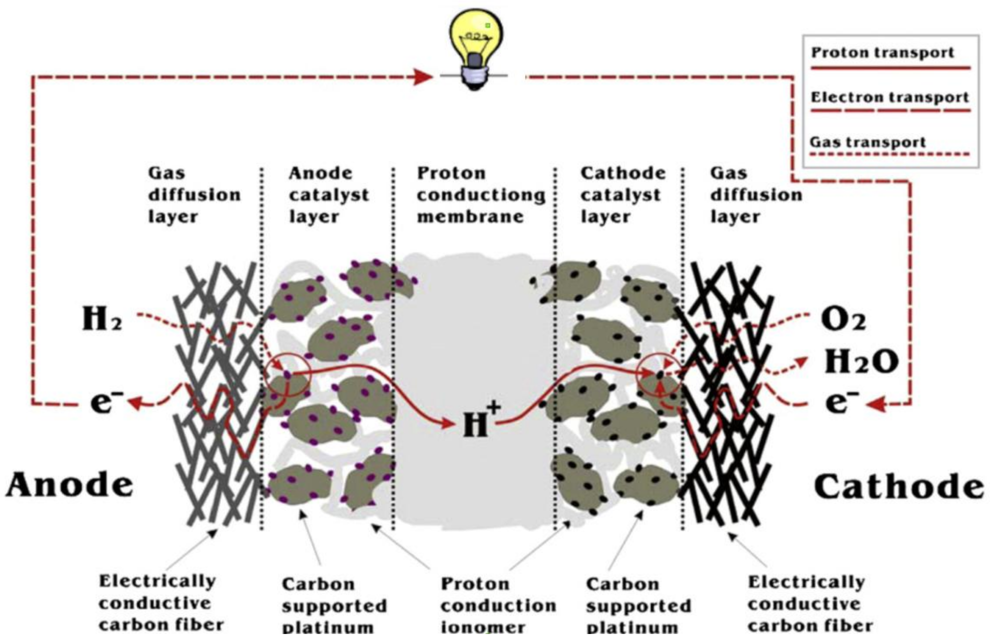
How fuel cells work



Anode side reaction:

$$2H_2 \rightarrow 4H^+ + 4e^-$$

Cathode side reaction:

$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$

Net reaction:

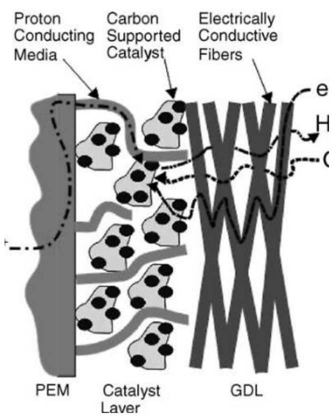
$$2H_2 + O_2 \rightarrow 2H_2O$$

- A fuel cell is a device that converts chemical potential energy into electrical energy

- A PEM (Proton Exchange Membrane) cell uses hydrogen gas (H2) and oxygen gas (O2) as fuel

- The products of the reaction in the cell are water, electricity, and heat

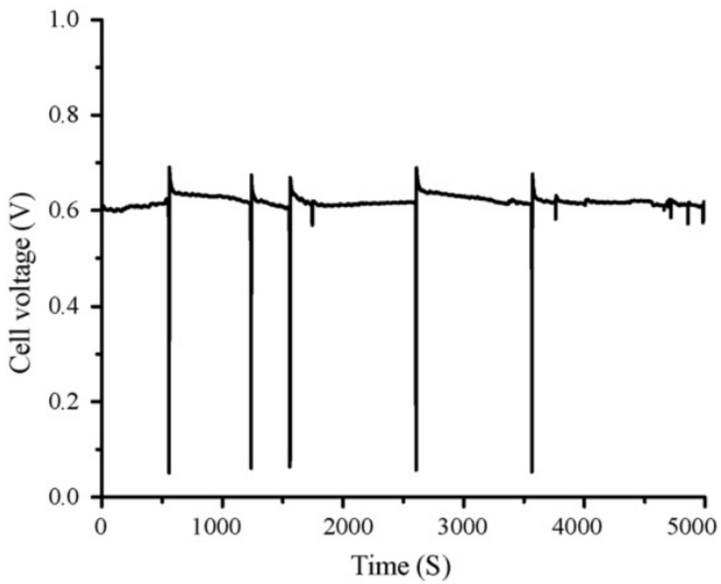
Water flooding in fuel cells



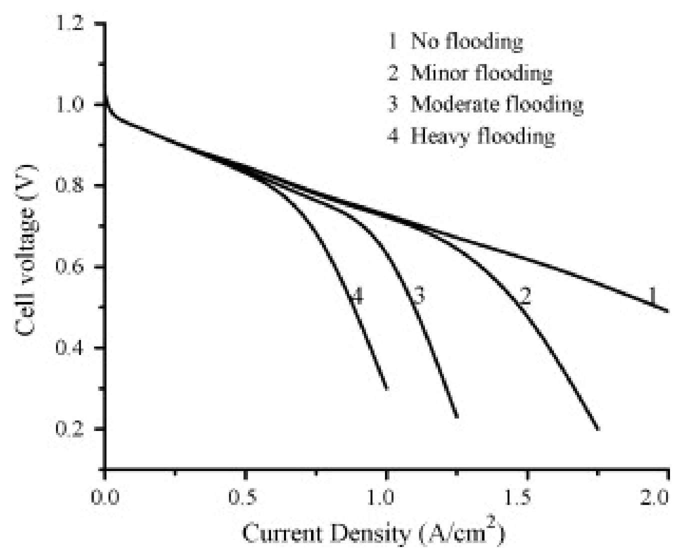
-Hydration in necessary for fuel cell operation

- Excess water fills the pores and blocks the access of reactants

-Water management influences cell efficiency

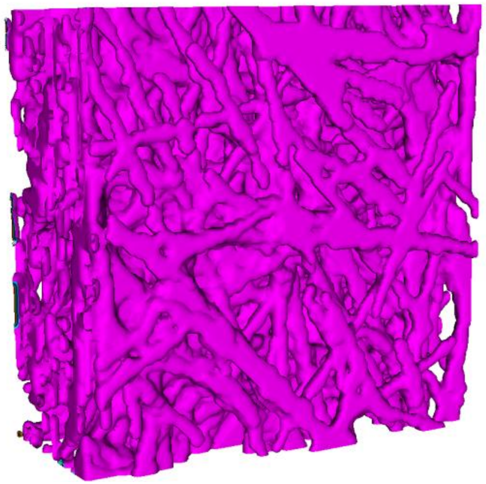


A typical water flooding pattern in a PEM fuel cell



Polarization curves of a PEM fuel cell: the effect of water flooding

Modeling of water flow dynamics in GDL



Carbon cloth and carbon paper for Gas Diffusion Layer (GDL)

Thickness: 200-400 micron
Fiber diameter: ~10 micron
Pore size: ~80 micron

Goal:

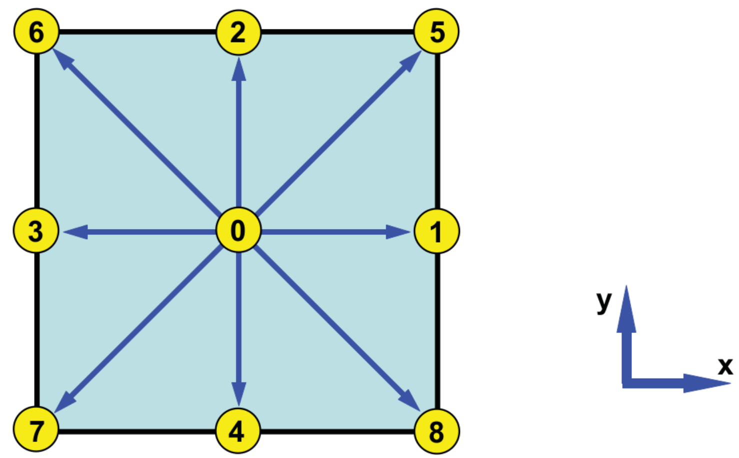
Modeling of two-phase flows in a real GDL structure

Pore-scale-based models for water transport and perspectives on design

Develop fuel cells with optimized geometry and water management parameters

Lattice Boltzmann Method (LBM)

- Ideal to handle complicated boundary porous media
- Ideal to handle complex flows e.g. mutliphase
- Easy for parallel computing



D2Q9 lattice scheme

Boltzmann's equation:

$$\frac{\partial F_i}{\partial \hat{t}} + \boldsymbol{c}_i \bullet \hat{\nabla} F_i = -\frac{1}{\hat{\tau} \cdot \varepsilon}\left(F_i - F_i^{(eq)}\right)$$

$$F_i\left(\boldsymbol{x} + \boldsymbol{c}_i \cdot \Delta t, t + \Delta t\right) - F_i\left(\boldsymbol{x}, t\right) = -\frac{1}{\tau}\left(F_i - F_i^{(eq)}\right)$$

* LBM assumes that particles are s constrained to move in a lattice

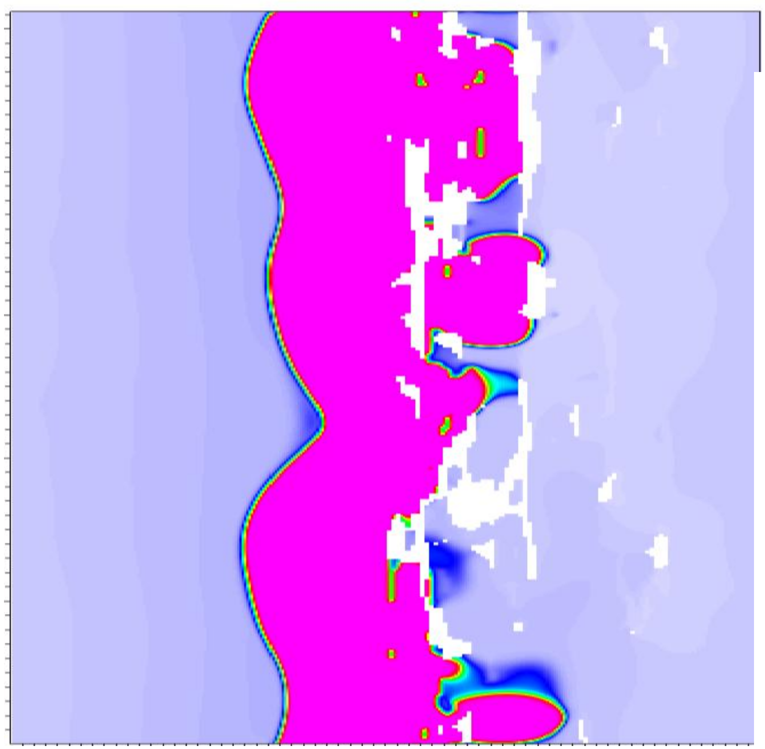
Macroscopic quantities:

$$\rho\left(\boldsymbol{x}, t\right) = \sum_i F_i\left(\boldsymbol{x}, t\right)$$

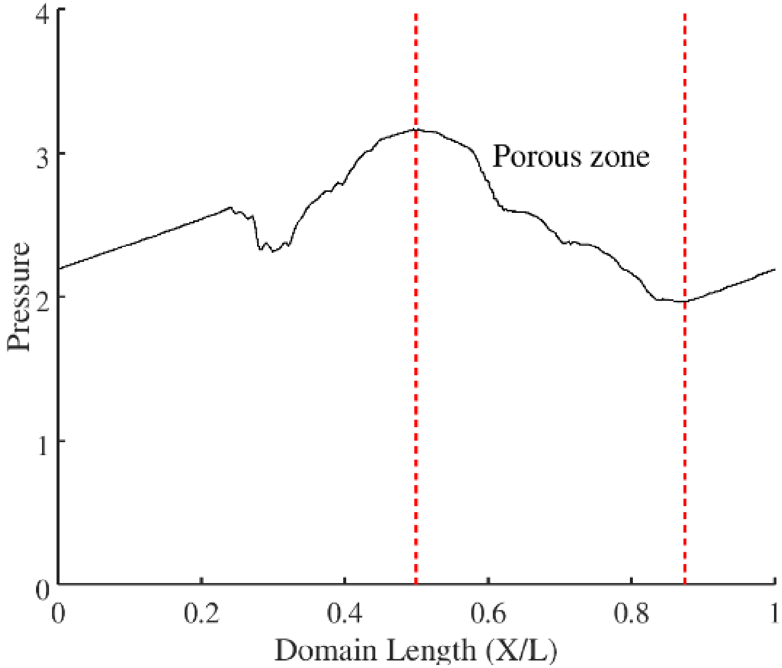
$$j\left(\boldsymbol{x}, t\right) = \rho\left(\boldsymbol{x}, t\right) \cdot \boldsymbol{u}\left(\boldsymbol{x}, t\right) = \sum_i \boldsymbol{c}_i \cdot F_i\left(\boldsymbol{x}, t\right)$$

Results: Pressure variation along GDL

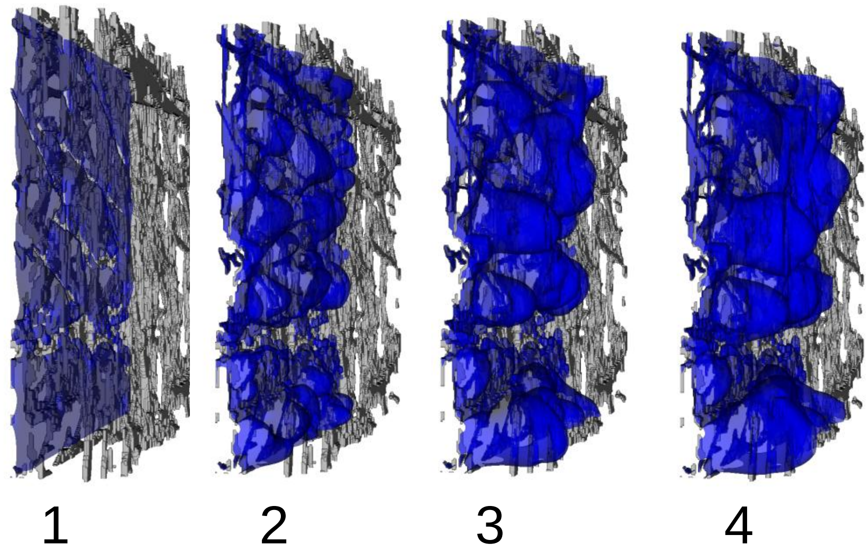
- Pressure drop is applied on the flow
- Pressure increases behind the GDL untill it starts to penetrate
- Pressure decreases in porous zone

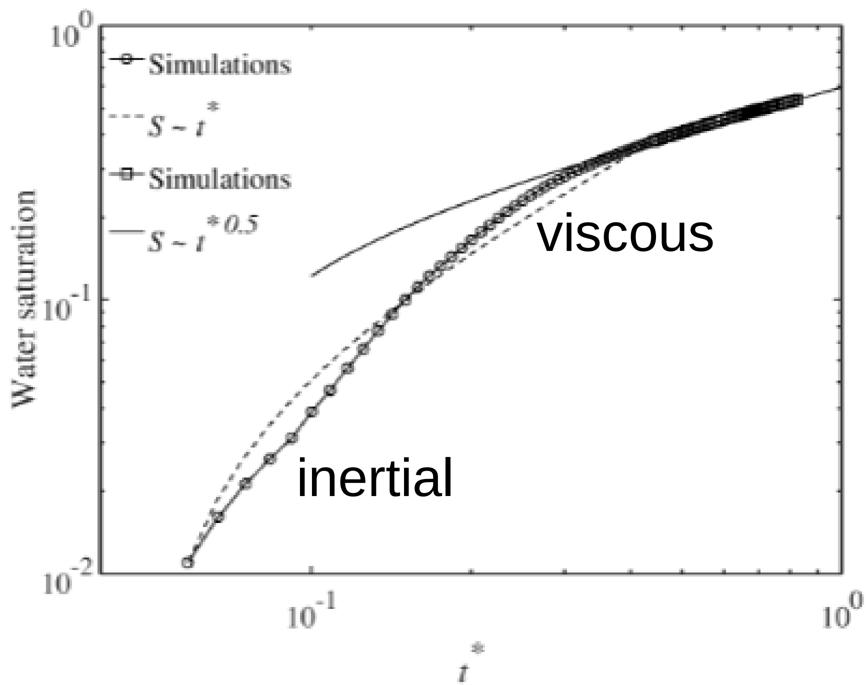


Flow distribution



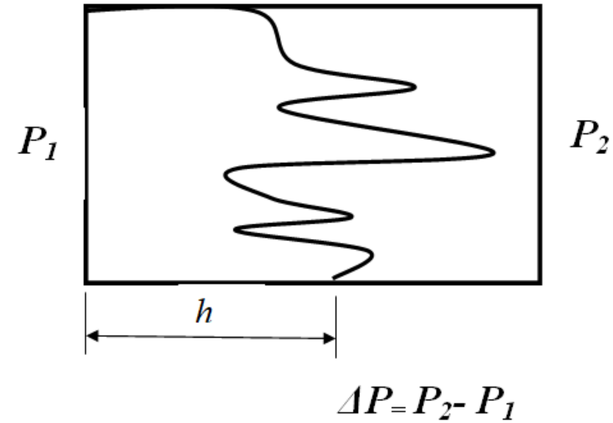
Results: Liquid propagation in GDL





Conventional approach:

Flow in porous media is described by **Darcy's law**:



$$\overline{V} = \frac{K}{\mu_w}\frac{\Delta P}{h}$$

$$\frac{h}{t} = \frac{K}{\mu_w}\frac{\Delta P}{h}$$

$$h = \sqrt{\left(\frac{K}{\mu_w}\Delta P\right) t}$$

$$S \sim \sqrt{t}$$

Summary

- Fuel cells description
- Water management in fuel cells
- Results of LBM simulations
- Models developed for both inertial & viscous regimes
- Darcy's Law cannot capture liquid kinetics in inertial regime