Second model

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January 2020

Geometry

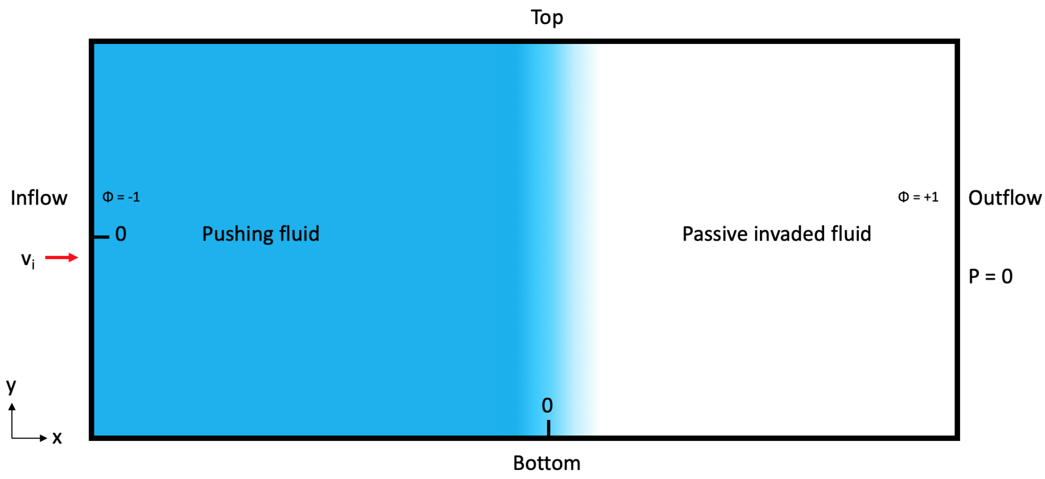

Figure 1: Geometry of the system

Simplifications

In this first model, we set $k = 0$ and $\alpha = 0$. The 'growth' of the fluid is due to an inflow on the left of the space.

Equations

$$\vec{\nabla} p + \phi \vec{\nabla} \mu = -\beta \theta_c(\phi) \vec{v}$$

$$\vec{\nabla} \cdot \vec{v} = 0$$

$$\frac{\partial \phi}{\partial t} + (\vec{v} \cdot \vec{\nabla}) \phi = M \nabla^2 \mu$$

$$\mu = \frac{\kappa}{\xi^2}(\phi^3 - \phi) - \kappa \nabla^2 \phi$$

Parameters

- β passive friction of the fluid on the left (pushing)
- $\theta(\phi) = \frac{1}{2}[(1-\phi)+(1+\phi)\theta]$ linear continuous dimensionless friction coefficient (linear from [1–3] but no justification)
- $\theta = \frac{\beta'}{\beta}$ friction ratio, has to be > 1 (less viscous invading more viscous)
- M is the mobility of the phase (here taken as a constant [2, 4], can be $M(\phi) \sim 1-\phi^2$ [1, 3])
- κ is the mixing energy
- ξ is the width of the interface

Initial conditions

For the phase

$$\phi(\vec{r}, t=0) = \phi_0(x) = tanh\left(\frac{x}{\sqrt{2}\xi}\right)$$
$$\mu(\vec{r}, t=0) = 0$$

For the flow

$$\vec{v}(\vec{r}, t=0) = v_i\hat{x}$$
$$p(\vec{r}, t=0) = P_{in}(\frac{1}{2} - \frac{x}{L}) \ \ (L\ length\ of\ the\ box)$$

Boundary conditions

For the phase

$$\vec{\nabla}\phi(\vec{r}, t) \cdot \vec{n} = 0\ on\ \partial\Omega_{t/b}$$
$$\vec{\nabla}\mu(\vec{r}, t) \cdot \vec{n} = 0\ on\ \partial\Omega_{t/b}$$
$$\phi = -1\ on\ \partial\Omega_{left}$$
$$\phi = +1\ on\ \partial\Omega_{right}$$
$$\mu = 0\ on\ \partial\Omega_{left/right}$$

For the flow

$$\vec{v}(\vec{r}, t) = v_i\hat{x}\ on\ \partial\Omega_{left}$$
$$p(\vec{r}, t) = 0\ on\ \partial\Omega_{right}$$
$$\vec{v} \cdot \vec{n} = 0\ on\ \partial\Omega_{top/bottom}$$
$$\vec{\nabla}p \cdot \vec{n} = 0\ on\ \partial\Omega_{top/bottom}$$

Dimensionless

New dimensionless parameters

- $l = \sqrt{\frac{\gamma}{\beta v_i}}$
- $\tau = \frac{l}{v_i}$
- $p^* = \beta l v_i$
- $\mu^* = \frac{\kappa}{\xi^2}$
- $\theta = \frac{\beta'}{\beta}$
- and we have $\gamma = \frac{2\sqrt{2}}{3}\frac{\kappa}{\xi}$

Dimensionless equations

For the flow

$$\vec{\nabla} p + \frac{\mu^*}{\beta l v_i}\phi\vec{\nabla}\mu = -\theta_c(\phi)\vec{v}$$
$$\vec{\nabla}\cdot\vec{v} = 0$$

For the phase

$$\frac{\partial\phi}{\partial t} + \vec{v}\cdot\vec{\nabla}\phi = \frac{M\mu^*}{l_v i}\nabla^2\mu$$
$$\mu = \phi^3 - \phi - \frac{\xi^2}{l^2}\nabla^2\phi$$

Dimensionless numbers

Cahn number

We introduce the Cahn number [1, 2, 5, 6] $K = \frac{\xi}{l}$

Capillary number [2, 5]

$$\frac{\mu^*}{\beta v_i l} = \frac{\kappa}{\xi^2\beta v_i l} = \frac{3}{2\sqrt{2}}\frac{\gamma}{\xi\beta l v_i}$$

Capillary number $Ca = \frac{viscous}{surf.tension}$

$$Ca = \frac{2\sqrt{2}}{3}\frac{\xi\beta l v_i}{\gamma} = \frac{2\sqrt{2}}{3}\frac{\xi}{l}\frac{\beta l^2 v_i}{\gamma}$$

We introduce the natural capillary number for a sharp interface [2] $Ca^* = \frac{\beta l^2 v_i}{\gamma}$

$$Ca = \frac{2\sqrt{2}}{3} K Ca^*$$

With our choice of l, we notice that $Ca^* = 1$ and then $Ca = \frac{2\sqrt{2}}{3}K$

Péclet number [1–3, 6, 7]

$$\frac{M\mu^*}{l v_i} = \frac{M\kappa}{\xi^2}\frac{1}{l v_i}$$

- $D = \frac{M\kappa}{\xi^2}$ has the dimension of a diffusion coefficient for the phase
- Péclet number $Pe = \frac{advection}{diffusion}$

$$Pe = \frac{v_i l}{D} = \frac{v_i l}{M\kappa/\xi^2}$$

Dimensionless equations with dimensionless numbers

For the flow

$$\vec{\nabla} p + \tfrac{1}{Ca}\phi\vec{\nabla}\mu = -\theta(\phi)\vec{v}$$
$$\vec{\nabla}\cdot\vec{v} = 0$$

For the phase

$$\tfrac{\partial\phi}{\partial t} + \vec{v}\cdot\vec{\nabla}\phi = \tfrac{1}{Pe}\nabla^2\mu$$
$$\mu = \phi^3 - \phi - K^2\nabla^2\phi$$

Summary of the dimensionless problem

Geometry

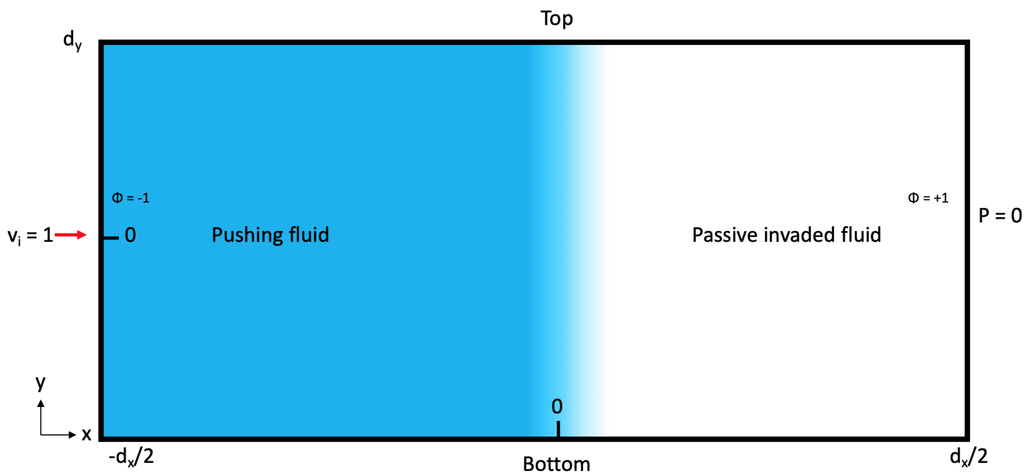

Figure 2: Geometry of the system

Initial conditions

For the phase

$$\phi(\vec{r}, t=0) = \phi_0(x) = tanh\left(\frac{x}{\sqrt{2K}}\right)$$
$$\mu(\vec{r}, t=0) = 0$$

For the flow

$$\vec{v}(\vec{r}, t=0) = 1 \cdot \hat{x}$$
$$p(\vec{r}, t=0) = \frac{d_x}{2} - x$$

Boundary conditions

For the phase

$$\vec{\nabla}\phi(\vec{r}, t) \cdot \vec{n} = 0 \; on \; \partial\Omega_{t/b}$$
$$\vec{\nabla}\mu(\vec{r}, t) \cdot \vec{n} = 0 \; on \; \partial\Omega_{t/b}$$
$$\phi = -1 \; on \; \partial\Omega_{left}$$
$$\phi = +1 \; on \; \partial\Omega_{right}$$
$$\mu = 0 \; on \; \partial\Omega_{left/right}$$

For the flow

$$
\begin{aligned}
\vec{v}(\vec{r},t) &= 1 \cdot \hat{x} \ on \ \partial\Omega_{left} \\
p(\vec{r},t) &= 0 \ on \ \partial\Omega_{right} \\
\vec{v} \cdot \vec{n} &= 0 \ on \ \partial\Omega_{top/bottom} \\
\vec{\nabla} p \cdot \vec{n} &= 0 \ on \ \partial\Omega_{top/bottom}
\end{aligned}
$$

Dimensionless equations

$$
\begin{gathered}
\vec{\nabla} p + \frac{1}{Ca}\phi\vec{\nabla}\mu = -\theta(\phi)\vec{v} \\
\vec{\nabla} \cdot \vec{v} = 0 \\
\frac{\partial\phi}{\partial t} + \vec{v} \cdot \vec{\nabla}\phi = \frac{1}{Pe}\nabla^2\mu \\
\mu = \phi^3 - \phi - K^2\nabla^2\phi
\end{gathered}
$$

Numerical values

Physics

Péclet number

In order to ensure 'instantaneous' local equilibrium/to converge like the sharp interface, we need $\frac{1}{Pe}$ to be as small as possible [1, 2, 8]. Take $Pe = O(1/K)$.

Capillary number

$Ca = \frac{2\sqrt{2}}{3} K Ca^*$ with $Ca^* = 1$ in our case (choice of l)

Computing values

Mesh size element

Smallest mesh size element $h = 0.1 - 0.2$ from [8], but we will try smaller ones in order to have a good resolution of the interface

Cahn number

From [2, 8, 9] we need $0.5h \leq \xi/l \leq 2h$ Meaning $K \sim 0.05 - 0.4$

Initial perturbation [2, 7]

We initiate the phase with a regular perturbation $\phi(t=0) = th(\frac{x+\delta x}{\sqrt{2}K})$ with $\delta x = h_0 sin(ky)$ and $\lambda = 2\pi/k$

- To fall into the linear phase, we need $h_0/\lambda \ll 1$ (in practice, $h_0/\lambda = 0.01 - 0.06$)

- The wave disturbance must not see the interface width $h_0/K \gg 1$ (in practice, $h_0/K = 10 - 40$)

This means that we have to change the value of ϕ and μ in the initial conditions.

- If $|x| > a * h_0$, we have $\mu = 0$ and $\phi = tanh(\frac{x}{\sqrt{2}K})$
- If $|x| \leq a * h_0$, we have $\phi = tanh(\frac{x+\delta x}{\sqrt{2}K})$ with $\delta x = h_0 sin(\frac{2\pi}{\lambda}y)$, then we need to have

$$\mu = \frac{K\delta x}{\sqrt{2}}(\frac{2\pi}{\lambda})^2(1-\phi^2) + (h_0\frac{2\pi}{\lambda}cos(\frac{2\pi}{\lambda}y))^2\phi(1-\phi^2)$$

In practice, we choose $1 < a < 2$

Comparison with theory

We call $\sigma(q)$ the growth rate of the fingers, with q the wave length of the fingers.
According to the theory, we have:

$$\sigma(q) = \frac{\theta - 1 - q^2}{\theta + 1}q$$

The wave length that will be selected and that we should see is the one with the fastest growing fingers, meaning the biggest σ.

$$\begin{aligned}
\frac{\partial\sigma(q)}{\partial q} &= \frac{\theta-1}{\theta+1} - \frac{3q^2}{\theta+1} = 0 \\
\Leftrightarrow q_{chosen} &= \sqrt{\frac{\theta-1}{3}} \\
\Leftrightarrow \sigma_{chosen} &= \frac{\theta-1}{\theta+1}\sqrt{\frac{\theta-1}{3}} - \left(\frac{\theta-1}{3}\right)^{3/2}\frac{1}{\theta+1}
\end{aligned}$$

Initially, the interface is $H = \delta x_0$, with time it will be $H(t) = \delta x_0 + \delta h(t)$ and with $\delta h(t) \propto exp(\sigma_{chosen}t) \Leftrightarrow ln(\delta h(t)) \propto \sigma_{chosen}t$.
To begin with, we choose $\lambda = q_{chosen}$ to make sure the fingers are growing, and then we will choose different λ to see if we can get the appropriate q_{chosen} after some time.

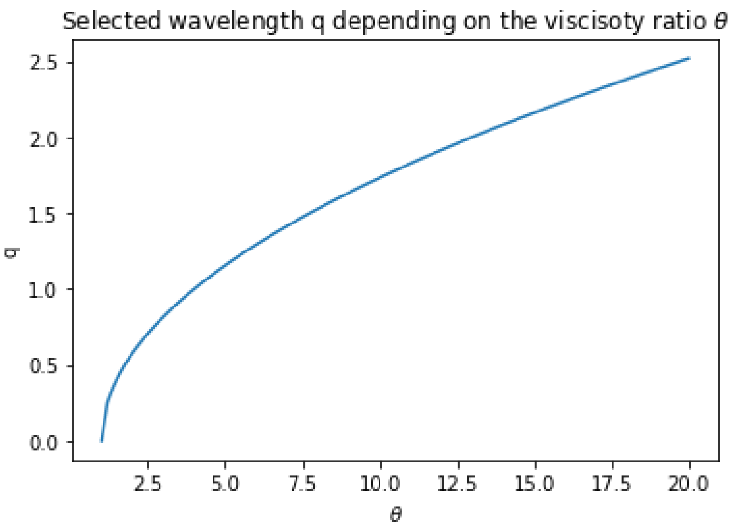

Figure 3: Wave length depending on the viscosity

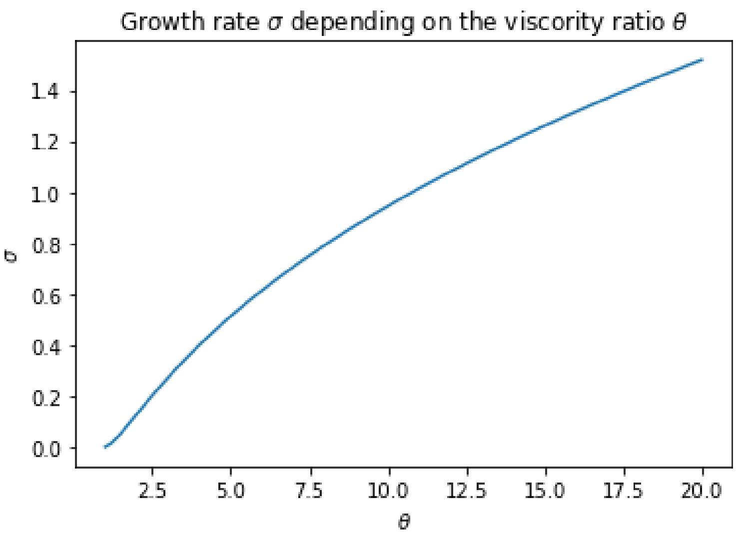

Figure 4: Growth rate depending on the viscosity

Variational problem

Solving the flow

Test functions $\vec{v_t} \in \mathbb{R}^2$ and $p_t \in \mathbb{R}$

$$\vec{\nabla} p + \theta_c(\phi)\vec{v} = -\frac{1}{Ca}\phi\vec{\nabla}\mu$$
$$\Rightarrow \int_\Omega \vec{\nabla} p \cdot \vec{v_t} + \theta_c(\phi)\vec{v} \cdot \vec{v_t} = \int_\Omega -\frac{1}{Ca}\phi\vec{\nabla}\mu \cdot \vec{v_t}$$

$$\vec{\nabla} \cdot \vec{v} = 0$$
$$\Rightarrow \int_\Omega p_t \vec{\nabla} \cdot \vec{v} = 0$$

$$\begin{aligned} &\int_\Omega \theta_c(\phi)\vec{v}\cdot\vec{v_t} + \vec{\nabla}p\cdot\vec{v_t} + p_t\vec{\nabla}\cdot\vec{v} = -\int_\Omega \frac{1}{Ca}\phi\vec{\nabla}\mu\cdot\vec{v_t} \\ \Leftrightarrow &\int_\Omega \theta_c(\phi)\vec{v}\cdot\vec{v_t} - p\vec{\nabla}\cdot\vec{v_t} - \vec{\nabla}p_t\cdot\vec{v} + \int_{\partial\Omega} p\vec{v_t}\cdot\vec{n} + p_t\vec{v}\cdot\vec{n}dS = -\int_\Omega \frac{1}{Ca}\phi\vec{\nabla}\mu\cdot\vec{v_t} \end{aligned}$$

$$\begin{aligned} \int_{\partial\Omega} p\vec{v_t}\cdot\vec{n} + p_t\vec{v}\cdot\vec{n}dS &= \int_{\partial\Omega_{in}} p\vec{v_t}\cdot\vec{n} + p_t\vec{v}\cdot\vec{n}dS + \int_{\partial\Omega_{out}} p\vec{v_t}\cdot\vec{n} + p_t\vec{v}\cdot\vec{n}dS + \int_{\partial\Omega_{top/bot}} p\vec{v_t}\cdot\vec{n} + p_t\vec{v}\cdot\vec{n}dS \\ &= \int_{\partial\Omega_{in}} p_t\vec{v}\cdot\vec{n}dS + \int_{\partial\Omega_{top/bot}} p\vec{v_t}\cdot\vec{n}dS \\ &= \int_{\partial\Omega_{in}} -p_t dS + \int_{\partial\Omega_{top/bot}} p\vec{v_t}\cdot\vec{n}dS \end{aligned}$$

Because

- p_{out} is know so $p_t = 0$ on $\partial\Omega_{out}$ and $p_{out} = 0$, then $\int_{\Omega_{out}} = 0$
- $\vec{v}\cdot\vec{n} = 0$ on $\partial\Omega_{top/bot}$
- $\vec{v}$ is known on $\partial\Omega_{in}$ so $\vec{v_t} = 0$ on $\partial\Omega_{in}$ and $\vec{v}\cdot\vec{n} = -1$ because the normal goes outward

Then

$$\begin{aligned} \int_\Omega \theta_c(\phi)\vec{v}\cdot\vec{v_t} - p\vec{\nabla}\cdot\vec{v_t} - \vec{\nabla}p_t\cdot\vec{v} + \int_{\partial\Omega_{top/bot}} p\vec{v_t}\cdot\vec{n}dS = -\int_\Omega \frac{1}{Ca}\phi\vec{\nabla}\mu\cdot\vec{v_t} + \int_{\partial\Omega_{in}} p_t dS \\ \Leftrightarrow a((\vec{v},p),(\vec{v_t},p_t)) = L((\vec{v_t},p_t)) \end{aligned}$$

Solving the phase

Test functions $\phi_t \in \mathbb{R}$ and $\mu_t \in \mathbb{R}$.

$$\begin{aligned} &\frac{\partial\phi}{\partial t} + \vec{v}\cdot\vec{\nabla}\phi - \frac{1}{Pe}\nabla^2\mu = 0 \\ \Rightarrow &\int_\Omega \frac{\partial\phi}{\partial t}\phi_t + \phi_t\vec{v}\cdot\vec{\nabla}\phi - \frac{1}{Pe}\phi_t\nabla^2\mu = 0 \\ \Leftrightarrow &\int_\Omega \frac{\partial\phi}{\partial t}\phi_t + \phi_t\vec{v}\cdot\vec{\nabla}\phi + \frac{1}{Pe}\vec{\nabla}\mu\cdot\vec{\nabla}\phi_t = 0 \end{aligned}$$

Because $\int_{\partial\Omega}\phi_t\vec{\nabla}\mu\cdot\vec{n}dS = 0$

- $\vec{\nabla}\mu\cdot\vec{n} = 0$ on $\partial\Omega_{t/b}$
- ϕ is know on $\partial\Omega_{left/right}$ so $\phi_t = 0$ on $\partial\Omega_{left/right}$

$$\mu - (\phi^3 - \phi) + K^2\nabla^2\phi = 0$$
$$\Rightarrow \int_\Omega \mu\mu_t - (\phi^3 - \phi)\mu_t + K^2\mu_t\nabla^2\phi = 0$$
$$\Leftrightarrow \int_\Omega \mu\mu_t - (\phi^3 - \phi)\mu_t - K^2\vec{\nabla}\phi \cdot \vec{\nabla}\mu_t = 0$$

Because $\int_{\partial\Omega} \mu_t\vec{\nabla}\phi \cdot \vec{n} dS = 0$

- $\vec{\nabla}\phi \cdot \vec{n} = 0$ on $\partial\Omega_{t/b}$
- μ is know on $\partial\Omega_{left/right}$ so $\mu_t = 0$ on $\partial\Omega_{left/right}$

Time-Discretization

We now discretize the time: $dt = t_{n+1} - t_n$ and $\mu_{n+\rho} = (1-\rho)\mu_n + \rho\mu_{n+1}$ (with $\rho = 0.5$, Crank Nicholson method)

$$\boxed{\begin{array}{l} \int_\Omega \theta_c(\phi)\vec{v} \cdot \vec{v_t} - p\vec{\nabla} \cdot \vec{v_t} - \vec{\nabla}p_t \cdot \vec{v} + \int_{\partial\Omega_{top/bot}} p\vec{v_t} \cdot \vec{n} dS = -\int_\Omega \frac{1}{Ca}\phi_n\vec{\nabla}\mu_n \cdot \vec{v_t} + \int_{\partial\Omega_{in}} p_t dS \\ \int_\Omega (\phi_{n+1} - \phi_n)\phi_t + dt \times \phi_t\vec{v} \cdot \vec{\nabla}\phi_n + \frac{dt}{Pe}\vec{\nabla}\mu_{n+\rho} \cdot \vec{\nabla}\phi_t = 0 \\ \qquad \int_\Omega \mu_{n+1}\mu_t - (\phi_{n+1}^3 - \phi_{n+1})\mu_t - K^2\vec{\nabla}\phi_{n+1} \cdot \vec{\nabla}\mu_t = 0 \end{array}}$$

Current solver

Currently : solve the flow with a Krylov solver with MUMP.
Solve the 2 equations for the phase together with a Newton solver (non linear).

Algorithm

1. Initiate the phase with the initial conditions
2. Solve for the flow everywhere
3. Solve for the phase everywhere
4. Back to 2.

Dimensions

- $\beta = 10^{15} - 10^{16} Pa.s.m^{-2}$
- $\gamma = 10^{-3} - 10^{-2} Pa.m$

- $v_i = 10^{-8} - 10^{-6} m/s$ (we choose it to be a bit bigger than normal cell migration speed)
- For $\beta = 10^{15}$, $\gamma = 10^{-3}$ and $v_i = 10^{-8}$ we have $l = 10^{-5} m = 10 \mu m$
- The typical size of an epithelial cell would be $10 \mu m$

We ideally want to try in boxes of (dimensionless) dimensions (100 x 100) - (200 x 200) to hope and see something.