

Homogenization of contact line dynamics

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Abstract

This paper considers the effects of substrate inhomogeneity on the motion of the three phase contact line. The model employed assumes the slowness of the contact line in comparison to capillary relaxation. The homogenization of this free boundary problem with a spatially periodic velocity law is considered. Formal multiple scales analysis yields a local, periodic problem whose time-averaged dynamics correspond to the homogenized front velocity. A rigorous understanding of the long time dynamics is developed using comparison techniques. Computations employing boundary integral equations are used to illustrate the consequences of the analysis. Advancing and receding contact angles, pinning and anisotropic motion can be predicted within this framework.

In many realistic circumstances, the static and dynamic wetting properties of liquids are substantially influenced by imperfections in the solid surface. Heterogeneities result in contact lines with a fine scale structure that may lead to pinning of the evolving front and hysteresis of the overall fluid shape.

Understanding the role that surface imperfections play is part of larger theoretical effort to determine the macroscopic manifestations of microscopic contact line features [4, 15, 40]. Classical fluid mechanics is by itself insufficient to describe the moving contact line [30], and the additional physical ingredients needed are still controversial. Modeling and theoretical studies include notions of slip boundary conditions [26, 28], continuum models [15, 43, 49], rheological modifications [25, 51], and atomistic simulations [19, 27] (see [4, 40] for more extensive accounts). There is also considerable

technological importance in understanding the role of wetting on patterned substrates [11, 17, 35, 46].

The model studied here is based on the slowness of the contact line in comparison to the time for capillary relaxation, known as the quasistatic limit. This represents possibly the simplest nontrivial global model for contact line motion, and therefore provides a good starting point for examining surface heterogeneity. In this limiting case, the fluid pressure is constant, and the fluid’s geometry can therefore be described as a “capillary” surface. Motion arises from an imbalance of surface forces at the contact line itself, which can be modeled by a constitutive velocity-contact angle law. This approximation has been utilized in many previous studies [2, 20–22, 26, 29, 31, 38, 41].

The static effects of surface heterogeneity have been studied for some time. Early heuristic theories considered the averaged effect of rough surfaces and chemical heterogeneities on the equilibrium contact angle [7, 52]. These laws have known limits of applicability, however ([4] Chapter 9, [3]). More recent studies have considered this problem from the point of view of mechanics [4, 32], statistics [14, 39], and gamma convergence techniques [1].

In the dynamic case, much less is understood. Flows over heterogeneous surfaces have been studied experimentally [11, 12, 36, 37, 45] and computationally [47, 48]. Theoretical arguments, on the other hand, have been limited to cases with simplified geometries [33, 44] or deal specifically with the dynamic coating transition [24].

Homogenization of free boundary and front propagation problems is an evolving field (see, e.g. [5, 9, 53]). The strategy we adopt is a combination of formal asymptotic calculations coupled with a detailed understanding of the “inner” or “cell” problem. The existence and uniqueness of the homogenized velocity is studied rigorously. A Green’s function formulation is used for numerical computation to illustrate the analytical results.

1 Problem formulation

We consider a fluid droplet on a macroscopically flat surface whose height is assumed to be a graph $h(x, y)$. The function h has bounded support Ω , whose boundary is the contact line Γ . In the small angle limit [6], the linearized contribution of surface energy is given by

$$\gamma \int_{\Omega} 1 + |\nabla h|^2 dx \tag{1}$$

where γ is the liquid-vapor surface energy, which is presumed constant here. The minimizer of this expression, subject to the constraint of constant volume, is the quasi-steady droplet shape. Finding the minimizer amounts to solving the Euler-Lagrange problem

$$\Delta h = \lambda, \quad h|_{\Gamma} = 0, \quad \int_{\Omega} h d\mathbf{x} = M \equiv \text{volume}, \quad (2)$$

where λ is a Lagrange multiplier, essentially just the negative hydrostatic pressure. We remark that body forces such as gravity can be added to this model [21] without compromising the homogenization procedure.

The “apparent” contact angle θ is defined on the boundary of Ω (again in the small angle limit) as

$$\theta = -\frac{\partial h}{\partial \mathbf{n}}, \quad \mathbf{n} = \text{outward normal of } \Gamma. \quad (3)$$

The motion of Γ is then specified by prescribing the normal velocity, denoted $d\Gamma/dt$, as a function of this angle and the spatial location of the contact line:

$$\frac{d\Gamma}{dt} = F(\theta; \mathbf{x}) = F(-\partial h/\partial \mathbf{n}; \mathbf{x}). \quad (4)$$

The function F is a constitutive law relating the contact line velocity to the apparent contact angle θ . Generally speaking, F must be continuous and an increasing function of θ so that there is a local “equilibrium” angle $\theta_e(\mathbf{x})$ where $F(\theta_e(\mathbf{x}); \mathbf{x}) = 0$. Some additional technical restrictions will be placed on F to obtain the rigorous results of section 4. Common examples found in the literature are

$$F = \theta^3 - \theta_e^3, \quad (\text{Cox [8], Voinov [50]}) \quad (5)$$

$$F = \theta(\theta^2 - \theta_e^2), \quad (\text{deGennes [16] }). \quad (6)$$

The spatial dependence of F arises as a consequence of substrate inhomogeneities. We focus here on two-dimensional periodicity with some small period ϵ :

$$F(\theta; \mathbf{x} + \epsilon \mathbf{k}) = F(\theta, \mathbf{x}), \text{ for all } \mathbf{k} \in \mathbb{Z}^2. \quad (7)$$

The purpose of this paper is to examine the homogenized limit $\epsilon \rightarrow 0$ by deriving an effective velocity law that is independent of ϵ .

The free boundary problem (2),(4) forms the basis for our study. While a complete and rigorous analysis has not been performed on this particular

model, it has much in common with well-understood problems such as zero surface tension Hele-Shaw flow [13, 34]. This paper’s scope is restricted just to smooth solutions of (2),(4). We anticipate that a generalized notion of non-smooth solutions is possible, akin to the theory of viscosity solutions which has been developed for a variety of second order nonlinear problems [10, 18, 34].

2 Formal multiple scales analysis

The goal of this paper is to derive a free boundary problem of the form (2),(4) in the limit $\epsilon \rightarrow 0$, where the contact angle-velocity relation is replaced by a homogenized version

$$\frac{d\Gamma}{dt} = F_{\text{hom}}(\theta, \mathbf{n}). \quad (8)$$

The dependence on the normal direction \mathbf{n} to the contact line stems from the anisotropy introduced by periodicity of F . In particular, F_{hom} will inherit the four-fold symmetry from the periodic heterogeneity. (Other types of periodicity, hexagonal, rhombic, etc. should of course lead to other types of symmetry in the homogenized velocity.) The strategy we adopt is to use a combination of spatial matched asymptotics and a multiple-scales ansatz in time to derive a dynamic “cell problem”. This problem must be solved independently, either analytically or numerically, and is studied at length in later sections.

Expansions in the interior of Ω (“outer problem”) and near the contact line Γ (“inner problem”) are sought. We will introduce the “fast” time variable $\tau = \epsilon^{-1}t$. For the outer problem (in the bulk of the droplet), the expansion has the form

$$h = H_0(\mathbf{x}, t) + \epsilon H_1(\mathbf{x}, t, \tau) + \mathcal{O}(\epsilon^2), \quad \lambda = \lambda_0 + \mathcal{O}(\epsilon). \quad (9)$$

At leading order, the boundary value problem (2) reads

$$\Delta H_0 = \lambda_0, \quad H_0|_{\Gamma_0} = 0, \quad \int_{\Omega_0} H_0 d\mathbf{x} = M \equiv \text{volume}, \quad (10)$$

where Ω_0, Γ_0 are the limiting values of support of h and contact line as $\epsilon \rightarrow 0$. The motion of Γ_0 will be deduced by asymptotic matching and time averaging.

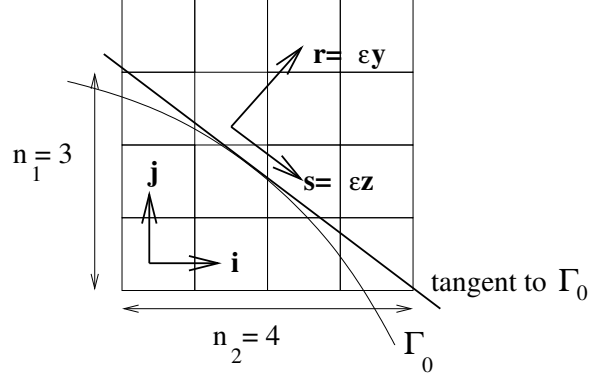


Figure 1: Coordinate system used for matched expansion. In this example, the normal vector is parallel to $3\mathbf{i} + 4\mathbf{j}$.

The contact line Γ is expanded in ϵ by supposing that it admits a local parameterization (with parameter η) of the form

$$\mathbf{g}(\eta, t) = \mathbf{g}_0(\eta, t) + \epsilon \mathbf{g}_1(\eta, t, \tau) + \mathcal{O}(\epsilon^2). \quad (11)$$

The leading order interface position Γ_0 is parameterized by $\mathbf{g}_0(\eta, t)$. The correction term \mathbf{g}_1 is meant to capture temporal fluctuations about the mean dynamics, and is therefore assumed bounded as $\tau \rightarrow \infty$. A time derivative of the boundary condition $h(\mathbf{g}(\eta, t), t) = 0$ yields

$$\frac{\partial h}{\partial t}(\mathbf{g}, t) + \frac{\partial h}{\partial \mathbf{n}}(\mathbf{g}, t) \left(\frac{\partial \mathbf{g}}{\partial t} \cdot \mathbf{n} \right) = 0. \quad (12)$$

In the multi-scale expansion, time derivatives become $\partial_t + \epsilon^{-1} \partial_\tau$; therefore expanding (12) in ϵ gives at leading order

$$\left(\frac{\partial H_0}{\partial t} + \frac{\partial H_1}{\partial \tau} \right) \Big|_{\Gamma_0} - \theta_M \left(\frac{\partial \mathbf{g}_0}{\partial t} + \frac{\partial \mathbf{g}_1}{\partial \tau} \right) \cdot \mathbf{n} = 0, \quad (13)$$

where \mathbf{n} is the normal to the leading order interface and we define the “macroscopic” contact angle as

$$\theta_M \equiv - \frac{\partial H_0}{\partial \mathbf{n}} \quad (14)$$

For the inner problem, a local rectilinear coordinate system (r, s) is used (see fig. 1). The coordinate s varies in direction tangent to a point $\mathbf{x}_0 \in \Gamma_0$

and r is in the negative normal direction so that $r > 0$ is the fluid's interior. We can suppose that the normal \mathbf{n} at \mathbf{x}_0 is in a “rational” direction, in other words $\mathbf{n} \parallel n_1 \mathbf{i} + n_2 \mathbf{j}$ where $n_1, n_2, \in \mathbb{Z}$. This ensures that F is periodic with period $\epsilon p_n \equiv \epsilon \sqrt{n_1^2 + n_2^2}$ in r and s .

We expect that small disturbances in the contact line with wavelength ϵ will lead to disturbances on the free surface which decay away into the interior exponentially in r/ϵ . This motivates an expansion near the contact line of the form

$$h = \epsilon h_1(y, z, \tau) + \mathcal{O}(\epsilon^2), \quad y = \epsilon^{-1} r, \quad z = \epsilon^{-1} s. \quad (15)$$

where h_1 is assumed p_n -periodic in z . We can define the “leading order” contact line as $\Gamma_\epsilon = \{h_1 = 0\}$. The moving boundary problem (2), (4) written in the inner coordinate system is to leading order

$$\Delta h_1 = 0, \quad h_1|_{\Gamma_\epsilon} = 0, \quad \frac{d\Gamma_\epsilon}{dt} = F(-\partial h_1 / \partial \mathbf{n}; y, z). \quad (16)$$

The velocity law is p_n periodic in y and z and it depends on the leading order normal direction \mathbf{n} :

$$F(\theta; y + k_1 p_n, z + k_2 p_n) = F(\theta; y, z) \text{ for all } (k_1, k_2) \in \mathbb{Z}^2 \quad (17)$$

The Laplace problem in (16) is solved in a simply connected subset of the channel $(-\infty, \infty) \times [0, p_n]$ which extends to $y = +\infty$ (see fig. 2). The boundary conditions on h_1 are

$$h_1(z, y, \tau) = h_1(z + p_n, y, \tau), \quad (18)$$

$$\lim_{y \rightarrow \infty} \frac{\partial h_1}{\partial y} = \theta_M = -\frac{\partial H_0}{\partial n}. \quad (19)$$

The first arises from the assumption of periodicity in z , whereas the far field boundary condition is given by matching so that the asymptotic slope of h_1 is the macroscopic contact angle θ_m .

To complete the analysis, the dynamics of the inner and outer solutions need to be connected. Computing $\partial h / \partial t$ for the both expansions and equating at order $\mathcal{O}(1)$ gives the matching condition

$$\frac{\partial h_1}{\partial \tau}(y, z, \tau) \sim \left(\frac{\partial H_0}{\partial t} + \frac{\partial H_1}{\partial \tau} \right) \Big|_{\Gamma_0}, \quad y \rightarrow \infty. \quad (20)$$

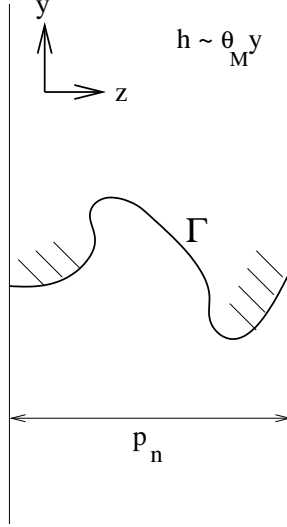


Figure 2: Diagram of the free boundary "cell" problem.

Using (13) this becomes

$$\lim_{y \rightarrow \infty} \frac{\partial h_1}{\partial \tau} = \theta_M \left(\frac{\partial \mathbf{g}_0}{\partial t} + \frac{\partial \mathbf{g}_1}{\partial \tau} \right) \cdot \mathbf{n}. \quad (21)$$

We can now average over the fast scale by applying $T^{-1} \int_0^T d\tau$ to equation (21)

$$T^{-1} \int_0^T \lim_{y \rightarrow \infty} \frac{\partial h_1}{\partial \tau} d\tau = \theta_M \frac{\partial \mathbf{g}_0}{\partial t} \cdot \mathbf{n} + T^{-1} \int_0^T \frac{\partial \mathbf{g}_1}{\partial \tau} \cdot \mathbf{n} d\tau \quad (22)$$

Taking the limits $\epsilon \rightarrow 0, T \rightarrow \infty$ in such a way that $T\epsilon \rightarrow 0$, the term involving \mathbf{g}_1 drops out since it is assumed bounded in τ . We obtain the homogenized front velocity

$$F_{\text{hom}}(\theta, \mathbf{n}) = \frac{\partial \mathbf{g}_0}{\partial t} \cdot \mathbf{n} = \theta_M^{-1} \lim_{T \rightarrow \infty} T^{-1} \int_0^T \lim_{y \rightarrow \infty} \frac{\partial h_1}{\partial \tau} d\tau, \quad (23)$$

where h_1 is found by solving the free boundary problem (16),(18), (19).

3 A comparison principle

The main tool for investigating the limit (23) is a comparison principle similar to the one used by Kim [34] to construct viscosity solutions of Hele-Shaw and

Stefan problems [34]. We focus here only on smooth solutions, which can be expected for mild heterogeneities. This makes the analysis considerably more transparent, although similar results should hold for nonsmooth solutions provided they obey the same comparison principle.

Following [34], we define notions of super- and subsolutions.

Definition 1 (*Super- and subsolutions*) *Suppose that $h(y, z, t)$ is a smooth function, p_n -periodic in z and $\{h > 0\}$ is a simply connected subset of $(-\infty, \infty) \times [0, p]$. Let $\Gamma(t) = \{h = 0\}$ be a smooth, nonintersecting curve which is differentiable in time (in the sense that it admits a differentiable parameterization). Then h is a supersolution (respectively subsolution) if*

1. $\Delta h \leq (\geq) 0$ on the set $\{h > 0\}$.
2. There exists y^* so that $h(y, z) > 0$ when $y > y^*$ and $\lim_{y \rightarrow \infty} \partial h / \partial y \geq (\leq) \theta_M$.
3. $d\Gamma/dt \geq (\leq) F(-\partial h / \partial \mathbf{n}; \mathbf{x})$ for $x \in \Gamma$.

We also have a notion of comparing two functions (typically super- or subsolutions).

Definition 2 (*separation of functions*) *Suppose that h_1, h_2 are smooth functions, p -periodic in z and $\{h_{1,2} > 0\} = \Omega_{1,2}(t)$ are simply connected subsets of $(-\infty, \infty) \times [0, p]$. Then if $\Omega_1(t)$ is a proper subset of $\Omega_2(t)$, we say that h_1 and h_2 are separated at time t , and write $h_1 \prec h_2$.*

It is convenient to rephrase the Laplace problem (16) by introducing the change of variables $w = h_1 - \theta_M y$ so that we have the boundary conditions

$$w|_{\Gamma_\epsilon} = -\theta_M y, \quad \lim_{y \rightarrow \infty} w(y, z) = w_\infty. \quad (24)$$

Note that the homogenized velocity can be written as

$$F_{\text{hom}}(\theta, \mathbf{n}) = \theta_M^{-1} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{dw_\infty}{dt} dt. \quad (25)$$

The far field value w_∞ should be regarded as an unknown of the problem, and can be bounded by the values w takes on Γ_ϵ :

Proposition 1 1. If w solves $\Delta w = 0$ on $\Omega(t)$ with boundary conditions (24),

$$\min_{\Gamma_\epsilon} w \leq w_\infty \leq \max_{\Gamma_\epsilon} w.$$

2. Let h_1 and h_2 be sub- and supersolutions, respectively. If $h_1 \prec h_2$ then for the corresponding functions $w_{1,2} = h_{1,2} - \theta_M y$ we have

$$\lim_{y \rightarrow \infty} w_1 \leq \lim_{y \rightarrow \infty} w_2.$$

Proof. For (1) The upper bound is obtained by setting $g = w - \max_{\Gamma_\epsilon} w$ and applying the Phragmén - Lindelöf principle ([42], p. 97), which gives $g \leq 0$ in Ω_ϵ . The lower bound is similar.

For (2), we observe that $w_2 + \theta_M y$ takes on nonnegative boundary values on any finite domain $\{h_2 > 0\} \cap \{y < y^*\}$, so it follows that $w_2 \geq -\theta_M y$ and $w_2 \geq w_1$ on $\{h_1 = 0\}$. The Phragmén - Lindelöf principle applied to $w_2 - w_1$ on the domain Ω_1 implies $w_1 > w_2$ in $h_1 > 0$. \square

We can now establish the main tool for analysis of the cell problem.

Proposition 2 (*Comparison principle*) Let h_1 and h_2 be sub- and supersolutions, respectively, and suppose that $h_1 \prec h_2$ at time $t = 0$. Then either $h_1 = h_2$ after some positive time or $h_1 \prec h_2$ for all $t > 0$.

Proof. Set $\Omega_{1,2} = \{h_{1,2} > 0\}$ and let $\Gamma_{1,2}$ be the respective boundaries. If $\Omega_1(t) \subset \Omega_2(t)$ does not hold for all $t \geq 0$, then there exists a maximal time T for which this happens, and a contact point $P \in \Gamma_{1,2}(T)$. It follows that the normal velocity of Γ_1 is greater than or equal to that of Γ_2 at P . The monotonicity of the velocity function F implies that at P ,

$$\frac{\partial h_1}{\partial n} \leq \frac{\partial h_2}{\partial n}. \quad (26)$$

The difference $h = h_1 - h_2$ satisfies Laplace's equation with the boundary condition $h = -h_2 \leq 0$ on Γ_1 . If $h \equiv 0$ on Γ_1 , then uniqueness implies that both solutions will remain identical for $t > T$. If not, proposition 1 implies there is a large y^* so that that $h(y, z) < 0$ if $y > y^*$. Then h must obtain its maximum on the boundary of the bounded domain $D = \Omega_1 \cup \{y < y^*\}$. This maximum can't occur on the periodic boundaries ($z = 0$ or $z = p_n$) of D . If it did, one could simply shift the domain in z so that the maximum point was in the interior. A maximum therefore occurs at the contact point P . Because of the assumed smoothness of the boundary of D , the Hopf maximum principle ([42], p. 65) shows that $\partial u / \partial n$ is strictly positive at the contact point P , which contradicts (26). \square

4 The homogenized front velocity

This section establishes the existence of the limit in (23) and explores some of its properties. The following assumptions are placed on $F(\theta, \mathbf{x})$ to get control over the front width:

- (1) $F(\theta, \mathbf{x})$ is continuous, strictly increasing in θ
- (2) For any $\theta_M > 0$, there exists constants $C_1, C_2, C_3 > 0$ so that

$$\mu - C_3 + C_1\theta \leq F(\theta, \mathbf{x}) \leq C_2 \left(\frac{\theta - \theta_M}{\theta_M} \right), \quad \mu = \min_{\mathbf{x}} F(\theta_M, \mathbf{x}). \quad (27)$$

The second condition ensures that (A) the front velocity will get large for steep contact angles and (B) the front recedes fast enough for shallow contact angles. Using (27), control over the front width can be obtained:

Proposition 3 (*Bound on front width*) *Suppose that $h(y, z, t)$, $\Gamma_\epsilon(t) = \{h = 0\}$ is a smooth, non-self-intersecting solution of (16) - (19). Let $W = \max_\Gamma y - \min_\Gamma y$. If the front velocity satisfies the conditions (27) there exists an upper bound B so that if $W(0) \leq B$, $W(t) \leq B$ for all $t \geq 0$.*

The proof of this is deferred to the Appendix.

We can now prove the main result of this section, which establishes the existence of the limit in (23).

Theorem 1 *Suppose that $h(y, z, t)$, $\Gamma_\epsilon(t) = \{h = 0\}$ is a smooth, non-self-intersecting solution of (16) - (19), whose initial front $\Gamma_\epsilon(0)$ has width smaller than the bound guaranteed by proposition (3). Then we have*

1. *The following limit exists (i.e. the long time average front velocity):*

$$F_{\text{hom}}(\theta_M, \mathbf{n}) = \theta_M^{-1} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{dw_\infty}{dt} dt. \quad (28)$$

2. *The limit is unique: F_{hom} is independent of the initial condition.*
3. *$F_{\text{hom}}(\theta_M, \mathbf{n})$ is nondecreasing in θ_M .*

Proof.

Existence of the limit. For a solution $h = w + \theta_M y$ define the channel-averaged interface position and average velocity as

$$\bar{y}(T) = \frac{1}{p_n} \int_{\Gamma_\epsilon(T)} y dz, \quad v(T) \equiv \frac{\bar{y}(0) - \bar{y}(T)}{T}. \quad (29)$$

Proposition (1) and the boundary conditions (24) imply that

$$\bar{y}(T) - B \leq -\theta_M^{-1} w_\infty(T) \leq \bar{y}(T) + B$$

where B is an upper bound on front width. Dividing by T , integrating and taking $T \rightarrow \infty$ we have

$$\lim_{T \rightarrow \infty} \frac{\bar{y}(0) - \bar{y}(T) - B}{T} \leq \theta_M^{-1} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{dw_\infty}{dt} dt \leq \lim_{T \rightarrow \infty} \frac{\bar{y}(0) - \bar{y}(T) + B}{T}$$

which implies the equality of limits

$$\lim_{T \rightarrow \infty} v(T) = \theta_M^{-1} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{dw_\infty}{dt}. \quad (30)$$

Since the front velocity $F(\theta, \mathbf{x})$ is bounded from below, we can define

$$v^* = \liminf_{T \rightarrow \infty} v(T).$$

For any $\delta > 0$, there is a time T_δ so that

$$v(T_\delta) \leq v^* + \delta. \quad (31)$$

Let M be a positive integer so that $\bar{y}(T_\delta) + B \leq Mp_n$. By periodicity, $h_1 = h(y - Mp_n, z, T - T_\delta)$ is also a solution. Using proposition 2, $h \prec h_1$ for all $T > T_\delta$. It follows that the position of front Γ_ϵ has the bound

$$\bar{y}(T) - \bar{y}(0) \leq n(\bar{y}(T_\delta) - \bar{y}(0)) + B + p_n, \quad (n-1)T_\delta \leq T \leq nT_\delta$$

for any $n \in \mathbb{Z}^+$. Dividing by T and using (29) and (31),

$$v(T) \leq \frac{n}{n-1}(v^* + \delta) + \frac{B + p_n}{(n-1)T_\delta}.$$

This implies that for any $\delta > 0$,

$$\limsup_{T \rightarrow \infty} v(T) \leq v^* + \delta$$

which shows that $\lim_{T \rightarrow \infty} v(T) = v^*$.

Uniqueness of the limit. Suppose that h_1 and h_2 are solutions and $v_1(T), \bar{y}_1(T)$, etc. are average velocities and front positions. We can ensure that $h_1 \prec h_2$

initially by a suitable periodic translation which does not affect the long time average (28). Since $h_1 \prec h_2$ for all time, it follows that for large T ,

$$v_1(T) = \frac{\bar{y}_1(0) - \bar{y}_1(T)}{T} \leq \frac{\bar{y}_2(0) - \bar{y}_2(T)}{T} + \frac{\bar{y}_1(0) - \bar{y}_2(0)}{T} \leq v_2(T) + O(T^{-1}). \quad (32)$$

Similarly, by a suitable periodic translation we could ensure that $h_1(t) \prec h_2(t)$ so that $v_2(T) \leq v_1(T) + O(T^{-1})$. It follows that the long time limits must be equal.

Monotonicity. Suppose that h_1 is any solution corresponding to $\theta_M = \theta_1$ with initially bounded front width. Let h_2 be a solution corresponding to $\theta_M = \theta_2 > \theta_1$. We can guarantee that $h_1 \prec h_2$ at time $t = 0$ by suitable periodic translation in y . With respect to $\Theta_M = \theta_1$, h_2 is a supersolution, so $h_1 \prec h_2$ for all time $t > 0$. It follows that $F_{\text{hom}}(\theta_1, \mathbf{n}) \leq F_{\text{hom}}(\theta_2, \mathbf{n})$. \square

5 Integral equations and numerical examples

The problem (16)-(19), (24) can be written as a pair of integral equations to expedite numerical simulation of the cell problem and computation of F_{hom} . The Green's function appropriate for an infinite channel with periodic boundary conditions (see also [29]) is

$$G(y, z) = \frac{1}{4\pi} \ln \left[\sin^2 \left(\frac{\pi z}{p_n} \right) \cosh^2 \left(\frac{\pi y}{p_n} \right) + \cos^2 \left(\frac{\pi z}{p_n} \right) \sinh^2 \left(\frac{\pi y}{p_n} \right) \right]. \quad (33)$$

Taking the inner product with $\Delta w = 0$ on the domain $\Omega_\epsilon \cap \{y < y^*\}$ gives the standard integral representation

$$\begin{aligned} \int_{\Gamma_\epsilon \cup \{y=y^*\}} w(y, z) \frac{\partial G}{\partial n}(y - y_0, z - z_0) - G(y - y_0, z - z_0) \frac{\partial w}{\partial n}(y, z) ds(y, z) \\ = \begin{cases} w(y_0, z_0) & (y_0, z_0) \in \text{int } \Omega_\epsilon \\ \frac{1}{2} w(y_0, z_0) & (y_0, z_0) \in \Gamma_\epsilon. \end{cases} \end{aligned} \quad (34)$$

where n is the outward normal.

As $y \rightarrow \infty$, we have the asymptotics $G \sim y/2p_n + o(1)$ and $w \sim w_\infty + o(1)$.

Taking $y^* \rightarrow \infty$ in (34) leads to

$$\begin{aligned} \frac{w(y_0, z_0) - w_\infty}{2} &= \int_{\Gamma_\epsilon} w(y, z) \frac{\partial G}{\partial n} (y - y_0, z - z_0) \\ &\quad - G(y - y_0, z - z_0) \frac{\partial w}{\partial n} (y, z) ds(y, z), \quad (y_0, z_0) \in \Gamma_\epsilon. \end{aligned} \quad (35)$$

A similar calculation taking $y^* \rightarrow \infty$ and then $y_0 \rightarrow \infty$ gives another equation

$$w_\infty = \frac{1}{p_n} \int_{\Gamma_\epsilon} y \frac{\partial w}{\partial n} - w n_y ds. \quad (36)$$

where n_y is the y component of the normal vector. Equations (35-36) form a system to be solved for unknowns $\partial w / \partial \mathbf{n}$, w_∞ . This allows the contact angle $\theta = -\partial w / \partial \mathbf{n} \cdot \theta_M n_y$ and the associated normal interface velocity to be computed. Other details concerning the discretization of integrals and the time stepping procedure have been reported elsewhere [21].

5.1 Example: array of large defects

The practical consequences of the theory which has been developed can now be illustrated. A simple nonuniform velocity law can be constructed using the Cox-Voinov law (5) where the equilibrium contact angle θ_e has spatial dependence. Assuming that the (y, z) coordinates are aligned with the underlying periodicity, this example supposes

$$\theta_e = \begin{cases} .6 & (z - \pi)^2 + (y - \pi)^2 < 1.5^2 \\ .3 & \text{otherwise} \end{cases} \quad (37)$$

With this orientation the (rescaled) spatial periodicity is taken as $p_n = 2\pi$. To investigate anisotropy, we also conducted simulations where the orientation was rotated by 45° and the corresponding spatial periodicity was $2\sqrt{2}\pi$. This particular example is meant to model a flow over a rectangular array of circular “defects” - regions which are less wetting than the rest of the solid surface. All computations used initial data that was just a flat interface $y = 0$, although the uniqueness of the homogenized velocity should mean that this choice is more or less inconsequential.

Figure 3 shows typical front evolution when the normal to the macroscopic front is aligned with the array. In figure 4 the normal is instead at a 45° -angle

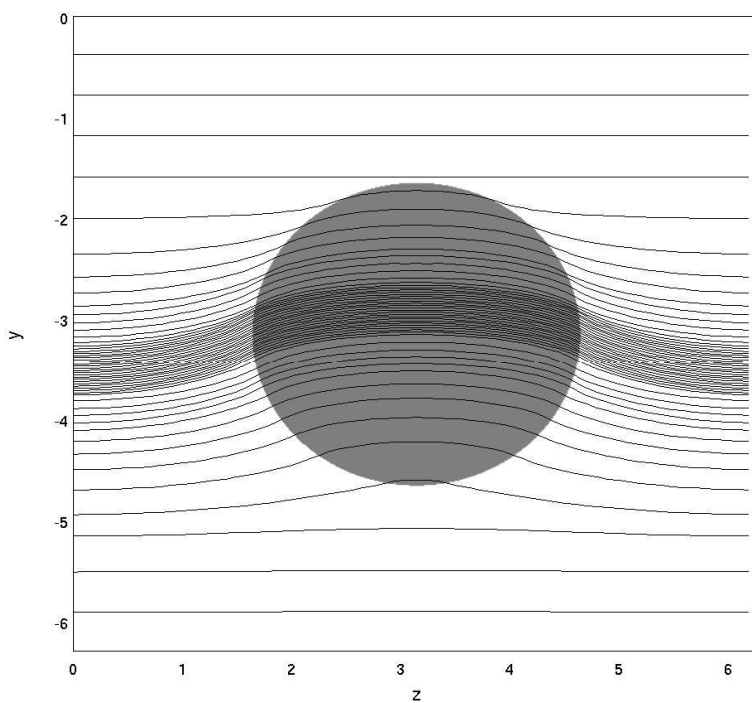


Figure 3: Front motion when $\theta_m = .48$, slightly above the pinning threshold. The y coordinate is aligned with the underlying spatial periodicity in this example. The shaded regions are where the contact angle is higher (less wetting). Contours are roughly spaced in equal time intervals.

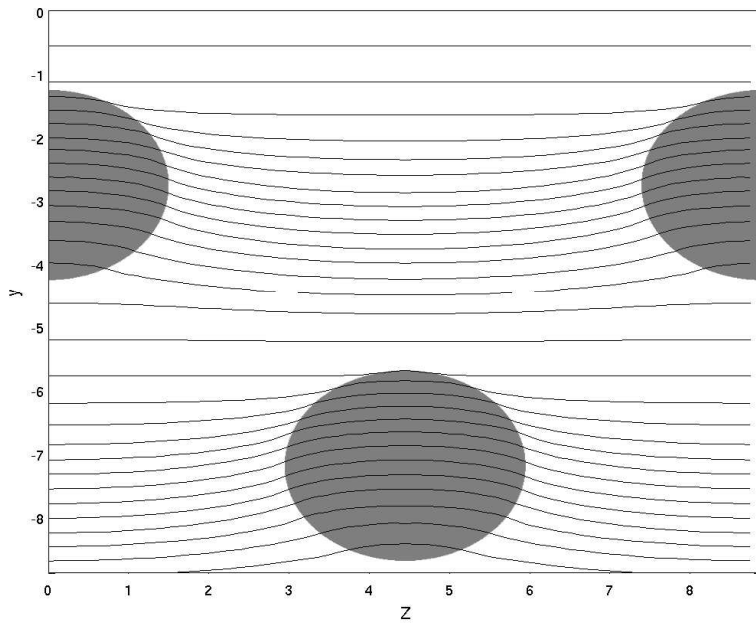


Figure 4: Front motion when the y coordinate is oriented at a 45° angle to the underlying spatial periodicity ($\theta_m = 0.48$).

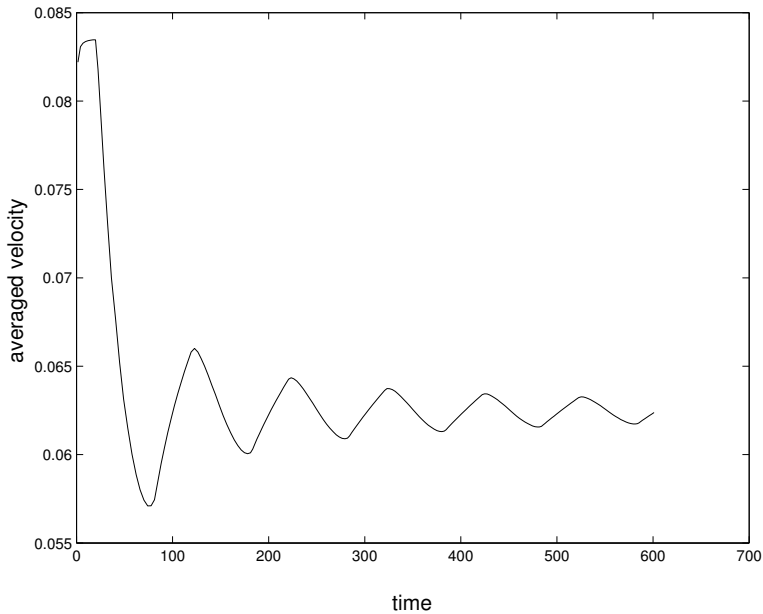


Figure 5: Time averaged front velocity as a function of time ($\theta_m = .48$).

to the array. The time averaged front motion (see 29) typically oscillates and converges (somewhat slowly) to a long time limit (figure 5). Nonlinear regression was used to extrapolate this limit to avoid unnecessarily lengthy computation.

The long-time averaged velocities $F(\theta_m, \mathbf{n})$ were computed for many values of θ_M for both orientations (figure 6). Over a closed interval of θ_M , the front is pinned and the averaged velocity is zero. The endpoints of this interval can be thought of as the receding and advancing contact angles. Anisotropy is present in both the overall velocities and in the interval on which pinning occurs. Experiments on periodically structured surfaces have also found this [12, 23].

5.2 Example: small randomly placed defects

As a second more elaborate example, we consider smaller randomly placed defects, (still arranged periodically), with the same velocity law (5). Figure 7 shows typical front motion. The homogenized front speed (figure 8) was computed as before. The pinning interval is markedly smaller than the

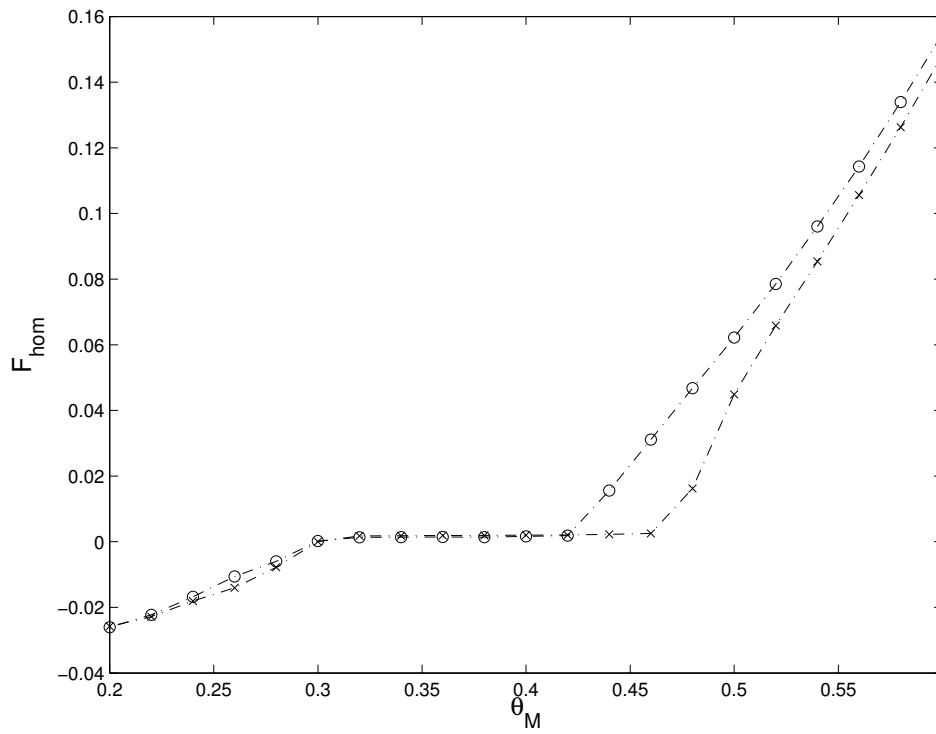


Figure 6: Homogenized front velocities. The x's denote computations for orientation angle 0° and the circles for orientation angle 45° .

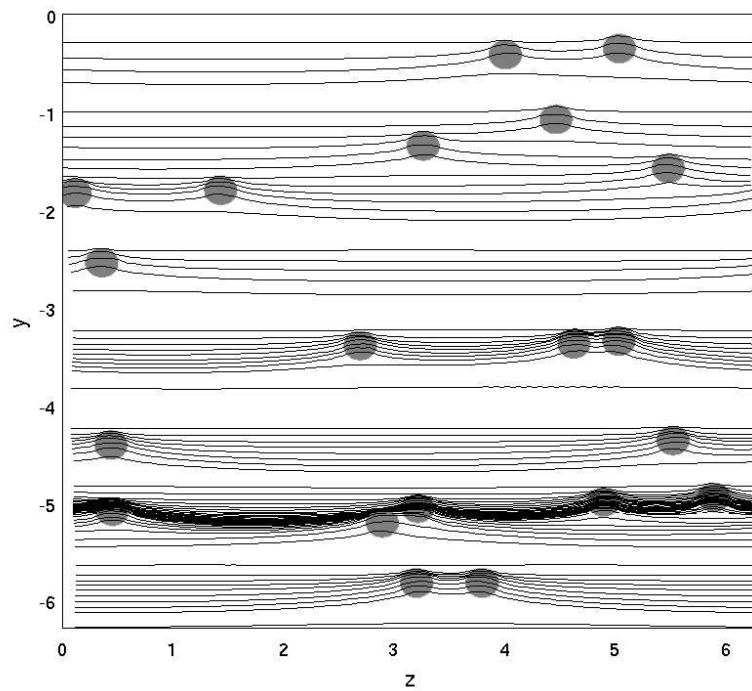


Figure 7: Front motion for $\theta_m = 0.5$. There were 20 defects of radius 0.15. Slowing of the front around defects is modified by the lateral spacing.

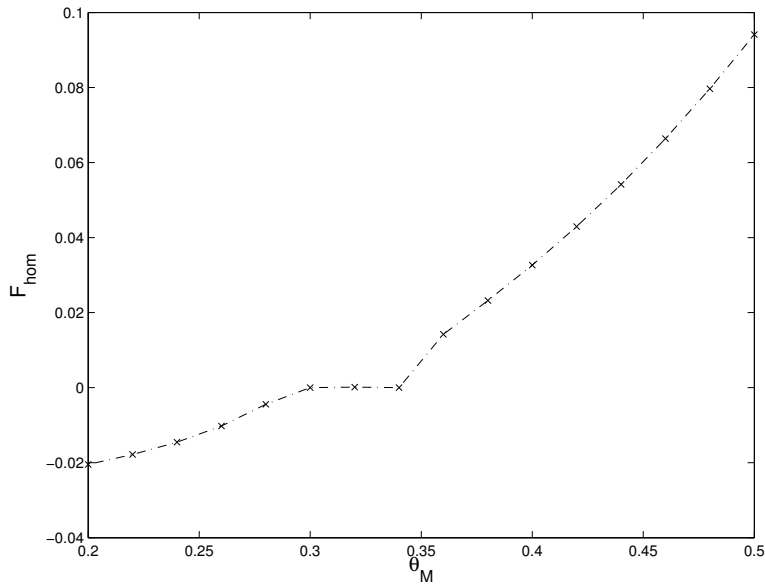


Figure 8: Homogenized front velocities for the case of many defects. The x's denote actual computations, and the dashed line is an interpolation.

case with larger defects. The average front motion is, on the other hand, quantitatively similar.

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Appendix: proof of bound on front width

The proof relies on comparison functions which control the normal derivatives at extreme points on Γ . Constants C, β are generic and assumed independent of W .

Proof. Let $(x_m, y_m), (x_M, y_M) \in \Gamma$ be points on the interface where the minimum and maximum, respectively, of y is achieved. Then w is harmonic in $[0, p] \times [y_M, +\infty)$ and has a Green's function representation

$$w(x_0, y_0) - w_\infty = \int_0^p G_0(x, y_M, x_0, y_0)(w(x, y_M) - w_\infty)dx, \quad y_0 > y_M$$

where $G_0 = G(x, y, x_0, y_0) - G(x, -y, x_0, y_0)$. It is easily verified that G_0 satisfies a bound of the form $\|G_0\|_{L^1(x)} < C \exp(-\beta y)$, so it follows that w satisfies a pointwise estimate

$$\begin{aligned} |w(x, y) - w_\infty| &\leq C \|w(x, y_M) - w_\infty\|_{L^\infty} \exp(-\beta[y - y_M]) \\ &\leq C \theta_M W \exp(-\beta[y - y_M]). \end{aligned} \quad (38)$$

In the last step the maximum principle was used to obtain $|w - w_\infty| \leq \max(|w_\infty + \theta y_m|, |w_\infty + \theta y_M|) \leq W \theta_M$.

We now construct the linear comparison functions

$$u_1 = -\theta_M y_m + s_1(y - y_m), \quad s_1(L) = \frac{C \theta_M W \exp(-\beta[L - y_M]) + \theta_M y_m + w_\infty}{L - y_m} \quad (39)$$

$$u_2 = -\theta_M y_M + s_2(y - y_M), \quad s_2(L) = \frac{-C \theta_M W \exp(-\beta[L - y_M]) + \theta_M y_m + w_\infty}{L - y_M} \quad (40)$$

for some parameter L which will be determined. Using the estimate (38), the maximum principle implies that $u_2 \leq w \leq u_1$ on the domain $\Omega \cup [0, p] \times [y_m, L]$. In particular, $w = u_1$ at (x_m, y_m) and $w = u_2$ at (x_M, y_M) so that the normal derivatives at the extreme points satisfy

$$\frac{\partial w}{\partial y}(x_m, y_m) \leq s_1(L), \quad L > y_M, \quad (41)$$

$$\frac{\partial w}{\partial y}(x_M, y_M) \geq s_2(L), \quad L > 0. \quad (42)$$

To make the rest more attractive, introduce $\rho = (y_M + w_\infty/\theta_M)/W$. The maximum principle implies $-\theta_M y_M \leq w_\infty \leq -\theta_M y_m$ so that $0 \leq \rho \leq 1$.

For the first estimate, set $\lambda = (L - y_m)/W$ so that

$$\frac{\partial w}{\partial y}(x_m, y_m) \leq \theta_M \frac{C \exp(-\beta W[\lambda - 1]) + \rho - 1}{\lambda}, \quad \lambda > 0. \quad (43)$$

Now choose λ so that $C \exp(-\beta W[\lambda - 1]) = 1/W$, which gives

$$\frac{\partial w}{\partial y}(x_m, y_m) \leq \theta_M \frac{1/W + \rho - 1}{1 + \ln(CW)/(\beta W)} \leq \theta_M (1/W + \rho - 1) \quad (44)$$

for large enough W . For the second estimate, set $\lambda = (L - y_M)/W$ and obtain

$$\frac{\partial w}{\partial y}(x_M, y_M) \geq \theta_M \frac{\rho - C \exp(-\beta W \lambda)}{\lambda}, \quad \lambda > 0. \quad (45)$$

Choosing λ so that $C \exp(-\beta W \lambda) = 1/W$ gives

$$\frac{\partial w}{\partial y}(x_m, y_m) \geq \theta_M \frac{W\rho - 1}{\ln(CW)/\beta}. \quad (46)$$

Finally, (44), (46) and (27) are combined to give a bound on dW/dt :

$$\begin{aligned} dW/dt &= f(\theta_M + dw/dy(x_m, y_m), x_m, y_m) - f(\theta_M + dw/dy(x_M, y_M), x_M, y_M) \\ &\leq C_1 \theta_M (1/W + \rho) - C_3 + C_2 \frac{1 - W\rho}{\ln(CW)/\beta}. \end{aligned} \quad (47)$$

For large enough W , this expression is negative for all $\rho \in [0, 1]$. \square

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