quad \bar{c} = \frac{c}{c_0} \quad \bar{x} = \frac{x}{L} \quad c_0 = \frac{kL^2}{D_2} \]

\[ T_0 = \left( \frac{QD_2 \rho v^2}{D_1 n} \right)^{1/2} \quad \bar{\epsilon} = \frac{\epsilon}{c_0} \quad \bar{T} = T/T_0 \]

\[ \bar{\epsilon}_0 = \frac{kL^2 Q}{D_1} \quad \bar{S}_N = \left( \frac{k^2 L^4 Q \rho}{D_1 D_2 \rho v^2} \right)^{1/2} = \sqrt{\bar{S}} \]
\[ \bar{\xi} = \frac{\xi}{\xi_0} \quad \bar{e} = \frac{e}{e_0} \quad Sc = \frac{\nu}{D_2} \]

\[ e_0 = \left( \frac{D_1 \alpha \nu^2}{D_2 Q_h} \right)^{1/2} \quad Pr = \frac{\nu}{D_1} \quad 5.2.20 \]

When this is done, the resulting equations are (dropping the bars once again):

\[ \frac{dK}{dt} = -\int_V (\nu \cdot D \cdot \nabla \cdot \nabla \cdot \nabla \cdot S_{N \xi} \cdot \nabla \cdot \nabla \cdot \nabla) dV \quad 5.2.21 \]

\[ Pr \frac{d\theta}{dt} = -\int_V (PrS_{N \xi} \cdot \nabla \cdot \nabla \cdot \nabla \cdot \nabla) dV \quad 5.2.22 \]

\[ Sc \frac{d\psi}{dt} = -\int_V (ScS_{N e} \cdot \nabla \cdot \nabla \cdot \nabla \cdot \nabla) dV \quad 5.2.23 \]

The function which determines stability can now be defined as:

\[ E = (K + \lambda_T Pr \theta + \lambda_e Sc \psi) \quad \lambda_T, \lambda_e \text{ coupling parameters} \quad 5.2.24 \]

The statement for stability is simply that the time derivative of this quantity should be less than zero.

\[ \frac{dE}{dt} = \frac{d}{dt} [K + \lambda_T Pr \theta + \lambda_e Sc \psi] < 0 \quad 5.2.25 \]

This states that the total energy of the perturbations in the system must vanish as time goes to infinity. As
mentioned previously this function is not really an energy, but it is a legitimate Liapunov function in the application of Liapunov's second or direct method.

There are two basic methods which have been used to evaluate the problem posed in the previous paragraph. The first consists of finding bounds for the integrals on the right hand sides of equations 5.2.21-5.2.23. This method has been used by various workers for several different problems (35, 20, 82, 100). The idea is quite simple and requires only a moderate amount of work. Unfortunately the results are normally very conservative, depending on how well the bounds can be obtained.

The second method requires the application of the Calculus of Variations (30, 78) to equations 5.2.21-5.2.23. It entails the selection of a variational principle for this system of equations and evaluation of this principle to give conditions under which equation 5.2.25 is satisfied. This method is somewhat more complicated, but it should yield less conservative results. Therefore, the variational method was the one used in the present work.

A variational principle for the problem at hand can be written as:

\[- \{ \int_V [v \cdot D \cdot v + S_{N\alpha} v v + \lambda_T P r S_N T v \cdot v \cdot v \xi ] + \lambda e S c S_N e v \cdot v c ] d V \} = \text{MAX} \]

5.2.26
This principle holds for a set of functions which satisfy the boundary conditions, the equation of continuity, and appropriate differentiability conditions. Also the above equation is subject to the following normalization constraint:

\[ \int_V \left[ \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla \right] dV = 1 \quad 5.2.27 \]

Equation 5.2.26 represents the rate at which energy is extracted from the system. The first term is the energy extracted from the bulk flow, and the remaining terms give the energy extracted from the active stress term. The principle 5.2.26 thus gives the condition that the rate of energy extraction is a maximum. This should be the least stable situation.

Equations 5.2.26-5.2.27 can be combined by the use of Lagrange multipliers to give the variation:

\[ \delta \int_V \left[ \frac{1}{S_N} \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla \right] dV \]

\[ + \frac{1}{S_L} \int_V \left[ \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla + \lambda \nabla \cdot \nabla \right] dV \]

\[ - 2p(x) \nabla \cdot \nabla dV \} = 0 \quad 5.2.28 \]

The Euler equations for this system are found by application of the Calculus of Variations again. The resulting equations are:
\[ v^2 v \cdot v_0 (x) = -\frac{S_\lambda}{2} \frac{v \cdot \tau}{\tau} + \frac{Pr S_\lambda}{2} T \frac{v}{v} \xi \]

\[ + \lambda e \frac{Sc S_\lambda}{2} e v c \]

5.2.29

\[ \lambda_T v^2 T = \frac{S_\lambda}{2} Pr v \cdot v \xi - \frac{2S_\lambda}{2} v \cdot (v c \cdot E) \]

5.2.30

\[ \lambda_e v^2 e = \frac{S_\lambda}{2} Sc v \cdot v c - \frac{2S_\lambda}{2} v \cdot (v \xi \cdot E) \]

5.2.31

\[ v \cdot v = 0 \]

5.2.32

In finding these equations the fact that the present problem is one of quiescent initial state has been used to give \( \xi = 0 \). The tensor \( \xi \) is the rate of deformation tensor for the perturbation \( v \) and is given by:

\[ \xi = \frac{1}{2} [vv + (vv)^T] \]

Also used in the derivation of these equations was a linearization assumption. The tensor \( \tau_a \) (equation 5.2.7) contains terms which are non-linear in the perturbations (for example \( v v \xi T \)). To simplify calculations later, these terms were assumed negligible. This assumption is similar to that made for infinitesimal disturbances in linear theory. The equations 5.2.29-5.2.32 are thus the energy equations which will give conditions for the stability of the system when subjected to small disturbances. A similar
assumption was used by Gupta (35) in treating Couette flow of second order fluids.

One final step is taken in the analysis of equations 5.2.29-5.2.32. The coupling parameters \( \lambda_T \) and \( \lambda_e \) are set equal to each other (\( \lambda_T = \lambda_e = \lambda \)). This simply assigns equal weight to the concentration and temperature contributions. With this fact new variables \( \bar{T} = \sqrt{\lambda} T \) and \( \bar{e} = \sqrt{\lambda} e \) are defined and substituted into the equations 5.2.29-5.2.31. The resulting system (once again dropping the bars) is:

\[
\nabla^2 \eta - \nabla p(x) = -\frac{S_\lambda}{2\sqrt{\lambda}} \nabla \cdot \eta \alpha + \frac{\lambda \text{Pr} S_\lambda}{2\sqrt{\lambda}} \nabla \eta \xi
+ \frac{\lambda S \text{Sc} S_\lambda}{2\sqrt{\lambda}} e \nabla \eta \xi
\]

5.2.33

\[
\nabla^2 T = \frac{S_\lambda}{2\sqrt{\lambda}} \text{Pr} \nabla \cdot \eta \xi - \frac{S_\lambda}{\sqrt{\lambda}} \nabla \cdot (\nabla \eta \cdot \xi)
\]

5.2.34

\[
\nabla^2 e = \frac{S_\lambda}{2\sqrt{\lambda}} \text{Sc} \nabla \cdot \nabla \eta \xi - \frac{S_\lambda}{\sqrt{\lambda}} \nabla \cdot (\nabla \xi \cdot \xi)
\]

5.2.35

This set of equations is reduced further by setting the parameter \( \lambda \) equal to one. Since this multiplier is arbitrary, this selection represents only one of the infinity of possibilities. The final set of equations thus defines an eigenvalue problem for the quantity \( S_\lambda / 2 \). Since for this particular case the exchange of stabilities can be
proved (see Chapter 8 and Appendix B), the energy equations can be compared to the linear equations governing the marginal state. This comparison reveals that the eigenvalue in the energy equations, \( S_{\lambda}/2 \), corresponds to the square root of the active stress number, \( \sqrt{\mathcal{S}} \). The determination of this eigenvalue and its comparison to the linear result is discussed in the numerical results chapter (Chapter 7).
CHAPTER 6

NUMERICAL METHODS

Section 6.1. Introduction

Three numerical methods were used in analyzing the sequence of equations obtained from non-linear theory. First a variational or Galerkin method was used to find an initial approximation to the linear eigenvalue. This eigenvalue was then refined by means of an orthogonal integration method proposed by Davey (13); hereafter referred to as Davey's method. Once the linear eigenvalue was found the method of complementary functions combined with Conte's method was used to find the four eigenfunctions necessary to calculate the second (or first non-linear) eigenvalue.

Section 6.2. Galerkin Method

The Galerkin method is a member of the broader class of methods known as Weighted Residuals. Finlayson (22) provides a good and easily read reference for many of the methods contained in this class. These methods have been used frequently for many problems in fluid mechanics and reactor analysis (23,49,2,101).
All of the weighted residual methods involve the use of a set of trial functions, \( \{ T_i \} \), to approximate the solution to a differential equation \( u = \sum a_i T_i \). If the set of trial functions is complete, the solution to a self-adjoint system of equations can be approximated exactly if the number of functions used is large enough (23). The selection of trial functions is really an art. Normally these functions are selected such that they satisfy the boundary conditions of the system. The functions chosen in this way must satisfy only the boundary conditions given. Care must be taken not to satisfy any other conditions which are not conditions given by the problem. Lee and Reynolds (49) discuss the selection of trial functions for the Orr-Sommerfeld problem.

Once the trial functions have been selected, the approximate solution, \( u = \sum a_i T_i \), is substituted into the differential equation. A residual \( (R) \) is formed, since in general the approximate solution will not satisfy the equation identically. The coefficients \( a_i \) are then chosen to make a weighted average of the residual equal to zero over the space. This weighted average is defined as the integral inner product of a weighting function and the residual. A set of weighting functions, containing the same number of elements as the set of trial functions used, thus enables one to determine the \( a_i \)'s.

In the Galerkin method, the weighting functions are
selected to be the trial functions. The Galerkin method as applied to an eigenvalue problem is now outlined. Consider the linear eigenvalue problem:

\[ Lu + \lambda Nu = 0 \quad \text{L, N are differential operators} \]
\[ B_k u = 0 \quad \text{On boundary} \quad 6.2.1 \]

In general the problem has solutions only for discrete values of \( \lambda \). As used in this current work, the purpose is to approximate the eigenvalues \( \lambda \). An approximate solution of the form \( u = \sum a_i T_i \) is used, with the resulting residual given by:

\[ R = \sum_{i=1}^{N} (a_i Lu_i + \lambda a_i Nu_i) \quad 6.2.2 \]

This residual is then made orthogonal to each of the trial functions:

\[ \sum_{i=1}^{N} a_i [(u_j, Lu_i) + \lambda (u_j, Nu_i)] = 0 \]
\[ j=1,2,...N; \quad (a,b) = \int_{1}^{2} ab \, dy \quad 6.2.3 \]

In order for the above system to have a solution for the \( a_i \)'s, the following determinantal equation must be satisfied:

\[ \det[A_{ji} + \lambda B_{ji}] = 0, \quad A_{ji} = (u_j, Lu_i), \quad B_{ji} = (u_j, Nu_i) \quad 6.2.4 \]
This is the same as finding the eigenvalues of the algebraic eigenvalue problem:

$$Aa = -\lambda Ba$$  \hspace{1cm} 6.2.5

The eigenvalues of this problem are thus the approximations to the eigenvalues of the differential equation.

Wilkinson (107) provides a good reference for the solution of eigenvalue problems of this type. The method used in this work is to find the inverse of $B$ (assumed to exist) and multiply through by this inverse. The resulting system is:

$$B^{-1}Aa = -\lambda Ia$$  \hspace{1cm} 6.2.6

The eigenvalues of the matrix $B^{-1}A$ must now be found. In order to do this, the matrix is reduced to Hessenberg form by the use of Givens rotations and then further reduced to triangular form using the QR algorithm. The eigenvalues are then found on the diagonal of the matrix. The program used in this process was one written by Rinzel and Funderlic (72). These methods are outlined in Wilkinson and further elaboration is out of place here.

Section 6.3. Davey's Method

The method outlined by Davey (13) is a complete orthonormalization method belonging to the general class
of shooting or marching methods. Two references for this class of methods are Keller (45) and Roberts and Shipman (74). Davey applied his technique to the Orr-Sommerfeld equation, however the basic concept can be extended to equations of higher differential order such as those encountered in this work. In the original paper, Davey discusses the comparison of his technique with other well known methods such as those of Keller and Godunov.

The concept of shooting methods in solving two point boundary value problems is to find the initial conditions which give the same solution as the boundary conditions. In doing this the problem is handled as if it were an initial value problem. If n initial conditions are required and r boundary conditions have been specified already, then n-r initial conditions are missing. These missing conditions are found by integrating the equations forward using an orthogonal set of initial values and then finding the required conditions by manipulation of the solutions given by this set. One final integration forward is required using the known boundary conditions and the calculated missing conditions. For linear problems the process can be simplified somewhat. The final integration does not have to be performed because the desired solution can be constructed from a linear combination of the solutions given by the set of initial conditions.

Consider now the differential eigenvalue problem
given in Chapter 4 (equation 4.2.20). For the present section also consider the boundary conditions
\[ \phi = D\phi = \beta = \Omega = 0 \quad \text{at} \quad y = \pm 1/2 \quad 6.3.1 \]

For each point \( y \) contained in the range of integrations, the eight-dimensional vector space \( z = \{\phi, D\phi, D^2\phi, D^3\phi, \beta, D\beta, \Omega, D\Omega\} \) is defined. A non-standard inner product for this space is given by
\[
\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{8} a_k b_k.
\]

The equation 4.2.20 will be integrated using a finite difference method with \( m \) steps of size \( h (h=1/m) \). In this section a predictor-corrector algorithm was used with a Runge-Kutta starter (Appendix A).

If the integration is started with some initial conditions \( z_0 \), the value of \( z \) at \( y = ih \), \( z_i \), and the value at \((i+1)h\), \( z_{i+1} \), are related by a transfer matrix \( A^{i+1} \); where
\[
z_{i+1} = A^{i+1} z_i \quad (A^{i+1} \text{ is an } 8 \times 8 \text{ matrix}) \quad 6.3.2
\]

The elements of \( A^{i+1} \) may be determined by letting \( z_i \) have separately the eight values
\[
\{1,0,0,0,0,0,0,0\}, \{0,1,0,0,0,0,0,0\}, \ldots
\]
\[
\{0,0,0,0,0,0,0,1\}, \quad 6.3.3
\]
and performing the integration from i to i+1. The columns of $A^{i+1}$ are just the eight vectors $z_{i+1}$ which correspond to the initial eight $z_i$'s. The transfer matrix $A^P$ can be found for each integration step in this manner. The method is called complete orthonormalization because of the use of orthogonal conditions for $z_i$ at each step.

The relation between the initial vector $z_0$ at $y = -1/2$ and the final vector $z_m$ at $y = +1/2$ is

$$z_m = Bz_0 \quad \text{where} \quad B = A^mA^{m-1}...A^2A^1$$ \hspace{1cm} (6.3.4)

In practice it is not necessary to evaluate the individual transfer functions, $A_i$'s, unless the function $z$ is desired at every point. As the method is used in this work, the unknown quantity is the eigenvalue of the linear problem. All that is needed in this case is that the eight vectors arising from the orthogonal starting conditions remain linearly independent as the integration proceeds. If they do not, the final transfer matrix, $B$, may be deformed so as to be of little or no use.

The resolution of this problem is to interrupt the integration a few times in order to assure this linear independence. If the integration is broken into q divisions and restarted each time with orthogonal conditions, the final transfer matrix becomes

$$B = B^q B^{q-1}...B^2B^1.$$ \hspace{1cm} (6.3.5)
Using the boundary conditions given earlier, equation 6.3.4 can be written as

\[
\begin{bmatrix}
0 \\
0 \\
x \\
x \\
0 \\
x
\end{bmatrix}
= 
\begin{bmatrix}
x \\
x \\
x \\
x \\
x \\
x
\end{bmatrix}
\begin{bmatrix}
x \\
x \\
x \\
x \\
x \\
x
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
x \\
x \\
0 \\
x
\end{bmatrix}
\]

6.3.6

In order for this expression to have a solution the 4 x 4 submatrix represented by the dots in the main matrix must have a zero determinant. This determinant is just a function of the system parameters; in this case Pr, Sc, S, \(\kappa^2\), and \(c^{(0)}\). It is desired to evaluate this determinant as accurately as possible. One way to do this is outlined below.

The third, fourth, sixth, and eighth columns of \(B^1\) are orthogonalized with respect to the previously defined inner product. Every column of \(B^1\) is then normalized. This new matrix called \(C\) is left multiplied by \(B^2\) and the orthogonalization and normalization process is repeated. This is repeated successively for \(B^3\) through \(B^m\) until the final \(C\) has been obtained. The final matrix is a modification of \(B\) such that columns three, four, six and eight
are orthonormal. The singular nature of the submatrix has not been changed. The required determinant is an analytic function of the system parameters, and an iterative technique can be used to find the eigenvalue (or other parameter) which sets the determinant equal to zero.

The iterative method used in this work was to start with the Galerkin eigenvalue as a first approximation and perform the above described process for this value. Two other points, one on either side of the Galerkin value, were also evaluated. These three points provided the basis for a quadratic fit, and the roots of this quadratic equation were found. Using the correct root as a starting point, the iteration was continued until sufficient accuracy was achieved.

Section 6.4 Complementary Functions and Conte's Method

Section 6.4.1. Introduction

The final step in the non-linear analysis was to determine the four eigenfunctions necessary to calculate $c^{(2)}$ (Figure 4). The method which was used for this purpose was once again a shooting method. Several of these methods were considered, and the one which was chosen was the method of complementary functions.

The particular reason for selecting the method of
complementary functions was its slightly easier implementation compared with the other methods. The other two methods which were seriously considered were the Method of Adjoints and Miele's Method of Particular Solutions. The Method of Adjoints requires the use of the adjoint differential equation. One of its strengths is its automatic generation of an iterative process for non-linear equations. This factor does not come into play here since the equations of interest are linear. The method of particular solutions is similar to the complementary functions technique. The main stumbling block here is that this method requires integration of the entire inhomogeneous problem for each member of the set of initial conditions. The method used only requires this integration be done once (the other integrations being done using the homogeneous analog).

As mentioned in Section 6.2 it is sometimes necessary to stop the integration to assure linear independence of the elements of the set of solutions. The reason for this procedure is that oftentimes a differential operator will have characteristic values which differ greatly in magnitude. If this is the case, then one element of the solution set will grow much more rapidly than the others. By numerical round off error all of the other elements may be malformed by introduction of a small portion of this rapidly growing element. As the integration proceeds, the elements will become increasingly closer to being parallel.
When this happens, the information given by these elements is practically useless.

Two of the methods most commonly used to insure the linear independence of the solution vectors are Kaplan's filtering method and Conte's method. Conte's method was used for this work and will be discussed later in this section. The filtering technique of Kaplan (44) involves the subtraction of a fraction of the rapidly growing solution from the other more slowly growing solutions at each point. This fraction is determined by forcing the difference to satisfy a second differential equation used as the filter. The resulting solutions are nearly orthogonal and are linearly independent. For the Orr-Sommerfeld problem the filter is the inviscid Orr-Sommerfeld operator. The main reason this method was not used was that it was felt that a good natural filter did not exist for the active stress problem. Any appropriate filter would have been somewhat artificial.

Section 6.4.2. Method of complementary functions

The method of complementary functions is a formal method used to find the missing initial conditions needed to turn the two point boundary value problem into an initial value problem. The description of the method which follows parallels that of Roberts and Shipman (74).
by the set of $n$ linear ordinary differential equations

\[
\dot{y} = A(t)y + f(t) \quad y(t) \text{ is } n \times 1 \text{ vector}
\]

\[
A(t) \text{ is } n \times n \text{ matrix}
\]

\[
f(t) \text{ is } n \times 1 \text{ vector} \quad 6.4.1
\]

with the boundary conditions

\[
y_i(t_0) = c_i \quad i = 1, 2, \ldots, r
\]

\[
y_{i_m}(t_f) = c_{i_m} \quad m = 1, 2, \ldots, n-r \quad 6.4.2
\]

The homogeneous analog to the above equation is

\[
\dot{u}(t) = A(t)u(t) \quad 6.4.3
\]

The homogeneous equation is integrated $n-r$ times with the initial conditions

\[
\begin{align*}
\left\{ 
\begin{array}{ll}
\not_0 (t_0) = 1 & i = r+m \\
0 & i \neq r+m
\end{array}
\right. \\
, \quad m = 1, 2, \ldots, n-r \quad 6.4.4
\end{align*}
\]

The subscript $i$ indicates the component of the $u$ vector, and the superscript $m$ indicates the number of the integration. Define a particular solution $v(t)$ which is the solution to the equation

\[
\dot{v}(t) = A(t)v(t) + f(t) \quad 6.4.5
\]
with the initial conditions

\[ v_i(t_0) = y_i(t_0) = c_i \quad i=1,2,\ldots,r \]

\[ v_i(t_0) = 0 \quad i=r+1,\ldots,n \quad 6.4.6 \]

The solution \( y(t) \) to the original problem 6.4.1 can then be expressed as a function of the \((n-r)\) homogeneous solutions and the one particular solution

\[ y_i(t) = \sum_{j=1}^{n-r} b_j u_i^{(j)}(t) + v_i(t) \quad i=1,2,\ldots,n. \quad 6.4.7 \]

The coefficients \( b_j \) can be determined by applying the above expansion at \( t = t_f \) and using the known conditions there

\[ y_m(t_f) = \sum_{j=1}^{n-r} b_j u_i^{(j)}(t_f) + v_i(t_f) \quad m=1,2,\ldots,n-r \quad 6.4.8 \]

The only unknowns in these equations are the \( b_j \)'s. The result is a linear algebraic equation for these coefficients. This equation can be written as:

\[ D \text{ is } (n-r) \times (n-r) \text{ matrix with elements } D_{mj} = u_{im}^{(j)}(t_f) \]

\[ b \text{ is } (n-r) \times 1 \text{ vector} \]

\[ c \text{ is } (n-r) \times 1 \text{ vector with elements } c_m = y_{im}(t_f) = c_{im} \]

\[ v \text{ is } (n-r) \times 1 \text{ vector} \quad 6.4.9 \]
After solving for the $b_j$'s, two methods can be employed to find the final solution $y(t)$. If the values of $u^{(j)}$ have been kept along with $v(t)$, equation 6.4.7 can be used to find the solution. The $b_j$'s can also be seen to correspond to the missing initial conditions $y_i(t_0)$ ($i=r+1,\ldots,m$)

$$y_i(t_0) = \sum_{j=1}^{n-r} b_j u^{(j)}_i(t_0) + v_i(t_0) \quad i=r+1,\ldots,n$$

$$v_i(t_0) = 0 \quad i=r+1,\ldots,n \quad 6.4.10$$

$$u^{(j)}_i(t_0) = \begin{cases} 1 & i=r+j \\ 0 & i\neq r+j \end{cases}, j=1,2,\ldots,n-r$$

and

$$y_i(t_0) = b_{i-r} \quad i=r+1,\ldots,n$$

These missing conditions can be combined with the known initial conditions, and a final integration can be performed to find $y(t)$.

In this paper the first of these two methods was employed. The homogeneous solutions were stored along with the particular solution. The matrix equation 6.4.9 was solved for the $b$'s by means of a linear equation solver which employed an LU decomposition using Gaussian elimination (Moler (55)). The solution was then constructed according to equation 6.4.7.
Section 6.4.3. Conte's method

Conte's method was used to do the orthonormalization of the vectors obtained by the method of complementary functions. The method consists of doing a complete Gram-Schmidt orthonormalization on the homogeneous vectors. The Gram-Schmidt process is a very well known process and is described in any good text on linear algebra (Noble (57)). Using this set of orthonormal vectors, the "orthogonal complement" of the particular solution is found. This complement is formed by subtracting out a linear combination of the orthonormal homogeneous vectors.

In practice the process is to do a Gram-Schmidt orthonormalization on the entire system with the particular solution as the last vector. The process is stopped before the normalization of this last vector is done. In this way the vector representing the particular solution is orthogonal to the homogeneous solution vectors, but it is not normalized. In addition the homogeneous solutions have not been modified by introducing any of the particular solution.

Consider n interruptions of the integration to do the orthonormalization. Assume for simplicity that the last orthonormalization is done at the final boundary. This gives n integration blocks to be used in solving the system. The starting conditions for the (m+1)st block will be the orthonormal set of vectors given by the mth orthonormalization.
The Gram-Schmidt process may be represented in matrix form by

\[ z = P_y \]  \hspace{1cm} 6.4.11

\( z \) is \( N \times 1 \) vector with elements orthonormal vectors \( z^{(1)}, \ldots, z^{(N)} \)

\( y \) is \( N \times 1 \) vector with elements original vectors \( y^{(1)}, \ldots, y^{(N)} \)

\( P \) \( N \times N \) matrix lower triangular form, giving the linear operations done on \( y \) to form \( z \).

Assume that in the process of integrating the differential system, the orthonormalization is performed \( m \) times. The matrix \( P_f \) thus represents all of the linear manipulations done on the vector set as the integration was carried out.

\[ P_f = p_{n_f}^{p_{n_f-1}} \ldots p_2^{p_1} \]  \hspace{1cm} 6.4.12

The vectors \( y_f \) are used to determine the missing initial conditions in the method of complementary functions. These are the vectors which would have been obtained had the integration been done without orthonormalization.

\[ y_f = P_f^{-1} z_f \]

\[ \begin{cases} 
    y_f & \text{vectors at integration} \\
    z_f & \text{end}
\end{cases} \]  \hspace{1cm} 6.4.13

The stored vectors must also be reconstructed in
order to provide the correct system for linear combination to form the final solution. This reconstruction is done step by step as the integration proceeds. The vectors from the first block are correct. The vectors at each point in the second block must be multiplied by \((p_1^{-1})^{-1}\) in order to retrieve the proper solutions. The above process for the \(r^{th}\) block \((r \geq 2)\) is to multiply the vectors at each point by \((p_1^{-1}p_1^{-2}...p_1^{-2})\) in order to regenerate the required solutions.

Section 6.5. Finding the Eigenvectors

The basic theory used to calculate the eigenvectors was outlined in the previous section. The actual application of this theory is quite straightforward. The formulae for the numerical integration methods mentioned in this section can be found in Appendix A. Two good references for these procedures are Collatz (10) and Lapidus and Seinfeld (47).

The logic for the calculations done in finding the eigenvectors is outlined briefly in Figure 5. The first step was to find the linear eigenvector \(\phi^{(1;1)}\). Since this vector forms the inhomogeneous part of the non-linear equations, high accuracy was required. An eighth order Predictor-Corrector was used with an eighth order Runge-Kutta starter. Four hundred steps were used to get this solution, and four orthonormalizations were found to be adequate.
FIGURE 5. COMPUTATIONAL FLOW CHART
FIGURE 5 - CONTINUED
The other three eigenvectors \( \phi_A, \phi^{(0;2)}, \phi^{(2;2)} \) were all found using a fifth order Predictor-Corrector with a fourth order Runge-Kutta starter. Two hundred steps were used in these calculations with four orthonormalizations performed.
CHAPTER 7

NUMERICAL RESULTS AND DISCUSSION

The numerical results obtained in this work fall into three general categories; the linear stability results, the non-linear stability results, and the energy result. The sections in this chapter are arranged in this order. In addition the first two sections are further divided into subsections concerned with buoyancy effects, active stress effects, and combined active stress and buoyancy effects. Most of the results are presented in graphical form with discussion centered around these visual aids.

Section 7.1. Linear Stability Results

The neutral curves in this section were found by estimating their position using Galerkin techniques. The approximate combination of parameters was found for which the real part of the linear eigenvalue was zero. This was done for several wave numbers. The results were then refined using Davey's method. In this application of Davey's method the eigenvalue was set, and iteration was done on another parameter (for example the active stress number). The critical
number and mode were found from the minimum value given by a cubic fit to four wave numbers and their corresponding neutral numbers.

Section 7.1.1 Buoyancy effects

The linear system for the problem with gravity effects and no active stress was given in Chapter 4 (equation 4.2.21). The first application of this system was to calculate the neutral curve for the Bénard problem. This was done essentially as a check of the programs, and the curve is presented in Figure 7.1. The agreement with the values presented in Chandrasekhar (7) was excellent. This curve is also the neutral curve for the problem of combined heat and mass transfer with no chemical reaction. In this case the Rayleigh number is actually the sum of the two Rayleigh numbers \( R_1 + R_2 \).

For the problem of combined heat and mass transfer Figure 7.1 represents the neutral curve for stationary marginal states. If the density effects are in opposite directions, overstability is possible and the figure is no longer valid. A further discussion of this behavior can be found in Chapter 8. This problem assumes no chemical reaction in the system. The driving force in the buoyancy term is thus the gradient set up by constant but unequal values of temperature and concentration on the boundaries. The Rayleigh
FIGURE 7.1. NEUTRAL CURVE FOR THE BENARD PROBLEM
numbers therefore have their usually defined values

\[ R_i = \alpha_i \Delta c_i g L^3 / D_i \nu, \quad (i=1,2) \]

where \( \Delta c_i \) is the difference in the boundary values for species \( i \). The other terms have been defined earlier in this paper.

The first results for a chemically reactive system were obtained for constant and equal values of temperature and concentration on the boundaries. In this case there is no characteristic gradient \( \Delta c_i \) to be used as a driving force. The driving force is the temperature or concentration profile set up by chemical reaction with diffusion. The Rayleigh numbers in this situation must therefore be defined in a non-standard way. The gradients \( \Delta c_i \), \( i=1,2 \), are replaced by terms labeled \( c_0 \) and \( \xi_0 \). These terms are related to the reaction rate on the boundaries and to the diffusivities of the species in question. In reality they are the non-dimensionalizing variables for concentration and temperature which were discussed in Section 2.3.

For a zeroth order reaction the Rayleigh numbers are given by

\[ R_1 = \alpha_1 k Q L^5 g / D_1^2 \nu; \quad R_2 = \alpha_2 k L^5 g / D_2^2 \nu; \]

\[ Q = \frac{|\Delta H|}{\rho C_p}. \]
A typical neutral curve for this case is seen in Figure 7.2. This curve is once again for stationary marginal states. The sum of the two Rayleigh numbers is still the parameter governing the stability of the system. For a Prandtl number of 0.1 and a Schmidt number of 100, the neutral sum is 37,300 for a wave number of 4, and for a Prandtl number of 10 and a Schmidt number of 100 the sum is 37,400. The difference can easily be explained by the fact that the latter value was not refined using Davey's method. In spite of this fact there is much less than one percent difference.

The Rayleigh numbers for a first order reaction case are given by

\[ R_1 = \alpha_1 k c_1 Q L_1^5 g/D_1^2 \nu \]
\[ R_2 = \alpha_2 k c_1 L_1^5 g/D_2^2 \nu \].

A typical curve for this case is also shown in Figure 7.2. The sum of the Rayleigh numbers is no longer the only parameter of interest. Since there is a coupling of heat and mass transfer through the chemical reaction, there should also be a coupling in the buoyancy effect. This coupling comes out to be a term like \( \text{Gr}_1 \text{Sc} \) where \( \text{Gr}_1 \) is the heat Grashof number. In a sense this term is an additional Rayleigh number in the system. It represents the buoyancy effect of heat (Grashof number) combined with the mass transfer in the system (Schmidt number). In the next chapter it is seen that this
term has actually only a small effect on the neutral numbers for the system. The sum of the Rayleigh numbers \((R_1 + R_2)\) is therefore a reasonable first approximation to use as a governing parameter.

The first order case is less stable than the zero order case. Inspection of the Rayleigh numbers for the two cases reveals that they are defined differently depending on the reaction order. The difference lies in the fact that the reaction rate at the surface, which is contained in the Rayleigh numbers, is not the same for the two cases. In the first order case the term is \(k_1 c_1\), where \(k_1\) is a rate constant and \(c_1\) is the concentration at the surface. For the zero order case the reaction rate is given by the rate constant \(k_0\). The fact remains that in either case the term of interest does represent the surface reaction rate. The two cases are therefore directly comparable if the surface reaction rate is considered to be the key parameter.

Mathematically the difference in the steady states for the two cases can help to explain the differences in stability. The gradients of the temperature and concentration steady states for a first order reaction are larger in magnitude across the entire interval than those for the zero order reaction (except at the centerline where they are all equal to zero). This means that the coefficients in the governing equations which contain these quantities will be larger for the first order reaction. The larger coefficients
**Figure 7.2.** Mass Grashof Number Neutral Curves for Constant Equal Wall Conditions

*0th Order Reaction*
- \( \text{Pr} = 0.1 \)
- \( \text{Sc} = 100.0 \)
- \( \text{Gr}_1 = 10000.0 \)
- \( \xi_1 = \xi_2 = 1 \)

*1st Order Reaction*
- \( \text{Pr} = 0.1 \)
- \( \text{Sc} = 100.0 \)
- \( \text{Gr}_1 = 5000.0 \)
- \( \xi_1 = \xi_2 = 1 \)
may cause a destabilization. Another destabilizing effect may arise from the fact that the linear equations for a first order reaction contain two extra terms compared with the equations for a zero order reaction. These terms occur because of the dependence of the first order reaction rate on concentration. There is also a coupling of temperature and concentration because of the chemical reaction.

The instability caused by the density gradient in the body force term may be reinforced somewhat by the first order reaction. In the zero order case a perturbation in the concentration has no effect on the reaction rate. The disturbance is therefore neither increased nor decreased by the presence of reaction. In the first order case a perturbation will be reinforced because of the reaction rate dependence on the concentration. Perturbations in the concentration arising from the convection in the system may therefore be strengthened by the presence of the first order reaction.

The magnitudes of the Rayleigh numbers for the reaction cases appear to be quite large in comparison to those in the no reaction case. If a temperature difference based on the maximum temperature in the reacting system versus the bounding temperature is used, it can be shown that this difference is of the same order of magnitude as the gradient in the no reaction problem. A similar result for the concentration can also be shown. The large values in the reaction cases are
therefore simply due to the difference in definitions. Consider now the following example. The parameters chosen are roughly those for small molecules diffusing in water. The heat of reaction in this example is in the neighborhood of ten kilocalories.

\[ \nu = 10^{-2} \text{ cm}^2/\text{sec} \quad \alpha_2 = 10^{-2} \text{ cm}^3/\text{mole} \]

\[ D_1 = 10^{-3} \text{ cm}^2/\text{sec} \quad L = 10^{-1} \text{cm} \]

\[ D_2 = 10^{-5} \text{ cm}^2/\text{sec} \quad g = 10^3 \text{ cm/sec}^2 \]

\[ \alpha_1 = 10^{-2} \text{ °C}^{-1} \quad Q = 10^4 \text{ cm}^3 \text{ °C/mole} \]

For a zeroth order reaction

\[ R_2 = \alpha_2 g L^5 k / D_2^2 \nu = 10^8 k \]

\[ R_1 = \alpha_1 g L^5 k Q / D_1^2 \nu = 10^8 k \]

\[ R_1 + R_2 \approx 2k10^8 \times 3 \times 10^4 \text{ (neutral condition)} \]

\[ \therefore k \approx 10^{-4} \text{ mole/cm}^3\text{sec} \]

\[ \xi_{ss} = \frac{1}{2} \left( \frac{1}{4} - y^2 \right) \quad \xi_{\text{max}} = 0.125 \]

\[ \tilde{\xi}_1 = \text{value at boundary (dimensional)} \]
\[ \xi_m = \tilde{\xi}_1 = \xi_0 \xi_{\text{max}} \quad \text{(dimensional)} = \Delta \tilde{\xi} \]

\[ \xi_0 = kQL^2/D_1 = 10 \]

\[ \therefore \Delta \tilde{\xi} = 1.25 \, ^\circ \text{C} \]

For the no reaction case

\[ R_1 = \alpha_1 g\Delta \xi L^3/D_1 \nu = 10^3 \Delta \xi \]

\[ R_1 = 10^3 \quad \text{(neutral)} \]

\[ \therefore \Delta \xi = (10^0)^\circ \text{C} \approx 1 \, ^\circ \text{C} \]

Therefore the two differences are of the same order.

Figure 7.3 shows the effect of non-equal constant conditions on the boundaries. These results agree very well with those given by Sparrow, et al. (84). They looked solely at the problem of one specie, not two. In the problem treated here the Grashof (Rayleigh) numbers are defined as they were in the no reaction case, since there are characteristic gradients for temperature and concentration.

The parameters \( N_{s_i}, i = 1, 2 \), measure the deviation from the linear situation. These parameters are given by

\[ N_{s_1} = \tilde{S}_1 L^2/D_1 (\xi_1 - \xi_2) \quad N_{s_2} = \tilde{S}_2 L^2/D_2 (c_1 - c_2) \]
Figure 7.3. Grashof number neutral curves for non-linear temperature and concentration

Pr = 1
Sc = 100
Gr₂ = 4

A - Nₛ = 0
B - Nₛ = 10
C - Nₛ = 20
\( \tilde{S}_1 \) and \( \tilde{S}_2 \) are uniformly distributed source terms for heat and mass respectively. The steady states in this situation are given by

\[
\bar{c}_i = \left( \frac{1}{2} + \frac{N_{S_1}}{8} \right) - x - N_{S_1} x^2/2;
\]

\[
\bar{c}_i = (c_1 - c_2)/(c_1 - c_2)
\]

The \( N_s \)'s here are twice those defined by Sparrow et al. The factors \( \tilde{S}_1 L^2/D_1 \) and \( \tilde{S}_2 L^2/D_1 \) are just the non-dimensionalizing variables for temperature and concentration which are used in the zero order reaction case with equal boundary values.

A value of \( N_{S_1} \) of twelve gives a centerline value for \( \bar{c}_i \) of two. The form of the expression for \( \bar{c}_i \) shows that this means that the difference between the centerline value and the value at the upper wall is twice that between the lower and upper walls (linear gradient). The values of \( N_{S_1} \) used in the figure are of the same order as this value of twelve. For this range of parameters, inspection of Figure 7.3 reveals that the linear gradient and the nonlinear terms have the same order effect on the results. In light of the previous discussion this is very reasonable behavior. The curves shown are for equal values of \( N_{S_1} \) and \( N_{S_2} \) so that the governing parameter for the system is once again \( (R_1 + R_2) \).
Section 7.1.2. Active stress effects

The linear system governing the active stress problem was given in equation 4.2.20. The first problem studied here was for constant equal wall conditions for temperature and concentration and zero slip for velocity. The steady states for a zero and first order reaction with these boundary conditions are given in equations 2.3.11 through 2.3.16. These steady states for a source term are shown in Figure 7.4.

As mentioned in Chapter 3 the solution to the system governing the above problem can be separated into two modes. The mode which is the less stable one is for an even stream function (called the even mode). The other mode is for an odd stream function (odd mode). The neutral curves for the even mode for two different sets of Prandtl and Schmidt numbers are shown in Figures 7.5 and 7.6. These curves are for the case of both species being produced (both source).

In the zero order problem the governing parameter for stability is $S(Pr+Sc)$ where $S$ is the active stress number defined earlier. This is equivalent to the number $(R_1+R_2)$ in the buoyancy problem. The first order case does not have this combined parameter as a governing parameter. As in the buoyancy problem there is an additional term in the governing expression for the first order reaction. The
FIGURE 7.4. TEMPERATURE STEADY STATES FOR CONSTANT WALL CONDITIONS
Figure 7.5. Active stress neutral curves for constant equal wall conditions.
Figure 7.6. Active Stress Neutral Curves for Constant Equal Wall Conditions
results in Chapter 8 show that this additional term is small.

Once again the first order case is less stable than the zero order case. The effect here is less pronounced than it was in the buoyancy problem. The nature of the active stress operator causes this reduction in effect. The derivative of the steady state temperature (concentration) is contained in the concentration (temperature) operator in the equation of motion as well as in the stream function operator in the heat (mass) equation.

Figure 7.7 shows the neutral curve for the collapsed number $S(Pr+Sc)$ for the zero order reaction. A corresponding figure for the first order case cannot rigorously be drawn.

The results for the active stress problem with the above boundary conditions do not show any oscillatory marginal states. Chapter 8 and Appendix B discuss this situation in more detail. The result is that when the production terms are parallel (either both sources or both sinks), the marginal states are stationary for either reaction order. If the terms are antiparallel, the zero order system is unconditionally stable. The first order system is also very nearly unconditionally stable.

Using the antisymmetric form of the active stress tensor (Chapter 2), Lin and McIntire (52) found oscillatory marginal states for parallel plate geometry. Finlayson and
Scriven (21) found a similar result using cylindrical geometry. They also comment on the stationary behavior for the deviatoric active stress tensor in this geometry.

The neutral curves for an odd mode for one choice of Prandtl and Schmidt numbers are shown in Figure 7.8. This mode is indeed more stable than the even mode. The difference is not overwhelming, however. Other problems (the Bénard problem for instance) show a much greater difference between the two solutions. The critical wave number for the odd mode is also larger than that for the even mode.

The next change which was made was to look at the situation where both species are being consumed (both sinks). Figure 7.9 shows the temperature steady state for the case where both terms are sinks with a first order reaction. As a comparison it also shows the situation for a mass sink and a heat source. In either case the steady states are given by hyperbolic cosines (equations 2.3.15 and 2.3.16). The steady states for sink terms with a zero order reaction are just the negative of those for source behavior.

Figure 7.10 illustrates one situation where both reaction terms are sinks. Comparison of this figure with Figure 7.5 in which both reaction terms are sources reveals the following. The neutral curve is the same for the two cases when a zero order reaction is involved. The reason for this is the previously mentioned result that the only
**Figure 7.8.** Active stress neutral curves for constant equal wall conditions (odd solution)
TEMPERATURE STEADY STATES FOR 1ST ORDER REACTION - CONSTANT
EQUAL WALL CONDITIONS \( q_2 = -1 \)

FIGURE 7.9
FIGURE 7.10. ACTIVE STRESS NEUTRAL CURVES FOR CONSTANT EQUAL WALL CONDITIONS
difference in steady states for the two cases is a sign change. This is a result of the fact that the reaction rate for a zero order reaction is independent of concentration. The effect of the sign change is eliminated by the presence of the active stress mechanism. With this mechanism dependent on the gradients of temperature and concentration, it makes no difference whether a specie is being consumed or produced.

The situation for a first order reaction is different from that for a zero order reaction. In this case the steady states differ by more than a sign change if sinks rather than sources are used. They are actually different functions. The derivatives of the steady states for a first order sink case are everywhere smaller in magnitude than the corresponding derivatives for a zero order reaction. They are therefore smaller than the derivatives for a first order source case as well. The first order sink case is thus more stable than either the zero order sink (Figure 7.10) or the first order source (Figure 7.5). Another contributing factor is that the additional coupling terms in the linear equations for a first order reaction are opposite in sign for the sink case compared with the source case. These terms will therefore have a stabilizing rather a destabilizing effect.

The next case which was considered was once again sources for both reaction terms. However, now the boundary
conditions were assumed to be those of constant non-equal temperature (concentration) on the two walls. In this problem the same definition of non-dimensionalizing variables was used as in the equal conditions case. Two additional parameters ($\Delta \xi$ and $\Delta c$) were defined to set the differences between the dimensionless values of temperature or concentration at the two walls. A steady state for this problem is compared to one for the equal boundaries case in Figure 7.11. The steady states for a zero order reaction with the non-equal conditions are

$$\overline{c} = \frac{1}{2} \left( \frac{1}{4} - y^2 \right) + \Delta cy; \quad \overline{c} = c - \frac{c_1 + c_2}{2} \quad \text{and} \quad \Delta c = c_2 - c_1$$

$$\overline{\xi} = \frac{1}{2} \left( \frac{1}{4} - y^2 \right) + \Delta \xi y; \quad \overline{\xi} = \xi - \frac{\xi_1 + \xi_2}{2}$$

and $\Delta \xi = \xi_2 - \xi_1$.

Figure 7.12 shows some neutral curves for the non-equal boundaries problem. All of the lines in this figure are for a zero order reaction. Similar results are anticipated for a first order reaction. Three different situations are examined in this figure. The neutral curve for equal boundaries is presented for comparison. Curve A represents the situation of equal values for $\Delta c$ and $\Delta \xi$. Curve B is for $\Delta \xi = 0$ (equal conditions), and $\Delta c$ has the same value as in Curve A. Curve C is the reverse of Curve B, since $\Delta c = 0$.
Figure 7.11. Temperature steady states for 0th order reaction non-equal wall conditions.

A $- \Delta \xi = 0$
B $- \Delta \xi = -0.1$
Figure 7.12. Active Stress Neutral Curves for 0th Order Reaction - Non-Equidistant Wall Conditions
and $\Delta \xi$ is the same as in Curve A. The least stable situation is where both profiles are not symmetric about $y = 0$ (Curve A). The case of equal temperature and non-equal concentration (Curve B) is slightly less stable than the opposite case (Curve C). The reason for this is that the Schmidt number is larger than the Prandtl number. The effect is only a small one because of the nature of the active stress operators which was mentioned earlier (i.e. the coupling of temperature and concentration).

The curves in Figure 7.13 represent the steady state temperature for another set of boundary conditions. In this case the upper plate is insulated, and there is no heat flux. A similar condition is used for concentration (impermeable wall). Once again the reaction terms are assumed to be sources. The kinematic conditions here are still no slip on fixed walls.

The neutral curves obtained for this situation are presented in Figure 7.14. It is immediately obvious that this situation is much less stable than the case where both boundaries are held at constant temperature and concentration (Figure 7.5). From a physical standpoint the presence of a flux has a stabilizing effect. The movement of species into or out of the system helps to damp out the effect of fluctuations in the steady state. When there is no flux of species into or out of the system, these fluctuations can cause the concentration to build up on the boundary. The boundary
FIGURE 7.13. TEMPERATURE STEADY STATES FOR ZERO FLUX AT $y = 1/2$

$\frac{d}{dt} = 0$

$\frac{d}{dt} = 1$

$\frac{d}{dt} = 1/2$

1st Order Reaction

0th Order Reaction
FIGURE 7.14. ACTIVE STRESS NEUTRAL CURVES FOR ZERO FLUX AT $\gamma = 1/2$

$Pr = 0.1$
$Sc = 100.0$
$Gr_1 = Gr_2$
$x_1 = x_2 = 1$
condition of constant wall values does not allow any build up to occur. The accumulation of species at the boundary is equivalent to increasing the concentration gradient between the walls, which is a destabilizing effect.

Figure 7.15 presents a similar situation for mass and heat, however the velocity conditions have been changed. In this problem the upper plate is treated as a flat free surface. The tangential shear stress here is equal to zero. Since the shear stress at the wall represents a momentum flux from the system, the zero tangential stress is equivalent to zero momentum flux. The similarity to the case of zero heat and mass flux is evident. From this argument it is expected that the current problem would be less stable than the previous one. Comparison of Figures 7.14 and 7.15 reveals that this is indeed true.

The preceeding system can be solved by consideration of the odd mode for the two fixed boundaries case (Figure 7.8). If the first half of the interval (-1/2 to + 1/2) for the latter problem is considered, the boundary conditions are the same for the two problems. The fixed-free case is therefore the same problem as the odd mode with a characteristic length of L/2 instead of L. The parameters in the system which depend on L must therefore be modified accordingly. The active stress number and wave number for instance are divided by sixteen and two respectively.
**Figure 7.15.** Active stress neutral curves for zero flux and free surface at $\gamma = 1/2$

- $Pr = 0.1$
- $Sc = 100.0$
- $Gr_1 = Gr_2 = 0.0$
- $\xi_1 = \xi_2 = 1$
Section 7.1.3. Active stress with buoyancy

Combination of the two systems discussed in Sections 7.1.1 and 7.1.2 yields the problem of active stress with buoyancy effects as well. In this case there are two mechanisms contributing to the instability of the system. A few examples of the combined effects are given in this subsection. Both of the problems dealt with here are for fixed walls and constant equal conditions of temperature and concentration at these walls. The reaction terms used are source terms for both species.

Figure 7.16 illustrates neutral curves for a first order and a zero order reaction for the case of parallel effects of temperature and concentration on density. The buoyancy effects and active stress effects reinforce each other. The neutral curves lie below those for the active stress and buoyancy problems treated separately. The critical wave numbers fall in between those of the buoyancy problem and the active stress problem. The marginal states in this case are stationary.

The next figure in this section (Figure 7.17) shows the results for antiparallel density effects. The marginal states here are also stationary. The possibility of overstability should exist because of the antiparallel density effects. A numerical search of the five parameters (Pr, Sc, R₁, R₂, S) governing this system in order to find oscillatory
Figure 7.16. Active/Grashof Neutral Curves for Constant Equal Wall Conditions

0th Order Reaction

1st Order Reaction

Pr = 0.1
Sc = 100.0
Gr₁ = 10000.0
Gr₂ = 160.0
ξ₁ = ξ₂ = 1

Pr = 0.1
Sc = 100.0
Gr₁ = 5000.0
Gr₂ = 50.0
ξ₁ = ξ₂ = 1
FIGURE 7.17. ACTIVE/GRASHOF NEUTRAL CURVES FOR CONSTANT EQUAL WALL CONDITIONS
states was really out of the question at this point. The next chapter treats the possibility of overstability in a little more detail.

Comparison of Figures 7.16 and 7.17 indicates that the sum of the Rayleigh numbers is still a parameter of interest. This is evidenced by the fact that the systems in Figure 7.16 are less stable than those in Figure 7.17. Looking at the zero order case the sum of the Rayleigh numbers in 7.16 is 17,000 while that in 7.17 is -15,000. Because of the symmetry of the steady state in this case, the sign difference has no effect on the buoyancy problem. The first order reaction situation shows a similar result. The two mechanisms, although reinforcing each other, do not interact in a complex way. This fact could be deduced from inspection of the governing equations. There are no cross terms involving the gravity effects and the active stress effects.

Estimation of the relative importance of the two effects is a difficult task since the active stress number contains the parameter h (active stress coefficient) about which nothing is really known. A continuation of the numerical example given in Section 7.1.1 may help in understanding the problem. The orders of magnitude for the Rayleigh number and active stress number are $10^4$ and $10^0$ respectively. Since the Rayleigh number is of the same order of magnitude
as in the buoyancy problem the following can be written.

\[ k = 10^{-4} \]

\[ S = k^2 L^4 Qh / \rho \nu^2 D_1 D_2 \approx 1.0 \]

\[ \therefore \tilde{h} = h / \rho \approx 10^{-4} \]

The quantity \( \tilde{h} \) which represents the active stress contribution to the stress tensor is in this case quite small. This is the result when the buoyancy and active stress mechanisms contribute nearly equally to the instability.

The value of the active stress coefficient given by this example is strongly dependent on the other parameters of the system. If the rate constant \( k \) is allowed to vary and the parameter \( \tilde{h} \) is held fixed, the following results (all other parameters remain the same). If the value of \( \tilde{h} \) is greater than \( 10^{-4} \), the active stress mechanism will predominate. The reason is that the rate constant \( k \) needed to give instability by active stress is smaller than the value of \( 10^{-4} \) needed to give instability through the effect of buoyancy. Conversely if the value of \( \tilde{h} \) is less than \( 10^{-4} \), the buoyancy mechanism will predominate.

Section 7.2. Non-Linear Results

The methods used to find the numerical results reported in this section have been described earlier. One more
detail of the computation is mentioned here. Since the boundary conditions used in this work are all of a homogeneous nature, there remains one degree of freedom in solving the non-linear system of equations. This can be satisfied by arbitrarily setting the amplitude of the disturbance, which in turn normalizes the eigenfunctions. Another method is to normalize the linear eigenfunction in some way. In this way the non-linear eigenfunctions and eigenvalue are also determined. This latter method was the one used in this work.

For problems whose solution was of an even or odd nature the linear eigenfunction was normalized by setting the value of the stream function or its derivative at the centerline.

\[ \phi^{(1;1)} = 1 \quad \text{at} \quad y = 0 \]

\[ D\phi^{(1;1)} = 1 \quad \text{at} \quad y = 0 \]

For other problems a value at the end of the integration was set such that the stream function at the centerline was of order one. For example, using fixed boundaries the second derivative of the stream function at the upper plate was selected such that this condition was satisfied. It must be remembered in comparing equilibrium amplitudes that they were found using different normalizing conditions. One possible way to make the definitions consistent is to normalize
the maximum value of the stream function in the interval to one. For the even mode this occurs at the centerline. A difficulty here is that for each problem, in general, the maximum may occur at a different point.

In the tables presenting the non-linear results the column labeled $a_{M}^{(2)}$ has as its entries the eigenvalues obtained by normalizing the maximum value to one. The amplitudes reported are those calculated from the original $a^{(2)}$'s. When these amplitudes are used in calculating the stream functions, the effect of the method of normalization is balanced out.

Section 7.2.1. Buoyancy effect

As in the preceding section, the first results discussed here are for the Bénard problem. In this problem it is known that supercritical equilibrium states exist, and cellular convection is the result of the instability. Some results from non-linear theory for this problem are presented in Table 7.1. The theoretical results do predict supercritical equilibrium states. The amplitude $A_e$ grows as the Prandtl number is decreased at constant Rayleigh number. This indicates that the convection is more violent for small Prandtl numbers. In fact for very low Prandtl number ($Pr = 0.025$ for mercury), Turner (95) mentions that steady flows are not seen. The transition is to turbulent flow after the critical point is reached.
Table 7.1. Nonlinear Eigenvalues
Fixed-Fixed Boundaries
Benard Problem

<table>
<thead>
<tr>
<th>Pr</th>
<th>R₁</th>
<th>Wave #</th>
<th>a₀</th>
<th>a(2)</th>
<th>Aₑ</th>
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<table>
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<th>Wave #</th>
<th>a₀</th>
<th>a(2)</th>
<th>Aₑ</th>
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<td>1.3054</td>
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<td>16.6360</td>
<td>-2.28132</td>
<td>2.7004</td>
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Constant equal boundaries for temperature and concentration
Pr = 0.1  Sc = 100.0  l₁ = 1  l₂ = 1

<table>
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<th>Order</th>
<th>Wave #</th>
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<th>R₂</th>
<th>S</th>
<th>a₀</th>
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<td>0.012064</td>
<td>-5739.4</td>
<td>-2768.6</td>
<td>0.00145</td>
</tr>
</tbody>
</table>

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A recent experimental investigation by Farhadieh and Tankin (19) provides some good data for comparison. They reported temperature profiles at several places in a convection cell; upstream, midcell, and downstream. Some streamlines and isotherms for this problem can be found in the book by Turner. Experimental streamlines and isotherms can be seen in the photographs of Farhadieh and Tankin.

Figures 7.18, 7.19, and 7.20 show the temperature profiles, streamlines, and isotherms calculated in this work for the Bénard problem. The results reported here are for a Prandtl number of 2.0 and a Rayleigh number of 6450. Several values of Prandtl number were used (Table 7.1), and the value of 2.0 gave results quite close to those reported by Farhadieh and Tankin. The value of Prandtl number used in their work was 6.8. They compare their results to some theoretical results obtained by Royal (75). These results were for both a different Prandtl number and a different Rayleigh number than those used in the experimental work. It is felt in the present work that varying only the Prandtl number in order to match the experimental results is a very satisfactory outcome.

Figure 7.18 shows the temperature profiles calculated in this work as well as the experimental midcell profile observed by Farhadieh and Tankin. The reversal of the profiles is an interesting feature of the problem which has been observed by the above authors and others. The isotherms in
FIGURE 7.18. TEMPERATURE PROFILES IN BENARD CELL

\[ \kappa = 3.117 \quad R_1 = 6450 \quad Pr = 2.0 \]
Figure 7.19. Streamlines in Benard Cells

\( \kappa = 3.117 \quad R_1 = 6450 \quad Pr = 2.0 \)
FIGURE 7.20. ISOHERMS FOR BENARD CELLS

\( \kappa = 3.117 \quad R_l = 6450 \quad Pr = 2.0 \)
Figure 7.20 show this reversal even more dramatically. The upstream and downstream profiles of Figure 7.18 were chosen to be those at $\theta = 0.4\pi$ and $\theta = -0.4\pi$ respectively. These represent positions near the boundaries of a cell. The agreement between this rather simple theory and experiment is considered quite good.

Figure 7.19 illustrates the streamlines for this particular problem. These are the patterns for two dimensional roll cells which are the initial cells observed experimentally. There is a repeating pattern of two cells, one rotating clockwise and the other counter clockwise. Comparison of these streamlines with the isotherms in Figure 7.20 shows the rising and falling of the hot (H) and cold (C) fluid regions. In the steady state the streamlines are equal to the pathlines and actually represent particle paths in the fluid.

The remainder of Table 7.1 presents a few results for the buoyancy problem with chemical reaction present. The boundary conditions and parameters used are given in the table. It can be seen that supercritical equilibrium states are possible here also. The values of the amplitudes obtained are rather small since the parameters chosen are not far from the neutral values (Figure 7.2). For the problems in the table the imaginary parts of the eigenvalues $c^{(0)}$ and $c^{(2)}$ are zero, so that the supercritical states are stationary in time. Comparison of the first and zero order reaction
cases again reveals very little difference for comparable distances from the neutral curve.

Figures 7.21 and 7.23 show streamlines for the chemically reactive fluid under the influence of gravity. The first figure is for a first order reaction, and the second is for a zero order reaction. Comparison of the two figures shows that there is very little difference between the flow patterns in the two cases. This is not unexpected since the steady states for the two problems are quite similar (Figure 7.4), and the governing equations are therefore similar.

The streamlines in both cases are compressed in the upper half of the region. This is in the direction opposite to the force of gravity. The reason for this behavior is that the least dense spot in the fluid at rest is in the middle of the region. The lower half of the fluid therefore has a stable density gradient. The instabilities arise initially in the upper half of the system. The convection in the upper half is thus stronger than that in the lower half. In fact, the convection in the bottom of the system is caused by its interaction with the top. The result that one of the closed streamlines is contained entirely within the region from \( y = 0 \) to \( y = 1/2 \) is evidence of this behavior. Were the reaction terms sinks, the density gradients would be reversed; and it is anticipated that the effect on the streamlines would also be reversed.
FIGURE 7.21. STREAMLINES FOR 1ST ORDER REACTION BCUOANCY PROBLEM (VALUES X 10^2)

\[ \Theta(x, y) \]

- \( \Theta_1 = 100 \)
- \( \Theta_2 = 180 \)
- \( \Theta_1 = 180 \)
- \( \Theta_2 = 1 \)

- \( Pr = 0.1 \)
- \( Sc = 100 \)
- \( \kappa = 3.5 \)
- \( Gr_1 = 5000 \)
- \( Gr_2 = 1 \)

Y-axis range: 0.5 to -0.5
Figure 7.22. Concentration profiles for the situation in Figure 7.21.
FIGURE 7.23. STREAMLINES FOR 0TH ORDER REACTION BUOYANCY PROBLEM (VALUES x 10^2)

Pr = 0.1  Sc = 100  \kappa = 3.5  Gr_1 = 10000  Gr_2 = 400  \varepsilon_1 = \varepsilon_2 = 1
Figures 7.22 and 7.24 show the upstream and downstream concentration profiles for the buoyancy problem. The profiles are represented as the deviations from the steady state situation. The deviations are quite small since the conditions used are near the neutral curves. The deviations in the temperature profiles are even smaller than the concentration deviations. This is due to the small value of Prandtl number which was used. In the zero order case the temperature profiles calculated were almost identical to the steady state situations. Because of the interaction of temperature and concentration in the first order case, the temperature deviations here were noticeable. They were in the same direction as the concentration effects and were still nearly two orders of magnitude smaller. Because of their similarity to the concentration profiles (and small values) no temperature profiles are presented.

The upstream and downstream profiles represent the regions where the deviations from steady state are the greatest. This is the same situation as was observed in the Bénard problem. Because of the small deviations observed no isotherms or isoconcentration lines are presented. They would be very close to the steady state lines.

Inspection of the profiles in Figures 7.22 and 7.24 helps to reinforce the previous discussion about the flow situation. The deviations from steady state are much greater in the upper half of the system where the convection is more
severe. In the bottom half of the region more dense fluid is actually rising (and less dense falling). This is caused by the fact that convection in this region is due to interaction with the upper region. In these results the density decreases with concentration so that the less dense fluid is the one of higher concentration.

Section 7.2.2. Active stress

The non-linear eigenvalues for the active stress problem are summarized in Tables 7.2 through 7.6. Inspection of these tables reveals that all of the problems checked possess supercritical equilibrium states. In addition, for all of the problems considered the secondary flow is stationary not oscillatory. This results from the fact that both $b^{(0)}$ and $b^{(2)}$ are equal to zero.

Using the antisymmetric model for active stress given in Section 2.1, Lin and McIntire (52) reported oscillatory supercritical states. Qualitatively their results are acceptable, however several minor errors in the article make it impossible to judge the quantitative validity of the results. The equilibrium amplitudes given by their results are quite large. This could be a function of the method chosen for normalization however.

The trend in the results in the tables is that the magnitude of $a^{(2)}$ decreases as the parameters increase above
### Table 7.2. Nonlinear Eigenvalues

**Fixed - Fixed Boundaries**

Constant equal boundaries for temperature and concentration  
Pr = 0.1  Sc = 100.0  \( \varepsilon_1 = 1 \)  \( \varepsilon_2 = 1 \)

<table>
<thead>
<tr>
<th>Order</th>
<th>Wave #</th>
<th>R₁</th>
<th>R₂</th>
<th>S</th>
<th>a(0)</th>
<th>a(2)</th>
<th>a_M(2)</th>
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### Table 7.3. Nonlinear Eigenvalues

**Fixed - Fixed Boundaries**

Constant equal boundaries for temperature and concentration  
Pr = 1.0  Sc = 10.0  \( \varepsilon_1 = 1 \)  \( \varepsilon_2 = 1 \)

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<th>R₂</th>
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<th>a(2)</th>
<th>a_M(2)</th>
<th>A_e</th>
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<tr>
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<td>0.29248</td>
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<td>-51.616</td>
<td>0.0753</td>
</tr>
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</table>
Table 7.4. Nonlinear Eigenvalues  
Fixed - Fixed Boundaries (Odd Mode)  
Constant equal boundaries for temperature and concentration  
Pr = 0.1  Sc = 100.0  \varepsilon_1 = 0  \varepsilon_2 = 1

<table>
<thead>
<tr>
<th>Order</th>
<th>Wave #</th>
<th>R₁</th>
<th>R₂</th>
<th>S</th>
<th>a(0)</th>
<th>a(2)</th>
<th>a_M(2)</th>
<th>A_e</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.0</td>
<td>0.0</td>
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<td></td>
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<td>-3141.7</td>
<td>0.0206</td>
</tr>
<tr>
<td>1</td>
<td>8.0</td>
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<td>0.0</td>
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<td>-137.2</td>
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<td></td>
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<tr>
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</tr>
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</table>

Table 7.5. Nonlinear Eigenvalues  
Fixed - Fixed Boundaries  
Constant equal boundaries for temperature and concentration  
Pr = 0.1  Sc = 100.0  \varepsilon_1 = -1  \varepsilon_2 = -1

<table>
<thead>
<tr>
<th>Order</th>
<th>Wave #</th>
<th>R₁</th>
<th>R₂</th>
<th>S</th>
<th>a(0)</th>
<th>a(2)</th>
<th>a_M(2)</th>
<th>A_e</th>
</tr>
</thead>
<tbody>
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<td>0.0</td>
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<td></td>
<td></td>
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<td>0.0</td>
<td>31.0</td>
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<td></td>
<td></td>
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<tr>
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<td>0.0</td>
<td>0.0</td>
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<td>-5951.5</td>
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<td>-6086.5</td>
<td>-6086.5</td>
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</tbody>
</table>
Table 7.6. Nonlinear Eigenvalues

Fixed - Free Boundaries
Zero flux at the free boundary - constant conditions at the fixed boundary
Pr = 0.1  Sc = 100.0  $\lambda_1 = 1$  $\lambda_2 = 1$

<table>
<thead>
<tr>
<th>Order</th>
<th>Wave #</th>
<th>R₁</th>
<th>R₂</th>
<th>$S$</th>
<th>$a_0$</th>
<th>$a_1$</th>
<th>$a_M(2)$</th>
<th>$A_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
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<td>0.0</td>
<td>0.0</td>
<td>2.0625</td>
<td>-0.013325</td>
<td>-801.7</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>0.0</td>
<td>0.0</td>
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<td>-567.8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
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<td>0.0</td>
<td>0.0</td>
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<td>0.00515</td>
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</tr>
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<td>1.59375</td>
<td>-0.012074</td>
<td>-548.8</td>
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<td></td>
</tr>
<tr>
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<td>0.0</td>
<td>1.59375</td>
<td>-0.012859</td>
<td>-641.6</td>
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<td></td>
</tr>
<tr>
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<td>0.00566</td>
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<tr>
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<td>0.021169</td>
<td>-557.2</td>
<td>-3120.0</td>
<td>0.00616</td>
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</tbody>
</table>
the neutral conditions. This is reasonable behavior. As the system deviates more and more from the neutral situation, the results indicate the establishment of more violent convection. Eventually the amplitude may become large enough such that a two term approximation in the expression for \( \frac{dA}{dt} \) may not be a good one.

Comparison of Tables 7.2 and 7.3 reveals the effect of Prandtl and Schmidt numbers on the non-linear eigenvalue. In the zero order reaction case the parameter \( S(Pr + Sc) \) is the important one in determining instability. The effect on the non-linear eigenvalue of the Prandtl and Schmidt numbers can be judged by holding this quantity nearly constant while varying these physical parameters. This procedure is equivalent to what was done in the Bénard problem (see Table 7.1). The effect of Prandtl and Schmidt numbers in the active stress problem is similar to the effect of Prandtl number in Bénard convection.

Figures 7.25 through 7.38 show some further results of the non-linear stability analysis for the active stress problem. Figures 7.25, 7.27, 7.29, 7.33, 7.35, and 7.36 represent streamlines for several different parameter and boundary conditions. Figure 7.32 shows two isoconcentration lines for two active stress problems. The remaining figures in this section are concentration profiles for the active stress problems. Once again these profiles represent the deviations from the steady state situations.
All of the problems tested resulted in cellular convection qualitatively similar to that in the Bénard problem. The cellular patterns repeat in groups of two cells (four for an odd mode); one rotating clockwise and one counter clockwise. Since the evaluations were done for parameter values near the neutral values, the values of the streamlines are quite small.

Figures 7.25 and 7.27 show the difference between the streamlines for a first order reaction and those for a zero order reaction. These curves are for fixed boundaries with constant equal wall values for temperature and concentration. Looking at the figures almost no difference is discernable. The actual co-ordinates of the streamlines reveal only very minor differences in the positions. The values of the streamlines for the zero order case are larger than those in the first order case. This indicates more violent convection, and is largely due to the difference in equilibrium amplitudes. The lines $\theta = \pi/2$ and $\theta = -\pi/2$ are lines of symmetry for both reaction cases. The cells are not quite symmetric about the centerline $(y = 0)$ because of the effect of the non-linear eigenfunctions which are used in the calculation of the stream function. The linear eigenfunction is symmetric, and the non-linear eigenfunctions cause it to deviate from this symmetric behavior. The reason that the deviation is so small is that the parameter values are near those for the neutral situation.
FIGURE 7.25. STREAMLINES FOR ACTIVE STRESS PROBLEM 1ST ORDER REACTION (VALUES x 10^2)

\[ \kappa = 4.5 \quad Pr = 0.1 \quad Sc = 100 \quad S = 21 \]
FIGURE 7.26. CONCENTRATION PROFILES FOR SITUATION IN FIGURE 7.25
FIGURE 7.27. STREAMLINES FOR ACTIVE STRESS PROBLEM 0TH ORDER REACTION
(VALUES x 10^2)
\( \kappa = 4.5 \)  \( Pr = 0.1 \)  \( Sc = 100 \)
\( S = 27.5 \)
FIGURE 7.28. CONCENTRATION PROFILES FOR SITUATION IN FIGURE 7.27
FIGURE 7.29. STREAMLINES FOR ACTIVE STRESS PROBLEM 1ST ORDER REACTION
VALUES x 10^2
κ = 6.5  Pr = 0.1  Sc = 100  S = 21
Figures 7.26 and 7.28 show the concentration profiles corresponding to the flow patterns given in Figure 7.25 and 7.27. The two situations again are very similar. The profiles shown are for positions upstream and downstream in the cell. The profiles are nearly symmetric about the centerline. One of the reasons for this is the proximity to the neutral conditions which was mentioned earlier. Another reason for this is that the driving forces for the convection in this case are symmetric in the steady state. It makes no difference how the physical system is oriented. This can be compared with the results shown in Figures 7.22 and 7.24 for the buoyancy problem. In this case the profiles in the two regions are widely different.

Figures 7.25 and 7.29 show the effect of the wave number on the cellular patterns. Each streamline is elongated in the y direction as the wave number in the θ direction is increased. These streamlines are for a first order reaction, however the behavior should be independent of the reaction order. The same effect is therefore anticipated for a zero order reaction.

Figure 7.30 illustrates the concentration profiles for the larger wave number. The deviations are larger than those shown in Figure 7.26 (smaller wave number) because of a larger equilibrium amplitude than existed in the prior case. The shapes of the profiles are very similar since near the boundaries of the cell the streamlines do not differ
greatly. As the center of the cell is approached, there should be more difference in shape because the streamlines differ more for the two cases near the middle of the cell.

Figure 7.31 shows the difference in shape for concentration profiles near midcell. These are the profiles at $\theta = 0.1 \pi$ and $\theta = -0.1 \pi$. The shapes are shown by normalizing the profiles so that the maximum deviation in each case is one. It can be seen that the deviation for the larger wave number is greater near the upper and lower surfaces. This is because the streamlines are elongated in the $y$ direction compared with those for the lower wave number.

The next figure (7.32) displays two isoconcentration lines for the problem of fixed boundaries and equal constant wall conditions. One line for both a first order reaction and a zero order reaction is shown. As mentioned previously the deviation from the steady state isoconcentration lines is small. The steady state in each case is a straight line of $y = -0.1$. Because of the small deviation no other lines are presented although they could be found. The profiles present a good picture of what is happening in the system. The deviations in temperature are even smaller than those in concentration. This is the same result as was seen in the reactive buoyancy problem, and the discussion given there carries over to this situation as well. For this reason no isotherms or temperature profiles are drawn for any of these problems.
FIGURE 7.31. NORMALIZED CONCENTRATION PROFILES FOR PROBLEMS IN FIGURES 7.25 AND 7.29
Figure 7.32. Isoconcentration lines for active stress problems in figures 7.25 and 7.27.
One example of the streamlines for an odd mode is shown in Figure 7.33. There are four cells in the repeating pattern in this case. Each cell and its adjacent three cells rotate in opposite directions. The line $y = 0$ is a flat free surface boundary for the linear problem. The addition of non-linear effects causes this boundary to deform.

Figure 7.34 shows the concentration profiles for the odd mode of Figure 7.33. The profiles are considerably different from those for an even mode. The existence of two cells in the region from $y = -1/2$ to $y = 1/2$ causes the shape of the profiles shown. Consider the curve labeled upstream in the figure. In reality this curve is upstream for the lower cell and downstream for the upper cell. In the lower cell less concentrated fluid is rising and in the upper cell it is falling. The curve labeled downstream is therefore downstream for the lower cell and upstream for the upper cell. Here more concentrated fluid is falling in the bottom cell and rising in the top cell.

Figures 7.35 and 7.36 show streamlines for the case of a free boundary at the upper surface with zero flux of temperature and concentration across this surface. The lower surface is still fixed with constant temperature and concentration. As mentioned in the previous section the solutions to these problems can be found from the solutions of the odd mode problems. In practice the shape of the upper boundary could be found, however this was not done here. In these
FIGURE 7.33. STREAMLINES FOR ACTIVE STRESS PROBLEM 1ST ORDER REACTION

ODD MODE (VALUES x 10^2)

κ = 8    Pr = 0.1    Sc = 100    S = 28.5
FIGURE 7.35. STREAMLINES FOR ACTIVE STRESS PROBLEM 0\textsuperscript{TH} ORDER REACTION
ZERO FLUX-FREE SURFACE AT $\gamma = 1/2$ (VALUES $\times 10^2$)

$\kappa = 4$  $Pr = 0.1$  $Sc = 100$  $S = 2.1875$
ZERO FLUX - FREE SURFACE AT \( y = \frac{1}{2} \) (VALUES \( \times 10^2 \))

\[ \kappa = 4, \quad Pr = 0.1, \quad Sc = 100, \quad S = 1.78125 \]

FIGURE 7.36. STREAMLINES FOR ACTIVE STRESS PROBLEM 1ST ORDER REACTION
problems the proximity to the neutral curve should cause the deformation of this boundary to be small. The different boundary conditions at the two surfaces cause the streamlines to deviate drastically from the near symmetric lines in the fixed-fixed case. The center of the middle cell is shifted away from the point \( y = 0 \) and \( \theta = 0 \) in the direction of the upstream flow and toward the fixed boundary. The streamlines are also farther apart in the direction of the free surface. The reason behind these observations is that the driving forces for the convection, that is the derivatives of the steady state temperature and concentration, are larger near the fixed wall than they are near the free surface. Once again the similarity of the zero and first order cases is evident.

The next two figures (7.37 and 7.38) show the concentration profiles for these fixed-free (zero flux) boundary conditions cases. At the line \( y = 1/2 \) there is a deviation from the steady state concentration. As mentioned earlier this deviation is possible because of the specification of zero flux at the free boundary. The upstream and downstream curves show that the more concentrated fluid is falling and the less concentrated is rising.

Section 7.2.3. Active stress with buoyancy

A few results for the combined problem of active stress with buoyancy are presented in Table 7.7. Once again
FIGURE 7.37. CONCENTRATION PROFILES FOR SITUATION IN FIGURE 7.35

FIGURE 7.38. CONCENTRATION PROFILES FOR SITUATION IN FIGURE 7.36
Table 7.7. Nonlinear Eigenvalues
Fixed - Fixed Boundaries
Constant equal boundaries for temperature and concentration
Pr = 0.1   Sc = 100.0   $\lambda_1 = 1$   $\lambda_2 = 1$

<table>
<thead>
<tr>
<th>Order</th>
<th>Wave #</th>
<th>$R_1$</th>
<th>$R_2$</th>
<th>$S$</th>
<th>$a^{(0)}$</th>
<th>$a^{(2)}$</th>
<th>$a_M^{(2)}$</th>
<th>$A_e$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>18000.0</td>
<td>16.0</td>
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<td>-5751.5</td>
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<tr>
<td>0</td>
<td>5.5</td>
<td>1000.0</td>
<td>18000.0</td>
<td>18.0</td>
<td>0.015853</td>
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<td>-4668.4</td>
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<tr>
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<tr>
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<td>5000.0</td>
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<td>0.013934</td>
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<td>0.00161</td>
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</tbody>
</table>

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the combination of parameters used gives supercritical equilibrium situations. These states are of a stationary nature. The density effects of temperature and concentration are in parallel directions for the cases shown in the table.

Figure 7.39 illustrates some streamlines for a first order reaction problem with this combined effect. The lines are very similar to those for the buoyancy problem alone (Figure 7.21). The near symmetry of the streamlines in the active stress problem has been disrupted by the introduction of the gravity effects. Because of the similarity of the streamlines for a zero order reaction to those for a first order reaction in the two problems treated separately, it is expected that the lines for the combined problem for a zero order reaction will be very close to those presented here for a first order reaction.

The concentration profiles for this combined problem are shown in Figure 7.40. Comparison with Figure 7.22 shows the similarity to those for the buoyancy problem.

Section 7.3. Energy Result

The eigenvalue problem presented in Chapter 5 was solved using a one term Galerkin expansion to find the quantity $S_a/2$. This simple expansion gives a rough estimate of the value of this parameter and does yield an interesting result. The problem treated was the active stress problem without buoyancy effects and with a zero order chemical
FIGURE 7.39. STREAMLINES FOR ACTIVE STRESS/GRASHOF PROBLEM 1ST ORDER REACTION
(VALUES x 10^2)
\[ \kappa = 4.5 \quad Pr = 0.1 \quad Sc = 100 \quad Gr_1 = 5000 \quad Gr_2 = 50 \quad S = 13 \]
FIGURE 7.40. CONCENTRATION PROFILES FOR SITUATION IN FIGURE 7.39
reaction. The boundary conditions were zero slip with constant equal values for temperature and concentration on the boundaries.

The one term Galerkin approximation gives the following expression for the eigenvalue \( N = \frac{S_{\lambda}}{2} \).

\[
N^2[((Sc+Pr)(1+a) + b(Sc^2+Pr^2) + 2c] = d
\]

The coefficients \( a, b, c, \) and \( d \) are just constants given by the evaluation of integrals in the Galerkin method. The value of \( d \) is the same for the energy method as for the linear stability method. The linear method for this problem would yield \( a = b = c = 0 \).

Evaluation of the constants \( a, b, \) and \( c \) for the energy method reveals that all three of these coefficients are positive. The energy result will therefore be smaller than the linear result. For a wave number of 5 the above expression is

\[
N^2[2(Sc+Pr) + 0.0164(Sc^2+Pr^2) + 122] = 3646
\]

Substituting into this expression the values of \( Pr = 0.1 \) and \( Sc = 100 \), the resulting value of \( N^2 \) is

\[
N^2 = 7.5.
\]

As mentioned in Chapter 5, this value is equivalent to the active stress number \( S \). The linear neutral number for a wave number of 5 is approximately 26.
The fact that the energy result is less than the linear result indicates the possibility of subcritical instabilities in the system. The results from non-linear theory do not support this possibility. Only supercritical equilibrium states were found.

In deriving the energy equations for the system a linearizing assumption was made. The effect of this assumption on the results is difficult to determine. It is possible that a more complete analysis of the non-linear energy equations may yield a result closer to that given by linear stability theory. The possibility also exists that the energy result is merely a conservative one for the system in question. The result obtained from this method is a sufficient condition for stability with respect to small disturbances. The small disturbances condition must be added because of the linearization which was done in the equations. The linear stability results give sufficient conditions for instability with respect to small disturbances.
CHAPTER 8

OVERSTABILITY

Section 8.1. Introduction

As mentioned in the previous chapter, the active stress problem cannot exhibit overstability for a zeroth order reaction and does not appear to show overstability for a first order reaction. The addition of the effect of gravity on the system could cause it to have overstable behavior. Several authors (64,37,56,1) have found that a system with temperature and concentration gradients can exhibit oscillatory marginal states, if the effects of the changes in temperature and concentration on density are oppositely directed. This is equivalent to setting $s$ in equation 2.2.2 equal to -1 if the gradients are in the same direction. Most work has been done with a fluid heated from below, and the phrase stabilizing solute gradient is used to describe the concentration effect. Problems in this general class are known as thermohaline convection problems.

Nield (56) derived conditions for overstability for a thermohaline convection problem using the mathematically convenient boundary conditions of free surfaces. In fact most work done in this area has dealt with these boundary
conditions. Yih (110) claims to do linear stability analysis for fixed boundaries, but uses expansion functions satisfying the free surface conditions. Shirtcliffe (83) did some experimental work on a thermohaline problem with a salt gradient. He used the form for the conditions for overstability derived by Nield, even though different boundary conditions were used (fixed-free versus free-free). The Soret effect, or thermally driven diffusive flow, was studied by Hurle and Jakeman (37) among others. They treated this problem theoretically with rigid and free boundaries. Platten and Chavepeyer (64) and Caldwell (6) did experimental work on this system.

In this chapter a general form of the conditions for overstability is explored for the thermohaline problem with or without chemical reaction. The numerical values of coefficients in this expression are calculated for the case of fixed walls with constant concentration and temperature at the surfaces. The problem of overstability with active stress and buoyancy is also explored.

The method used in this chapter to find the conditions for overstability is a one term Galerkin expansion in the equations of interest. The Galerkin method in this case is equivalent to the local potential method introduced by Glansdorff and Prigogine (32). The equivalence of these methods is demonstrated by Schecter (79). Admittedly a one term expansion will only give a very approximate result, but
the basic form of the equations is correct. Another method which could be used is outlined by Nield (56). His method is a modified Fourier series expansion which employs the use of the boundary conditions to find the unknown Fourier coefficients.

Section 8.2. Buoyancy Effects

The situation of convective instabilities arising from the effect of gravity is considered here. The general form of these equations is, from linear stability theory:

\[
\begin{bmatrix}
(D^2 - \kappa^2)^2 & -Gr_1 \kappa^2 & -Gr_2 \kappa^2 \\
-\lambda (D^2 - \kappa^2) & -PrD\xi_0 & (D^2 - \kappa^2) - Pr\lambda \\
-ScDc_0 & (D^2 - \kappa^2) & +\iota_2 - Sc\lambda
\end{bmatrix}
\begin{bmatrix}
\phi \\
\varepsilon \\
\Omega
\end{bmatrix} = 0 \quad 8.2.1
\]

\(\xi_0\) and \(c_0\) are the steady state temperature and concentration respectively, and \(\iota_1\) and \(\iota_2\) indicate once again source or sink behavior. In the above equations \(Gr_2\) has incorporated into it the quantity \(s\) in equation 2.2.2.

When the one term Galerkin analysis is done, the solution of the above system becomes equivalent to solving
\[
\begin{vmatrix}
  a_{11} - \lambda b_{11} & -Gr_1 a_{12} & -Gr_2 a_{13} \\
  Pr a_{21} & a_{22} - Pr\lambda b_{22} & a_{23} \\
  Sc a_{31} & 0 & a_{33} - Sc\lambda b_{33}
\end{vmatrix}
= 0. \quad 8.2.2
\]

For the situation where \( \beta \) and \( \Omega \) have the same boundary conditions and the same source or sink behavior, this can be written as

\[
\begin{vmatrix}
  a_{11} - \lambda b_{11} & -Gr_1 a_{12} & -Gr_2 a_{12} \\
  Pr a_{21} & a_{22} - Pr\lambda b_{22} & a_{23} \\
  Sc a_{31} & 0 & a_{33} - Sc\lambda b_{22}
\end{vmatrix}
= 0. \quad 8.2.3
\]

If the opposite source behavior is used \( a_{21} = -a_{31} \), and the only difference in the analysis is this sign change. Equation 8.2.3 when multiplied out gives

\[
-\lambda^3(b_{11}b_{22}^2PrSc) + \lambda^2(PrSc a_{11}b_{22}^2 + Pr b_{11}b_{22}a_{33}
+ Sc a_{22}b_{11}b_{22}) - \lambda(a_{11}a_{22}b_{22}^2Sc + a_{11}a_{33}^2b_{22}Pr
+a_{22}a_{33}b_{11} + ScR_1 a_{12}a_{21}b_{22} + PrR_2 a_{12}a_{21}b_{22}
+ R_1 a_{12}a_{21}a_{33} + R_2 a_{12}a_{21}a_{22} - Gr_1 Sc a_{12}a_{21}a_{23}
+ a_{11} a_{22} a_{33} = 0. \quad 8.2.4
\]
$R_1$ and $R_2$ are the heat and mass Rayleigh numbers respectively. $\lambda$ is in general a complex number.

If $\lambda$ is now written $\lambda = \lambda_r + i\lambda_i$, the neutral condition is $\lambda_r = 0$. The real and imaginary parts of 8.2.4 give for this case:

**Real**

$$\omega^2 (PrSc \ a_{11} b_{22}^2 + Pr \ b_{11} b_{22} a_{33} + Sc \ a_{22} b_{11} b_{22})$$

$$- (R_1 a_{12} a_{21} a_{33} + R_2 a_{12} a_{21} a_{22} - Gr_1 Sc \ a_{12} a_{21} a_{23})$$

$$+ a_{11} a_{22} a_{33} = 0 \quad 8.2.5$$

**Imag.**

$$\omega [\omega^2 b_{11} b_{22} PrSc - (a_{11} a_{22} b_{22} Sc + a_{11} a_{33} b_{22} Pr)$$

$$+ a_{22} a_{33} b_{11} + ScR_1 a_{12} a_{21} b_{22}$$

$$+ PrR_2 a_{12} a_{21} b_{22})] = 0 \quad 8.2.6$$

For steady convection $\omega_i = 0$, and the real equation yields the following

$$(R_1 + \frac{a_{22}}{a_{33}} R_2) - Gr_1 Sc \ \frac{a_{23}}{a_{33}} = - \frac{a_{11} a_{22}}{a_{12} a_{21}} \quad 8.2.7$$

The system is unstable if the above equality becomes the inequality
\[(R_1 + \frac{a_{22}}{a_{33}} R_2) - Gr_1 Sc \frac{a_{23}}{a_{33}} > - \frac{a_{11} a_{22}}{a_{12} a_{21}}\]

For unsteady convection $\omega_1 \neq 0$, and the solution to equations 8.2.5 and 8.2.6 is

\[
\frac{Sc^2 R_1}{(Sc + \frac{1}{c_2})(Pr + \frac{a_{22}}{a_{33}} Sc)} + \frac{Pr^2 R_2}{(Pr + \frac{a_{22}}{c_2 a_{33}})(Pr + \frac{a_{22}}{a_{33}} Sc)}
\]

\[
+ \frac{b_{11} a_{23}}{a_{11} b_{22} (Pr + \frac{a_{22}}{c_2 a_{33}})(Sc + \frac{1}{c_2})(Pr + \frac{a_{22}}{a_{33}} Sc)}
\]

\[
= -\frac{a_{11} a_{33}}{a_{12} a_{21}}
\]

\[c_2 = \frac{a_{11} b_{22}}{b_{11} a_{33}}\]

The conditions for overstability or oscillatory neutral states are now that inequality 8.2.8 is not satisfied and that the following inequality is satisfied:

LHS of Equation 8.2.9 > RHS of Equation 8.2.9.

Consider now either a zeroth order reaction or no reaction. Then equations 8.2.8 and 8.2.10 become (in this case $a_{23} = 0$ and $a_{22} = a_{33}$),

\[(R_1 + R_2) > -\frac{a_{11} a_{22}}{a_{12} a_{21}}\]
or

\[
\frac{\text{Sc}^2 R_1}{(\text{Sc}+1/c_2)(\text{Pr}+\text{Sc})} + \frac{\text{Pr}^2 R_2}{(\text{Pr}+1/c_2)(\text{Pr}+\text{Sc})} > \frac{-a_{11}a_{22}}{a_{12}a_{21}}. \tag{8.2.13}
\]

These equations compare with Nield's for free boundaries and constant temperature and concentration on the surfaces. In his analysis \(c_2 = 1\) and the right hand sides of equations 8.2.12 and 8.2.13 are both equal to \((27/4)\pi^4\).

For the case of no reaction with fixed boundaries and constant concentration and temperature, the critical Rayleigh number is 1707.762 at a wave number of 3.117. This critical Rayleigh number corresponds to the right hand sides of the inequalities. In this case the least stable mode is one in which \(\phi\), \(\beta\) and \(\Omega\) are all even. A one term Galerkin expansion gives the following results for equations 8.2.12 and 8.2.13 evaluated at the above critical wave number.

\[
(R_1 + R_2) > 1750 \quad \text{Stationary} \tag{8.2.14}
\]

and

\[
\frac{\text{Sc}^2 R_1}{(\text{Sc}+1/1.94)(\text{Pr}+\text{Sc})} + \frac{\text{Pr}^2 R_2}{(\text{Pr}+1/1.94)(\text{Pr}+\text{Sc})} > 1750 \quad \text{Oscillatory} \tag{8.2.15}
\]

Using this expression the area in which overstability is expected can be determined. By examining equations 8.2.14 and
8.2.15 it can be seen that the two Rayleigh numbers must have opposite signs in order to have an instability which is oscillatory. If a positive Rayleigh number is defined as one which has a destabilizing effect, the antiparallel effect which is required can be accomplished in two ways.

(1) The density changes due to concentration and temperature are in the same direction and the gradients are antiparallel.

(2) The density changes are opposite and the gradients are parallel.

Some results for Case (2) are given in Table 8.1. In this case equations 8.2.14 and 8.2.15 provide a good estimation of the actual situation. For this problem overstability can exist, and the conditions which give it can be found quite well using equations 8.2.14 and 8.2.15.

The zeroth order reaction case for fixed boundaries and constant concentration and temperature at the surfaces is similar to the no reaction result. The numerical values are different since in this case the steady state is parabolic and the quantities \( \phi \), \( \beta \) and \( \Omega \) are neither even nor odd functions. Using the one term Galerkin technique, equations 8.2.14 and 8.2.15 are for this case (for a wave number of 4)

\[
(R_1 + R_2) > 40526 \quad \text{Stationary} \quad 8.2.16
\]

\[
\frac{Sc^2 R_1}{(Sc+1/1.6)(Pr+Sc)} + \frac{Pr^2 R_2}{(Pr+1/1.6)(Pr+Sc)} > 40526 \quad \text{Oscillatory} \quad 8.2.17
\]
In this situation also, the Rayleigh numbers must have opposite effects. For the reaction case the situations corresponding to cases (1) and (2) above are:

(1) Density changes are in the same direction and antiparallel source terms exist.

(2) The density changes are in opposite directions and parallel source terms are present.

Equations 8.2.16 and 8.2.17 provide a fairly good approximation in this case as well. Some results confirming the existence of overstability for this particular situation are given in Table 8.2. For both the no reaction case and the zeroth order case the critical parameter for stationary instability is the sum of the Rayleigh numbers $R_1 + R_2$.

The entire expansions 8.27 and 8.29 must be used for a first order reaction. These expressions are more complex, however the results should be similar to those for the zeroth order case. Equations 8.2.8 and 8.2.10 given by the usual one term Galerkin expansion are for this case (wave number of 4)

$$ (R_1 + 1.045 R_2) + 0.045 \frac{Gr_1}{Sc} > 33931.0 \quad 8.2.18 $$

$$ \frac{Sc^2 R_1}{(Sc+1/1.87)(.96 Pr+Sc)} + \frac{Pr^2 R_2}{(1.045)(.96Pr+1/1.87)(.96Pr+Sc)} $$

$$ - .0235 \frac{ScPrGr_1}{(.96 Pr+1/1.87)(Sc+1/1.87)(.96 Pr+Sc)} > 33931.0 \quad 8.2.19 $$
TABLE 8.1. OVERSTABILITY (MARGINAL OSCILLATORY STATES)**

\[ \text{Pr} = 1.0 \quad \text{Sc} = 100.0 \quad R_2 = -400.0 \]

NO CHEMICAL REACTION \hspace{1cm} \text{Wave #} = 3.117

<table>
<thead>
<tr>
<th>( R_1 )</th>
<th>( a(0) )</th>
<th>( b(0) )</th>
<th>\text{PNP}^1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1736.0</td>
<td>-0.75912x10^{-2}</td>
<td>0.74637</td>
<td></td>
</tr>
<tr>
<td>1737.0</td>
<td>-0.37756x10^{-2}</td>
<td>0.74550</td>
<td></td>
</tr>
<tr>
<td>1738.0*</td>
<td>-0.7630x10^{-5}</td>
<td>0.74420</td>
<td>1779.3</td>
</tr>
<tr>
<td>1739.0</td>
<td>0.38004x10^{-2}</td>
<td>0.74318</td>
<td></td>
</tr>
</tbody>
</table>

*Critical point

\(^1\)Value predicted from equation 8.2.15

TABLE 8.2. OVERSTABILITY (MARGINAL OSCILLATORY STATES)**

\[ \text{Pr} = 10.0 \quad \text{Sc} = 100.0 \quad R_2 = -10^4 \]

ZERO ORDER REACTION \hspace{1cm} \text{Wave #} = 4.0

<table>
<thead>
<tr>
<th>( R_1 )</th>
<th>( a(0) )</th>
<th>( b(0) )</th>
<th>\text{PNP}^1</th>
</tr>
</thead>
<tbody>
<tr>
<td>41000.0</td>
<td>-0.93170x10^{-1}</td>
<td>0.44574</td>
<td></td>
</tr>
<tr>
<td>42000.0</td>
<td>-0.45634x10^{-1}</td>
<td>0.41176</td>
<td></td>
</tr>
<tr>
<td>42959.0*</td>
<td>0.0</td>
<td>-0.57202</td>
<td>45827.0</td>
</tr>
<tr>
<td>43000.0</td>
<td>0.19356x10^{-2}</td>
<td>0.37033</td>
<td></td>
</tr>
<tr>
<td>44000.0</td>
<td>0.49444x10^{-1}</td>
<td>0.31861</td>
<td></td>
</tr>
</tbody>
</table>

*Neutral point

\(^1\)Value predicted from equation 8.2.17

** These results were obtained using a three term Galerkin expansion. This expansion gives a good approximation for the Bénard problem.

***These results were found using a five term Galerkin approximation.
Due to the added complexity of these equations the bounds given are not as good as those for no reaction or a zeroth order reaction. The basic similarity to the zeroth order situation, however, would indicate overstability is possible. No test results were obtained here.

Section 8.3. Active Stress - No Buoyancy

For the active stress problem the linear system is given by equation 4.2.20. The Galerkin expression equivalent to equation 8.2.3 can be written down immediately as

\[
\begin{vmatrix}
 a_{11} - \lambda b_{11} & -S_c b_{12} & -S_c b_{12} \\
 Pr a_{21} & a_{22} - Pr \lambda b_{22} & a_{23} \\
 Sc a_{21} & 0 & a_{33} - Sc \lambda b_{22}
\end{vmatrix} = 0
\quad 8.3.1
\]

This system is once again for the problem of the same boundary conditions on concentration and temperature and parallel sources. The least stable situation is when \( \phi \) is even and \( \beta \) and \( \Omega \) are odd.

For a zeroth order reaction the conditions for over-stability can be written as

\[
S(Pr + Sc) < -a_{11} a_{22} / c_{12} a_{21}
\quad 8.3.2
\]

and
$$S\left( \frac{\text{PrSc}^2}{(\text{Sc}+1/c_2)(\text{Pr}+\text{Sc})} + \frac{\text{Pr}^2\text{Sc}}{(\text{Pr}+1/c_2)(\text{Pr}+\text{Sc})} \right)$$

$$> - \frac{a_{11}a_{22}}{c_{12}a_{21}}.$$  

8.3.3

The quantity $c_2$ is numerically positive as it was in the previous section. Using this fact equation 8.3.3 can be rewritten

$$S(a \text{ Pr}+b \text{ Sc}) > -\frac{a_{11}a_{22}}{c_{12}a_{21}} \quad 0 < a,b < 1.$$  

8.3.4

Comparison of equations 8.3.2 and 8.3.4 yields obviously and immediately the conclusion that overstability is impossible for this case (the case of parallel sources). The critical parameter for instability is thus $S(\text{Pr} + \text{Sc})$.

For the case of antiparallel sources the possibility of overstability must be explored. If the same signs as above for $c_{12}$ and $a_{21}$ are retained, the two possibilities for this case are

$$\det \begin{bmatrix}
  a_{11} - \lambda b_{11} & -\text{Sc}_{12} & \text{Sc}_{12} \\
  -\text{Pr} a_{21} & a_{22} - \text{Pr}\lambda b_{22} & 0 \\
  \text{Sc} a_{21} & 0 & a_{22} - \text{Sc}\lambda b_{22}
\end{bmatrix} = 0,$$
\[
\begin{vmatrix}
  a_{11} - \lambda b_{11} & Sc_{12} & -Sc_{12} \\
  Pr a_{21} & a_{22} - Pr\lambda b_{22} & 0 \\
  -Sc a_{21} & 0 & a_{22} - Sc\lambda b_{22}
\end{vmatrix}
= 0.
\]

The solutions of these two possibilities are identical. The condition for stationary marginal states is

\[-S(Pr + Sc) > -a_{11} a_{22}/c_{12} a_{21}\]

Since the same sign behavior as before is retained, the right hand side of this inequality is positive while the left hand side is negative. Therefore, no stationary marginal states can exist for this situation. This equation can never be satisfied for positive active stress number. The solution for overstability for this case is

\[-S\left(\frac{PrSc^2}{(Sc+1/c_2)(Pr+Sc)} + \frac{Pr^2Sc}{(Pr+1/c_2)(Pr+Sc)}\right)\]

\[> -a_{11} a_{22}/c_{12} a_{21}\]

Once again the right hand side is positive and the left negative. This means that the system with antiparallel sources and the same boundary conditions for temperature and concentration is always stable in a linear analysis. These two conditions on the stability of the system with active stress and...
a zero order reaction are proved in Appendix B by more conventional techniques.

For a first order reaction with parallel sources the conditions for overstability are

\[ S(Pr + \frac{a_{22}}{a_{33}} Sc) - SSc \frac{a_{23}}{a_{33}} < -a_{11}a_{22}/c_{12}a_{21} \quad \text{8.3.7} \]

and

\[ S[ \frac{PrSc^2}{(Sc+1/c_2)(\frac{a_{33}}{a_{22}} Pr+Sc)} + \frac{Pr^2Sc}{\frac{a_{33}}{a_{22}} Pr+1/c_2)(\frac{a_{33}}{a_{22}} Pr+Sc)} \right] > -a_{11}a_{22}/c_{12}a_{21} \cdot \quad \text{8.3.8} \]

These equations can be rewritten as

\[ S(Pr + \frac{a_{22}}{a_{33}} Sc) - D < F \quad \text{8.3.9} \]

and

\[ S(a \cdot Pr + b \frac{a_{22}}{a_{33}} Sc) + E > F \quad 0 < a, b < 1 \quad \text{8.3.10} \]
Close inspection of the term \( E \) in the second inequality reveals an interesting fact. The denominator is lower bounded by the expression \( \Pr \text{Sc} \left( \frac{a_{33}}{a_{22}} \Pr + \text{Sc} \right) \). Substituting this expression into the term, an upper bound is obtained of the form

\[
\frac{b_{11}a_{23}a_{33}}{a_{11}b_{22}a_{22}} \frac{S}{(\frac{a_{33}}{a_{22}} \Pr + \text{Sc})} = G \frac{S}{(\frac{a_{33}}{a_{22}} \Pr + \text{Sc})}
\]

Numerically the coefficient \( G \) turns out to be quite small (its magnitude is \( O(10^{-2}) \)). The second inequality is now written as

\[
S\left(a \Pr + b \frac{a_{22}}{a_{33}} \text{Sc}\right) + G \frac{S}{(\frac{a_{33}}{a_{22}} \Pr + \text{Sc})} > F
\]

\[
0 < a, b < 1 \text{ and } G \ll 1 \quad 8.3.11
\]

The second term on the left hand side is thus very small compared with the first term on the left hand side for most reasonable values of \( \Pr \) and \( \text{Sc} \). If both of these quantities are very small this term could become important.

The first inequality can now be written as

\[
S\left(\Pr + \frac{a_{22} - a_{23}}{a_{33}} \text{Sc}\right) < F. \quad 8.3.12
\]

Again numerical inspection reveals that the term \( \frac{a_{22} - a_{23}}{a_{33}} \) is
quite close to one. A good approximation to the first inequality is thus

$$S(Pr + Sc) < F$$  \hspace{1cm} 8.3.13

This is of the same form as the zeroth order result. The second inequality is nearly in the form of the zeroth order result also. As previously mentioned the deviating term will normally be very small. The zeroth order behavior thus provides a good approximation for this system. It is therefore unlikely that overstability will exist for the first order case. In addition, the antiparallel source case should be very nearly unconditionally stable in a linear sense. Because of the similarity between this situation and the zeroth order reaction, a curve for the collapsed neutral number $S(Pr + Sc)$ could be written for the first order as well. The curve for this case would technically be an approximate one however. Figure 7.7 for the zero order reaction is an exact relation.

Section 8.4. Active Stress with Buoyancy

In this section the problem of a system undergoing a zero order chemical reaction with both active stress and gravity will be considered. The results from Sections 8.2 and 8.3 can be combined to yield the conditions on overstability. It should be remarked that the forms of the equations can be
combined, however in this case the functions are neither even nor odd. This fact must be used in evaluating the coefficients in the inequalities. The inequalities for overstability are

\[(R_1 + R_2) + \frac{c_{12}}{a_{12}} S(Pr-Sc) < -\frac{a_{11} a_{22}}{a_{21} a_{12}}\]  \hspace{1cm} (8.4.1)

and

\[\frac{Sc^2 R_1}{(Sc+1/c_2)(Pr+Sc)} + \frac{Pr^2 R_2}{(Pr+1/c_2)(Pr+Sc)} + \frac{c_{12}}{a_{12}} S \]

\[\left( \frac{Pr^2 Sc}{(Pr+1/c_2)(Pr+Sc)} + \frac{Sc^2 Pr}{(Sc+1/c_2)(Pr+Sc)} \right)\]

\[> -\frac{a_{11} a_{22}}{a_{21} a_{12}}\]  \hspace{1cm} (8.4.2)

Because of the introduction of the gravity effects, overstability may be possible.

The above system of inequalities can be written as

\[(R_1 + R_2) + \frac{c_{12}}{a_{12}} S(Pr+Sc) < -\frac{a_{11} a_{22}}{a_{21} a_{12}}\]  \hspace{1cm} (8.4.3)

and

\[(aR_1 + bR_2) + \frac{c_{12}}{a_{12}} S(aPr + bSc) > -\frac{a_{11} a_{22}}{a_{21} a_{12}}\]  \hspace{1cm} (8.4.4)

One way to obtain overstability would be to use antiparallel
density effects. Some preliminary numerical work was attempted here. Unfortunately the values given by a one term Galerkin expansion are not accurate enough to yield an easily identifiable set of parameters which will give overstability. A few sets of parameters were tried but to no avail. The eigenvalues which showed non-zero imaginary parts when the real parts were negative had zero imaginary parts as the real part when through zero. A more complete search should yield conditions which give overstability.
CHAPTER 9

CONCLUDING REMARKS

It has been shown that the deviatoric active stress mechanism proposed by Finlayson and Scriven can lead to convective instabilities in parallel plate geometry. The system is unstable with either zero or first order reactions occurring in the fluid. The results for source terms for the two reacting species show the first order case to be less stable than the zero order case. The situation is reversed for sink terms for the reacting species.

Various boundary conditions were tried for the active stress problem. The situation where the two boundaries are at different constant values of temperature and concentration is less stable than when they are held at equal values. The results here were for fixed walls at both surfaces. The case of fixed walls with zero fluxes of temperature and concentration at one wall is less stable than the case of constant wall conditions. If the zero flux surface is a free surface the stability is lessened again. The fluxes of temperature, concentration, and momentum thus represent stabilizing influences on the system.

The marginal states for the active stress problem are
stationary for all of the problems tested. This was observed in the numerical results for the system. It was also proved by a combination of a theoretical and a numerical approach for a few of the problems tested.

The parameter governing the linear stability of the zero order reaction active stress problem is $S(\text{Pr} + \text{Sc})$ (where $S$ is the active stress number) if the boundary conditions for temperature and concentration are equivalent. This parameter is only an approximate governing parameter for a first order reaction system. The cause of this is the coupling of the reacting species in the transport equations. The interaction of the species adds another dimension to the problem.

Inspection of the non-linear stability results shows that secondary steady states (supercritical equilibrium) exist for all of the active stress problems which were studied. In this analysis this state is characterized by roll cell convection in the transformed $(\theta, y)$ co-ordinate system ($\theta$ is a combination of the $x$ and $z$ directions and possibly containing a time term). In the problems analyzed here the secondary steady states are all stationary. This means that the time term in $\theta$ is zero.

The streamlines for the case of fixed walls with constant equal values of temperature and concentration are nearly symmetric about $y = 0$ in the active stress problem (for the less stable even mode). The problems analyzed were near
the neutral curves so that the non-linear effects on the streamlines were small. These are the effects which would cause the deviation from symmetry since the linear eigenfunction for the streamfunction in this case is symmetric about \( y = 0 \).

The concentration profiles for this problem show that for the portion of a cell below \( y = 0 \) the less concentrated fluid is rising on one side and the more concentrated is falling on the other side. Above \( y = 0 \) the opposite occurs. This is a result of the symmetric steady states in this problem.

The more stable odd mode for these boundary conditions does not show this near symmetric nature. In this case the linear eigenfunction for the streamfunction is antisymmetric about \( y = 0 \). The results for this case can be immediately extended to the problem of a zero flux, free surface boundary at the upper plate. The streamlines in this case are compressed in the direction of the fixed boundary (lower plate). This is a result of the higher driving forces at this boundary (steeper gradients in temperature and concentration).

The effect of buoyancy on a chemically reactive system was also analyzed. The first problem tested was the Bénard problem of no chemical reaction. The results obtained from the non-linear stability analysis agree quite well with observed experimental results. Both isotherms and temperature profiles agree very well. The problem of no reaction with
antiparallel effects of temperature and concentration on density shows the possibility of oscillatory marginal states.

The problems with chemical reaction show some interesting behavior. Once again the possibility of oscillatory marginal states exists if the density gradients due to temperature and concentration are oppositely directed. If these gradients are in the same direction, the marginal states are stationary, and the boundary conditions for temperature and concentration are the same; the parameter governing linear stability for a zero order reaction is the sum of the Rayleigh numbers \(R_1 + R_2\). This sum is only an approximate parameter in a first order reaction because of the interaction of temperature and concentration. The effect of a non-linear gradient arising from a chemical reaction is very similar to that of the linear gradient due to diffusion.

The streamlines for the case where the reaction terms are sources (with parallel density effects) show that the convection begins in the upper half of the region. This is because the density gradient in the lower half is stable, while that in the upper half is unstable. The convection is therefore more vigorous in the upper portion. This can be seen by the fact that the concentration profiles here differ more from steady state than those in the lower half of the region. An interesting result of this effect is that in the portion below \(y = 0\) more dense fluid is rising and less dense fluid is falling. The interaction with the area above the centerline
causes this phenomenon.

The combined effects of gravity and active stress reinforce each other in their contributions to instability. They interact in a simple way so that no cross terms are involved in the parameters governing linear stability. For a given set of physical parameters either mechanism may predominate depending on the value of the undetermined active stress coefficient. When the two effects have nearly equal contribution to the linear stability result, the convection cells resemble those for the buoyancy problem. The addition of a gravity field may lead to the possibility of oscillatory marginal states.

The energy method which was used for one problem in the active stress system gives a result which appears to be very conservative. A linearization made in the procedure causes this result to be the energy result for small disturbances. This linearization may contribute to the solution being conservative.

Suggestions for Future Work

The deviatoric active stress mechanism is capable of yielding stationary secondary flow patterns for the boundary conditions used. This steady flow is one form of streaming which has been observed in living cells.

There are some additional problems which may be of interest for future research. Some of them may give the
possibility of oscillatory flows with the deviatoric active stress tensor. The consideration of a heterogeneous chemical reaction at one or both surfaces may be of importance in biological systems. Also the possibility of surface effects could be of interest. Two of these would be the contributions from surface tension and surface elasticity. The role of surface effects in biological cells is an interesting and challenging area. Some work by Kamiya and Kuroda (43) and Donaldson (16) indicates that the motive force for the onset of the streaming in cells may have its origins near the surface. The nature of this motive force is really unknown.

In the constitutive relation for the active stress tensor for this problem the consideration of a non-Newtonian kinematic base may be an important problem. Some experimental evidence (Donaldson (16) and Kamiya and Kuroda (43)) indicates that a relatively simple power law model may give a good approximation to the behavior of the protoplasm. They also indicate that the possibility of a yield stress (such as in a Bingham plastic) may be important.
BIBLIOGRAPHY


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APPENDIX A

NUMERICAL INTEGRATION

In this appendix the forms of the integration methods used in the numerical section of this work are presented. The expansion functions used in the Galerkin method are also presented.

Runge-Kutta Integration Formulae

Gill's Form (Fourth Order)

\[ y_{n+1} = y_n + \frac{1}{6}(k_1 + (2-\sqrt{2})k_2 + (2+\sqrt{2})k_3 + k_4) \]

\[ k_1 = hf(x_n, y_n) \]

\[ k_2 = hf(x_n + \frac{1}{2} h, y_n + \frac{1}{2} k_1) \]

\[ k_3 = hf(x_n + \frac{1}{2} h, y_n + (\sqrt{2}-1)/2 k_1 + (2-\sqrt{2})/2 k_2) \]

\[ k_4 = hf(x_n + h, y_n - \frac{\sqrt{2}}{2} k_2 + (1 + \frac{\sqrt{2}}{2} ) k_3) \]

This form of the Runge-Kutta integration method has the advantage of minimizing round-off error.
Eighth Order Form

\[ y_{n+1} = y_n + \frac{1}{840} \left( 41k_1 + 27k_4 + 272k_5 + 27k_6 + 216k_7 + 216k_9 + 41k_{10} \right) \]

\[ k_1 = hf(x_n, y_n) \]

\[ k_2 = hf(x_n + \frac{4}{27} h, y_n + \frac{4}{27} k_1) \]

\[ k_3 = hf(x_n + \frac{2}{9} h, y_n + \frac{1}{18} (k_1 + 3k_2)) \]

\[ k_4 = hf(x_n + \frac{1}{3} h, y_n + \frac{1}{12} (k_1 + 3k_3)) \]

\[ k_5 = hf(x_n + \frac{1}{2} h, y_n + \frac{1}{8} (k_1 + 3k_4)) \]

\[ k_6 = hf(x_n + \frac{2}{3} h, y_n + \frac{1}{54} (13k_1 - 27k_3 + 42k_4 + 8k_5)) \]

\[ k_7 = hf(x_n + \frac{1}{6} h, y_n + \frac{1}{4320} (389k_1 - 54k_3 + 966k_4 - 824k_5 + 243k_6)) \]

\[ k_8 = hf(x_n + h, y_n + \frac{1}{20} (-231k_1 + 81k_3 - 1164k_4 + 656k_5 - 122k_6 + 800k_7)) \]
\[ k_9 = hf(x_n + \frac{5}{6} h, y_n + \frac{1}{288} (-127k_1 + 18k_3 - 678k_4 + 456k_5 - 9k_6 + 576k_7 + 4k_8)) \]

\[ k_{10} = hf(x_n + h, y_n + \frac{1}{820} (1481k_1 - 81k_3 + 7104k_4 - 3376k_5 + 72k_6 - 5040k_7 - 60k_8 + 720k_9)) \]

**Predictor corrector formulae**

**Fifth order predictor**

\[ y_{n+1} = y_n + \frac{h}{24} (55y'_n - 59y'_{n-1} + 37y'_{n-2} - 9y'_{n-3}) \]

**Eighth order predictor**

\[ y_{n+1} = y_n + \frac{h}{60,480} (198,721y'_n - 447,288y'_{n-1} + 705,549y'_{n-2} - 688,256y'_{n-3} + 407,139y'_{n-4} - 134,472y'_{n-5} + 19,087y'_{n-6}) \]

**Fifth order corrector**

\[ y_{n+1} = y_n + \frac{h}{24} (9y'_{n+1} + 19y'_n - 5y'_{n-1} + y'_{n-2}) \]
Eighth order corrector

\[ y_{n+1} = y_n + \frac{h}{60,480} \left( 19,087y'_{n+1} + 65,112y'_n \right. \]
\[ - 46,461y'_{n-1} + 37,504y'_{n-2} - 20,21 y'_{n-3} \]
\[ + 6312y'_{n-4} - 863y'_{n-5} \) \]

Expansion functions used in the Galerkin method

**Fixed Boundaries Stream Function**

**Even** \[ \phi = \left( \frac{1}{4} - y^2 \right)^2 y^{2n-2} \]

**Odd** \[ \phi = \left( \frac{1}{4} - y^2 \right)^2 y^{2n-1} \]

**Either** \[ \phi = \left( \frac{1}{4} - y^2 \right)^2 y^{n-1} \]

**Constant conditions for heat and mass**

**Either heat or mass since they are the same functions**

**Odd** \[ \beta = \left( \frac{1}{4} - y^2 \right) y^{2n-1} \]

**Even** \[ \beta = \left( \frac{1}{4} - y^2 \right) y^{2n-2} \]

**Either** \[ \beta = \left( \frac{1}{4} - y^2 \right) y^{n-1} \]

*Zero flux for heat or mass at the y = 1/2 boundary*
Either heat or mass

\[ \beta = (1 - (x - 0.5)^2)(x - 0.5)^{2n-2}. \]
APPENDIX B

EXCHANGE OF STABILITIES

In this appendix the exchange of stabilities will be proved for the problem of active stress and a zero order reaction. The boundary conditions used are $\phi = D\phi = 0$ at $y = \pm 1/2$, and $\beta = \Omega = 0$ at $y = \pm 1/2$. The method used here is a fairly classical approach compared to the approach which was used in Chapter 8. The equations governing the linear stability system are ($\phi = \phi^{(1;1)}$, $\beta = \beta^{(1;1)}$, $\Omega = \Omega^{(1;1)}$).

\begin{align}
(1) & \quad \frac{c^{(0)}(D^2 - \kappa^2)\phi}{S\kappa^2} - \frac{(D^2 - \kappa^2)^2\phi}{S\kappa^2} - i\kappa_2 y (D^2 - \kappa^2)\beta \\
& \quad - i\kappa_1 y (D^2 - \kappa^2)\Omega = 0
\end{align}

\begin{align}
(2) & \quad i\kappa_1 \phi + c^{(0)}\beta - \frac{(D^2 - \kappa^2)\beta}{Pr} = 0
\end{align}

\begin{align}
(3) & \quad i\kappa_2 \phi + c^{(0)}\Omega - \frac{(D^2 - \kappa^2)\Omega}{Sc} = 0
\end{align}

Multiply (1) by $\phi^*$ which is the complex conjugate of $\phi$ and integrate over the region $y = -1/2$ to $y = 1/2$. 

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\[ \int_{-1/2}^{1/2} \left[ \frac{c^{(o)}}{S \kappa^2} \phi^*(D^2 - \kappa^2)\phi - \frac{1}{S \kappa^2} \phi^*(D^2 - \kappa^2)^2 \phi \right. \\
\left. - i \varepsilon_2 \gamma_y \phi^*(D^2 - \kappa^2) - i \varepsilon_1 \gamma_y \phi^*(D^2 - \kappa^2) \Omega \right] dy = 0 \]

\[ \int_{-1/2}^{1/2} |\tilde{D}\phi|^2 dy - \frac{1}{S \kappa^2} \int_{-1/2}^{1/2} |\tilde{D}^2 \phi|^2 dy \\
- i \varepsilon_2 \int_{-1/2}^{1/2} \gamma_\beta \tilde{D}^2 \phi^* dy - 2i \varepsilon_2 \int_{-1/2}^{1/2} \beta D\phi^* dy \\
- i \varepsilon_1 \int_{-1/2}^{1/2} \gamma_\Omega \tilde{D}^2 \phi^* dy - 2i \varepsilon_1 \int_{-1/2}^{1/2} \Omega D\phi^* dy = 0 \]

\( \tilde{D} \) is defined by the expression \( \tilde{D}^2 = (D^2 - \kappa^2) \) and \( |a|^2 = aa^* \).

Define \( (a, b) = \int_{-1/2}^{1/2} abdy \) and \((4)'\) can be written as

\[ \int_{-1/2}^{1/2} (\tilde{D} \phi, \tilde{D} \phi^*) - \frac{1}{S \kappa^2} (\tilde{D}^2 \phi, \tilde{D}^2 \phi^*) - i \varepsilon_2 (\gamma_\beta, \tilde{D}^2 \phi^*) \\
- 2i \varepsilon_2 (\beta, D\phi^*) - i \varepsilon_1 (\gamma_\Omega, \tilde{D}^2 \phi^*) - 2i \varepsilon_1 (\Omega, D\phi^*) = 0 \]

Multiply \((2)\) by \((D^2 - \kappa^2)\beta^* \) and \((3)\) by \((D^2 - \kappa^2)\Omega^* \) and integrate these equations over the region. The resulting equations are

\[ i \varepsilon_1 (\gamma_\beta^*, \tilde{D}^2 \phi) + 2i \varepsilon_1 (\beta^*, D\phi) - c^{(o)} (\tilde{D}_\beta, \tilde{D}_\beta^*) \\
- \frac{1}{P_T} (\tilde{D}^2 \beta, \tilde{D}^2 \beta^*) = 0 \]
and

\[ (7) \quad i\lambda_2(y\Omega^*,\tilde{D}^2\phi) + 2i\lambda_2(\Omega^*,D\phi) - c^{(o)}(\tilde{D}\Omega,\tilde{D}\Omega^*) \]

\[ - \frac{1}{S\varepsilon} (\tilde{D}^2\Omega,\tilde{D}^2\Omega^*) = 0 \]

Add (5), (6), and (7) together to yield the equation

\[ (8) \quad -c^{(o)} \left[ \frac{1}{S\kappa} (\tilde{D}\phi,\tilde{D}\phi^*) + (\tilde{D}\beta,\tilde{D}\beta^*) + (\tilde{D}\Omega,\tilde{D}\Omega^*) \right] \]

\[ - \frac{1}{S\kappa} (\tilde{D}^2\phi,\tilde{D}^2\phi^*) - \frac{1}{P\tau} (\tilde{D}^2\beta,\tilde{D}^2\beta^*) \]

\[ - \frac{1}{S\varepsilon} (\tilde{D}^2\Omega,\tilde{D}^2\Omega^*) - i[\lambda_2(y\beta,\tilde{D}^2\phi^*) + 2\lambda_2(\beta,D\phi^*)] \]

\[ + \lambda_1(y\Omega,\tilde{D}^2\phi^*) + 2\lambda_1(\Omega,D\phi^*) - \lambda_1(y\beta^*,\tilde{D}^2\phi) \]

\[ - 2\lambda_1(\beta^*,D\phi) - \lambda_2(y\Omega^*,\tilde{D}^2\phi) - 2\lambda_2(\Omega^*,D\phi) \]

\[ = 0 \]

Write this equation as

\[ (9) \quad -c^{(o)}I_0 - \frac{1}{S\kappa} I_1 - \frac{1}{P\tau} I_2 - \frac{1}{S\varepsilon} I_3 - iI_4 = 0 \]

Inspection of equations (8) and (9) reveals the following: \( I_0, I_1, I_2, \) and \( I_3 \) are all real and positive, and \( I_4 \) can be written as

\[ I_4 = [\lambda_2(y\beta,\tilde{D}^2\phi^*) - \lambda_1(y\beta,\tilde{D}^2\phi^*) + 2\lambda_2(\beta,D\phi^*)] \]
\[-2\lambda_1 (\beta, D\phi^*) + \lambda_1 (\gamma \Omega, D^2 \phi^*) - \lambda_2 (\gamma \Omega, D^2 \phi^*)^* \]

\[+ 2 \lambda_1 (\Omega, D\phi^*) - 2 \lambda_2 (\Omega, D\phi^*)^*] \]

The two possibilities for the number \(\lambda_1\) and \(\lambda_2\) are

\[\lambda_1 = \lambda_2 \text{ or } \lambda_1 = -\lambda_2\]

The first of these yields the fact that \(I_4\) is imaginary since 
\(a - a^*\) is imaginary. This means that \(c^{(0)}\) in equation (9) must 
be real and there is no possibility of oscillatory marginal 
states.

If \(\lambda_1 = -\lambda_2\) the integral \(I_4\) is real since \(a + a^*\) is 
real. Separation of equation (9) into real and imaginary 
parts gives for the real part of the equation

\[-a^{(0)} I_0 = \frac{1}{Sk} I_1 + \frac{1}{Fr} I_2 + \frac{1}{Sc} I_3\]

From what is known about \(I_0, I_1, I_2,\) and \(I_3\) this equation 
says that \(a^{(0)}\) must be negative. This means that the situa-
tion of antiparallel reaction source terms \((\lambda_1 = -\lambda_2)\) is 
unconditionally stable to infinitesimal disturbances.