

Second model

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Geometry

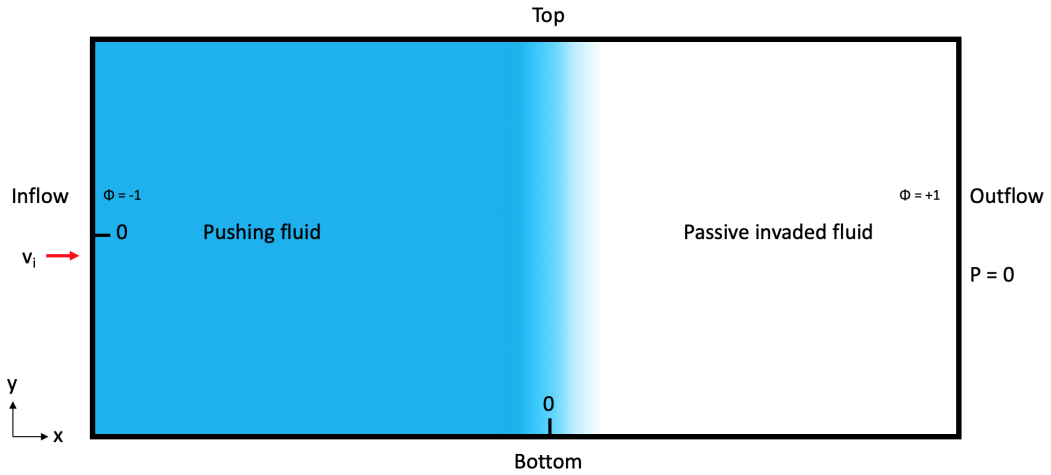


Figure 1: Geometry of the system

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

$$\begin{aligned}\vec{\nabla} p + \phi \vec{\nabla} \mu &= -\beta \theta_c(\phi) \vec{v} \\ \vec{\nabla} \cdot \vec{v} &= 0 \\ \frac{\partial \phi}{\partial t} + (\vec{v} \cdot \vec{\nabla}) \phi &= M \nabla^2 \mu \\ \mu &= \frac{\kappa}{\xi^2} (\phi^3 - \phi) - \kappa \nabla^2 \phi\end{aligned}$$

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

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

For the flow

$$\begin{aligned}\vec{v}(\vec{r}, t = 0) &= v_i \hat{x} \\ p(\vec{r}, t = 0) &= P_{in}\left(\frac{1}{2} - \frac{x}{L}\right) \quad (L \text{ length of the box})\end{aligned}$$

Boundary conditions

For the phase

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

For the flow

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

Dimensionless

New dimensionless parameters

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

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

- $D = \frac{M\kappa}{\xi^2}$ 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

$$\begin{aligned} \vec{\nabla} p + \frac{1}{C_a} \phi \vec{\nabla} \mu &= -\theta(\phi) \vec{v} \\ \vec{\nabla} \cdot \vec{v} &= 0 \end{aligned}$$

For the phase

$$\begin{aligned} \frac{\partial \phi}{\partial t} + \vec{v} \cdot \vec{\nabla} \phi &= \frac{1}{Pe} \nabla^2 \mu \\ \mu &= \phi^3 - \phi - K^2 \nabla^2 \phi \end{aligned}$$

Summary of the dimensionless problem

Geometry

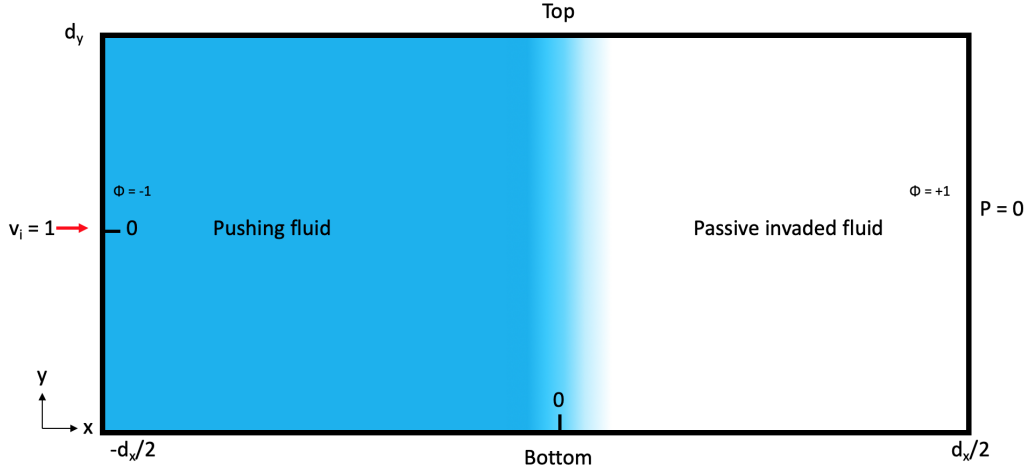


Figure 2: Geometry of the system

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

$$\vec{v}(\vec{r}, t = 0) = 1 \cdot \hat{x}$$

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

Boundary conditions

For the phase

$$\vec{\nabla}\phi(\vec{r}, t) \cdot \vec{n} = 0 \text{ on } \partial\Omega_{t/b}$$

$$\vec{\nabla}\mu(\vec{r}, t) \cdot \vec{n} = 0 \text{ on } \partial\Omega_{t/b}$$

$$\phi = -1 \text{ on } \partial\Omega_{left}$$

$$\phi = +1 \text{ on } \partial\Omega_{right}$$

$$\mu = 0 \text{ on } \partial\Omega_{left/right}$$

For the flow

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

Dimensionless equations

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

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

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

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.

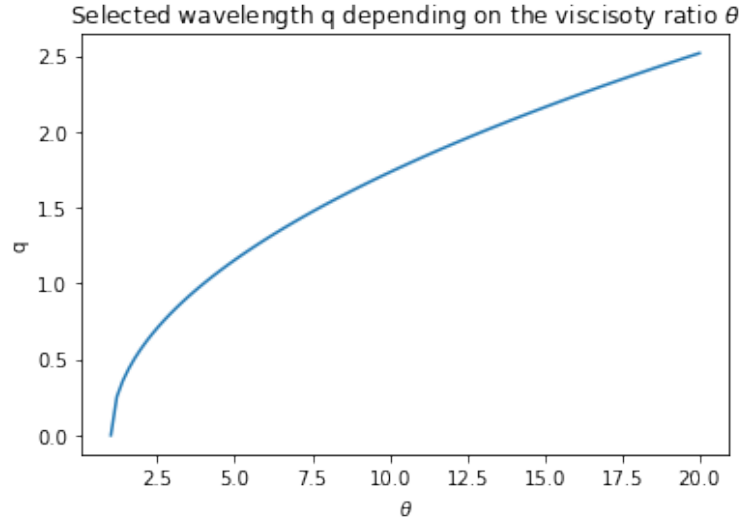


Figure 3: Wave length depending on the viscosity

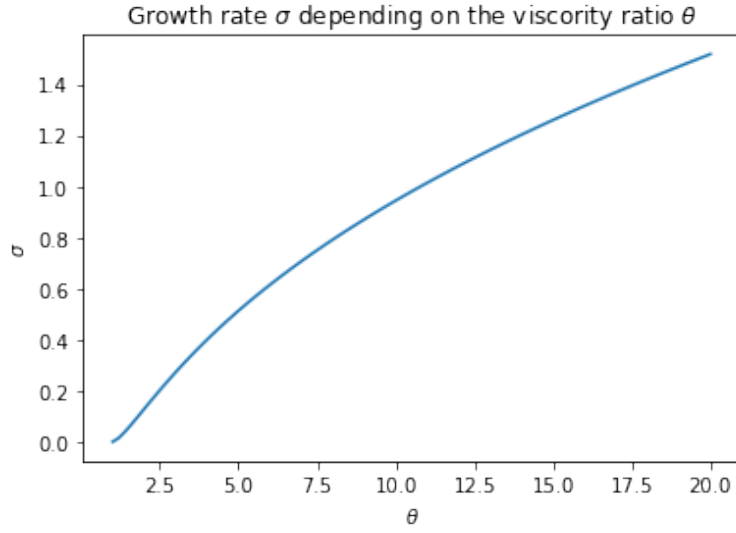


Figure 4: Growth rate depending on the viscosity

Variational problem

Solving the flow

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

$$\begin{aligned} \vec{\nabla} p + \theta_c(\phi) \vec{v} &= -\frac{1}{Ca} \phi \vec{\nabla} \mu \\ \Rightarrow \int_{\Omega} \vec{\nabla} p \cdot \vec{v}_t + \theta_c(\phi) \vec{v} \cdot \vec{v}_t &= \int_{\Omega} -\frac{1}{Ca} \phi \vec{\nabla} \mu \cdot \vec{v}_t \\ \vec{\nabla} \cdot \vec{v} &= 0 \\ \Rightarrow \int_{\Omega} p_t \vec{\nabla} \cdot \vec{v} &= 0 \end{aligned}$$

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

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

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 $\partial\Omega_{left/right}$

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

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 known 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)

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

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.

References

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