Two-dimensional Filtration of Nitrogen and Pentane (C_5H_{12})

1 Physical model

Darcy's law:

$$\boldsymbol{v}_i = -\frac{1}{\mu_i}\hat{K} \cdot f_\alpha(s) \cdot \nabla P \tag{1}$$

where $\hat{K}$, the specific permeability. It depends only on the geometry of the medium. We assume isotropy of space, so K is a scalar. μ is the dynamic viscosity.

i - component.

α - phase. (If we had multiple phases, then it would be f_α)

As an approximation, $f_\alpha(s) = s^2$ for the first component, and $f_\alpha(s) = (1-s)^2$ for the second.

The continuity equation for each component becomes:

$$\varphi\frac{\partial \rho_i}{\partial t} + div(\rho_i \boldsymbol{v}_i) = 0 \tag{2}$$

where $\rho_i = \frac{m_i}{V}$.

We use the Tait equation to relate liquid density to pressure:

$$\frac{\hat{\rho} - \rho_0}{\hat{\rho}} = C \log_{10}\frac{B+P}{B+P_0} \tag{3}$$

where $C = 0.2105$, $\rho_0 = \frac{1}{67.28\frac{m^3}{mol}}$, $P_0 = 0.1MPa$, $B = 35MPa$, in the case of C_5H_{12}.

Ideal gas equation of state:

$$P = \frac{RT}{M}\hat{\rho} \tag{4}$$

2 Boundary and Initial Conditions

On the first iteration, we set an initial pressure and molar composition. Then, we derive the velocities from the pressure gradient using Darcy's law and the saturation from the densities and molar composition.

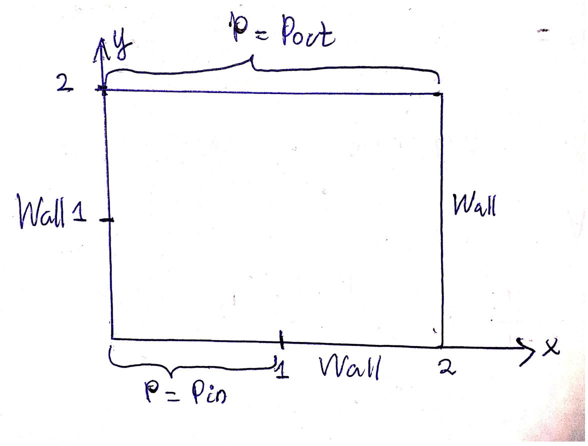

Figure 1: Boundary Conditions

2.1 Pressure

BC:

$$\begin{cases} P = P_{in} & \text{at } y = 0 \text{ and } x \in [0, 1] \\ P = P_{out} & \text{at } y = 2 \\ \frac{\partial P}{\partial x} = 0 & \text{at } x = 0, 2 \\ \frac{\partial P}{\partial y} = 0 & \text{at } y = 0 \text{ and } x \in [1, 2] \end{cases}$$

IC:

$$\begin{cases} P = P_{out} & \text{at outlet} \\ P = P_{in} & \text{at inlet} \\ P = P_0 & \text{everywhere else} \end{cases}$$

2.2 Velocities

IC: Darcy 2-nd order.
BC:

$$\begin{cases} u = 0 & \text{at } x = 0, 2 \\ v = 0 & \text{at } y = 0 \text{ and } x \in [1, 2] \\ \text{Darcy (2-nd Order FD)} & \text{at } y = 2 \\ \text{Darcy (2-nd Order FD)} & \text{at } y = 0 \text{ and } x \in [0, 1] \end{cases}$$

2.3 Density

We derive the densities from the equations of state.

2.4 Saturation

Boundary condition on the inlet as the molar composition ψ:

$$\frac{m_1}{m_2} = \frac{\psi}{1 - \psi} \frac{M_1}{M_2}$$

where M_1 and M_2 represent the molar mass of each component.

We can derive the densities from the equations of state, then we can find the saturation.

$$\hat{\rho}_1 = \frac{m_1}{sV}, \qquad \hat{\rho}_2 = \frac{m_2}{(1-s)V}$$

$$\frac{\hat{\rho}_1}{\hat{\rho}_2} = \frac{m_1}{m_2}\frac{1-s}{s} = \frac{\psi M_1}{(1-\psi)M_2}\frac{1-s}{s}$$

$$s = \left(\frac{\hat{\rho}_1 M_2(1-\psi)}{\hat{\rho}_2 M_1 \psi} + 1\right)^{-1}$$

On outlet:

$$\frac{\partial \alpha}{\partial \boldsymbol{n}} = 0$$

Or,

$$\frac{\partial s}{\partial \boldsymbol{n}} = 0$$

3 Discretization Scheme

3.1 Continuity Equation

$$\varphi\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x}u + \frac{\partial \rho}{\partial y}v + \frac{\partial u}{\partial x}\rho + \frac{\partial v}{\partial y}\rho = 0$$

$$\varphi\frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\Delta t} + \frac{\rho^n_{i+1,j} - \rho^n_{i-1,j}}{2\Delta x}u_{i,j} + \frac{\rho^n_{i,j+1} - \rho^n_{i,j-1}}{2\Delta y}v_{i,j} + \frac{u_{i+1,j} - u^n_{i-1,j}}{2\Delta x}\rho^n_{i,j} + \frac{v^n_{i,j+1} - v^n_{i,j-1}}{2\Delta y}\rho^n_{ij} = 0$$

3.2 Darcy's Law

$$u^n_{i,j} = -\frac{K}{\mu}f_\alpha(s^n_{i,j})\frac{P^n_{i+1,j} - P^n_{i-1,j}}{2\Delta x}$$

$$v^n_{i,j} = -\frac{K}{\mu}f_\alpha(s^n_{i,j})\frac{P^n_{i,j+1} - P^n_{i,j-1}}{2\Delta y}$$

3.2.1 BC

$$v^n_{i,1} = -\frac{K}{\mu}f_\alpha(s^n_{i,1})\frac{-3P^n_{i,1} + 4P^n_{i,2} - P^n_{i,3}}{2\Delta x} \qquad \text{(Inlet)}$$

$$v^n_{i,ny} = -\frac{K}{\mu}f_\alpha(s^n_{i,ny})\frac{-3P^n_{i,ny} + 4P^n_{i,ny-1} - P^n_{i,ny-2}}{(-2\Delta x)} \qquad \text{(Outlet)}$$

3.3 Predictor-Corrector

1. Predictor

   (a) Continuity Equation

$$\tilde{\rho}_{i,j}^{n+1} = \rho_{i,j}^n - \frac{\Delta t}{\varphi}\left(\frac{\rho_{i+1,j}^n - \rho_{i-1,j}^n}{2\Delta x}u_{i,j} + \frac{\rho_{i,j+1}^n - \rho_{i,j-1}^n}{2\Delta y}v_{i,j}\right.$$
$$\left. + \frac{u_{i+1,j} - u_{i-1,j}^n}{2\Delta x}\rho_{i,j}^n + \frac{v_{i,j+1}^n - v_{i,j-1}^n}{2\Delta y}\rho_{ij}^n\right)$$

$$\tilde{\rho}_{i,j}^{n+1} = \rho_{i,j}^n + F_\rho^n \Delta t$$

   (b) Compute Pressure $\tilde{P}^n$

   (c) Enforce boundary conditions for pressure, density, and saturation.

   (d) Darcy's Law (???)

$$\tilde{u}_{i,j}^n = -\frac{K}{\mu} f_\alpha(\tilde{s}_{i,j}^n)\frac{\tilde{P}_{i+1,j}^n - \tilde{P}_{i-1,j}^n}{2\Delta x}$$

$$\tilde{v}_{i,j}^n = -\frac{K}{\mu} f_\alpha(\tilde{s}_{i,j}^n)\frac{\tilde{P}_{i,j+1}^n - \tilde{P}_{i,j-1}^n}{2\Delta y}$$

   (e) Enforce boundary conditions for velocity.

2. Corrector

   (a) Continuity Equation

$$\tilde{F}^{n+1} = -\frac{1}{\varphi}\left(\frac{\tilde{\rho}_{i+1,j}^{n+1} - \tilde{\rho}_{i-1,j}^{n+1}}{2\Delta x}\tilde{u}_{i,j} + \frac{\tilde{\rho}_{i,j+1}^{n+1} - \tilde{\rho}_{i,j-1}^{n+1}}{2\Delta y}\tilde{v}_{i,j}\right.$$
$$\left. + \frac{\tilde{u}_{i+1,j} - \tilde{u}_{i-1,j}^{n+1}}{2\Delta x}\tilde{\rho}_{i,j}^{n+1} + \frac{\tilde{v}_{i,j+1}^{n+1} - \tilde{v}_{i,j-1}^{n+1}}{2\Delta y}\tilde{\rho}_{ij}^{n+1}\right)$$

$$\rho_{i,j}^{n+1} = \rho_{i,j}^n + \frac{F_\rho^n + \tilde{F}_\rho^{n+1}}{2}\Delta t$$

   (b) Compute Pressure P^n

   (c) Enforce boundary conditions for pressure, density, and saturation.

   (d) Darcy's Law

$$u_{i,j}^n = -\frac{K}{\mu} f_\alpha(s_{i,j}^n)\frac{P_{i+1,j}^n - P_{i-1,j}^n}{2\Delta x}$$

$$v_{i,j}^n = -\frac{K}{\mu} f_\alpha(s_{i,j}^n)\frac{P_{i,j+1}^n - P_{i,j-1}^n}{2\Delta y}$$

4 Finding Pressure using Binary Search

The function find_pressure takes as arguments ρ_1 and ρ_2, which are defined as

$$\rho_1 = \frac{m_1}{V}, \qquad \rho_2 = \frac{m_2}{V}.$$

We try to find the zero of the following function, that takes the pressure as an argument:

$$f(P) = \frac{\hat{\rho}_2 - \rho_0}{\hat{\rho}_2} - C \log_{10} \frac{B+P}{B+P_0}.$$

Here, $\hat{\rho}_2 = \frac{m_2}{(1-s)V}$. In order to determine $\hat{\rho}_2$, we first find $\hat{\rho}_1$ using the EoS, and from there, we are able to find the saturation $s = \frac{\rho_1}{\hat{\rho}_1}$. Lastly, we determine $\hat{\rho}_2 = \frac{\rho_2}{1-s}$.

5 Algorithm

Euler method for discretization with respect to time.

Second order scheme in space, with the use of ghost cells.

1. Calculate densities for each component using EOS.
2. Find the pressure and saturation with the help of the Newton Raphson method.
3. Use Darcy's law to calculate velocities.

6 Units and Parameters

Table 1: Parameters for our simulation.

Temperature	$298\ K$
P_{in}	$10^6 Pa$
P_{out}	$10^5 Pa$
Porosity, φ	0.7
Specific Permeability, K	10^{-12}
Dynamic Viscosity of Ideal Gas, μ_1	$1.8 \cdot 10^{-5}\ Pa \cdot s$
Dynamic Viscosity of Pentane, μ_2	$2,14 \cdot 10^{-4}\ Pa \cdot s$
Molar Mass of Ideal Gas, M_1	$0.028\ \frac{kg}{mol}$
Molar Mass of Pentane, M_2	$0.07215\ \frac{kg}{mol}$
Molar Composition at Inlet, ψ	0.3

7 Conventions

1. Density:

$$\rho_i = \frac{m_i}{V}, \qquad \hat{\rho}_i = \frac{m_i}{s_i V}.$$

8 TODO

1. ~~Fix: μ is different for each component.~~

2. ~~Calculate the velocities in the first iteration with a first order scheme. Then, everything is calculated as normal.~~

3. ~~The boundary condition $\frac{dv}{dn} = 0$ is usually used when solving the Navier-Stokes equation. In the case of filtration with Darcy's equation, we can either set the velocities explicitly or derive them from the pressure gradient on the boundaries and from the Darcy's equation on the inside.~~

4. ~~Create boundary condition on the inlet as the molar composition:~~

$$\frac{m_1}{m_2} = \frac{\psi}{1-\psi}\frac{M_1}{M_2},$$

   ~~where M_1 and M_2 represent the molar mass of each component. This way, we are essentially giving a boundary condition on the saturation, since we can derive the densities from the equations of state.~~

5. ~~Change order of indexing: column major storage in memory.~~

6. ~~Use naming conventions consistent with Julia base.~~

7. Use Real instead of T in functions' parameters.

8. Create modules.

9. ~~Change density convention on 'BC: Saturation'.~~

10. ~~Bug: The density functions don't take into account the saturation!~~

11. ~~Fix: When initializing the system, it turns out that the pressure doesn't converge with the gas EoS. (Although it aligns with the liquid EoS).~~

12. ~~Replace binary search with a more efficient algorithm.~~

13. Profile and optimize code.

14. Upgrade to predictor-corrector.