14

Additional applications of the Cahn-Hilliard model

14.1 Cahn-Hilliard equations: a characterization

It seems that before presenting a list of applications and contexts in which the Cahn-Hilliard equation arises, we must clarify a bit more precisely just what features we should like to see in an equation before we shall assert that the equation is indeed a *Cahn-Hilliard equation.* Although an absolute answer may not be so clear, we can give a working definition to be adopted throughout the present section.

In saying that a particular equation constitutes a *Cahn-Hilliard equation*, we should like the equation to be of the form:

$$u_t = \nabla \cdot Q(u)\nabla[f'(u) + \triangle u], \tag{14.1}$$

so that $\mu := f'(u) + \triangle u$ is the first variation of

$$\int_\Omega \{f(u) + \frac{1}{2}|\nabla u|^2\}\, dx, \tag{14.2}$$

where

(i_1) $Q(u) \geq 0$, and

(ii_1) $f(u)$ has the form of a double well potential; i.e., there exists $\{a, b\}$ such that $f(a) = f(b)$ and $f(u) > f(a) = f(b)$ for $u \neq a$ or b.

Here, $Q(u)$ and $f(u)$ are assumed to be smooth functions such that $Q \in \mathcal{C}(R)$ and $f \in \mathcal{C}^1(R)$, although, as we shall see shortly, somewhat less regularity can be required.

Note that equation (14.1) remains unchanged if $f'(u)$ is replaced by $f'(u) + \lambda$ where $\lambda \in R$ is arbitrary. This implies that the requirement (ii_1) is unnecessarily restrictive and can be replaced by the more general condition

Fig. 14.1. A sketch of the double tangency condition.

(ii$'_1$) there exists a constant $\lambda \in R$ such that

$$g(u) = f(u) + \lambda u \tag{14.3}$$

constitutes a double well potential.

Given then the function $f'(u)$, how is one to ascertain the existence of a suitable λ? Let us suppose for the moment that $f'(u) \in \mathcal{C}(R)$ and hence that $g(u)$ as defined by (14.3) is a smoothly defined $\mathcal{C}^1(R)$ function for any $\lambda \in R$. If $g(u)$ has the form of a double well potential with minima at $u = a$ and at $u = b$, then

$$\begin{cases} g(a) = g(b), \\ g'(a) = g'(b) = 0, \\ g(u) > g(a) = g(b) \ \text{ for } \ u \neq a \ \text{ or } \ b. \end{cases} \tag{14.4}$$

Hence (14.4) in conjunction with (14.3) implies that

$$\begin{cases} f(a) + \lambda a = f(b) + \lambda b, \\ f'(a) + \lambda = f'(b) + \lambda = 0, \\ f(u) + \lambda u > f(a) + \lambda a = f(b) + \lambda b \ \text{ for } \ u \neq a \ \text{ or } \ b. \end{cases} \tag{14.5}$$

From (14.5), we may conclude that

$$\frac{f(b) - f(a)}{b - a} = f'(a) = f'(b), \tag{14.6}$$

that there exists a line with slope $\lambda = \frac{f(a) - f(b)}{b - a}$ which is tangent to $f(u)$

at the points $u = a$ and $u = b$, and that the function $f(u)$ lies strictly above this line away from the points of tangency, a and b. If $f \in \mathcal{C}^1(R)$, and there exists a double tangent to $f(u)$, i.e. a straight line which lies below $f(u)$ which is tangent to $f(u)$ at precisely two points, then (14.6) holds, as does (14.5) with $\lambda = \frac{f(b)-f(a)}{b-a}$. Therefore (14.4) also holds with $g(u)$ defined via (14.3) with $\lambda = \frac{f(b)-f(a)}{b-a}$. Thus (14.5) can be considered as the formulation of a *double tangency condition,* and (ii_1') can be reformulated as

(ii_1'') $f(u)$ satisfies the double tangency condition (14.5). See Figure 14.1.

It is possible to generalize the discussion above to accommodate less smooth functions. Note that in the context of the double obstacle problem discussed in Section 10, $Q \in \mathcal{C}([a, b])$ and $f \in \mathcal{C}([a, b]) \cap \mathcal{C}^1((a, b))$, for some $-\infty < a < b < \infty$, and

(i_2) $Q(a) = Q(b) = 0$, $Q(u) > 0$ for $u \neq a$ or b,

(ii_2) the line

$$y(u) = \Big[\frac{f(b) - f(a)}{b - a}\Big]u + \Big[\frac{f(a)b - f(b)a}{b - a}\Big] \tag{14.7}$$

serves as a double tangent to $f(u)$ in *generalized sense* that $f(a) = y(a)$, $f(b) = y(b)$, $f(u) > y(u)$ for $u \in (a, b)$, and $y'(a)$ ($y'(b)$) belongs to the *tangent cone* [53] of $f(u)$ at $u = a$ ($u = b$).

It is also of some interest to make some intermediary considerations, since for example in the case of the degenerate Cahn-Hilliard equation, (i_2) and (ii_2) are satisfied with $0 < a < b < 1$, and (14.5) is satisfied for $u \in (0, 1)$. One possible example of such intermediary considerations, which shall be relevant in some of the examples which are given in the present chapter, can be stated as follows

There exist constants $\{a, b, c\}$, $\infty < a < b \le c \le \infty$, such that

(i_3) $Q \in \mathcal{C}([a, c])$, $Q(a) \ge 0$, $Q(u) > 0$ for $a < u < c$, and $Q(c) = 0$ if $c < \infty$, and

(ii_3) $f \in \mathcal{C}([a, c]) \cap \mathcal{C}^1((a, c])$, and (14.7) constitutes a double tangent to $f(u)$ in the generalized sense of (ii_2) discussed above.

If (i_3)-(ii_3) hold, it is easy to verify that λ, the slope of the double tangent line, satisfies

$$\lambda = \frac{f(b) - f(a)}{b - a} = -f'(b), \tag{14.8}$$

and tangency holds at b. Condition (14.8) constitutes an easy necessary condition which can be readily checked. The requirements in (i_3) on the vanishing of Q are imposed in order to guarantee that supp $u(x, t) \subset (a, c]$. It may or may not be necessary to require that $Q(a) = 0$; see the discussion in Chapter 11. An analogous discussion can be readily given with the rôles of a and b interchanged.

Within the framework of the existence theory, what regularity is required of $Q(u)$? of $f(u)$? Return after relevant sections are written, etc.

14.2 Biofilms

Recently Klapper & Dockery [58], have shown that the degenerate Cahn-Hilliard equation can arise in the context of modeling the structure of biofilms. The world is full of microorganisms such as bacteria, fungi, and protozoa, and commonly these microorganisms live within an organic structure known as a biofilm. For simplicity we shall refer to bacteria, although our conclusions are pertinent to many of other microorganisms which live within biofilms. Within the biofilm, the bacteria are encased within a matrix of extracellular polymers which they have excreted. This encasing layer allows the bacteria to thrive and allows them to protect themselves from disinfectants and other elements which might do them harm. These biofilms are to be found almost everywhere in our everyday surroundings, such as in kitchens, bathrooms, etc., and as such constitute a perhaps an all too unavoidable topic of interest. For an overview, see Costerton [24].

The model which is presented in [58], while it cannot explain biofilm generation, allows some of the key features of the structure of biofilms to be explained. According to their theory, the structure which can be seen in biofilms is a result of cohesion forces which also give rise to the "stickiness" of biofilms.

Let us now outline the key features of their model. The basis of their model is a two phase biomass-solvent theory, where the biomass phase includes both the bacteria and other ambient microorganisms as well as the extracellular encasing polymer material mentioned earlier. The variables $\phi_b(x, t)$, $\mathbf{u}_b(x, t)$ and $\phi_s(x, t)$, $\mathbf{u}_s(x, t)$, are employed, where ϕ_b and ϕ_s represent the volume fraction of the bacteria and of the solvent respectively, and $\mathbf{u}_b$ and $\mathbf{u}_s$ represent the velocities of the two phases, the bacterial phase and the solvent phase. Note that since ϕ_b and ϕ_s represent the volume fractions in a two phase flow model, they must

Fig. 14.2. A photo of a biofilm (details), reproduced curtesty of (details).

satisfy

$$\phi_b + \phi_s = 1. \tag{14.9}$$

Since a two phase flow model is being considered, mass conservation and momentum balance equations must be satisfied by each of the two phases. With regard to the mass conservation equations, taking the densities of the biomass phase, ρ_b, and of the solvent phase, ρ_s, to be constant, and neglecting any possible growth of one phase at the expense of the other, one obtains that

$$\frac{\partial \phi_b}{\partial t} + \nabla \cdot (\phi_b \mathbf{u}_b) = 0, \tag{14.10}$$

$$\frac{\partial \phi_s}{\partial t} + \nabla \cdot (\phi_s \mathbf{u}_s) = 0. \tag{14.11}$$

With regard to the momentum, neglecting inertial and convective effects, they propose to consider the equations

$$0 = \zeta(\mathbf{u}_b - \mathbf{u}_s) - \phi_b \nabla p + \phi_b \nabla \cdot \Pi^{(c)} + \nabla \cdot \Pi^{(b)}, \tag{14.12}$$

$$0 = -\zeta(\mathbf{u}_b - \mathbf{u}_s) - \phi_s \nabla p + \nabla \cdot \Pi^{(s)}. \tag{14.13}$$

Here $\Pi^{(c)}$, $\Pi^{(b)}$, $\Pi^{(s)}$ represent stress tensors, to be described shortly, p represents a hydrostatic pressure, and ζ represents a drag coefficient. The drag coefficient is taken to be of the form $\zeta = \zeta_0 \phi_s \phi_b$ where ζ_0 is a positive constant, since the drag effect can expect to vanish as the two phase flow degenerates into a one phase flow.

Their assumptions on the stress tensors may be explained as follows. Since the solvent can be expected to behave as a Newtonian fluid, clearly it is reasonable to take $\Pi^{(s)}$ as the standard Newtonian shear stress. Clearly also the stress tensor for the biomass phase must contain a component, which we shall denote here as $\Pi^{(b)}$, which represents the viscoelastic stress tensor of the biomass, and if the biofilm is being examined on a time scale which is not too short, then the elastic component in $\Pi^{(b)}$ may be neglected and $\Pi^{(b)}$ may also be taken as the standard Newtonian shear stress. A less classical element in the description of the stresses for the biomass phase is contained in the term $\Pi^{(c)}$, which perports to represent the stresses which arise as a result of cohesion (or "sticky") forces in the system. More specifically, the assumption is that there is a cohesion energy for the system which may be prescribed by

$$E = \int \{f(\phi_b) + \frac{1}{2}\kappa|\nabla\phi_b|^2\}\, dV, \tag{14.14}$$

where f is a homogeneous "cohesion" free energy, κ is a gradient energy coefficient, and $\Omega \subset R^n$, $n = 2, 3$, denotes the volume containing the two phase biomass/solvent layer. Within the context of biofilms, it is reasonable to assume that the "homogeneous cohesion free energy" $f(\phi_b)$ satisfies

(i) $f(0) = 0$,
(ii) $f(\phi_b)$ has a global minimum at $\phi_{b,0}$, and $\phi_{b,0} > 0$.
(iii) $f(\phi_b)$ has a unique inflection point at $\bar{\phi}_b$, where $0 < \bar{\phi}_b < \phi_{b,0}$,

Then, in analogy with the Cahn-Hilliard theory presented in §2, the "cohesion" stress tensor, $\Pi^{(c)}$, is taken to be the Fréchet derivative of the cohesion free energy, which can be interpreted as the "driving force" arising as a result of the tendency towards "local relaxation" of the cohesion energy. Assuming that there is no biomass flux into or out of the biofilm, then $\mathbf{n} \cdot \nabla(\phi_b \mathbf{u}_b) = 0$ along the boundary of Ω, and hence

$$\Pi^{(c)} \equiv \frac{\delta E}{\delta \phi_b} = f'(\phi_b) - \kappa \triangle \phi_b. \tag{14.15}$$

We now show how, by making certain reasonable assumptions, the equations above reduce under appropriate assumptions to the degenerate Cahn-Hilliard equation. Subtracting $\phi_b \times$ (14.13) from $\phi_s \times$ (14.12) and

Fig. 14.3. A sketch of a free energy which would be appropriate for modeling biofilms.

using (14.9), we find that

$$\mathbf{u}_b - \mathbf{u}_s = -\frac{1}{\zeta}[\phi_s \phi_b \nabla \cdot \Pi^{(c)} + \phi_s \nabla \cdot \Pi^{(b)} - \phi_b \nabla \cdot \Pi^{(s)}]. \tag{14.16}$$

Adding (14.10) and (14.11) and recalling (14.9), we obtain that

$$\nabla \cdot \mathbf{u} = 0, \tag{14.17}$$

where $\mathbf{u} \equiv \phi_b \mathbf{u}_b + \phi_s \mathbf{u}_s$ represents a mean velocity of the two phase flow system, and (14.17) expresses the incompressibility of the system in terms of the mean velocity. Adding (14.12) and (14.13), we get that

$$\nabla p = \phi_b \nabla \cdot \Pi^{(c)} + \nabla \cdot (\Pi^{(s)} + \Pi^{(b)}). \tag{14.18}$$

Note that (14.10) may be written in terms of $\mathbf{u}$ and $\mathbf{u}_b - \mathbf{u}_s$,

$$\frac{\partial \phi_b}{\partial t} + \nabla \cdot (\phi_b \mathbf{u}) = -\nabla \cdot [\phi_s \phi_b (\mathbf{u}_b - \mathbf{u}_s)]. \tag{14.19}$$

Using now (14.17), we obtain that

$$\frac{\partial \phi_b}{\partial t} + \mathbf{u} \cdot \nabla \phi_b = -\nabla \cdot [\phi_s \phi_b (\mathbf{u}_b - \mathbf{u}_s)]. \tag{14.20}$$

If, as is reasonable to assume for a two phase flow that is possibly undergoing phase separation, there is much more "relative" flow than "net" flow, then $|\mathbf{u}| \ll |\mathbf{u}_b - \mathbf{u}_s|$ and (14.20) is well approximated by

$$\frac{\partial \phi_b}{\partial t} = -\nabla \cdot [\phi_s \phi_b (\mathbf{u}_b - \mathbf{u}_s)]. \tag{14.21}$$

Substituting (14.16) into (14.21),

$$\frac{\partial \phi_b}{\partial t} = -\frac{1}{\zeta_0}\nabla \cdot [\phi_s \phi_b \nabla \cdot \Pi^{(c)} + \phi_s \nabla \cdot \Pi^{(s)} - \phi_b \nabla \cdot \Pi^{(s)}]. \tag{14.22}$$

Assuming now that the effects of the cohesion forces are large compared to the effects of the compressive stresses, (14.22) reduces to

$$\frac{\partial \phi_b}{\partial t} = -\frac{1}{\zeta_0}\nabla \cdot [\phi_s \phi_b \nabla \cdot \Pi^{(c)}]. \tag{14.23}$$

Recalling the definition of $\Pi^{(c)}$ and using (14.9), the degenerate Cahn-Hilliard equation,

$$\frac{\partial \phi_b}{\partial t} = -\frac{1}{\zeta_0}\nabla \cdot [\phi_b(1-\phi_b)\nabla \cdot \{f'(\phi_b) - \kappa \triangle \phi_b\}], \tag{14.24}$$

is obtained.

Exercises

14.1 Define

$$\bar{f}(\phi_b) = a\, \phi_b^3(\phi_b/4 - b).$$

a) Show that $\bar{f}(\phi_b)$ satisfies the conditions (i)-(iii) if a, $b > 0$.

b) Show that $\bar{f}(\phi_b)$ has a unique inflexion point and that it is located at $\phi_b = 2b$.

c) Show that there exists a unique value of ϕ_b^m such that

$$\phi_b^m \bar{f}'(\phi_b^m) = \bar{f}(\phi_b^m),$$

and that $\phi_b^m = 8b/3$.

d) Draw a phase diagram based on $\bar{f}(\phi_b)$ in terms of the variable b as a (temperature like) control parameter and the mean mass $\frac{1}{|\Omega|}\int_\Omega \phi_b \, dx$, indicating the spinodal, the limit of coexistence, and the stable region.

How is it that the applications and explanations are roughly the same, yet the scaling is so different?)

Fig. 14.4. A sketch of a thin layer of viscous film lying on a flat substrate in an inert gas.

14.3 An augmented thin film equation

The classical thin film equation

$$h_t + \frac{1}{\overline{c}}\nabla \cdot \left[\frac{h^3}{3}\nabla \triangle h\right] = 0, \tag{14.1}$$

was developed by Sharma & Ruckenstein [91] in 1986 to describe the time evolution of a thin film or layer of a viscous liquid on a flat surface, see Figure 14.4. Here $h = h(x, y, t)$ denotes the (dimensionless) height of the viscous film. The derivation of (14.1) is based on the Navier-Stokes equations and the lubrication approximation, as we shall explain shortly. The coefficient $\overline{c}$ in (14.1) is a *scaled capillary number* which can be prescribed more explicitly as $\overline{c} = (\frac{L}{a})^3 \frac{U_0 \mu}{\sigma}$, where a is a typical film height, L is a length scale characterizing spatial variation along the film, U_0 is a typical horizontal velocity, and μ and σ are respectively the viscosity and the surface tension, which are taken here to be constant.

Often, however, in many applications, additional physical effects are present which cannot be neglected to leading order. Such additional physical effects may include, for example, gravity, van der Waals forces, thermo-capillarity effects or evaporation. In such situations, (14.1) no longer adequately describes the evolution of the film height, though by considering the governing equations and re-running through the lubrication approximation arguments, it is often possible to obtain a suitable *augmented thin film equation.* For an overview of this approach, see the ample review article by Oron, Davis & Bankoff [84] which appeared in 1997. See also the discussion in [81] for background.

Such possibilities are of interest to us here in the context of this book since, when certain physical effects are taken into account, a *Cahn-Hilliard equation* arises as the resultant augmented thin film equation. This, in particular, is what happens when the effects of *gravity* and *thermo-capillarity* are taken into account. To be more specific, when gravitational and thermo-capillarity effects are taken into account, the equation

$$h_t+\frac{1}{\overline{c}}\nabla\cdot\Big[\frac{h^3}{3}\nabla\triangle h\Big]+\nabla\cdot\Big\{\Big[-\frac{1}{3}Gh^3+\frac{1}{2}MB\frac{h^2}{(1+Bh)^2}\Big]\nabla h\Big\}=0 \quad (14.2)$$

is obtained, where $\overline{c}$ is as defined earlier, $G=\frac{\rho g a^2}{\mu U_0}$ is a *gravitational coefficient*, $B=\frac{\alpha_{th}a}{k_{th}}$ is the *Biot number*, and $M=(\frac{\triangle\sigma}{\mu U_0})\frac{2\pi a}{\lambda}$ is a *Marangoni number.* In the definition of the Biot number, α_{th} and k_{th} denote the coefficients which appear in *Newton's cooling law*

$$k_{th}\nabla\theta\cdot\vec{n}+\alpha_{th}(\theta-\theta_\infty)=0, \quad (14.3)$$

which is assumed to hold along the upper surface of the thin film. In (14.3), θ denotes the value of the temperature along the upper surface of the film, θ_∞ denotes value of the temperature in the gas above the film, k_{th} is a coefficient of thermal diffusivity, α_{th} is a specific heat capacity, and $\vec{n}$ is a unit normal pointing outwards from the film along the gas-film interface. In the definition of the Marangoni number,

$$\triangle\sigma=\sigma_{|_{\theta_\infty}}-\sigma_{|_{\theta_0}}, \quad (14.4)$$

where θ_0 denotes the temperature of the solid substrate. With regard to the surface tension, the constitutive assumption that $\sigma=\sigma(\theta)$ has been adopted here to account for thermo-capillarity effects. In thin films heated from below, typically $\triangle\sigma>0$. See Figures 14.4 and 14.5.

We note that, as defined, B and G are positive, and as explained above, for films heated from below M can be expected to be positive. We shall now see that under the assumption that B, G, $M>0$, equation (14.2) has all the characteristics of a Cahn-Hilliard equation as outlined in Section 14.1. Let us rewrite (14.2) as

$$h_t+\nabla\cdot\Bigg[\Big(\frac{h^3}{3}\Big)\Big\{\frac{1}{\overline{c}}\nabla\triangle h-\Big[G-\frac{3}{2}\frac{MB}{h}\frac{1}{(1+Bh)^2}\Big]\nabla h\Big\}\Bigg]=0.$$

Fig. 14.5. The thermal boundary conditions above and below the thin viscous film.

In other words,

$$h_t = \nabla \cdot \Big[Q(h)\nabla\Big\{\frac{1}{\bar{C}}\triangle h + f'(h)\Big\}\Big], \tag{14.5}$$

where

$$Q(h) = \frac{1}{3}h^3,$$

and

$$f(h) = \frac{G}{2}h^2 - \frac{3}{2}MBh\ln\Big[\frac{h}{1+Bh}\Big].$$

By considering Figure 14.4, we see that in the context of thin films, it is necessary to require that $h = h(x,\, y,\, t) \geq 0$. Moreover, it would be reasonable to formulate a Cauchy problem with compact support or a boundary value problem with, say, periodic boundary conditions or Neumann and no flux boundary conditions.

We are thus led to consider the criteria of Section 14.1 for (14.5) to constitute a Cahn-Hilliard equation on the interval $[0,\, \infty)$. Note first that $Q(u) \in \mathcal{C}([0,\, \infty))$ with $Q(0) = 0$ and $Q(u) > 0$ for $u > 0$. With regard to $f(u)$, we note that $f(u) \in \mathcal{C}([0,\, \infty)) \cap \mathcal{C}^1((0,\, \infty))$, and that for $B,\, G,\, M\, > 0$,

$$f(0) = 0, \quad f(u) > 0 \quad \forall u > 0, \tag{14.6}$$

$$f''(0) = -\infty, \quad f''(\infty) > 0, \quad f'''(u) > 0 \quad \forall u > 0, \tag{14.7}$$

and that there exists a unique $h^* > 0$ such that

$$f(h^*) = h^* f'(h^*). \tag{14.8}$$

From (14.6)-(14.8) it can be concluded using (14.6) that the double tangency condition is satisfied with tangency at the points $u = 0$ and $u = h^*$. Therefore by the discussion in Section 14.1, $g(u) = f(h) - f'(h^*)h$ is a double well potential on $[0, \infty)$, and thus (14.2) constitutes a Cahn-Hilliard equation.

This would seemingly be the whole story, but in considering the derivation of the equation (14.2) we shall see that it is convenient to introduce a particular scaling so that the value $h = 1$ shall assume somewhat of a special rôle. More specifically, in [97] a was taken as the mean height of the film, which, in analogy with the earlier discussion of the mean mass, is a conserved quantity and hence affects, for example, the set of steady states which are accessible as $t \to \infty$. We shall now outline how (14.2) may be derived, indicating in the process the derivation of (14.1).

The derivation of (14.2) is based on the incompressible Navier-Stokes equations and an energy balance equation. The incompressible Navier-Stokes equations may be written as

$$\rho\Big[\frac{\partial}{\partial t}\vec{v} + [\nabla\vec{v}]\vec{v}\Big] = -\nabla p + \mu\triangle\vec{v} - \nabla\phi, \tag{14.9}$$

$$\nabla \cdot \vec{v} = 0, \tag{14.10}$$

where $\vec{v}$ is the fluid velocity, ρ, p, and μ are respectively the density, the pressure, and the fluid viscosity, and $\phi = \rho g z$ is a gravitational force potential and g is the gravity coefficient. The notation $\vec{v} = (u_1, u_2, w)$, with $\vec{v} = \vec{v}(\vec{x}, t)$ and $\vec{x} = (x_1, x_2, z)$, has been adopted, since the vertical and horizontal components of the flow play distinguished rôles in the context of thin films, see Figure 14.4. The density ρ is taken to be constant, and equation (14.10) is known as the *equation of continuity*. See e.g. Chorin & Marsden [21] or Temam [95] for a general discussion. The energy balance equation may be written as

$$\rho c\Big[\frac{\partial}{\partial t}\theta + \vec{v} \cdot \nabla\theta\Big] = k_{th}\triangle\theta, \tag{14.11}$$

where $\theta = \theta(\vec{x}, t)$ denotes the temperature field, and c and k_{th} denote respectively the heat capacity and the coefficient of thermal conductivity, which are taken to be constant.

Equations (14.9)-(14.11) are to be considered in conjunction with appropriate boundary conditions on the solid substrate and along the free surface. Along the solid substrate, $z = 0$, and reasonable boundary conditions to impose are

$$\vec{n} \cdot \vec{v} = 0, \tag{14.12}$$

$$u_i - \beta \frac{\partial u_i}{\partial z} = 0, \quad i = 1, 2, \tag{14.13}$$

$$\theta = \theta_0. \tag{14.14}$$

In (14.12), $\vec{n}$ denotes a unit normal vector to the solid substrate, and (14.12) expresses the inability of the fluid to penetrate into the solid substrate. Condition (14.13) corresponds to the *Navier slip condition*, and β is a slip coefficient which is assumed to be constant. Condition (14.14) states that the solid substrate is held at a uniform temperature, θ_0. We shall assume the free surface of the thin film to be single valued and expressible as $z = h(x_1, x_2, t)$. Reasonable boundary conditions along the upper surface are

$$w - \sum_{i=1}^{2} u_i \frac{\partial h}{\partial x_i} = \frac{\partial h}{\partial t}, \tag{14.15}$$

$$-p = \kappa\sigma, \tag{14.16}$$

$$T \cdot \vec{n} \cdot \vec{t_i} = \vec{t_i} \cdot \nabla\sigma \Big[1 + [\, \vec{t_i} \cdot \nabla h \,]^2 \Big]^{-1/2}, \quad i = 1, 2, \tag{14.17}$$

$$k_{th}\, \vec{n} \cdot \nabla\theta + \alpha_{th}(\theta - \theta_\infty) = 0. \tag{14.18}$$

Condition (14.15) is the *kinematic condition* which states that the normal velocity of the fluid at the free surface coincides with the normal velocity of the free surface. In (14.16), κ denotes the mean curvature of the free surface. Condition (14.16) is known as *Laplace's equation*, and expresses a balance of normal forces. The next condition, (14.17), expresses a balance of the tangential forces along the upper surface of the thin film, and in (14.17), T denotes the Newtonian stress tensor [44], $\vec{n}$ is a unit normal to the free surface pointing outwards, and $\vec{t_i}$, $i = 1, 2$ correspond to an ortho-normal basis for the tangent plane to the free surface at $z = h(x_1, x_2, t)$. The final condition, (14.18), is *Newton's cooling law,* which we saw earlier as (14.3).

A critical step in obtaining (14.2) from the equations above is to integrate the equation of continuity (14.10) with respect to z from $z = 0$ to

Fig. 14.6. A sketch of a slipper lubrication bearing.

$z = h$, and then to use the boundary conditions for w given in (14.12), (14.15) to obtain that

$$\frac{\partial h}{\partial t} + \sum_{i=1}^{2} \frac{\partial}{\partial x_i} \int_0^h u_i \, dz = 0. \tag{14.19}$$

To obtain (14.2) from (14.19), it is necessary to express u_i, $i = 1, 2$, in terms of h. This can be accomplished by making appropriate scaling assumptions, in particular by adopting scaling assumptions which correspond to the *lubrication approximation* made by O. Reynolds in 1886 in the context of modeling *slipper bearings* [30], see Figure 14.6. One assumption shall be that the spatial variations in $x_1 \times x_2$ plane are much smaller that the spatial variation in the vertical z direction. This assumption can be formulated by stating that $0 < \epsilon \ll 1$, where $\epsilon = \frac{a}{L}$. As mentioned earlier, a useful way to scale the film height is to take a as the mean film height,

$$a = \frac{1}{\Omega} \int_\Omega h_0(x_1, x_2) \, dx_1 \, dx_2, \tag{14.20}$$

where Ω is the domain of definition of the problem and $h_0(x_1, x_2)$ corresponds to some prescribed initial conditions for (14.2). However, for the discussion at hand, the assumption (14.20) is in no way essential. In accordance with the discussion above, the dimensionless scaled variables

$$X_i = \frac{\epsilon}{a} x_i, \; i = 1, 2, \quad Z = \frac{1}{a} z, \quad T = \frac{\epsilon U_0}{a} t, \tag{14.21}$$

are introduced, where the time scale has been chosen so as to reflect the time scale for spatial evolution in the $x_1 \times x_2$ plane. Moreover, we shall set

$$U_i = \frac{1}{U_0} u_i,\ i = 1,\, 2, \quad W = \frac{1}{\epsilon U_0} w, \quad H = \frac{h}{a}, \quad \Theta = \frac{\theta - \theta_\infty}{\theta_0 - \theta_\infty}. \tag{14.22}$$

For slipper bearings, the analysis of Reynolds identified $p_x \sim \mu \frac{\partial^2 u}{\partial z^2}$ as the dominant balance, see Figure 14.6. Assuming this dominant balance to remain valid also in the thin film setting, we set

$$(\Phi,\, P) = \frac{\epsilon a}{\mu U_0}(\phi,\, p), \qquad \text{and} \qquad \sum = \frac{\epsilon}{\mu U_0}\sigma. \tag{14.23}$$

The analysis now proceeds by assuming regular perturbation expansions in ϵ for U, W, P, H, Θ, and by assuming that Re, $\overline{c}$, B, M, G, and β_0 are all $\mathcal{O}(1)$ as $\epsilon \to 0$, where $\overline{c}$, B, M, and G are as previously defined earlier and $Re = \frac{\rho U_0 a}{\mu}$, $\beta_0 = \frac{\beta}{a}$. To leading the governing equations are

$$\frac{\partial^2 U_i}{\partial Z^2} = \frac{\partial}{\partial X_i}(P + \Phi), \quad i = 1,\, 2, \tag{14.24}$$

$$0 = \frac{\partial P}{\partial Z} + G, \tag{14.25}$$

$$\frac{\partial^2 \Theta}{\partial Z^2} = 0, \tag{14.26}$$

$$\frac{\partial H}{\partial T} + \sum_{i=1}^{2} \left[\int_0^H U_i \, dz \right] = 0, \quad i = 1,\, 2. \tag{14.27}$$

At $Z = 0$, the boundary conditions to leading order are

$$U_i - \beta_0 \frac{\partial U_i}{\partial Z} = 0, \quad i = 1,\, 2, \tag{14.28}$$

$$\Theta = 1, \tag{14.29}$$

and at $Z = H(X_1,\, X_2,\, T)$, to leading order

$$\frac{\partial U_i}{\partial Z} = \frac{\partial \sum}{\partial X_i}, \quad i = 1,\, 2, \tag{14.30}$$

$$-P = \frac{1}{\overline{c}} \sum_{i=1}^{2} \frac{\partial^2 H}{\partial X_i^2}, \tag{14.31}$$

$$\frac{\partial \Theta}{\partial Z} + B\Theta. \tag{14.32}$$

To obtain (14.2), one may proceed as follows. Using (14.25)-(14.26) and (14.29), (14.31), (14.32), P and Θ may be expressed in terms of $H = H(X_1, X_2, T)$. Then using these expressions as well as (14.24), (14.28), and (14.30), it is possible to express U in terms of H. Plugging this expression for U into (14.27), (14.2) is now obtained.

Note that setting $B = G = M = 0$ in the above discussion yields the "regular" thin film equation, (14.1).

Exercises

14.1 Adapt the existence proof given in Chapter 11 to prove existence for (14.5) with Neumann and no flux boundary conditions. What can be said here in regard to uniqueness?

14.4 The rings of Saturn

As fate would have it, the Cahn-Hilliard equation appears not only in the context of modeling very small structures, such as in the microstructure of binary alloys and in biofilms, but also in modeling some very large structures, such as in certain patterning features which have been seen in the inner "B" ring which revolves around the planet Saturn. Saturn has rings which are observable with even a light telescope, and there is an outer "A" ring and an inner "B" ring which are separated by a gap known as the Cassini divide. While these general features have been known since the time of Kepler (**Is this correct ??**), it is only since the 1980-1981 missions of Voyager I and II that the structure of these rings became known in some detail. More specifically, both the A and the B ring exhibit some amount of structural irregularity. The irregularities in the structure of the A ring can be readily explained by considering the interaction of the ring with impinging satellites, however this explanation cannot be used in explaining the structural irregularities of the B ring. This is because interactions with satellites leave characteristic trails in their wake, and while such trails are seen in the A ring, they are not to be found in the B ring.

A bit unexpectedly, the explanation for the irregularities in the B ring which has been proposed by Tremaine [98] has certain similarities with the explanation which was given earlier for biofilms in §14.2 and it is within this context that the Cahn-Hilliard equation again appears. The B ring has an inner width $x_1 \approx 92,000\,\text{km}$ and an outer width

$x_2 \approx 122,000$ km. The features in the B ring appear to be axi-symmetric on scales which are presently accessible which are on the order of 50 km or more, and certain radial striations are discernable with a dominant wavelength of about $100 - 200$ km. It has been suggested by Tremaine [98] that the radial striations represent a radial variation between regions of "liquid" and "solid" within the ring. The composition of the rings is known to be made up of particles of varying sizes with an upper cut off of a few meters, and whether a region is to be considered a liquid or a solid depends on how the particles are glued together. The distinction between snow, sleet, ice, and mush, in general, even on Earth, is of a similar nature, and the ability of the particles to stick together is determined by certain (weak) cohesive forces. It is, for example, precisely such weak cohesive forces that bond ice particles together which are covered by a layer of frost.

Before pursuing the line of explanation outlined above, we remark that independent estimates of the viscosity and the scale of these features which are seen indicate that the features would have been washed out by viscosity millenia ago were they not being actively sustained by some mechanism. Moreover, explanations which have been developed to explain structures which occur in accretion disks yield inappropriate estimates for the viscosity, density, and the spatial and temporal variation when applied to the B ring of Saturn. However, certain elements of the explanations which were developed in that context nevertheless reappear here.

To get started we need some governing equations, and in the present context it is not unreasonable to adopt a certain variant of the incompressible Navier-Stokes equations, known as Hill's approximation [99]. This approximation can be obtained by writing out the incompressible Navier-Stokes equations using a rotating Cartesian coordinate system (x, y) whose origin $(0, 0)$ rotates around a central mass M at a distance R with an angular velocity $\Omega_K(R)$, and $\hat{e}_x$ points radially outward from the origin and $\hat{e}_y$ points in the direction of rotation. Here $\Omega_K(R)$ is the "Keplerian" angular velocity of a particle rotating around a central mass due to gravitational effects. By considering radial distances from the origin which are small compared with R ("Hill's approximation"), ignoring vertical variation in the system, taking μ to be the surface density, and assuming the system to be axi-symmetric, the following system of equations is obtained:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 3\Omega^2 x + 2\Omega v + \frac{1}{\mu}\frac{\partial}{\partial x}\sum\nolimits_{xx}, \tag{14.1}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} = -2\Omega u + \frac{1}{\mu}\frac{\partial}{\partial x}\sum\nolimits_{xy}, \tag{14.2}$$

$$\frac{\partial \mu}{\partial t} + \frac{\partial}{\partial x}(\mu u) = 0. \tag{14.3}$$

Here $\mathbf{v}(\mathbf{x}, \mathbf{t}) = u(x, t)\hat{\mathbf{e}}_x + v(x, t)\hat{\mathbf{e}}_y$ is the velocity in the rotating frame and $\sum_{ik}$ are the components of the vertically integrated stress tensor.

To understand the implications of these equations, we first note that they admit certain special solutions. These include a solution with zero stress gradients in which

$$\begin{gathered} u = 0, \quad v = -3\Omega x/2, \quad \tfrac{\partial}{\partial t}\mu = 0, \\ \sum\nolimits_{xx} = \text{constant}_1, \quad \sum\nolimits_{\mathrm{xy}} = \text{constant}_2, \end{gathered} \tag{14.4}$$

which corresponds to the Keplerian orbit of a particle about a point mass. There is also a zero shear solution,

$$\begin{gathered} u = 0, \quad v(x, t) = v_s = \text{constant}_1, \quad \tfrac{\partial}{\partial \mathrm{t}}\mu = 0, \\ \sum\nolimits_{xy} = \text{constant}_2, \quad \tfrac{\partial}{\partial \mathrm{x}}\sum\nolimits_{\mathrm{xx}} = -\mu(2\Omega \mathrm{v_s} + 3\Omega^2 \mathrm{x}), \end{gathered} \tag{14.5}$$

which describes the motion of a solid rotating disk. While neither of these solutions quite correspond to the motion of rings about a planet, they can be used to obtain certain predictions. The constant shear solution (14.4), which neglects compressibility, is known to be stable and hence cannot explain the striations seen in the B ring of Saturn. Thus some compressibility is apparently necessary. The zero shear solution, (14.5), which allows for compressibility but neglects rigidity, can be used to estimate the strength of the material which comprises the B ring. Suppose that the tensile stress of a ring of radius $\triangle x \approx 100 - 200\,\mathrm{km}$ satisfies (14.5), and that the tensile stress vanishes along the edges of the ring, where $x = x_1$ and $x = x_2$. Then the maximal tensile stress can be estimated as $\approx 1 \times 10^4\,\mathrm{dyn\,cm^{-2}}$. This value is high for solid ice and low for water, but gives a feasible estimate for ice rubble in which there are cohesive forces due to a thin layer of frost on the ice particles. Assuming the value $1 \times 10^4\,\mathrm{dyn\,cm^{-2}}$ to be realistic, the tensile strength of the material can be understood to limit the size of the ring striations.

To analyse the system (14.1)-(14.3) in greater depth, one needs appropriate constitutive assumptions. Tremaine [98] suggests proceeding as follows. Clearly the stress should dependent on the tangential shear, $s \equiv v_x$ as well as on the density, given here in terms of the variable μ. Since the weak cohesive forces described earlier are non-Newtonian in nature, it makes sense to assume that $\sum_{xy} = \sum_{xy}(\mu,\, s)$ and $\sum_{xx} = \sum_{xx}(\mu,\, s)$, where $\sum_{xy}$ and $\sum_{xx}$ are nonlinear functions. More specifically, it is reasonable to assume that $\sum_{xy} = 0$ if $s = 0$, and that $\sum_{xy}$ and s should have the same sign, though $\frac{\partial}{\partial s}\sum_{xy}$ may change sign. In fact, if $\frac{\partial}{\partial s}\sum_{xy} < 0$, then making the assumptions mentioned above and linearizing about the special solution (14.4), certain known instabilities may be reproduced. With regard to $\sum_{xx}$, it could indeed change sign depending on whether the material being described was more like a liquid or more like a solid (ice), though this possibility shall not be critical to the discussion which follows.

The idea now is to focus on "striated" solutions of (14.1)-(14.3) which are somewhat like (14.5), but which exhibit locally periodic structure in the x direction. Thus we are led to look for solutions of the form

$$\mathbf{v} = (0,\, v(x,t)), \quad x \in [x_1,\, x_2], \tag{14.6}$$

such that

$$v(x_2,\, t) = v(x_1,\, t), \quad s(x_2,\, t) = s(x_1,\, t), \quad t > 0. \tag{14.7}$$

Using (14.6) in (14.1)-(14.3) yields

$$0 = 3\Omega^2 x + 2\Omega v + \tfrac{1}{\mu}\tfrac{\partial}{\partial x}\textstyle\sum_{xx}, \tag{14.8}$$

$$\tfrac{\partial v}{\partial t} = \tfrac{1}{\mu}\tfrac{\partial}{\partial x}\textstyle\sum_{xy}, \tag{14.9}$$

$$\tfrac{\partial \mu}{\partial t} = 0. \tag{14.10}$$

From (14.10) it follows that $\mu = \mu(x)$, and (14.8) can be interpreted as prescribing the constitutive relation for $\sum_{xx}$ in terms of $v(x,\, t)$ and $\mu(x)$. For simplicity we may consider solutions in which μ is x independent. Note that if we proceed as before and require that $\sum_{xx} = 0$ at $x = x_1$ and $x = x_2$, then (14.8) implies that

$$\sum\nolimits_{xx}(x,\, t) = -2\mu\Omega \int_{x_1}^{x} v(\bar{x},\, t)\, d\bar{x} + \frac{3}{2}\mu\Omega^2(x^2 - x_1^2), \tag{14.11}$$

and hence that

$$\int_{x_1}^{x_2} v(\bar{x},\, t)\, d\bar{x} = \frac{3}{4}\Omega(x_2^2 - x_1^2). \tag{14.12}$$

It remains now to focus on (14.9). Differentiating (14.9) with respect to x, we obtain that

$$\frac{\partial s}{\partial t} = \frac{1}{\mu}\frac{\partial^2}{\partial x^2} g(s), \tag{14.13}$$

where $g(s) = \sum_{xy}(s)$. The μ dependence has been dropped for simplicity from $\sum_{xy}$, since μ has been assumed to be constant. Note that the periodicity of $v(x, t)$ in (14.7) implies upon integrating (14.13) that

$$\frac{\partial}{\partial x} g(s(x_2, t)) = \frac{\partial}{\partial x} g(s(x_1, t)), \tag{14.14}$$

and the periodicity of $s(x, t)$ in (14.13) implies that

$$g(s(x_2, t)) = g(s(x_1, t)). \tag{14.15}$$

From (14.13) it follows that steady states of (14.13) must satisfy

$$g(s(x)) = ax + b,$$

where a and b are constants. From (14.14), it follows that $a = 0$.

Note now that if we linearize (14.13) about some typical value of s which we shall denote by s_K, and if we assume in conjunction with our earlier discussion that $g'(s_K) < 0$, we obtain within the context of linear theory

$$s_t = \frac{1}{\mu} g'(s_K) s_{xx},$$

which clearly corresponds to backwards diffusion. Thus is appears that we are in a Cahn-Hilliard like setting with $\epsilon = 0$, and the conditions to be satisfied by g should now to be formulated.

Since the term g represents a shear stress, the following assumptions seem reasonable:

(i) $g(s) = -g(-s)$ (changing the direction of the shear should change the sign of the shear stress),
(ii) $g(0) = 0$ (there is no stress if there is no shear),
(iii) $\operatorname{sgn} g(s)/s = 1$ (positivity of the viscosity).

A simple example of a function which satisfies these conditions is

$$g(s) = s(as^2 + b|s| + c), \quad a, c > 0, \; b > -(3ac)^{1/2}. \tag{14.16}$$

It is easy to check that (14.16) yields two spinodal parameter regions rather than one, see Figure 14.7. This, however, has little net effect on the double tangent construction considerations discussed in Section 14.1, see Exercise 1 for details.

Fig. 14.7. The function $g(s)$ from (14.16

Two steps remain to be undertaken to complete the theory above. Firstly, it is necessary to identify the natural source of a "regularizing term, such as the ϵs_{xxxx} term which appears in the Cahn-Hilliard context in order to obtain a well-posed problem (The original problem prior to approximation was seemingly well posed). Although there may be numerous ways in which this could be accomplished, and easy way to reproduce an ϵs_{xxxx} term would be to proceed as in the biofilm discussion given in §14.2, by introducing a "cohesion energy" which includes gradient terms. Here, though, gradient term would reflect gradients in the shear rather than in the concentration. The inclusion of shear gradient energies has, however, been suggested already many years ago in the context non-Newtonian fluid mechanics in modelling non-simple fluids, [101]. A second step could be to return to the more general setting of (14.13) to the wider setting of (14.1)-(14.3), and to consider stability of the solution which has been identified within the more limited setting of (14.13) within this wider framework.

Exercises

14.1 Consider the function $g(u)$ defined in (14.16). Demonstrate that for any a, b, and c which satisfy the conditions given there, the double tangency condition (14.6) described in Section 14.1 holds on two intervals, $\{A_i, B_i\}$, $i = 1, 2$, which are not intersecting.

14.2 Suppose that we include in (14.13) the fourth order regularizing term ϵs_{xxxx} discussed above. Can the resultant equation be considered a Cahn-Hilliard equation in accordance with the discussion given in Section 14.1? What expression assumes the rôle here of the "mean concentration," and what is its value?