Third model - Includes activity

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Geometry

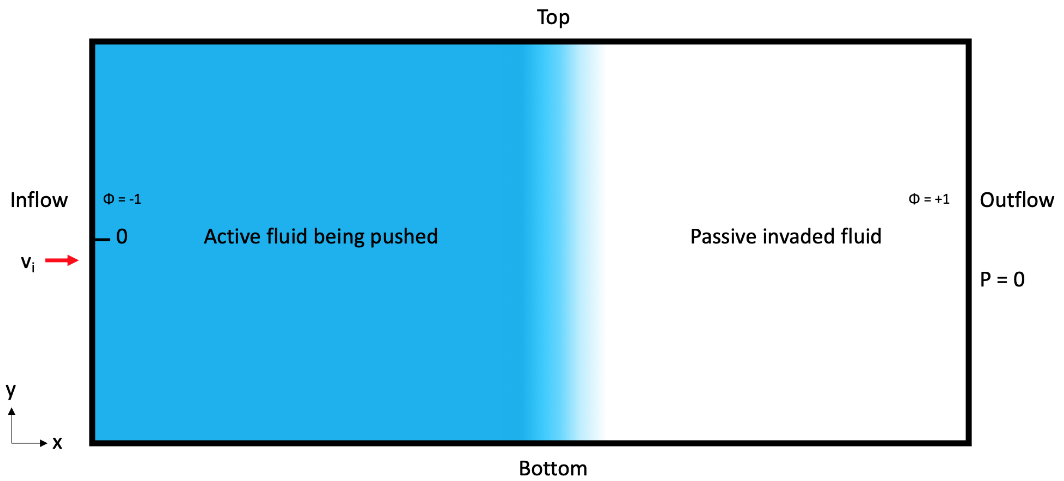

Figure 1: Geometry of the system

Simplifications

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

Equations

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

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

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

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

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)
- $I(\phi) = \frac{1}{2}(1-\phi)$, is 1 in the active fluid and 0 in the passive fluid
- $\theta = \frac{\beta'}{\beta}$ 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

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

For the flow

$$\begin{aligned}
\vec{v}(\vec{r}, t=0) &= v_i\hat{x} \\
p(\vec{r} > start, t=0) &= \beta' v_i(\frac{L}{2} - x) \\
p(\vec{r} < start, t=0) &= (\beta v_i - \alpha)(start - x) + \beta' v_i(\frac{L}{2} - start)
\end{aligned}$$

With L the length of the box and start the initial position of the interface (does not have to be zero).

Boundary conditions

For the phase

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

For the flow

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

Dimensionless

New dimensionless parameters

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

Dimensionless equations

For the flow

We drop the tilde of the dimensionless parameters

$$
\begin{aligned}
\vec{\nabla}p + \frac{\mu^*}{\beta l v_i}\phi\vec{\nabla}\mu &= -\theta_c(\phi)\vec{v} + \alpha I(\phi)\frac{\vec{v}}{\mid \vec{v} \mid} \\
\vec{\nabla}\cdot\vec{v} &= 0
\end{aligned}
$$

For the phase

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

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

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

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

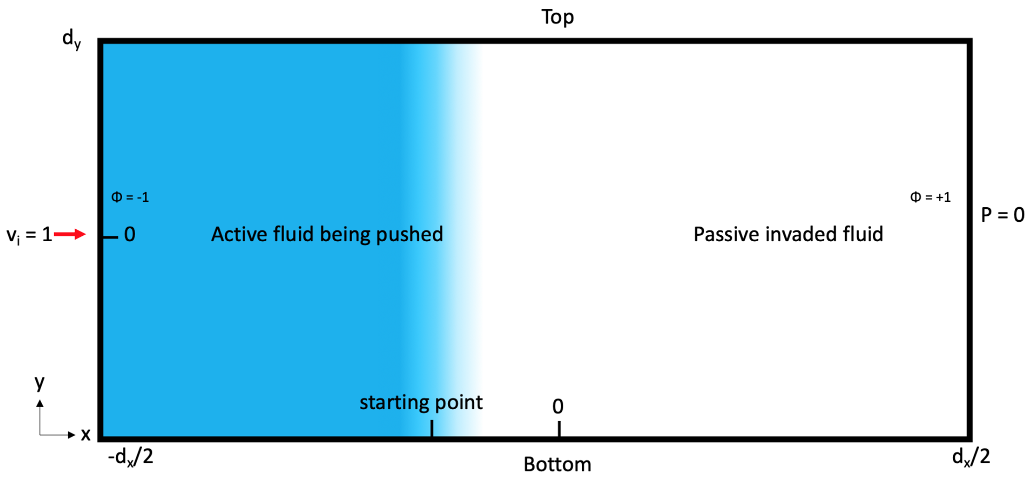

Figure 2: Geometry of the system

Initial conditions

For the phase

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

For the flow

$$\vec{v}(\vec{r}, t=0) = 1 \cdot \hat{x}$$
$$p(\vec{r} > start, t=0) = \theta(\frac{d_x}{2} - x)$$
$$p(\vec{r} < start, t=0) = (1-\alpha)(start - x) + \theta(\frac{d_x}{2} - start)$$

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

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

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 $\phi(t=0) = th(\frac{x+\delta x}{\sqrt{2K}})$ 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 $1 < a < 2$

New values

From [2], and CFL condition

- $h = \frac{1}{2^n}$ with $n = 6, 7, 8$
- $K = O(h^k)$ with $0 < k < 1$ (try $K = 10h$)
- $\Delta t \leq h^2 Pe/2$
- $\Delta t \leq h/v_i$

Comparison with theory

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

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

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

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

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 $k = 2\pi/\lambda = q_{chosen}$ to make sure the fingers are growing, and then we will choose different q to see if we can get the appropriate q_{chosen} after some time.

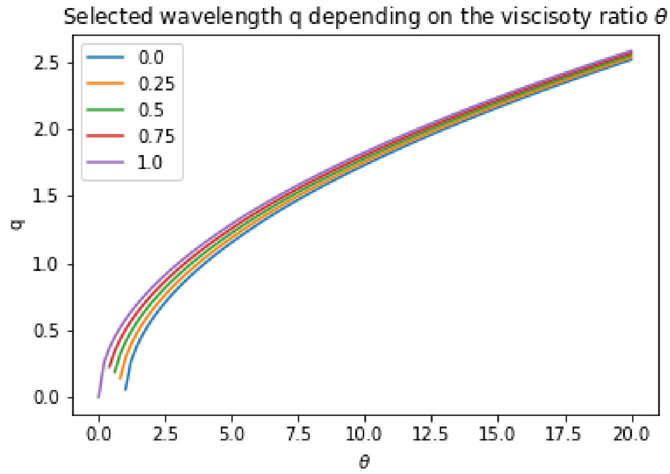

Figure 3: Wave length depending on the viscosity for various values of α (coloured lines)

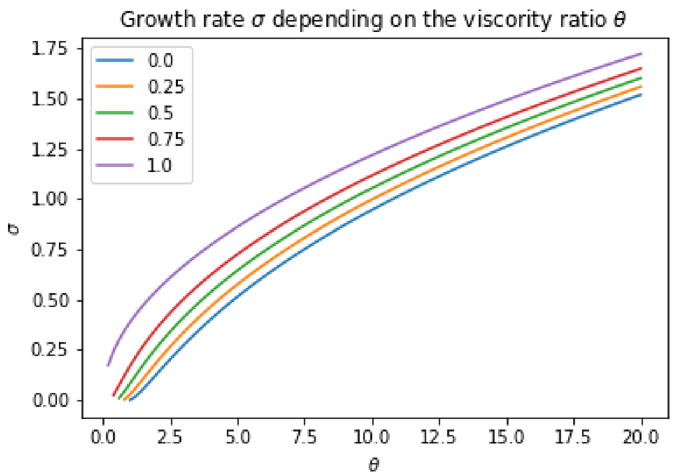

Figure 4: Growth rate depending on the viscosity for various values of α (coloured lines)

Variational problem

Solving the flow

Test functions $\vec{v_t} \in L(\mathbb{R}^2) \to L(\mathbb{R}^2)$ and $p_t \in L(\mathbb{R}) \to L(\mathbb{R})$

$$\vec{\nabla}p + \frac{1}{Ca}\phi\vec{\nabla}\mu + \theta_c(\phi)\vec{v} - \alpha I(\phi)\frac{\vec{v}}{\mid\vec{v}\mid} = 0$$

$$\Rightarrow \int_\Omega \vec{\nabla}p \cdot \vec{v_t} + \frac{1}{Ca}\phi\vec{\nabla}\mu \cdot \vec{v_t} + \theta_c(\phi)\vec{v} \cdot \vec{v_t} - \alpha I(\phi)\frac{\vec{v}}{\mid\vec{v}\mid} \cdot \vec{v_t} = 0$$

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

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

$$
\int_\Omega \theta_c(\phi)\vec{v}\cdot\vec{v_t} + \frac{1}{Ca}\phi\vec{\nabla}\mu\cdot\vec{v_t} + \vec{\nabla}p\cdot\vec{v_t} + p_t\vec{\nabla}\cdot\vec{v} - \alpha I(\phi)\frac{\vec{v}}{\mid\vec{v}\mid}\cdot\vec{v_t} = 0
$$

$$
\Leftrightarrow \int_\Omega \theta_c(\phi)\vec{v}\cdot\vec{v_t} + \frac{1}{Ca}\phi\vec{\nabla}\mu\cdot\vec{v_t} + \vec{\nabla}p\cdot\vec{v_t} - \vec{\nabla}p_t\cdot\vec{v} - \alpha I(\phi)\frac{\vec{v}}{\mid\vec{v}\mid}\cdot\vec{v_t} + \int_{\partial\Omega} p_t\vec{v}\cdot\vec{n}dS = 0
$$

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

Because

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

Then

$$
\int_\Omega \theta_c(\phi)\vec{v}\cdot\vec{v_t} + \frac{1}{Ca}\phi\vec{\nabla}\mu\cdot\vec{v_t} + \vec{\nabla}p\cdot\vec{v_t} - \vec{\nabla}p_t\cdot\vec{v} - \alpha I(\phi)\frac{\vec{v}}{\mid\vec{v}\mid}\cdot\vec{v_t} - \int_{\partial\Omega_{in}} p_t dS = 0
$$

Solving the phase

Test functions $\phi_t \in L(\mathbb{R}) \to L(\mathbb{R})$ and $\mu_t \in L(\mathbb{R}) \to L(\mathbb{R})$.

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

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 $\partial\Omega_{left/right}$

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

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 apply an implicit time scheme $\frac{\phi^{n+1}-\phi^n}{dt} = f(\phi^{n+1}, \mu^{n+1})$:

$$\int_\Omega \frac{\partial\phi}{\partial t}\phi_t + \phi_t\vec{v}\cdot\vec{\nabla}\phi + \frac{1}{Pe}\vec{\nabla}\mu\cdot\vec{\nabla}\phi_t = 0$$
$$\Leftrightarrow \int_\Omega \frac{\phi^{n+1}-\phi^n}{dt}\phi_t + \phi_t\vec{v}^n\cdot\vec{\nabla}\phi^{n+1} + \frac{1}{Pe}\vec{\nabla}\mu^{n+1}\cdot\vec{\nabla}\phi_t = 0$$

We first initiate ϕ and μ, and give $\vec{v}$ an initial value of 1.
Then, if we know the values of ϕ^n, μ^n, $\vec{v}^n$ and p^n, we first solve the phase and the chemical potential:

$$\int_\Omega \frac{\phi^{n+1}-\phi^n}{dt}\phi_t + \phi_t\vec{v}^n\cdot\vec{\nabla}\phi^{n+1} + \frac{1}{Pe}\vec{\nabla}\mu^{n+1}\cdot\vec{\nabla}\phi_t = 0$$
$$\int_\Omega \mu^{n+1}\mu_t - ((\phi^{n+1})^3 - \phi^{n+1})\mu_t - K^2\vec{\nabla}\phi^{n+1}\cdot\vec{\nabla}\mu_t = 0$$

We now know ϕ^{n+1} and μ^{n+1}, and then use these values to update the velocity and the pressure:

$$0 = \int_\Omega \theta_c(\phi^{n+1})\vec{v}^{n+1}\cdot\vec{v_t} + \frac{1}{Ca}\phi^{n+1}\vec{\nabla}\mu^{n+1}\cdot\vec{v_t} + \vec{\nabla}p^{n+1}\cdot\vec{v_t} - \vec{\nabla}p_t\cdot\vec{v}^{n+1} - \alpha I(\phi^{n+1})\frac{\vec{v^{n+1}}}{\mid \vec{v^{n+1}} \mid}\cdot\vec{v_t}$$
$$- \int_{\partial\Omega_{in}} p_t dS$$

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).

Dimensions

- $\beta = 10^{15} - 10^{16} Pa.s.m^{-2}$
- $\gamma = 10^{-3} - 10^{-2} Pa.m$
- $\alpha = 0 - 10^{10} Pa.m^{-1}$
- $v_i = 10^{-8} - 10^{-6} m/s$ (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 $l = 10^{-5}m = 10\mu m$ and $\alpha = 10^7$
- 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.

References

1. Badalassi, V., Ceniceros, H. & Banerjee, S. Computation of multiphase systems with phase field models. *Journal of Computational Physics* **190,** 371–397. ISSN: 00219991 (Sept. 2003).
2. Ceniceros, H. D., Nós, R. L. & Roma, A. M. Three-dimensional, fully adaptive simulations of phase-field fluid models. *Journal of Computational Physics* **229,** 6135–6155. ISSN: 00219991 (Aug. 2010).
3. Kim, J. Phase-Field Models for Multi-Component Fluid Flows. *Communications in Computational Physics* **12,** 613–661. ISSN: 1815-2406 (Sept. 2012).
4. Hernández-Machado, A., Lacasta, A. M., Mayoral, E. & Corvera Poiré, E. Phase-field model of Hele-Shaw flows in the high-viscosity contrast regime. *Physical Review E,* 046310. ISSN: 1063-651X. arXiv: `0309466 [cond-mat]` (Oct. 2003).
5. Cueto-Felgueroso, L. & Juanes, R. A phase-field model of two-phase Hele-Shaw flow. *Journal of Fluid Mechanics* **758,** 522–552. ISSN: 0022-1120 (Nov. 2014).
6. He, Q. & Kasagi, N. Phase-Field simulation of small capillary-number two-phase flow in a microtube. *Fluid Dynamics Research* **40,** 497–509. ISSN: 0169-5983 (July 2008).
7. Celani, A., Mazzino, A., Muratore-Ginanneschi, P. & Vozella, L. Phase-field model for the Rayleigh–Taylor instability of immiscible fluids. *Journal of Fluid Mechanics* **622,** 115–134. ISSN: 0022-1120. arXiv: `0806.0783` (Mar. 2009).
8. Ganapathy, H., Al-Hajri, E. & Ohadi, M. M. Phase field modeling of Taylor flow in mini/microchannels, Part I: Bubble formation mechanisms and phase field parameters. *Chemical Engineering Science* **94,** 138–149. ISSN: 00092509 (May 2013).
9. Yue, P., Feng, J. J., Liu, C. & Shen, J. A diffuse-interface method for simulating two-phase flows of complex fluids. *Journal of Fluid Mechanics* **515,** 293–317. ISSN: 0022-1120 (Sept. 2004).