Filtration of Ideal Gas and Pentane (C_5H_{12})

1 The Physics

We simulate 2d flow of ideal gas and C_5H_{12} through a porous medium with the help of 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.

All our BC are 2-nd order (thanks to ghost cells), except for the BC on velocity on the inlet and outlet, which end up 1-st order.

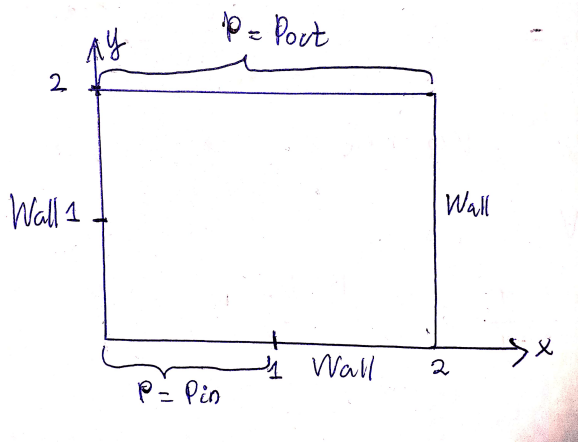

Figure 1: Boundary Conditions

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 1-st order.

BC:

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

2.3 Density

We derive the densities from the equations of state.

2.4 Saturation

Boundary condition on the inlet as the molar composition:

$$\psi = \frac{\nu_1}{\nu_2} = \frac{m_1}{M_1} \cdot \frac{M_2}{m_2},$$

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.

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

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

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

What about everywhere else???

On outlet:

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

Or:

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

3 Discretization Scheme

We use the finite difference method (FDM).

3.1 Continuity Equation

Second order in space. First order in time.

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

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

3.2 Darcy's Law

Second order in space.

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

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

4 Finding Pressure using Binary Search

The function findPressure 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. (TODO: upgrade to predictor-corrector).

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 binary search.
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 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:~~

$$\psi = \frac{\nu_1}{\nu_2} = \frac{m_1}{M_1} \cdot \frac{M_2}{m_2},$$

~~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.

   Functions are lowercase (maximum, convert) and, when readable, with multiple words squashed together. When necessary, use underscores as word separators.

7. Upgrade to predictor-corrector

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

9. Create modules.

10. Change density convention on 'BC: Saturation'.

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

8 Conventions

1. Density:

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