14

Multi-component convection diffusion

14.1 Convection with heating and salting below

In the standard Bénard problem the instability is driven by a density difference caused by a temperature difference between the upper and lower planes bounding the fluid. If the fluid layer additionally has salt dissolved in it then there are potentially two destabilizing sources for the density difference, the temperature field and the salt field. A similar scenario could be witnessed in isothermal conditions but with two dissolved salts such as sodium and potassium chloride. When there are two effects such as this the phenomenon of convection which arises is called *double diffusive convection*. For the specific case involving a temperature field and sodium chloride it is frequently referred to as *thermohaline convection*. There are many recent studies involving three or more fields, such as temperature and two salts such as NaCl, KCl. For the three or greater field case we shall refer to *multi-component convection*.

The driving force for many studies in double diffusive or multi-component convection is largely physical applications. For instance modelling geothermal reservoirs, e.g. in the Imperial valley in California, cf. (Cheng, 1978) the Wairakei system in New Zealand, cf. (Griffiths, 1981) near Lake Kinnert in Israel, cf. (Rubin, 1973) the Floridan aquifer, cf. (Kohout, 1965) and in the Salton sea geothermal system in California, cf. (Fournier, 1990), (Helgeson, 1968), (Oldenburg and Pruess, 1998), (Williams and McKibben, 1989), (Younker et al., 1982): a recent review of numerical techniques and their application in geothermal reservoir simulation may be found in (O'Sullivan et al., 2001). The Salton sea geothermal system in southern California is particularly interesting in that it involves convection of hypersaline fluids. For example, to model the Salton sea geothermal system (Oldenburg and Pruess, 1998) develop a model for convection in a Darcy porous medium where the mechanism involves temperature, NaCl, $CaCl_2$, and KCl. Other applications include the oceans, cf. (Stern, 1960), (Cathles, 1990), (Mellor, 1996), (Pedlosky, 1996), the Earth's magma, e.g. (Hansen and Yuen, 1989), (Carrigan and Cygan, 1986), (Huppert and Sparks, 1984). Drainage in a mangrove system, (van Duijn et al., 2001) is yet another area encompassing double diffusive flows. Solar ponds are a particularly promising means of harnessing energy from the Sun by preventing convective overturning in a thermohaline system by salting from below, cf. (Rothmeyer, 1980), (Tabor, 1980), (Zangrando, 1991). Bio-remediation, involving the introduction of micro-organisms to change the chemical composition of contaminants is a very important area, cf. (Celia et al., 1989), (Chen et al., 1994), (Suchomel et al., 1998). Contaminant movement or pollution transport is a further area of multi-component flow in porous media which is of much interest in environmental engineering, cf. (Curran and Allen, 1990), (Ewing et al., 1997), (Ewing, 1996), (Ewing, 1997), (Ewing and Weekes, 1998), (Franchi and Straughan, 2001). Other very important areas of double diffusive transport occur in oil reservoir simulation, cf. (Allen, 1984), (Allen, 1986), (Allen et al., 1988), (Allen et al., 1992), (Ludvigsen et al., 1990), and salinization, cf. (Gilman and Bear, 1996).

To describe nonlinear energy stability results in double-diffusive convection we begin by introducing the relevant equations. For a fluid, these have already been encountered in section 4.6. With no Soret effect the equations are

$$\dot{v}_i = -\frac{1}{\rho_0}\, p_{,i} + \nu\Delta v_i - gk_i\big(1 - \alpha[T - T_0] + \gamma[C - C_0]\big), \tag{14.1}$$

$$v_{i,i} = 0, \tag{14.2}$$

$$\dot{T} = \kappa\Delta T\,, \tag{14.3}$$

$$\dot{C} = \kappa_C\Delta C\,. \tag{14.4}$$

If we suppose equations (14.1-14.4) are defined on the spatial region $\mathbb{R} \times \{z \in (0,d)\}$ with $t > 0$, then with boundary conditions of fixed temperatures and salt concentrations, T_L, T_U, C_L, C_U, and no-slip velocity boundary conditions the steady solution in whose stability we are interested is

$$\bar{v}_i \equiv 0, \qquad \bar{T} = -\beta z + T_L, \qquad \bar{C} = -\beta_C z + C_L, \tag{14.5}$$

where the temperature and concentration gradients are given by

$$\beta = \frac{T_L - T_U}{d}\,, \qquad \beta_C = \frac{C_L - C_U}{d}\,. \tag{14.6}$$

Perturbations u_i, π, θ, ϕ to the steady fields $\bar{v}_i, \bar{p}, \bar{T}$ and $\bar{C}$ then satisfy the equations

$$u_{i,t} + u_j u_{i,j} = -\frac{1}{\rho_0} p_{,i} + \nu \Delta u_i + g\alpha k_i \theta - g\gamma k_i \phi, \tag{14.7}$$

$$u_{i,i} = 0, \tag{14.8}$$

$$\theta_{,t} + u_i \theta_{,i} = \beta w + \kappa \Delta \theta, \tag{14.9}$$

$$\phi_{,t} + u_i \phi_{,i} = \beta_C w + \kappa_C \Delta \phi. \tag{14.10}$$

In general, the thermal and salt diffusivities κ, κ_C are very different and this gives rise to interesting effects. We non-dimensionalize equations (14.7-14.10) with the time, velocity, temperature, concentration, length, scales of $\mathcal{T} = d^2/\kappa$, $U = \kappa/d$, $T^\sharp = (\beta\nu/\alpha g\kappa)^{1/2}U$, $C^\sharp = (\beta_C \nu/\gamma g \kappa_C)^{1/2}U$, and $L = d$. We introduce the Lewis number, Le, (the ratio of diffusivities), the thermal and salt Prandtl numbers, Pr, P_C, and the Rayleigh number and salt Rayleigh numbers, $Ra = R^2$, $Ra_S = R_C^2$, by

$$Le = \frac{\kappa}{\kappa_C}, \quad Pr = \frac{\nu}{\kappa_C}, \quad P_C = \frac{\nu}{\kappa_C}, \quad R^2 = \frac{g\alpha\beta d^4}{\kappa\nu}, \quad R_C^2 = \frac{\beta_C g\gamma d^4}{\kappa_C \nu}.$$

Then equations (14.7-14.10) assume the non-dimensional form

$$\frac{1}{Pr}(u_{i,t} + u_j u_{i,j}) = -\pi_{,i} + \Delta u_i + R k_i \theta - R_C k_i \phi, \tag{14.11}$$

$$u_{i,i} = 0, \tag{14.12}$$

$$\theta_{,t} + u_i \theta_{,i} = \hat{H} R w + \Delta \theta, \tag{14.13}$$

$$Le(\phi_{,t} + u_i \phi_{,i}) = \tilde{H} R_C w + \Delta \phi, \tag{14.14}$$

where $k_i = \delta_{i3}$ and (14.11-14.14) hold on the spatial region $\mathbb{R}^2 \times (0,1)$ with $t > 0$. The constants $\hat{H}$ and $\tilde{H}$ take values ± 1. If the fluid is heated from below, $T_L > T_U$, and then $\hat{H} = 1$, otherwise $\hat{H} = -1$, whereas if the fluid is salted below, $C_L > C_U$, so $\tilde{H} = +1$ with salting above yielding $\tilde{H} = -1$. The boundary conditions are

$$u_i = 0, \quad \theta = 0, \quad \phi = 0, \qquad z = 0, 1, \tag{14.15}$$

and u_i, π, θ, ϕ satisfy a periodic plane tiling pattern in x, y.

In this section we pay particular attention to the case of infinite Prandtl number, Pr. While this is an unphysical case it is very useful example for illustration of what can be achieved with an energy method. The equations for this case are

$$\pi_{,i} = \Delta u_i + R k_i \theta - R_C k_i \phi, \tag{14.16}$$

$$u_{i,i} = 0, \tag{14.17}$$

$$\theta_{,t} + u_i \theta_{,i} = \hat{H} R w + \Delta \theta, \tag{14.18}$$

$$Le(\phi_{,t} + u_i \phi_{,i}) = \tilde{H} R_C w + \Delta \phi. \tag{14.19}$$

The equivalent perturbation equations for a Darcy porous medium may be derived from e.g. (Nield and Bejan, 1999), (Lombardo et al., 2001b) and are

$$\pi_{,i} = -u_i + Rk_i\theta - R_C k_i\phi, \qquad u_{i,i} = 0, \tag{14.20}$$

$$\theta_{,t} + u_i\theta_{,i} = \hat{H}Rw + \Delta\theta, \tag{14.21}$$

$$Le(\epsilon\phi_{,t} + u_i\phi_{,i}) = \tilde{H}R_C w + \Delta\phi, \tag{14.22}$$

where the constant ϵ is given by $\epsilon = \varepsilon M$ with ε the porosity and $M = (\rho_0 c_p)_f/(\rho_0 c)_m$, this being the ratio of heat capacities in the fluid and the porous matrix.

We now return to equations (14.11-14.14). In equations (14.11-14.14) if the layer is salty above and heated below then both effects are destabilizing, $\tilde{H} = -1$, $\hat{H} = 1$ in (14.11-14.14) and the linearized system is symmetric, therefore, the linear and nonlinear boundaries coincide and no sub-critical instabilities can occur. This result was first established by (Shir and Joseph, 1968). If, however, the layer is salted below, which is a stabilizing effect, while the layer is simultaneously heated from below, which is a destabilizing effect, then the two opposing effects make an energy analysis decidely more complicated, to achieve sharp results.

The really interesting situation from both a geophysical and a mathematical viewpoint arises when the layer is simultaneously heated from below and salted from below. In this situation heating expands the fluid at the bottom of the layer and this in turn wants to rise thereby encouraging motion due to thermal convection. On the other hand, the heavier salt at the lower part of the layer has exactly the opposite effect and this acts to prevent motion through convective overturning. Thus, these two physical effects are competing against each other. Due to this competition, it means that the linear theory of instability does not always capture the physics of instability completely and (sub-critical) instabilities may arise before the linear threshold is reached, cf. (Hansen and Yuen, 1989), (Proctor, 1981), (Veronis, 1965). Due to the possibility of sub-critical instabilities occurring, it is very important to obtain (unconditional) nonlinear stability thresholds which guarantee bounds below which convective overturning will not occur. For the heated and salted below situation the equations are (14.11-14.14) with $\tilde{H} = \hat{H} = +1$. For precisely this problem (Joseph, 1970) introduced a new twist into the theory of energy stability; the idea of a *generalized energy*. He sets $\tau = Pc/Pr$, $R_C = \alpha R$ and then chooses

$$E(t) = \frac{1}{2}\|\mathbf{u}\|^2 + \frac{1}{2}\,\frac{Pr}{1+\tau}\big[\|\gamma\|^2 + \|\psi\|^2\big],$$

where

$$\gamma = \lambda_1\theta - \lambda_2\phi, \qquad \psi = \lambda_1\theta - \tau\lambda_2\phi, \tag{14.23}$$

and where λ_1, λ_2 are coupling parameters linked by the equation

$$\lambda_1 + \frac{1}{\lambda_1} - \frac{2\alpha\lambda_2}{(1+\tau)} = \alpha\Big(\frac{1}{\lambda_2} - \lambda_2\Big) + \frac{2\lambda_1\tau}{1+\tau}\,.$$

The above choice of energy is evidently necessary to produce a sharp result. Indeed, (Joseph, 1970) finds a stability boundary that is very close to the linear instability one. He indicates that sub-critical instabilities arise in precisely the region delimited by his energy analysis.

From the point of view of Lyapunov functionals, or generalized energies, in fluid mechanics, the paper of (Joseph, 1970) is a very important one. It is the first one I know of where such a *generalized energy* is employed *very effectively* to achieve sharp results evidently not attainable by a standard energy analysis. Joseph's paper has unquestionably had a major influence on the work in energy theory which has subsequently developed.

We now demonstrate some unconditional nonlinear energy stability results for the $Pr = \infty$ case described by equations (14.16-14.19). While we begin with $Le = 1$ we note that this is an instructive case. In this section as throughout much of the book, we concentrate on unconditional nonlinear stability results.

Suppose $Le = 1$ in (14.16-14.19) and take $\hat{H} = \tilde{H} = 1$, i.e. this is the tricky case of heating below and salting below. It is instructive to write the right hand side of (14.16-14.19) as a matrix system in (u_i, θ, ϕ), for then we see it has form

$$\begin{pmatrix} \Delta & 0 & 0 & 0 & 0 \\ 0 & \Delta & 0 & 0 & 0 \\ 0 & 0 & \Delta & R & 0 \\ 0 & 0 & R & \Delta & 0 \\ 0 & 0 & 0 & 0 & \Delta \end{pmatrix} \begin{pmatrix} u \\ v \\ w \\ \theta \\ \phi \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -R_C \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & R_C & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \\ \theta \\ \phi \end{pmatrix}$$

By writing the right hand side in this way the symmetric effect of R is evident as is the anti-symmetric effect of the salt field via R_C.

To progress with a nonlinear energy stability analysis we introduce a *natural variable* $a = R\theta - R_C\phi$. The introduction of this natural variable and its usefulness in the heated/salted below problem is due to (Mulone, 1994). Equations (14.16-14.19) may be rearranged to combine θ and ϕ into a as

$$\pi_{,i} = \Delta u_i + k_i a, \qquad u_{i,i} = 0, \tag{14.24}$$

$$a_{,t} + u_i a_{,i} = (R^2 - R_C^2)w + \Delta a. \tag{14.25}$$

The boundary conditions are

$$u_i = 0, \quad a = 0, \qquad z = 0, 1$$

with u_i, π and a satisfying the periodicity condition with period cell V.

We first suppose $R^2 < R_C^2$. Then we put $\mu = R_C^2 - R^2 > 0$. Multiply (14.24) by u_i and integrate over V and likewise multiply (14.25) by a and integrate over V to obtain the energy identities

$$0 =(a, w) - \|\nabla \mathbf{u}\|^2 \tag{14.26}$$

$$\frac{d}{dt}\frac{1}{2}\|a\|^2 = - \mu(w, a) - \|\nabla a\|^2. \tag{14.27}$$

By adding this with μ as a coupling parameter one finds

$$\frac{d}{dt}\frac{1}{2}\|a\|^2 = -(\|\nabla a\|^2 + \mu\|\nabla \mathbf{u}\|^2).$$

From this we can clearly deduce that

$$\|a(t)\|^2 \leq \|a(0)\|^2 \exp(-2\pi^2 t) \tag{14.28}$$

and it follows a decays to zero at least exponentially fast in L^2 measure.

Then, from (14.26), using the arithmetic - geometric mean inequality and Poincaré's inequality we have

$$\begin{aligned}\pi^2\|\mathbf{u}\|^2 \leq \|\nabla \mathbf{u}\|^2 = (a, w) \leq & \frac{1}{2\pi^2}\,\|a\|^2 + \frac{\pi^2}{2}\,\|\mathbf{u}\|^2 \\ \leq & \frac{1}{2\pi^2}\,\|a\|^2 + \frac{1}{2}\|\nabla \mathbf{u}\|^2 \,. \end{aligned} \tag{14.29}$$

Hence,

$$\pi^4\|\mathbf{u}\|^2 \leq \pi^2\|\nabla \mathbf{u}\|^2 \leq \|a\|^2. \tag{14.30}$$

Employing (14.28) we then find that $R^2 < R_C^2$ also guarantees $\|\mathbf{u}\|$ and $\|\nabla \mathbf{u}\|$ decay exponentially fast in addition to $\|a\|$. Physically this is what we expect. The heavier salting at the bottom of the layer is dominating the heating from below and preventing convective overturning. These results are unconditional, i.e. for all initial data.

Suppose now $R^2 > R_C^2$ and put $\gamma = R^2 - R_C^2 > 0$. By multiplying (14.24) by γ this system becomes

$$\gamma\pi_{,i} = \gamma\Delta u_i + \gamma k_i a, \qquad u_{i,i} = 0, \tag{14.31}$$

$$a_{,t} + u_i a_{,i} = \gamma w + \Delta a. \tag{14.32}$$

The right hand side is equivalent to

$$\begin{pmatrix} \gamma\Delta & 0 & 0 & 0 \\ 0 & \gamma\Delta & 0 & 0 \\ 0 & 0 & \gamma\Delta & \gamma \\ 0 & 0 & \gamma & \Delta \end{pmatrix} \begin{pmatrix} u \\ v \\ w \\ a \end{pmatrix}$$

In this manner the symmetry of the system is evident and so we can conclude that the linear instability boundary is the same as the (unconditional) nonlinear energy stability one and hence no sub-critical instabilities are possible. Nevertheless, it is very instructive to prove this directly. To do this multiply (14.31) by u_i, (14.32) by a and integrate each over V to derive the energy identities

$$\begin{aligned} 0 =& \gamma(a,w) - \gamma\|\nabla\mathbf{u}\|^2 \\ \frac{d}{dt}\frac{1}{2}\|a\|^2 =& \gamma(w,a) - \|\nabla a\|^2. \end{aligned}$$

Adding these yields the equation

$$\frac{dE}{dt} = I - D \tag{14.33}$$

where

$$E(t) = \frac{1}{2}\|a(t)\|^2, \quad I(t) = 2\gamma(w,a), \quad D(t) = \|\nabla a\|^2 + \gamma\|\nabla\mathbf{u}\|^2.$$

Thus if we define

$$\frac{1}{R_E} = \max_{\mathcal{H}} \frac{I}{D} \tag{14.34}$$

then we derive

$$\frac{dE}{dt} \le -D\left(1 - \frac{1}{R_E}\right). \tag{14.35}$$

Nonlinear stability ensues when $R_E > 1$. The Euler-Lagrange equations from (14.34) are easily seen to be

$$\begin{aligned} &R_E 2\gamma a k_i + 2\gamma\Delta u_i = 2\lambda_{,i} \\ &R_E 2\gamma w + 2\Delta a = 0. \end{aligned} \tag{14.36}$$

For the linear theory it is not difficult to show $\sigma \in \mathbb{R}$ and then the equations governing linear instability are

$$\begin{aligned} &\pi_{,i} = \Delta u_i + a k_i, \quad u_{i,i} = 0, \\ &0 = \gamma w + \Delta a. \end{aligned} \tag{14.37}$$

Since λ is a Lagrange multiplier we divide the first of (14.36) by γ and then for the threshold case $R_E = 1$ it is easily seen that (14.36) are the same as (14.37) and so the linear instability threshold is identical to the nonlinear energy stability one.

To complete the proof we argue from (14.35) as in the case $R_C^2 > R^2$ to show $\|a\|, \|\mathbf{u}\|, \|\nabla\mathbf{u}\|$ are bounded by a decreasing exponential function of time.

We now abandon the restriction $Le = 1$ and derive an unconditional stability result valid for any Lewis number. To achieve this we form energy identities from (14.16-14.19) as

$$0 = -\|\nabla\mathbf{u}\|^2 + R(\theta,w) - R_C(\phi,w) \tag{14.38}$$

$$\frac{d}{dt}\frac{1}{2}\|\theta\|^2 = R(w,\theta) - \|\nabla\theta\|^2 \tag{14.39}$$

$$\frac{d}{dt}\frac{1}{2}Le\|\phi\|^2 = R_C(w,\phi) - \|\nabla\phi\|^2. \tag{14.40}$$

Form now the combination (14.38)+μ(14.40) +λ(14.39) where μ, λ are now positive constants we are using as coupling parameters. This leads to the energy equation (14.33) where now

$$\begin{aligned}
E &= \frac{\lambda}{2}\|\theta\|^2 + \frac{\mu Le}{2}\|\phi\|^2 \\
I &= R(1+\lambda)(\theta, w) + R_C(\mu-1)(\phi, w) \\
D &= \|\nabla \mathbf{u}\|^2 + \lambda\|\nabla\theta\|^2 + \mu\|\nabla\phi\|^2.
\end{aligned} \tag{14.41}$$

We may now establish at least exponential decay of E provided $R_E^{-1} < 1$ where $R_E^{-1} = \max_{\mathcal{H}}(I/D)$. From (14.38) we also find

$$\begin{aligned}
\pi^2\|\mathbf{u}\|^2 \le \|\nabla\mathbf{u}\|^2 \le & \frac{R}{2\alpha}\|\theta\|^2 + \frac{R_C}{2\beta}\|\phi\|^2 + \left(\frac{R\alpha}{2} + \frac{R_C\beta}{2}\right)\|w\|^2 \\
\le & \frac{R}{2\alpha}\|\theta\|^2 + \frac{R_C}{2\beta}\|\phi\|^2 + \frac{1}{2\pi^2}(R\alpha + R_C\beta)\|\nabla\mathbf{u}\|^2
\end{aligned}$$

for positive constants α, β. Select $\alpha = \pi^2/2R$, $\beta = \pi^2/2R_C$ and then we deduce

$$\pi^2\|\mathbf{u}\|^2 \le \|\nabla\mathbf{u}\|^2 \le \frac{2R^2}{\pi^2}\|\theta\|^2 + \frac{2R_C^2}{\pi^2}\|\phi\|^2.$$

This relation shows that R_E^{-1} guarantees in addition to decay of $\|\theta\|$ and $\|\phi\|$, also decay of $\|\mathbf{u}\|$ and $\|\nabla\mathbf{u}\|$.

To calculate the nonlinear stability boundary it remains to calculate the Euler-Lagrange equations for the maximum of I/D and this we do in the threshold case $R_E = 1$. The relevant Euler-Lagrange equations for a Lagrange multiplier ζ are

$$\begin{aligned}
&R(1+\lambda)\theta k_i + R_C(\mu-1)\phi k_i + 2\Delta u_i = \zeta_{,i} \\
&R(1+\lambda)w + 2\lambda\Delta\theta = 0 \\
&R_C(\mu-1)w + 2\mu\Delta\phi = 0.
\end{aligned}$$

We may eliminate ζ to derive the equation

$$2\Delta^2 w + R(1+\lambda)\Delta^*\theta + R_C(\mu-1)\Delta^*\phi = 0,$$

where Δ^* is the horizontal Laplacian. While we could solve this eigenvalue system numerically we assume we are dealing with two surfaces free of tangential stress. In this way we may look for solutions of form $w = W \sin n\pi z\, f(x,y)$, $\theta = \Theta \sin n\pi z\, f(x,y)$, $\phi = \Phi \sin n\pi z\, f(x,y)$, where W, Θ, Φ are constant amplitudes and f is a horizontal planform satisfying $\Delta^* f = -a^2 f$, a being the wavenumber. This allows us to deduce the relation below

$$\frac{2(\pi^2n^2 + a^2)^3}{a^2} = \frac{R^2(1+\lambda)^2}{2\lambda} + \frac{R_C^2(\mu-1)^2}{2\mu}.$$

We see that for R^2 minimized in n we need $n = 1$. Since μ is a coupling parameter we choose it to make R^2 as large as possible and so take $\mu = 1$.

Thus

$$R^2 = \frac{4\lambda}{(1+\lambda)^2}\,\frac{(\pi^2+a^2)^3}{a^2}\,.$$

The critical Rayleigh number of this energy theory is found as

$$Ra_E = \max_{\lambda}\,\min_{a^2}\,R^2$$

for which we find $a^2 = \pi^2/2$ and $\lambda = 1$, then $Ra_E = 27\pi^4/4$.

Thus, for system (14.16-14.19) with stress free velocity boundary conditions we have shown that $R^2 < 27\pi^4/4$ guarantees exponential decay of $\|\mathbf{u}\|, \|\nabla\mathbf{u}\|, \|\theta\|$ and $\|\phi\|$ for all initial data regardless of the values of R_C and Le.

One can prove much more than the above results for the $Pr = \infty$ problem, at the expense of increasing the technical nature of the calculations, by introducing generalized energies. The idea is to use the methods of (Mulone, 1994), (Mulone and Rionero, 1998), (Lombardo et al., 2000), and (Lombardo et al., 2001a).

Detailed linear instability theory for the problem of convection with temperature and salt fields has been worked out by (Nield, 1968) for a porous medium and by (Baines and Gill, 1969) in a fluid.

As we have already pointed out (Joseph, 1970) is the first to use a generalized energy method to incorporate the stabilizing effect of salting below in a nonlinear energy stability analysis. (Joseph, 1970) treats system (14.11-14.14) with $\hat{H} = \tilde{H} = 1$ and works with the variables γ and ψ given by (14.23). His energy uses two functionals,

$$\Psi(t) = \frac{Pr}{2(1+\tau)}\,\|\psi\|^2 \qquad \text{and} \qquad E(t) = \frac{1}{2}\|\mathbf{u}\|^2 + \frac{Pr\,\tau}{(1+\tau)}\,\|\phi\|^2.$$

He derives a sharp stabilty threshold with stability guaranteed in the sense that

$$\lim_{t\to\infty}\int_0^t E(s)ds < \infty. \tag{14.42}$$

(Rionero and Mulone, 1987) provide a rigorous linearization principle for double-diffusive convection problems using energy ideas. (Mulone, 1991b) develops a conditional nonlinear energy stability analysis for the heated and salted below problem allowing the fluid also to be undergoing Poisueille or Couette flow. This work is extended by (Mulone, 1994) but he now develops a sharp unconditional result for the heated and salted below problem. The analysis of (Mulone, 1994) also derives exponential decay for the energy instead of the condition (14.42). It is in this paper where the use of the "natural" variable suggested by the density, namely

$$a = R\theta - R_C\phi$$

is used with great effect. (Mulone, 1994) develops a nonlinear energy stability theory based on the generalized energy functional

$$E(t) = \frac{1}{2}\|\mathbf{u}\|^2 + \frac{1}{2}\lambda_1 P_C \|a\|^2 + \frac{1}{2}\lambda_2 Pr\|\theta\|^2.$$

Very sharp nonlinear stability thresholds are derived and compared carefully with the linear instability boundaries. (Mulone and Rionero, 1998), (Mulone, 1998), (Lombardo et al., 2000), (Xu, 2000), and (Lombardo et al., 2001a) derive further sharp nonlinear stability boundaries for the heated and salted below problem for a fluid by employing other kinds of generalized energies. The decay obtained is always exponential in time. (Lombardo et al., 2001b) and (Lombardo and Mulone, 2002a) use not dissimilar generalized energies to derive sharp nonlinear stability boundaries in the analogous problem for a porous medium.

Further interesting nonlinear (conditional) energy stability results in double-diffusive convection are due to (Guo et al., 1994), (Guo and Kaloni, 1995a), (Guo and Kaloni, 1995c), (Qin et al., 1995). These writers derive nonlinear stability bounds for double-diffusive convection in a Brinkman porous medium, (Guo and Kaloni, 1995a), in a rotating layer in (Guo et al., 1994) and (Guo and Kaloni, 1995c), and incorporating penetrative convection in (Qin et al., 1995). (Guo and Kaloni, 1995b) develop a nonlinear unconditional analysis for the interesting problem in a porous medium when the convection is induced by temperature and concentration gradients which have a horizontal as well as a vertical component. This nonlinear energy theory complements the linearized instability theory of (Nield et al., 1993). In addition (Kaloni and Qiao, 1997a), (Kaloni and Qiao, 2000), (Qiao and Kaloni, 1997), (Qiao and Kaloni, 1998), have developed a series of interesting articles in which they establish *unconditional* nonlinear energy stability results for double diffusive problems but when the temperature and concentration gradients vary in the horizontal as well as the vertical directions. The analogous problems in a fluid and in a porous medium are investigated and throughflow effects are additionally incorporated. (Bardan and Mojtabi, 1998) and (Bardan et al., 2000) study a nonlinear double diffusive problem in a two-dimensional enclosure. The temperature and concentration gradients are horizontal and opposing. Subcritical instabilities are found and a careful bifurcation analysis is performed. (Charrier-Mojtabi et al., 1998) and (Karimi-Fard et al., 1999) investigate double diffusive convection in a rectangular container filled with saturated porous material. The driving forces are horizontal temperature and concentration gradients and in the case of (Karimi-Fard et al., 1999) the rectangular cavity is tilted. These are both very interesting articles and go into much detail about the bifurcation patterns which develop.

14.2 Convection with three components

We have already seen that the solution behaviour in the double-diffusive convection problem is more interesting than that of the single component situation in so much as new instability phenomena may occur which are not present in the classical Bénard problem. Nonlinear energy stability theory is correspondingly more complicated and mathematically richer. When temperature and two or more component agencies, or three different salts, are present then the physical and mathematical situation becomes increasingly richer. Very interesting results in triply diffusive convection have been obtained by (Pearlstein et al., 1989). The results of (Pearlstein et al., 1989) are in some ways remarkable. They demonstrate that for triple diffusive convection linear instability can occur in discrete sections of the Rayleigh number domain with the fluid being linearly stable in a region in between the linear instability ones. This is because for certain parameters the neutral curve has a finite isolated oscillatory instability curve lying below the usual unbounded stationary convection one. The shape of the oscillatory convection curve is topologically complex being approximately heart shaped which in turn leads to the possibility of complex dynamical behaviour. (Pearlstein et al., 1989) cite specific examples of convection in a triply diffusive system, in crystal growth, (Coriell et al., 1987), and the chemical application of (Noulty and Leaist, 1989).

(Straughan and Walker, 1997) derive the equations for non-Boussinesq convection in a multi - component fluid [1] and investigate the situation analogous to that of (Pearlstein et al., 1989) but allowing for a density nonlinear in the temperature field. In this way they also encompass penetrative convection.

(Pearlstein et al., 1989) treat triply diffusive convection with a density linear in all fields and they employ stress free boundary conditions. They find that the oscillatory instability curve has a perfectly symmetric shape about a vertical axis. In (Lopez et al., 1990) they study the equivalent problem with fixed boundary conditions and show that the effect of the boundary conditions breaks the perfect symmetry. In reality the density of a fluid is never a linear function of temperature, and so the work of (Straughan and Walker, 1997) applies to the general situation where the equation of state is one of the density being quadratic in temperature, T. This is important, since they find that departure from the linear Boussinesq equation of state changes the perfect symmetry of the heart shaped neutral curve of (Pearlstein et al., 1989). This means that one is never likely to actually see the interesting dynamics predicted by (Pearlstein et al.,

[1] Some of the material in this section is reprinted from Fluid Dynamics Research, Vol. 19, B. Straughan and D.W. Walker, Multi component diffusion and penetrative convection, pp. 77-89, Copyright (1997), with permission from Elsevier Science.

1989). In fact, (Pearlstein et al., 1989) find that one can have a "heart shaped" curve lying below the usual unbounded stationary convection one and it is isolated in that below the stationary convection curve and above the lobes of the heart shaped curve the system is linearly stable. The lobes of the heart shape have the same Rayleigh number but different wavenumbers which suggests instability could occur at a given Rayleigh number for *two* distinct values of the wavenumber. The breaking of symmetry by rigid boundary conditions, (Lopez et al., 1990), or due to a non-Boussinesq equation of state, (Straughan and Walker, 1997), does not allow this equal Rayleigh number lobe behaviour. (Straughan and Walker, 1997) do, however, find that in the non-Boussinesq situation one can have equal *minima* of the stationary convection curve and the isolated oscillatory convection curve. This is further described after (14.51). While (Lopez et al., 1990) also find the perfect symmetry of (Pearlstein et al., 1989) is broken, they do not find the dynamical behaviour of (Straughan and Walker, 1997).

The work of (Straughan and Walker, 1997) restricts attention to two stress free surfaces since this is likely to be a physically relevant case in astrophysics. However, this still does not permit the use of the analytical method of (Pearlstein et al., 1989) who also employed surfaces free of tangential stress. The coefficients of the differential equations for the instability eigenvalue problem in (Straughan and Walker, 1997) are functions of the spatial variables. This necessitates a numerical approach and so they employ a Chebyshev tau method. This appraoch yields as many eigenvalues as are desired and so the structure of the growth rate may be studied for more than the leading eigenvalue. In fact, (Straughan and Walker, 1997) find a change from a complex conjugate eigenvalue to a real one as the eigenvalues change positions in Rayleigh number parameter space.

(Straughan and Walker, 1997) develop a linearized instability analysis for the problem of penetrative thermal convection in a three-component fluid. They study the situation of a layer of fluid occupying the three - dimensional region $\mathbb{R}^2 \times \{0 < z < d\}$. The lower plane of the fluid layer is held at the fixed temperature $T = 0°\mathrm{C}$ while the upper boundary is maintained at a constant temperature $T_1 \geq 4°\mathrm{C}$. Thus for a working fluid of water which has a density maximum at approximately $4°\mathrm{C}$, penetrative convection can occur and convection which commences in the gravitationally unstable lower section of the layer may penetrate into the upper part. (Straughan and Walker, 1997) assume that the fluid occupying the layer has dissolved in it two or more different species of chemicals and so they have a three or more component fluid with the solvent being one component. The analysis of (Straughan and Walker, 1997) proceeds by developing the general theory for $5+A$ equations, A being the number of species components. We here present equations for the case of two species of chemicals. The mathematical picture is described by 7 partial differential equations for the velocity, pressure, temperature, and 2 species components, of concentrations C_1 and C_2. The governing partial differential equations are,

$$
\begin{aligned}
&\rho_0(v_{i,t} + v_j v_{i,j}) = -p_{,i} + \rho_0 \nu \Delta v_i - g\rho(T, C_1, C_2)k_i, \qquad v_{i,i} = 0,\\
&T_{,t} + v_i T_{,i} = \kappa \Delta T,\\
&C_{1,t} + v_i C_{1,i} = \kappa_1 \Delta C_1,\\
&C_{2,t} + v_i C_{2,i} = \kappa_2 \Delta C_2,
\end{aligned}
$$

where ρ_0 is a constant, $\mathbf{k} = (0,0,1)$, and where $v_i, p, \nu, g, \kappa, \kappa_\alpha$ denote, respectively, velocity, pressure, viscosity, gravity, thermal diffusivity, and solute diffusivity of component α. The density is quadratic in the temperature field and linear in the two concentrations, i.e.

$$
\rho = \rho_0\big[1 - \alpha_T(T-4)^2 + A_1(C_1 - \hat{C}_1) + A_2(C_2 - \hat{C}_2)\big], \tag{14.43}
$$

where $\hat{C}_1, \hat{C}_2$, are constants.

The boundary conditions equivalent to those of (Straughan and Walker, 1997) are

$$
\begin{aligned}
T &= 0, \quad C^1 = C^1_\ell, \quad C^2 = C^2_\ell, \qquad z = 0,\\
T &= T_1, \quad C^1 = C^1_u, \quad C^2 = C^2_u, \qquad z = d,
\end{aligned} \tag{14.44}
$$

for prescribed constants $T_1, C^\alpha_\ell, C^\alpha_u$, $\alpha = 1,2$. They adopt stress free velocity boundary conditions.

The steady (conduction) solution whose stability is under investigation is

$$
\bar{v}_i = 0, \quad \bar{T} = \beta z, \quad \bar{C}^1 = C^1_\ell - \frac{\Delta C^1}{d}\,z, \quad \bar{C}^2 = C^2_\ell - \frac{\Delta C^2}{d}\,z, \tag{14.45}
$$

with $\beta = T_1/d$, $\Delta C^\alpha = C^\alpha_\ell - C^\alpha_u$, $\alpha = 1,2$. With the scalings $t = t^* d^2/\kappa, \mathbf{x} = \mathbf{x}^* d, Pr = \nu/\kappa, U = \nu/d,\ P = \nu U \rho_0/d, \xi = 4/T_1,\ T^\sharp = U\sqrt{\nu/\kappa\alpha_T d g},\ C^\sharp_\alpha = U\sqrt{|\Delta C^\alpha|/\kappa g d A_\alpha}\,,\ \tau_\alpha = \kappa_\alpha/\kappa,\ H_\alpha = \mathrm{sgn}\,(\Delta C^\alpha)$, we define the Rayleigh number, R^2, and the solutal Rayleigh numbers R_1^2 and R_2^2 as

$$
R^2 = T_1^2\left(\frac{\alpha_T g d^3}{\nu\kappa}\right), \qquad R_1^2 = \frac{|\Delta C^1| d^3 g A_1}{\nu^2 \kappa}\,, \qquad R_2^2 = \frac{|\Delta C^2| d^3 g A_2}{\nu^2 \kappa}\,.
$$

The quantities $T^\sharp$ and $C^\sharp_\alpha$ are temperature and concentration scales. The non-dimensional perturbation equations to the conduction solution (14.45) become, with π being the pressure perturbation,

$$
\begin{aligned}
&Pr^{-1} u_{i,t} + u_j u_{i,j} = -\pi_{,i} + \Delta u_i - 2R\theta k_i(\xi - z)\\
&\qquad\qquad\qquad - (R_1 c_1 + R_2 c_2)k_i + Pr\theta^2 k_i,\\
&u_{i,i} = 0,\\
&\theta_{,t} + Pr\, u_i \theta_{,i} = -Rw + \Delta\theta,\\
&c^1_{,t} + Pr\, u_i c^1_{,i} = H_1 R_1 w + \tau_1 \Delta c_1,\\
&c^2_{,t} + Pr\, u_i c^2_{,i} = H_2 R_2 w + \tau_2 \Delta c_2.
\end{aligned} \tag{14.46}
$$

(Straughan and Walker, 1997) concentrate on cases where the H_α have different signs and they develop a systematic linear analysis. They do cite one nonlinear energy stability result. This shows that when all the salts in the steady state are "salting" from above, and the layer is heated from below, then the nonlinear energy stability boundary coincides with the linear instability one in the *non - penetrative convection case*, where the density is linear in T. Thus sub-critical bifurcation is not possible in that particular scenario. We can illustrate this in the case of two salt fields and then instead of (14.43) one considers the linear equation of state of (Pearlstein et al., 1989),

$$\rho = \rho_0\big[1 - \alpha_T(T - \hat{T}_0) + A_1(C_1 - \hat{C}_1) + A_2(C_2 - \hat{C}_2)\big]. \tag{14.47}$$

Thus, assume we have equations (14.46) but with the density relation (14.43) replaced by (14.47). The nonlinear, non-dimensional perturbation equations which one derives become

$$\begin{aligned}
&Pr^{-1}u_{i,t} + u_j u_{i,j} = -\pi_{,i} + \Delta u_i + R\theta k_i - (R_1c_1 + R_2c_2)k_i,\\
&u_{i,i} = 0,\\
&\theta_{,t} + Pr\, u_i\theta_{,i} = Rw + \Delta\theta,\\
&c^1_{,t} + Pr\, u_i c^1_{,i} = H_1R_1w + \tau_1\Delta c_1,\\
&c^2_{,t} + Pr\, u_i c^2_{,i} = H_2R_2w + \tau_2\Delta c_2.
\end{aligned} \tag{14.48}$$

When $H_1 = H_2 = -1$, equations (14.48) are symmetric and an unconditional nonlinear energy stability analysis in the energy

$$E(t) = \frac{1}{2Pr}\|\mathbf{u}\|^2 + \frac{1}{2}\|\theta\|^2 + \frac{1}{2} < c^1c^1 > + \frac{1}{2} < c^2c^2 >$$

leads to the same critical Rayleigh number as a linearized instability analysis. One shows the growth rate of linearized instability in this case is real and then the equations to be solved for the linear instability critical Rayleigh number threshold are

$$\begin{aligned}
&\Delta^2 w = -R\Delta^*\theta + \sum_{\alpha=1}^{2} R_\alpha \Delta^* c_\alpha,\\
&-Rw = \Delta\theta, \qquad R_\alpha w = \tau_\alpha \Delta c_\alpha, \quad \alpha = 1, 2.
\end{aligned}$$

One shows from this that

$$\frac{(\pi^2 + a^2)^3}{a^2} = R^2 + \frac{R_1^2}{\tau_1} + \frac{R_2^2}{\tau_2}\,.$$

Hence, due to symmetry in equations (14.48) the threshold for linearized instability and for nonlinear stability is the boundary

$$\frac{27\pi^4}{4} = R^2 + \frac{R_1^2}{\tau_1} + \frac{R_2^2}{\tau_2}\,. \tag{14.49}$$

We have just demonstrated this coincidence for stress free boundaries, but the method works and the result is also true in the fixed velocity boundary condition case (although the left hand side of (14.49) changes from $27\pi^4/4$).

(Straughan and Walker, 1997) develop a linearized instability analysis in the general case where (14.46) have A concentration equations rather than 2. They concentrate on the case of $A = 2$ where they have a temperature field and two concentrations, C_1, C_2, only when a numerical investigation of the instability boundary is sought. We here restrict attention to the problem of $H_1 = +1, H_2 = -1$, which means salting below (bottom heavy) in C_1 with salting above in C_2. Thus, the C_1 effect is stabilizing whereas C_2 is destabilizing. In addition, the temperature field destabilizes. Thus, there is competition between two destabilizing effects and one stabilizing effect. The linearized equations which one finds from (14.46) are, after eliminating π and seeking a time-dependence like $e^{\sigma t}$,

$$\begin{aligned}
&\sigma Pr^{-1}\Delta w = \Delta^2 w - 2R(\xi - z)\Delta^*\theta - R_1\Delta^* c_1 - R_2\Delta^* c_2\,,\\
&\sigma\theta = -Rw + \Delta\theta,\\
&\sigma c_1 = R_1 w + \tau_1\Delta c_1,\\
&\sigma c_2 = -R_2 w + \tau_2\Delta c_2,
\end{aligned}\tag{14.50}$$

where $\Delta^* = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

The normal mode form of equations arising from (14.50) is

$$\begin{aligned}
&(D^2 - a^2)\big[(D^2 - a^2) - \sigma Pr^{-1}\big]W + 2R(\xi - z)a^2\Theta\\
&\qquad\qquad\qquad\qquad + R_1 a^2\mathcal{C}_1 + R_2 a^2\mathcal{C}_2 = 0,\\
&\big[(D^2 - a^2) - \sigma\big]\Theta - RW = 0,\\
&\big[(D^2 - a^2) - \sigma\tau_1^{-1}\big]\mathcal{C}_1 + \frac{R_1}{\tau_1}\,W = 0,\\
&\big[(D^2 - a^2) - \sigma\tau_2^{-1}\big]\mathcal{C}_2 - \frac{R_2}{\tau_2}\,W = 0,
\end{aligned}\tag{14.51}$$

where $D = d/dz$, a is the wavenumber, and $W, \Theta, \mathcal{C}_1, \mathcal{C}_2$, are the $z-$dependent parts of w, θ, c_1 and c_2. The above presentation is different from that of (Straughan and Walker, 1997) and care must be taken in comparing the Rayleigh numbers above with those of (Straughan and Walker, 1997).

The numerical findings of (Straughan and Walker, 1997) are based on a Chebyshev tau analysis of (14.51) although the Rayleigh number interpretations are different. Many results are reported in this paper for various upper temperatures in the range 4°C - 8°C. We only report one result. This is highlighted in figure 14.1 which illustrates the neutral stability curves for a special case. The upper temperature is 7°C and the salt Rayleigh numbers are $R_1^2 = 950.964$, $R_2^2 = 814.1119$. The salt diffusivities have values $\tau_1 = 0.22$, $\tau_2 = 0.21$. It is important to note that in the steady state the system is bottom heavy in the species with the larger diffusion coefficient

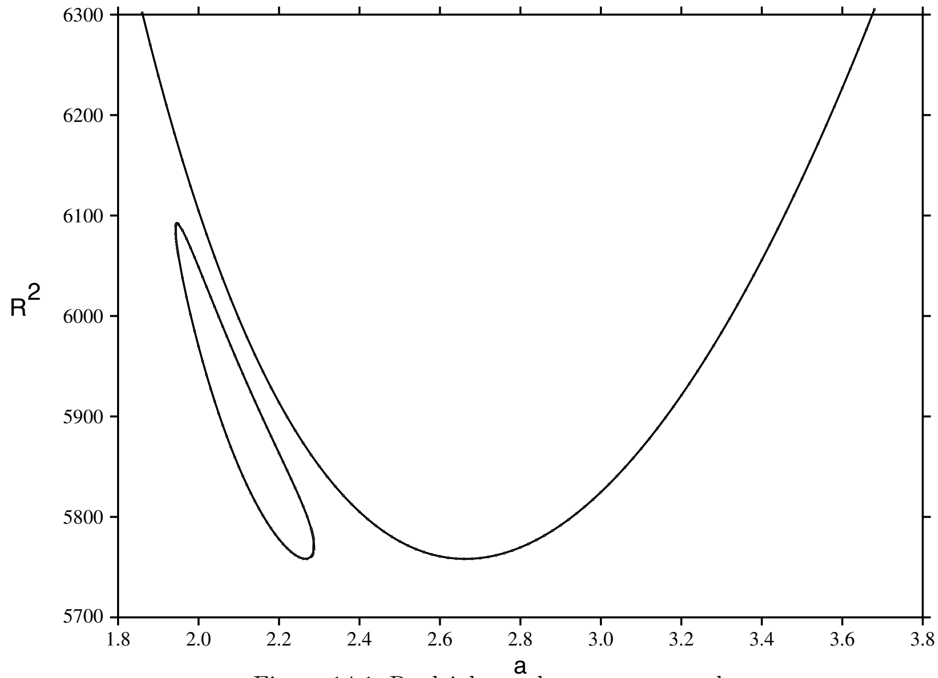

Figure 14.1. Rayleigh number vs. wavenumber

whereas it is top heavy in the species with the smaller diffusion coefficient, although the diffusion coefficients are close together in numerical value. Thus, this is essentially a stable configuration. However, temperature is destabilizing in the conduction state and this together with the competing concentration fields yields the complex dynamical behaviour depicted by figure 14.1. This allows the possibility for convection to commence simultaneously as stationary convection with a wavenumber $a = 2.66$ and as oscillatory convection with wavenumber $a = 2.27$. If R_1^2 is decreased, i.e. salting below decreased in species 1, then the oscillatory curve drops and the first occurrence of linear instability is via oscillatory convection. When R_1^2 is increased the opposite happens, the isolated closed curve rises and convection commences via stationary convection.

We have only shown the situation where the isolated oscillatory convection curve and the infinite stationary convection curve have the same minimum for one set of Rayleigh number parameters and one upper temperature, $T_1 = 7°$C. However, by careful numerical searching one can find other cases. For example, (Straughan and Walker, 1997) report a similar situation when the upper temperature T_1 is 8°C. The closed oscillatory convection curve becomes much thinner as T_1 increases. We could produce other examples where the isolated oscillatory convection curve and the infinite stationary convection curve have the same minimum for other T_1, with suitable R_1^2 and R_2^2 values.

So far we have only discussed the infinite layer situation. However, (Tracey, 1997) and (Straughan and Tracey, 1999), examine the equivalent class of problems in triply diffusive convection with a density quadratic in temperature, but when the layer is finite in extent, i.e. a box with lateral side walls. They also considered a fixed lower boundary condition. They were unable to find numerically parameter ranges where a situation like figure 14.1 holds when the upper and lower surfaces are both fixed (the continuous curves of figure 14.1 are necessarily replaced by points for the finite domain case). However, when the lower surface is fixed while the upper is free, a commonly occurring physical situation, they were able to find the analogous finite box behaviour to that of figure 14.1.

To my knowledge no energy theory has been applied to the systems studied by (Pearlstein et al., 1989) or (Straughan and Walker, 1997). However, (Tracey, 1997) has developed a very nice nonlinear energy stability theory for the equivalent problems in a Darcy porous medium.

(Tracey, 1997) begins with the equations

$$\begin{aligned}
&p_{,i} = -\frac{\mu}{k}\,v_i - gk_i\rho(T, C_1, C_2), \qquad v_{i,i} = 0,\\
&T_{,t} + v_iT_{,i} = \kappa\Delta T,\\
&C^1_{,t} + v_iC^1_{,i} = \kappa_1\Delta C^1,\\
&C^2_{,t} + v_iC^2_{,i} = \kappa_2\Delta C^2.
\end{aligned} \tag{14.52}$$

The density ρ has form, either,

$$\rho = \rho_0\big[1 - A(T - T_0) + A_1(C^1 - C^1_0) + A_2(C^2 - C^2_0)\big] \tag{14.53}$$

or, in the penetrative convection case with water as the saturating fluid

$$\rho = \rho_0\big[1 - A(T - 4)^2 + A_1(C^1 - C^1_0) + A_2(C^2 - C^2_0)\big] \tag{14.54}$$

where $A, A_1, A_2, T_0, C^1_0, C^2_0$ are constants.

We concentrate first on the density given by (14.53). For boundary conditions $T(0) = T_L, T(d) = T_U$, $C^\alpha(0) = C^\alpha_L, C^\alpha(d) = C^\alpha_U$, $\alpha = 1, 2$, with $v_3 = 0$ at $z = 0, d$ the conduction solution to (14.52) with density given by (14.53) is

$$\bar{T} = T_L - \beta z, \qquad \bar{C}^1 = C^1_L - \beta_1 z, \qquad \bar{C}^2 = C^2_L - \beta_2 z, \tag{14.55}$$

with $\beta = (T_L - T_U)/d$, $\beta^\alpha = (C^\alpha_L - C^\alpha_U)/d$, $\alpha = 1, 2$. The non-dimensional perturbation equations arising from this steady solution are (Tracey, 1997),

p. 14,

$$\pi_{,i} = -u_i + (R\theta - R_1\phi^1 - R_2\phi^2)k_i, \tag{14.56}$$
$$u_{i,i} = 0, \tag{14.57}$$
$$\theta_{,t} + u_i\theta_{,i} = HRw + \Delta\theta, \tag{14.58}$$
$$P_1(\phi^1_{,t} + u_i\phi^1_{,i}) = H_1R_1w + \Delta\phi^1, \tag{14.59}$$
$$P_2(\phi^2_{,t} + u_i\phi^2_{,i}) = H_2R_2w + \Delta\phi^2, \tag{14.60}$$

these equations holding on $\mathbb{R}^2 \times \{z \in (0,d)\} \times \{t > 0\}$ with the boundary conditions

$$w = \theta = \phi^1 = \phi^2 = 0, \qquad \text{on } z = 0, 1, \tag{14.61}$$

together with a plane tiling periodicity with period cell V.

(Tracey, 1997) develops a comprehensive linear instability analysis for (14.56-14.60). The linearized analysis is very detailed and yields many interesting effects including calculating the location of isolated oscillatory convection curves which lie below the standard unbounded stationary convection one. Our interest here centres mainly on his energy stability work. For this he first develops an L^2 analysis based on multiplying (14.56) by u_i, (14.58) by θ, (14.59) by ϕ^1, (14.60) by ϕ^2 and with coupling parameters λ, ξ, μ he derives

$$\frac{dE}{dt} = I - D \tag{14.62}$$

where

$$\begin{aligned} E =& \frac{1}{2}\lambda\|\theta\|^2 + \frac{1}{2}\xi P_1\|\phi^1\|^2 + \frac{1}{2}\mu P_2\|\phi^2\|^2 \\ I =& (\lambda H + 1)R(w,\theta) \\ &+ (\xi H_1 - 1)R_1(w,\phi^1) + (\mu H_2 - 1)R_2(w,\phi^2) \\ D =& \|\mathbf{u}\|^2 + \lambda\|\nabla\theta\|^2 + \xi\|\nabla\phi^1\|^2 + \mu\|\nabla\phi^2\|^2. \end{aligned} \tag{14.63}$$

This leads him to unconditional exponential decay results in $E(t)$ together with similar unconditional nonlinear stability in $\|\mathbf{u}(t)\|$. The Rayleigh number thresholds depend on the values of H, H_1, H_2, which are ± 1 depending on whether there is heating or salting above or below.

(Tracey, 1997) selects two cases. The first is $H = 1$, $H_1 = H_2 = -1$, so that there is heating below and salting above in both C_1 and C_2. All three effects are destabilizing and (14.56-14.60) defines a symmetric system. Thus, he derives the optimal result that the linear instability and nonlinear stability boundaries coincide and no sub-critical instabilities occur.

He then studies the very interesting case of $H = H_1 = 1$ with $H_2 = -1$. This is the competitive case where there is heating below, salting below in component 1 but salting above in component 2. For this situation (14.56-14.60) does not define a symmetric system. His energy theory based on

(14.63) for this particular case leads to the nonlinear stability boundary

$$R^2 + R_2^2 = 4\pi^2. \tag{14.64}$$

To improve on this threshold (Tracey, 1997) develops a very interesting generalized energy analysis. To do this he introduces the variables

$$\psi = \phi_1 + \phi_2 \qquad \text{and} \qquad \phi = \phi_1 - \phi_2. \tag{14.65}$$

He works with the generalized energy

$$E(t) = \frac{1}{2}\gamma_0\|\theta\|^2 + \frac{1}{2}\gamma_1\|\psi\|^2 + \frac{1}{2}\gamma_2\|\phi\|^2 \tag{14.66}$$

for coupling parameters $\gamma_0, \gamma_1, \gamma_2$. (Tracey, 1997) deduces exponential decay in $E(t)$ and $\|\mathbf{u}(t)\|$ from his energy equation and calculates the appropriate Euler-Lagrange equations for the Rayleigh number stability boundary.

The way the nonlinear energy stability boundary is computed and the improvement obtained over the standard energy boundary (14.64) is very interesting indeed. Many results are given in (Tracey, 1997), pp. 56-58, and the nature of these is depicted in the schematic figure 14.2. In figure 14.2 curve 3 represents the linear instability curve. Above this curve the steady solution is unstable. The kink is due to the occurrence of an isolated oscillatory convection curve. Curve 1 is the standard L^2 energy stability threshold given by (14.64). Between curves 1 and 3 would be the region of possible sub-critical instabilities. (Tracey, 1997) fixes γ_1, γ_2 and computes a nonlinear stability curve which gives a point on curve 2. By varying γ_1 and γ_2 one obtains the curve 2. Below this curve no instability can arise. Between curves 2 and 3 is now the region of possible sub-critical instabilities. This is a very strong energy stability result and is a major improvement over standard L^2 theory.

When the density is given by (14.54) (Tracey, 1997) adopts constant concentration boundary conditions and fixes $T_L = 0°\text{C}$ with $T_U = T_1^\circ\text{C}$ where $T_1 \geq 4°\text{C}$. This gives him the steady (conduction) solution $\bar{v}_i = 0$, $\bar{C}^\delta = C_L^\delta - \beta_\delta z$, $\delta = 1, 2$, and $\bar{T} = T_1 z/d$. The non-dimensional, nonlinear perturbation equations for this problem are

$$\begin{aligned}
&\pi_{,i} = -u_i - 2R(\xi - z)\theta k_i - R_1\phi^1 k_i - R_2\phi^2 k_i + \theta^2 k_i,\\
&u_{i,i} = 0,\\
&\theta_{,t} + u_i\theta_{,i} = -Rw + \Delta\theta,\\
&P_1(\phi^1_{,t} + u_i\phi^1_{,i}) = H_1 R_1 w + \Delta\phi^1,\\
&P_2(\phi^2_{,t} + u_i\phi^2_{,i}) = H_2 R_2 w + \Delta\phi^2.
\end{aligned} \tag{14.67}$$

A careful linear instability investigation is carried out by (Tracey, 1997) who finds parameters where the minimum of the isolated oscillatory convection curve is the same as that of the unbounded stationary convection one, in a manner similar to that depicted in figure 14.1.

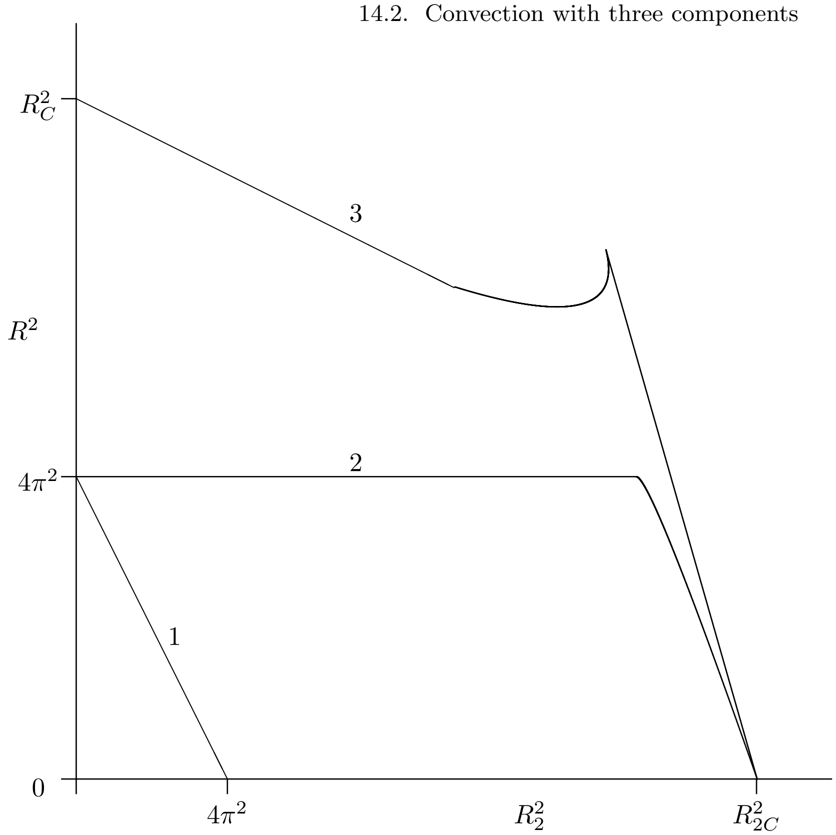

Figure 14.2. Stability and instability boundaries

A standard energy identity may be formed from (14.67) and we see that

$$\|\mathbf{u}\|^2 = -2R < (\xi - z)\theta w > -R_1(\phi^1, w) - R_2(\phi^2, w) + < \theta^2 w > . \quad (14.68)$$

The cubic term $\theta^2 w$ is troublesome if one desires to have an unconditional nonlinear stability theory. Hence, (Tracey, 1997) employs a weight in the velocity part of the energy, cf. section 17.1. He works with the energy

$$E(t) = \frac{1}{2} < \hat{\mu}\theta^2 > + \frac{1}{2}\lambda_1 P_1 \|\phi_1\|^2 + \frac{1}{2}\lambda_2 P_2 \|\phi_2\|^2,$$

for $\hat{\mu} = \mu - 2z$ with $\mu > 2, \lambda_1, \lambda_2$ coupling parameters. This choice of energy removes the cubic term of (14.68) and leads to a quadratic energy stability theory with equation (14.62) where now

$$I = -2R < (\xi - z)\theta w > + (\lambda_1 H_1 - 1)R_1(w, \phi_1) + (\lambda_2 H_2 - 1)R_2(w, \phi_2),$$
$$D = \|\mathbf{u}\|^2 + < \hat{\mu}|\nabla\theta|^2 > + \lambda_1\|\nabla\phi_1\|^2 + \lambda_2\|\nabla\phi_2\|^2.$$

He then derives conditions for exponential decay in the measure $E(t)$. Interestingly, a similar decay in u_i is not proven. Instead, it is shown that the nonlinear stability criteria yield

$$\int_0^\infty \|\mathbf{u}\|^2 ds < \infty,$$

i.e. $\|\mathbf{u}(t)\|^2 \in L^1(0,\infty)$.

The unconditional nonlinear stability thresholds derived for the quadratic density (14.54) model are computed for various parameters, see (Tracey, 1997), pp. 88-91. The nonlinear stability curves are not unlike curve 1 in figure 14.2 with not dissimilar linear instability curves.

14.3 Overturning and pollution instability

This section further analyses models for movement of a salt or pollutant in a layer of fluid. The motivation is not thermal convection as in sections 14.1, 14.2, but instead is directed toward applications in environmental or atmospheric physics where a polluted atmosphere at the Earth's surface is improved by convective motion overturning the air and mixing. When smog is present in a large city, convective overturning which brings in fresh air is welcome. References to other work in contaminant transport are given on page 239.

The model we discuss concerns a species (possibly pollutant) dissolved in a compressible fluid. The compressible fluid mixed with the species is regarded as a continuum mixture and the scenario is then transformed into one in which the fluid is incompressible. The models are due to (Graffi, 1955), (Kazhikhov and Smagulov, 1977), and (Beirao da Veiga, 1983). Various questions of existence, regularity and uniqueness are investigated by (Beirao da Veiga, 1983), (Beirao da Veiga et al., 1982), (Graffi, 1955), (Kazhikhov and Smagulov, 1977), (Prouse and Zaretti, 1987) and (Secchi, 1982). These papers place the Graffi, Kazhikhov - Smagulov, and Beirao da Veiga models on a sound mathematical footing. (Franchi and Straughan, 2001) develop a Graffi - Kazhikhov - Smagulov model to be applicable to convective overturning in a plane layer.

To describe the Graffi, Kazhikhov - Smagulov, and Beirao da Veiga models [2] we begin with a horizontal layer containing a mixture of two incompressible miscible fluids. Before mixing the densities of fluids 1 and 2 are ρ_{10} and ρ_{20}, respectively, while at point $\mathbf{x}$ and time t in the mixture they are $\rho_1(\mathbf{x},t)$ and $\rho_2(\mathbf{x},t)$. It is assumed that upon mixing the volume of the two individual incompressible fluids at the outset does not change

[2]Some of the material in this section is reprinted from Advances in Water Resources, Vol. 24, F. Franchi and B. Straughan, A comparison of the Graffi and Kazhikhov-Smagulov models for top heavy pollution instability, pp. 585-594, Copyright (2001), with permission from Elsevier Science.

and mathematically this is represented as,

$$\frac{\rho_1}{\rho_{10}} + \frac{\rho_2}{\rho_{20}} = 1 \,. \tag{14.69}$$

The total (mixture) density $\rho(\mathbf{x}, t) = \rho_1 + \rho_2$, and v_i^1 is the velocity of constituent 1 in the mixture while v_i^2 is that of constituent 2. The individual balance of mass equations are

$$\rho_{1,t} + (\rho_1 v_i^1)_{,i} = 0, \qquad \rho_{2,t} + (\rho_2 v_i^2)_{,i} = 0. \tag{14.70}$$

The models alluded to earlier require the introduction of w_i, which is the mean *mass* velocity, or barycentric velocity, viz.

$$\rho w_i = \rho_1 v_i^1 + \rho_2 v_i^2 \,. \tag{14.71}$$

By using equations (14.70) one can see that ρ and w_i satisfy the equation

$$\rho_{,t} + (\rho w_i)_{,i} = 0. \tag{14.72}$$

A further velocity, v_i, the mean *volume* velocity is defined by

$$v_i = \frac{\rho_1}{\rho_{10}}\, v_i^1 + \frac{\rho_2}{\rho_{20}}\, v_i^2. \tag{14.73}$$

Then, using (14.69) and (14.72) we derive the important relation that v_i is divergence free, i.e. $\partial v_i/\partial x_i = 0$.

(Franchi and Straughan, 2001) include a derivation of a fundamental relation of (Kazhikhov and Smagulov, 1977). This is stated in terms of the mass concentration, c, and volume concentration, α, of constituent 1 in the mixture given by

$$c = \frac{\rho_1}{\rho}\,, \qquad \alpha = \frac{\rho_1}{\rho_{10}}\,.$$

The fundamental relation of (Kazhikhov and Smagulov, 1977) is

$$w_i = v_i - \lambda\, \frac{\rho_{,i}}{\rho} \tag{14.74}$$

which follows from Fick's law of diffusion

$$v_i^1 = w_i - \lambda\, \frac{c_{,i}}{c}\,, \tag{14.75}$$

where λ is a (constant) diffusion coefficient, as described by (Franchi and Straughan, 2001).

Equation (14.74) is fundamental to further development since it allows the equations to be written in terms of the mixture velocities w_i and v_i rather than the velocity of individual constituents which appear in Fick's law.

We now describe the derivation of the Graffi, Kazhikhov-Smagulov, and Beirao da Veiga equations using relation (14.74).

The starting point involves the equations for flow of a compressible fluid with density ρ, velocity w_i, body force f_i and pressure p, under isothermal conditions, cf. section 15.2,

$$\rho(w_{i,t} + w_k w_{i,k}) = -p_{,i} + (\mu + \mu_2) w_{m,mi} + \mu \Delta w_i + \rho f_i, \tag{14.76}$$

$$\rho_{,t} + (\rho w_m)_{,m} = 0. \tag{14.77}$$

The quantities μ and μ_2 are viscosities of the compressible fluid and satisfy the restrictions $\mu \geq 0$ and $3\mu_2 + 2\mu \geq 0$, c.f. (Truesdell and Toupin, 1960), p. 719. In a mixture of two constituents w_i is interpreted as the barycentric velocity with ρ being the total density. The idea of the Graffi, Kazhikhov-Smagulov, and Beirao da Veiga models is to transform equations (14.76) and (14.77) with the aid of relation (14.74) into equations which involve the density ρ and mean volume velocity v_i so that the velocity field which appears, v_i, is divergence free.

One substitutes in equation (14.77) for w_i from (14.74) to derive

$$\rho_{,t} + \rho_{,i} v_i = \lambda \Delta \rho\,. \tag{14.78}$$

The momentum equation is a little more involved but the method is to use (14.74) to eliminate w_i from (14.76) and then use (14.78) on a $\rho_{,t}$ term. In this manner one derives

$$\begin{aligned} \rho(v_{i,t} + v_j v_{i,j}) - \underline{\lambda\big[\rho_{,j} v_{i,j} + v_j \rho_{,ij}\big]} &= -P_{,i} + \mu \Delta v_i \\ &+ \rho f_i + \underline{\lambda^2 \left[\frac{\rho_{,i} |\nabla \rho|^2}{\rho^2} - \frac{\rho_{,j} \rho_{,ij}}{\rho} - \frac{\rho_{,i} \Delta \rho}{\rho} \right]} \end{aligned} \tag{14.79}$$

where P is a generalized pressure given by

$$P = -\lambda \rho_{,t} + p + \lambda(\mu_2 + 2\mu) \Delta(\log \rho).$$

The theory of (Kazhikhov and Smagulov, 1977) is derived by discarding the underlined $O(\lambda^2)$ terms in (14.79), while the (Graffi, 1955) theory discards both the $O(\lambda^2)$ and $O(\lambda)$ underlined terms. The full equation (14.79)gives rise to the (Beirao da Veiga, 1983) model.

For the present discussion we are interested in instability in a horizontal layer under the influence of a downward vertical gravitational field. Hence let $f_i = -g k_i$ where g is gravity and **k**=(0,0,1). The equations for gravity driven convective motion according to the three theories are now given. For the Graffi theory we have

$$\begin{aligned} &\rho(v_{i,t} + v_j v_{i,j}) = -p_{,i} + \mu \Delta v_i - \rho g k_i \\ &v_{i,i} = 0 \\ &\rho_{,t} + v_i \rho_{,i} = \lambda \Delta \rho. \end{aligned} \tag{14.80}$$

The Kazhikhov-Smagulov theory gives rise to

$$\begin{aligned} &\rho v_{i,t} + \rho v_j v_{i,j} - \lambda\big[\rho_{,j} v_{i,j} + \rho_{,ij} v_j\big] = -P_{,i} + \mu \Delta v_i - \rho g k_i\,, \\ &v_{i,i} = 0, \\ &\rho_{,t} + \rho_{,i} v_i = \lambda \Delta \rho\,. \end{aligned} \tag{14.81}$$

Finally the Beirao da Veiga theory leads to the system

$$
\begin{aligned}
\rho(v_{i,t}+v_jv_{i,j}) - \lambda\big[\rho_{,j}v_{i,j}+v_j\rho_{,ij}\big] &= -P_{,i}+\mu\Delta v_i \\
&\quad -\rho g k_i + \lambda^2\left[\frac{\rho_{,i}|\nabla\rho|^2}{\rho^2} - \frac{\rho_{,j}\rho_{,ij}}{\rho} - \frac{\rho_{,i}\Delta\rho}{\rho}\right], \\
v_{i,i} &= 0, \\
\rho_{,t}+\rho_{,i}v_i &= \lambda\Delta\rho\,.
\end{aligned}
\tag{14.82}
$$

The work of (Franchi and Straughan, 2001) concentrates on the Kazhikhov-Smagulov model, equations (14.81). They study a layer of a mixture governed by equations (14.81) occupying the domain $\{z \in (0,d),(x,y)\in\mathbb{R}^2\}$, with gravity in the negative $z-$direction. The density is supposed known at the upper and lower surfaces with $\rho=\rho_L,\ z=0$, $\rho=\rho_U,\ z=d$, where $\rho_L<\rho_U,\ \rho_L,\rho_U$ constants. Their objective is to determine a critical “Rayleigh” number, $Ra_c \propto d^3(\rho_U-\rho_L)$, for which the fluid will convectively overturn once the Rayleigh number exceeds Ra_c.

The boundary conditions of (Franchi and Straughan, 2001) keep the lower surface, $z=0$, fixed, and since the fluid is viscous, $v_i=0$ there. On $z=d$ the surface is free of tangential stress and remains horizontal. The free surface boundary conditions correspond to $t_1=t_2=0$ on $z=d$, where t_α are components of the stress vector $t_i=n_jt_{ij}$ where t_{ij} denotes the stress tensor. The steady solution which satisfies the boundary conditions is

$$
\bar\rho = \left(\frac{\rho_U-\rho_L}{d}\right)z+\rho_L\,, \qquad \bar v_i\equiv 0\,. \tag{14.83}
$$

The steady pressure $\bar P$ is a quadratic function of z, given by

$$
\bar P = -g\left(\frac{\rho_U-\rho_L}{2d}\right)z^2+\rho_L z+p_0,
$$

where p_0 is a constant reference pressure. Perturbations (u_i,ρ,π) to $(\bar v_i,\bar\rho,\bar P)$ are introduced. (Franchi and Straughan, 2001) investigate linearized instability of the Graffi and Kazhikhov-Smagulov models. These writers introduce the Rayleigh number, Ra, the Graffi number, G, and Prandtl number, Pr, by

$$
Ra=\frac{gd^3(\rho_U-\rho_L)}{\mu\lambda} \qquad G=\frac{\mu\lambda}{gd^3\rho_L} \qquad Pr=\frac{\mu}{\lambda\rho_L}
$$

and for convenience define $R=\sqrt{Ra}$. The perturbation equations for linearized instability in the Kazhikhov-Smagulov model, about the steady solution (14.83), in terms of non-dimensional variables become

$$
\begin{aligned}
&\sigma(1+GRa\,z)u_i+R\rho k_i-\frac{GRa}{Pr}\frac{\partial u_i}{\partial z} = -\frac{\partial\pi}{\partial x_i}+\Delta u_i, \\
&u_{i,i}=0, \\
&\sigma Pr\rho+Rw=\Delta\rho,
\end{aligned}
\tag{14.84}
$$

these equations holding on $\{(x,y)\in\mathbb{R}^2\}\times\{z\in(0,1)\}$. The free surface boundary condition is

$$\frac{\partial^2 w}{\partial z^2}+\frac{2GR}{(1+GRa)}\,\Delta^*\,\frac{\partial\rho}{\partial z}=0. \tag{14.85}$$

The analogous equations which one finds from the Graffi theory are

$$\sigma(1+GRa\,z)u_i+R\rho k_i=-\frac{\partial\pi}{\partial x_i}+\Delta u_i, \tag{14.86}$$
$$u_{i,i}=0, \tag{14.87}$$
$$\sigma Pr\rho+Rw=\Delta\rho, \tag{14.88}$$

in $\{(x,y)\in\mathbb{R}^2\}\times\{z\in(0,1)\}$, with the free surface boundary condition

$$\frac{\partial^2 w}{\partial z^2}=0,\qquad \text{on } z=1. \tag{14.89}$$

(Franchi and Straughan, 2001) show that for the Graffi theory $\sigma\in\mathbb{R}$. Hence, the instability problem for the Graffi theory reduces to the classical one for Bénard convection with the lower surface being fixed but the upper surface is free of tangential stress. For this case the critical Rayleigh number, Ra_c, for linear instability is given by $Ra_c=1100.65$. One should, however, observe that the Graffi equations (14.86) - (14.89) are *not* the same as those of the classical Bénard problem,

For the Kazhikhov-Smagulov model equations (14.84) may be reduced to the following equations in w and ρ,

$$\begin{aligned}&\sigma\left[(1+GRa\,z)\Delta+GRa\,\frac{\partial}{\partial z}\right]w+R\Delta^*\rho=\Delta\left[\frac{G\,Ra}{Pr}\,\frac{\partial}{\partial z}+\Delta\right]w,\\&\sigma Pr\rho+Rw=\Delta\rho.\end{aligned} \tag{14.90}$$

In (Franchi and Straughan, 2001) the Prandtl number is kept fixed at the value 6. However, we note that equations (14.90) are, *a priori*, strongly dependent on the Prandtl number. In this book we investigate the quantitative effect of the Prandtl number.

The eigenvalue problem (14.90), (14.85) is solved numerically by Chebyshev tau and compound matrix methods in (Franchi and Straughan, 2001) for the value of $Pr=6$. They find that for small diffusion, i.e. small Graffi number, the Rayleigh number increases and thus the effect of the Kazhikhov-Smagulov terms is one of inhibiting instability. However, as G increases further (Franchi and Straughan, 2001) find a dramatic effect. They discover that the instability threshold remains essentially constant for $G\le 0.035$. Then, Ra rises rapidly for increasing G, and indeed, they find that Ra_{crit} apparently becomes infinite for $G\to G_{crit}\approx 0.0487^+$. They interpret this phenomenon of Ra_{crit} becoming infinite for $G\to G_{crit}$ as meaning that for $G>G_{crit}$ there is never convective overturning with the model developed from the Kazhikhov-Smagulov theory. This conclusion in (Franchi and Straughan, 2001) is based on calculation with $Pr=6$.

In this book we find that G_{crit} is strongly dependent on the value of the Prandtl number Pr.

We now present new numerical computations which investigate the behaviour of the Rayleigh number against the Graffi number, but for various values of Prandtl number other than 6. We select the value of 0.72 since this is appropriate for the working fluid being air, see (Batchelor, 1967), p. 597. We also employ the values $Pr = 9.5$ and $Pr = 11.2$, these being appropriate to water at temperatures of 10°C and 5°C, respectively. Since we might interpret overturning instability results in air as being physically important we expect the curves displayed here to be useful. Likewise, many oceans and lakes possess temperatures in the range $5 - 10$°C and so our density driven instability results should be of practical value.

In figures 14.3 - 14.8 we present numerical findings for the instability curves with the Rayleigh number, Ra, graphed against the Graffi number, G. Figures 14.3, 14.4 are for $Pr = 9.5$ which corresponds to water at 10°C. Figures 14.5, 14.6 are for $Pr = 11.2$ which corresponds to water at 5°C, while figures 14.7, 14.8 have $Pr = 0.72$ which is a value appropriate to air. The first figure of each pair, figures 14.3, 14.5, 14.7, displays the instability curve for small values of G. In these figures there is instability above the curve. In each of these we see a similar trend. The Rayleigh number rises then dips slightly before rising again. This is consistent with the behaviour found in (Franchi and Straughan, 2001) for $Pr = 6$. Of course, the rate of increase as a function of G for G close to 0 depends very strongly on Pr. When $Pr = 0.72$ this increase is small whereas it is relatively rapid for $Pr = 11.2$. The second figure of each pair, figures 14.4, 14.6, 14.8, show the instability curves as far as we have been able to compute. In each of these we see a similar trend, again confirming what (Franchi and Straughan, 2001) discovered for $Pr = 6$. There is instability above the curve in each of these figures but in each there is a critical value of G, $G_{crit}(Pr)$, such that instability does not appear to be witnessed for $G > G_{crit}$. The value of G_{crit} is strongly dependent on the Prandtl number. For $Pr = 0.72$ we find $G_{crit} \approx 0.0058457^+$, for $Pr = 9.5$ we find $G_{crit} \approx 0.07708^+$, while for $Pr = 11.2$, $G_{crit} \approx 0.09087^+$. This is a more comprehensive study than that of (Franchi and Straughan, 2001) and certainly underlines the dependence of the Kazhikhov-Smagulov equations (14.84) on the Prandtl number. Of course, the Prandtl number itself is defined in terms of the diffusion coefficient λ.

To explain the apparent singular behaviour Ra displays at G_{crit}, (Franchi and Straughan, 2001) argue that the Kazhikhov-Smagulov theory neglects $O(\lambda^2)$ diffusion terms. Hence, the Kazhikhov-Smagulov model is likely to be realistic only for small G. Our computations bear this out for a range of Prandtl numbers.

To overcome the infinite Rayleigh number behaviour observed with the Kazhikhov-Smagulov model we believe one must return to the full Beirao da Veiga equations (14.79) and retain all λ and λ^2 terms in the ensuing

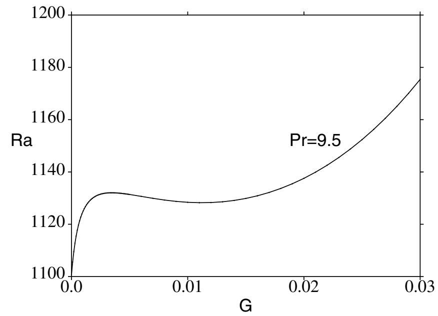

Figure 14.3. Rayleigh number, Ra, vs. Graffi number, G. Small G, $Pr = 9.50$.

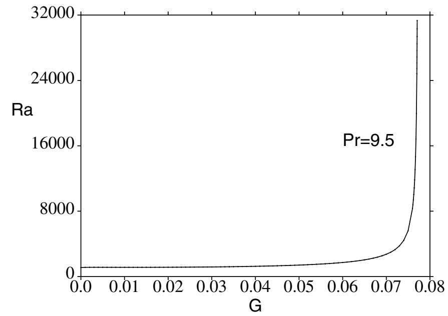

Figure 14.4. Rayleigh number, Ra, vs. Graffi number, G. Larger G, $Pr = 9.5$.

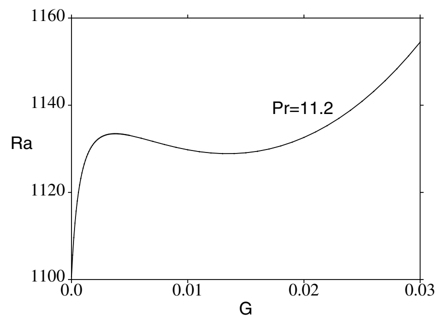

Figure 14.5. Rayleigh number, Ra, vs. Graffi number, G. Small G, $Pr = 11.2$.

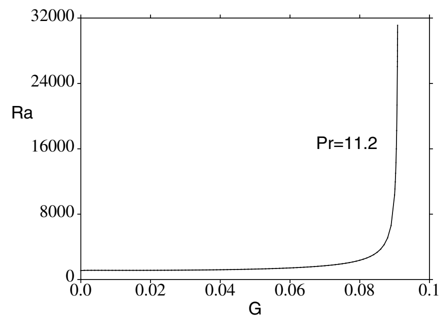

Figure 14.6. Rayleigh number, Ra, vs. Graffi number, G. Larger G, $Pr = 11.2$.

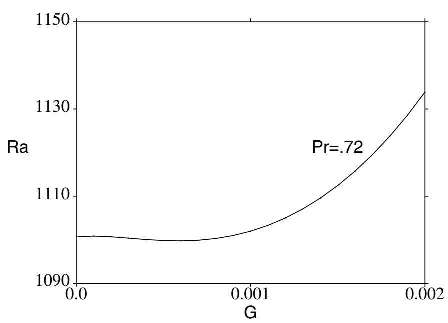

Figure 14.7. Rayleigh number, Ra, vs. Graffi number, G. Small G, $Pr = 0.72$.

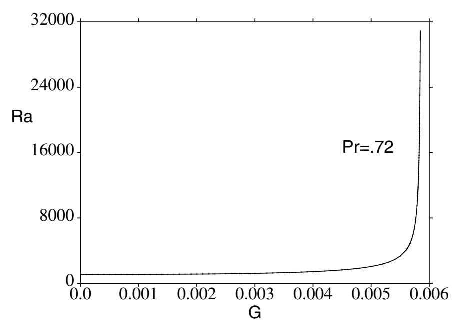

Figure 14.8. Rayleigh number, Ra, vs. Graffi number, G. Larger G, $Pr = 0.72$.

development. The linearized equations for top heavy pollution instability according to the Beirao da Veiga model (14.79) may be shown to be

$$\sigma\left[(1+G\,Ra\,z)\Delta w+GRa\,\frac{\partial w}{\partial z}+\frac{G^2R^3\Delta^*\rho}{(1+GRa\,z)}\right]+R\Delta^*\rho-\frac{GRa}{Pr}\,\Delta\frac{\partial w}{\partial z}$$
$$-\frac{G^3R^5}{Pr[1+GRa\,z]^2}\,\Delta^*\frac{\partial\rho}{\partial z}+\frac{G^2Ra^2}{Pr(1+GRa\,z)}\,\Delta^* w=\Delta^2 w,$$
$$\sigma Pr\rho+Rw=\Delta\rho.$$

The free surface boundary condition still has form

$$\frac{\partial^2 w}{\partial z^2}+\frac{2GR}{(1+GRa)}\,\Delta^*\,\frac{\partial\rho}{\partial z}=0,\qquad \text{on } z=1.$$

(Bresch et al., 2002) propose new Kazhikhov-Smagulov models and investigate questions of global existence of weak solutions.

14.4 Chemical convection

(Pons et al., 2000) review various chemistry experiments in which patterns are created in a layer of fluid due to chemical reactions inducing density gradients. They concentrate on a "blue bottle experiment" where the instability mechanism is gravity driven with the density being increased in the upper part of the fluid layer due to a chemical reaction. The reaction is an akaline oxidation of glucose by oxygen in which methylene blue acts as a catalyst and an indicator. The main oxidation product is gluconic acid and it is the accumulation of this in the upper layer of the fluid which initiates the convective overturning instability. The patterns which arise are very interesting.

A mathematical model for the experiment just outlined has been developed by (Bees et al., 2001). These writers refer to the instability thus arising as chemoconvection. Their model employs the Navier-Stokes equations with a Boussinesq approximation involving the density being a linear function of the concentration, A, of gluconic acid. Thus, they have

$$v_{i,t}+v_jv_{i,j}=-\frac{1}{\rho_0}\,p_{,i}-g\alpha Ak_i+\nu\Delta v_i,\qquad v_{i,i}=0 \tag{14.91}$$

where $\alpha=(\partial\rho/\partial A)|_{A_0}\rho_0^{-1}$ is the coefficient of expansion due to the dependence of ρ on gluconic acid. They study the situation of a free surface bounded below by a fixed surface corresponding to an experiment in an open Petri dish. (The effect of surface tension is neglected in (Bees et al., 2001).)

In addition to the balances of momentum and mass, equations (14.91), there are partial differential equations which describe the conservation of chemical species. These are given in the manner of interaction-diffusion equations of general form

$$C_{,t} + v_j C_{,j} = (D_C C_{,i})_{,i} + I_C \tag{14.92}$$

where C is the species concentration, allowance is made for variable diffusivity, D_C, and I_C represent the source terms for the reactions. The model of (Bees et al., 2001) involves four equations of type (14.92) for four chemical species believed dominant in the blue bottle reaction, namely the concentrations of the colourless reduced form of methylene blue, the blue oxidised form of methylene blue, gluconic acid, and oxygen, and these are denoted by W, B, A and Ω, respectively. Reasons for the precise forms of the interaction terms I_C which appear are given in (Bees et al., 2001). However, the relevant equations are

$$A_{,t} + v_i A_{,i} = (D_A A_{,i})_{,i} + k_2 B, \tag{14.93}$$
$$B_{,t} + v_i B_{,i} = (D B_{,i})_{,i} + 2k_1 \Omega W - k_2 B, \tag{14.94}$$
$$W_{,t} + v_i W_{,i} = (D W_{,i})_{,i} - 2k_1 \Omega W + k_2 B, \tag{14.95}$$
$$\Omega_{,t} + v_i \Omega_{,i} = (D_\Omega \Omega_{,i})_{,i} - k_1 \Omega W, \tag{14.96}$$

where k_1 and k_2 are reaction constants. (Bees et al., 2001) simplify their system by assuming that if $W + B$ is constant at some time, say $t = 0$, then by adding (14.94) and (14.95) one observes $W + B$ remains constant for all time. With this they eliminate W.

The seven equations (14.91) and what remains from (14.93) - (14.96) are non-dimensionalized with the groups $\kappa = 2k_1\Omega_0/k_2$, $\lambda = k_1 W_0/k_2$, $\delta = D_\Omega/D$, $\delta_A = D_A/D$, $Ra = g\alpha W_0 \bar{H}^3/\nu D$, $Sc = \nu/D$, where W_0 and Ω_0 are reference values of W and Ω and $\bar{H} = \sqrt{D/k_2}$ is a depth reflecting the depth of build up of gluconic acid near the open surface. The diffusion coefficients D, D_Ω and D_A are taken to be constant. The resulting non-dimensional equations are, (Bees et al., 2001),

$$Sc^{-1}(v_{i,t} + v_j v_{i,j}) = -P_{,i} - Ra\, A k_i + \Delta v_i, \tag{14.97}$$
$$v_{i,i} = 0, \tag{14.98}$$
$$A_{,t} + v_i A_{,i} = \delta_A \Delta A + B, \tag{14.99}$$
$$B_{,t} + v_i B_{,i} = \Delta B + \kappa\Omega(1 - B) - B, \tag{14.100}$$
$$\Omega_{,t} + v_i \Omega_{,i} = \delta\Delta\Omega - \lambda\Omega(1 - B), \tag{14.101}$$

holding on $\{(x, y) \in \mathbb{R}^2\} \times \{z \in (-d, 0)\} \times \{t > 0\}$. Here d is a scaled depth, so that $z = 0$ represents the upper (open) surface while $z = -d$ is the lower (fixed) surface. The boundary conditions are

$$v_i = 0, \qquad z = -d, 0, \tag{14.102}$$
$$\frac{\partial A}{\partial z} = \frac{\partial B}{\partial z} = \frac{\partial \Omega}{\partial z} = 0, \qquad z = -d, \tag{14.103}$$
$$\frac{\partial A}{\partial z} = \frac{\partial B}{\partial z} = 0, \quad \Omega = 1, \qquad z = 0, \tag{14.104}$$

together with free surface velocity boundary conditions at $z = 0$. The conditions on the chemical species are commensurate with no flux of A, B at the upper and lower surfaces, no flux of oxygen at the lower, and a continuous supply of oxygen at the upper surface, $z = 0$.

At this point (Bees et al., 2001) observe that the gluconic acid concentration never reaches steady state. They thus write

$$A(\mathbf{x}, t) =< A > (t) + a(\mathbf{x}, t)$$

where $< A >$ is a spatial average of A and $< a >= 0$. If we assume a spatial periodicity of the solution horizontal planforms then $< \cdot >$ may be interpreted as integration over a period cell V. The spatial average of (14.99) gives

$$\frac{\partial < A >}{\partial t} =< B >$$

and leads to

$$a_{,t} + v_i a_{,i} = \delta_A \Delta a + B- < B > .$$

The next step is to seek a steady solution to (14.97) - (14.104). (Bees et al., 2001) denote this steady solution by $v^i_{ss}(z), P_{ss}(z), a_{ss}(z), B_{ss}(z), \Omega_{ss}(z)$. They concentrate on a linearized instability analysis paying particular attention to stationary convection. The perturbations to this steady solution may be written as u_i, π, a, b, ω, where $v_i = v^i_{ss}(z) + u_i(\mathbf{x}, t)$, etc. We find it necessary to impose the constraint $< b >= 0$ to proceed. (This is, however, consistent with no flux boundary conditions.)

The linearized equations for stationary convection are presented in (Bees et al., 2001). However, if one goes through the requisite analysis we believe the following nonlinear perturbation equations may be deduced,

$$Sc^{-1}(u_{i,t} + u_j u_{i,j}) = -\pi_{,i} - Ra\, k_i a + \Delta u_i, \tag{14.105}$$

$$u_{i,i} = 0, \tag{14.106}$$

$$a_{,t} + u_i a_{,i} = -a'_{ss} w + \delta_A \Delta a + b, \tag{14.107}$$

$$b_{,t} + u_i b_{,i} = -B'_{ss} w + \Delta b + \kappa\big[\omega(1 - B_{ss}) - \Omega_{ss} b\big] - \underline{\kappa b \omega}, \tag{14.108}$$

$$\omega_{,t} + u_i \omega_{,i} = -\Omega'_{ss} w + \delta \Delta\omega - \lambda\big[\omega(1 - B_{ss}) - \Omega_{ss} b\big] + \underline{\lambda b \omega}, \tag{14.109}$$

where $'$ denotes d/dz. The boundary conditions are

$$\begin{aligned} &u_i = a_{,z} = b_{,z} = 0, \quad z = -d, 0; \\ &\omega = 0, \quad z = 0; \qquad \omega_{,z} = 0, \quad z = -d. \end{aligned} \tag{14.110}$$

As we have already stated, (Bees et al., 2001) develop a detailed linearized instability analysis of (14.105)-(14.110). They restrict attention to stationary convection, i.e. the growth rate σ in the linearized analysis is *a priori* set equal to zero. Oscillatory instabilities may be important in such a system. We add that it is not difficult to develop a *conditional* nonlinear energy stability analysis by multiplying (14.105) by u_i, (14.107) by a, (14.108) by

b, (14.109) by ω. The convective nonlinearities do not cause any problem and the conditional aspect arises only due to the $b\omega$ terms underlined in (14.108) and (14.109). Use of the Cauchy-Schwarz and Sobolev inequalities allows one to overcome these, but I have only seen how to obtain *conditional* nonlinear stability. One can form an equation for the variable $\phi = b + \kappa\omega/\lambda$ which removes the underlined quadratic terms. Whether a generalized energy analysis may be developed utilizing this variable, and which leads to *unconditional* nonlinear stability, is not clear to me.

We now mention recent work on swarming of bacteria in thin fluid films. This swarming behaviour may be regarded as an instability and since such effects are important in areas like food contaminantion the whole field is topical. (Bees et al., 2000) develop a very interesting model for the behaviour of the bacteria Serratia liquefaciens in a thin layer of growth culture. By studying the biology carefully they write down a model involving biological interactions and the fluid is described by a thin film approximation to the Navier-Stokes equations. The work of (Bees et al., 2000) is a stimulating paper in a very promising research area. They develop a numerical simulation using finite differences and to my knowledge no stability theory for their model has been developed.

To finish the present section we point out that nonlinear energy stability arguments, or Lyapunov functional arguments, have been effectively applied to Keller-Segel type biological models, see e.g. (Diaz and Nagai, 1995), (Diaz et al., 1989), (Gajewski and Zacharias, 1998), (Nagai et al., 1997), (Nagai et al., 2000), (Senba and Suzuki, 2000), (Senba and Suzuki, 2001). This represents an active and exciting area of research using energy stability arguments in bio-chemical systems and future work along these lines applied to models such as those of (Bees et al., 2000) will undoubtedly prove rewarding.

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