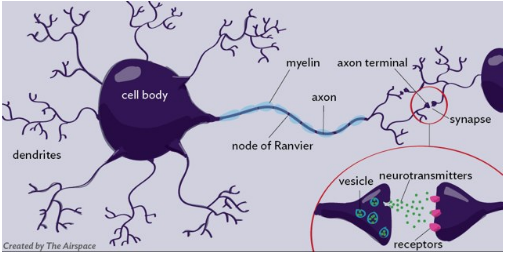
Mathematical modeling course
Fall 2014
Projects' presentation

28/10/2014

Project 1 : Modeling of synaptic transmission

- Signal transmission in a neuron



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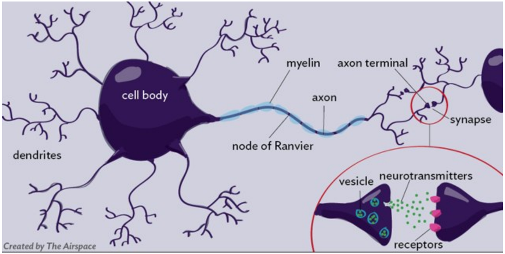

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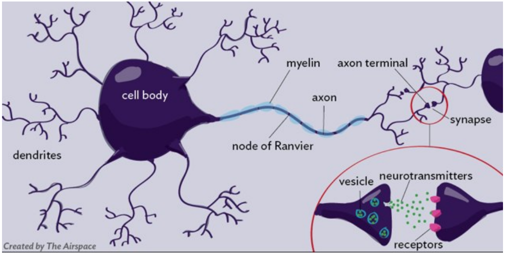
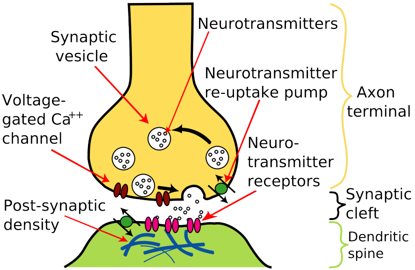


- Neurons are not hard-wired. Hypothesis defended by Fridtjof Nansen and formulated by Santiago Ramón y Cajal.
- 10^{11} neurons, 10^{14} synapses

Synapse

- Synaptic cleft, pre/post-synaptic terminal
- Neurotransmitters
- Receptors



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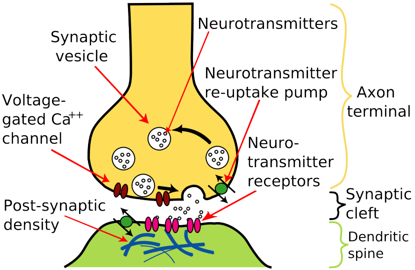

Example of neurotransmitters: dopamine, serotonin, noradrenaline, adrenaline.

Stochastic processes

The diffusion and reaction mechanisms are stochastic processes.

- Random walk or Brownian motion for the neurotransmitter molecules.

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- Random walk or Brownian motion for the neurotransmitter molecules.
- Receptor binding
$$\mathrm{R} + \mathrm{N} \rightleftharpoons \mathrm{R{-}N}.$$
The probability that a receptor R and neuron N reacts to bind together is related to the distance between the two and the time they remain close.

Concentration and expected values

- Brownian motion and diffusion equation.

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- Let $X(t)$ be the trajectory of a particle. We define the transition function
$$\phi_{\Delta t}(x,y) = P\left[X(t+\Delta t) = y | X(t) = x\right]$$
or
$$\phi_{\Delta t}(x,y) = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon} P\left[X(t+\Delta t) \in [y-\varepsilon, y+\varepsilon] | X(t) \in [x-\varepsilon, x+\varepsilon]\right].$$

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Let $f(t, x)$ be the probability density that the particle is at x in t,

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Morally speaking, we have

$$P\left[X(t+\Delta t) = x\right] = \sum_y P\left[X(t+\Delta t) = x | X(t) = y\right] P\left[X(t) = y\right].$$

We can show that

$$f(t+\Delta t, x) = \int_{-\infty}^{\infty} \phi_{\Delta t}(x,y) f(t,y)\, dy.$$

End of proof

We assume

- Translation invariance: $\phi_{\Delta t}(x, y) = \phi_{\Delta t}(y - x)$
- Isotropy: $\phi_{\Delta t}(z) = \phi_{\Delta t}(\|z\|)$ so that $\int z\phi_{\Delta t}(z)\,dz = 0$
- Brownian motion scaling

$$\phi_{\Delta t}(z) = \frac{1}{\sqrt{\Delta t}}\phi_1(\frac{z}{\sqrt{\Delta t}})$$

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$$\begin{aligned}\int_{-\infty}^{\infty} \phi_{\Delta t}(x-y) f(t,y)\,dy &= \int_{-\infty}^{\infty} \phi_{\Delta t}(y) f(t,x-y)\,dy \\ &= \int_{-\infty}^{\infty} \phi_{\Delta t}(y)(f(t,x) - \frac{\partial f}{\partial x}(t,x)y + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(t,x)y^2 + \dots)\,dy\end{aligned}$$

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$$= \int_{-\infty}^{\infty} \phi_{\Delta t}(y)(f(t, x) - \frac{\partial f}{\partial x}(t, x)y + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(t, x)y^2 + \ldots)\,dy$$

Hence,

$$f(t, x) + \Delta t\frac{\partial f}{\partial t} + \ldots = f(t, x) + \Delta t\alpha^2\frac{\partial^2 f}{\partial x^2} + \ldots.$$

where $\int_{-\infty}^{\infty} \phi(z)z^2\,dz = 2\alpha^2$ and we obtain the diffusion equation:

$$\frac{\partial f}{\partial t} = \alpha^2\frac{\partial^2 f}{\partial x^2}$$

Chemical reactions

- Probability to find one or more particle in a control volume ΔV is equal to
$$c\Delta V \text{ as } \Delta V \to 0$$

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For a particle A at a given place, we assume that the probability p that it reacts with a particle B in a period Δt is given by

$$p = \alpha \frac{V_a}{V} \Delta t + o(\Delta t)$$

where V is the total volume, V_a is an *interaction* volume and α denotes the probability that, once the particle are close enough, the reaction effectively takes place.

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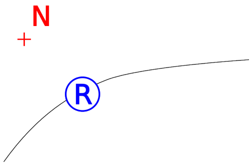
where k is the kinetic reaction constant.

Binding process on the membrane



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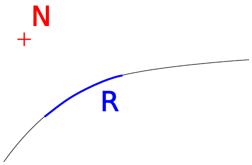

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You may want to consider a receptor density on the membrane (in $\mathrm{mol/m^2}$).

Main questions

Derive the modeling equations. Propose a numerical scheme to solve the equations. Propose a geometrical model for the synapse. Implement a numerical solver.

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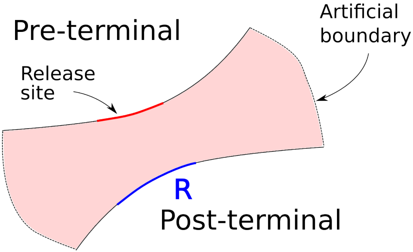
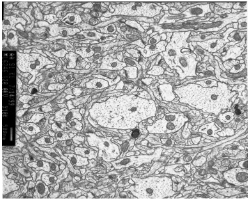
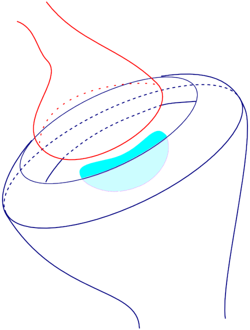
Derive the modeling equations. Propose a numerical scheme to solve the equations. Propose a geometrical model for the synapse. Implement a numerical solver.
Application: Estimate the time for a signal to be transmitted. To do so, you may consider the equilibrium state for the system in the case where the synaptic cleft is confined. Such equilibrium state yields the maximum number of receptors that in practice will be bound.

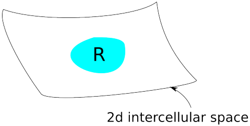


Follow-up question 1: Geometrical reduction

The intercellular space is very thin compared to the characteristic size of the cells. We want to exploit this fact and model the intercellular space as a 2-dimensional surface. By this geometrical reduction, we hope to increase the computation speed. It could be useful as the geometry of the intercellular space is typically very complex
How this reduction modify the modeling equations? Following the same steps as in the 3-dimensional case, implement a numerical solver for this case.







Follow-up question 2: Clearance of neurotransmitters

- The synaptic cleft need to cleared from neurotransmitters before a new signal can be transmitted.

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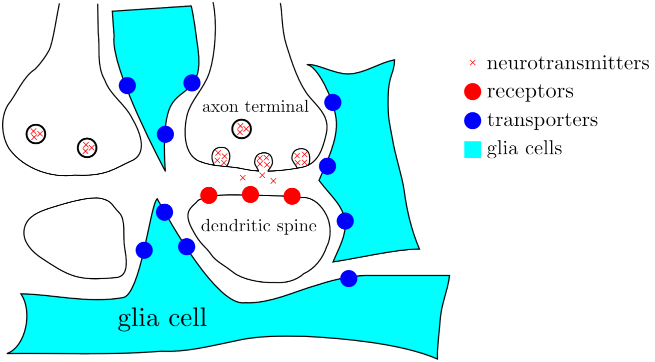

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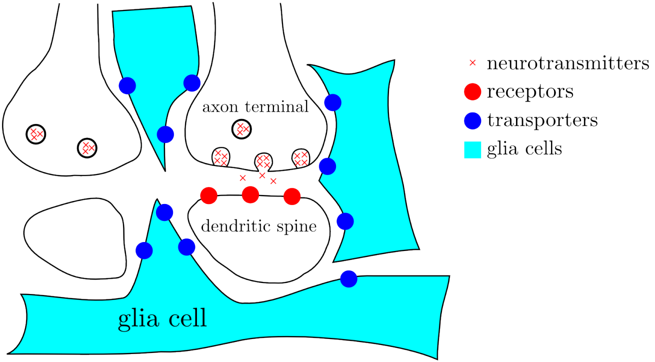


- *Estimate the clearance time. Estimate the probability of synaptic cross-talk.*

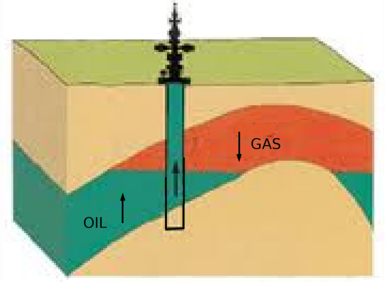
Follow-up question 3: Coupling with flow

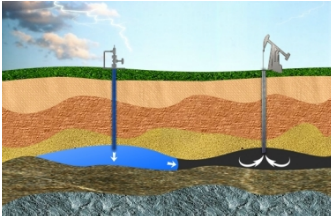
The intercellular space is filled with intercellular fluid. We want to study the effects of an underlying moving fluid on synaptic transmission. Derive the governing equations in this case and try to solve them.

Application: Estimate the influence of an underlying flow for synaptic cross-talk.

Project 2: Microbial Enhanced Oil Recovery (MEOR)

- *Primary* and *secondary* oil recovery





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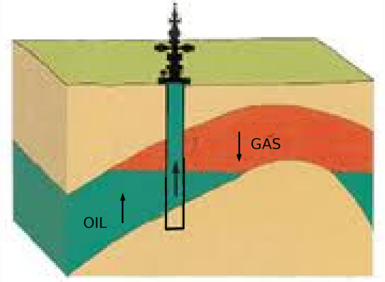

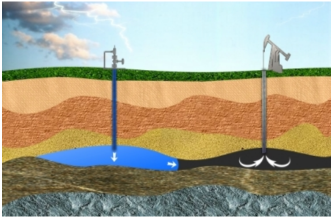

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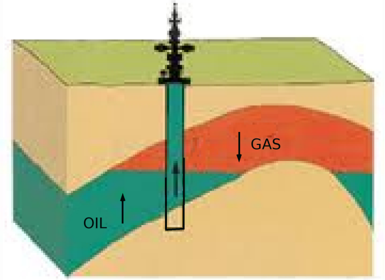
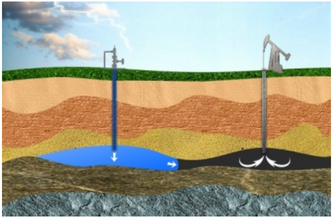
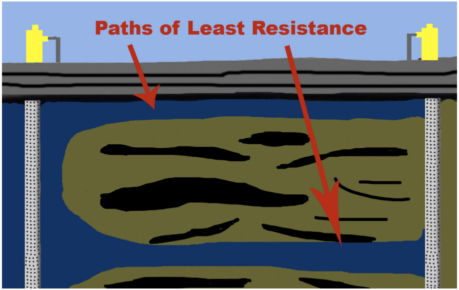




- Between 50% and 70% of the oil remains in place.
- *Enhanced* Oil Recovery (EOR): More advanced technologies to increase oil recovery.

Water channels

- Water flows in highest permeable regions and let large region of reservoir unswept.



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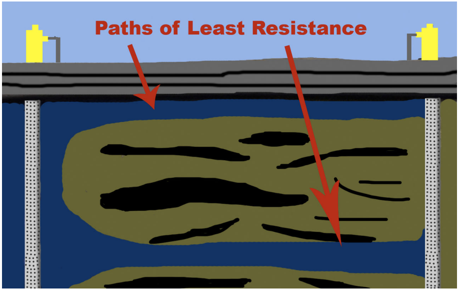
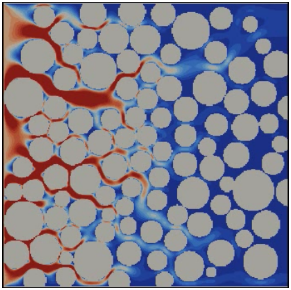


- EOR strategy: Diverge water from highly permeable regions.

Porous media flow



For incompressible single phase flow, we have essentially two parameters

- porosity
- permeability

Fluid flow equations

- Mass conservation equation

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- Momentum equation (Navier-Stokes)

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = -\nabla p + \mu \Delta \boldsymbol{u} + \rho \boldsymbol{g}$$

  - Kinetic forces: $\frac{1}{2} \int \rho \left\| \boldsymbol{u} \right\|^2 \, dxdt$
  - potential, elastic forces: $\frac{1}{2} \int \omega(\rho) \, dxdt$
  - viscous forces: $\frac{1}{2} \mu \int \left\| \nabla \boldsymbol{u} \right\|^2 \, dxdt$
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- If the fluid is incompressible,

$$\nabla \cdot \boldsymbol{u} = 0,$$

  If the fluid is compressible,

$$p = p(\rho) \qquad \text{(Legendre transform of } \omega.\text{)}$$

Euler and Stokes equation

- If we neglect the viscous forces, we obtain the Euler equation

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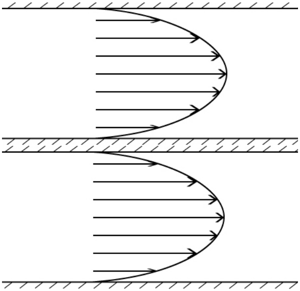
- In porous media, we use Stokes approximation.
- We cannot solve the equations at a pore level but there are large small scale velocity oscillation in a porous media.

Darcy's law

- Poisefeuille flow



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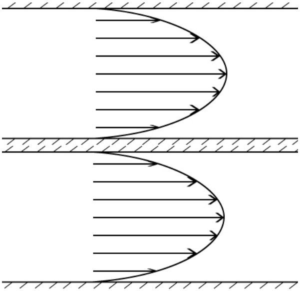
- Poisefeuille flow
- The analytical solution of the Stokes equations can be computed and we obtain that the gradient of P is constant, the velocity profile is a parabola, and

$$\frac{\Delta P}{\Delta x} = \frac{8\mu Q}{\pi r^4}$$



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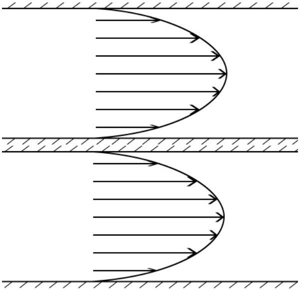

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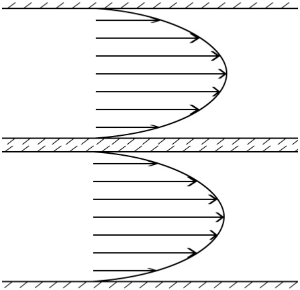

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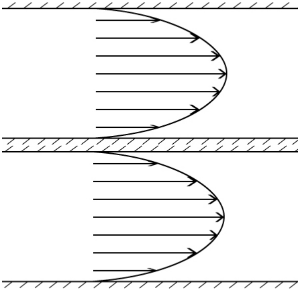

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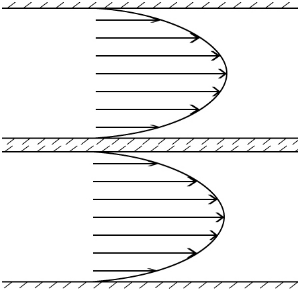

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- Viscous energy is now $\frac{\mu}{2}\int \frac{1}{K}\left\|u\right\|^2 dxdt$ (instead of $\frac{\mu}{2}\int \left\|u\right\|^2 dxdt$).

Porous media equation

- The porous media equations for an incompressible single phase are given by the mass conservation equation

$$\frac{\partial \phi}{\partial t} - \nabla \cdot \boldsymbol{u} = 0$$

and the Darcy's law

$$\boldsymbol{u} = -\frac{1}{\mu} \boldsymbol{K} \nabla P.$$

Microbial activity in the reservoir

- There exist stains of microbes which produce
  - biosurfactants (decrease surface tension),
  - biopolymers (improves mobility ratio),
  - biomass (clugging of high permeability region),
  - acids, solvents (increase permeability),
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  at reservoir conditions.
- MEOR: Add microbes, or stimulate microbes in place, to enhance oil recovery.

Main question (1)

- Population model without flow:

  We first focus on the microbial activity, assuming that the substrate where the microbes live is immobile. We need a population model for the microbes. Derive such model. The model should account for the following observations: Microbes reproduce themselves and eventually die. Their reproduction rate depends on the availability of nutrients and they will usually compete for nutrients. We may consider one or several, possibly competing, species.

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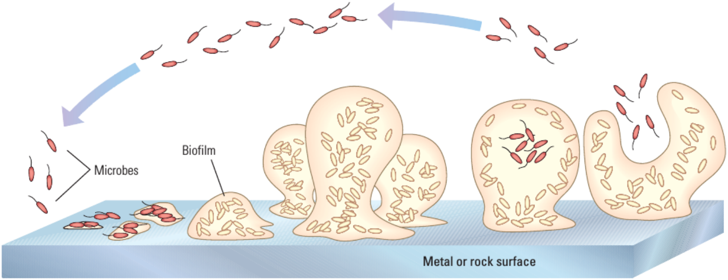
- Parameters:
  - population size N,
  - concentration of nutrients c_i,
  - reproduction rate, death rate.
- Find a model with an equilibrium.

Main question (2)

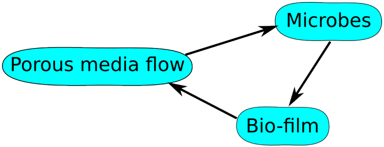
- Modeling of microbial accumulation:

  The microbes can produce bio-films which enable them to stick to the rock and colonize a region. This is the origin of clogging, whose consequence is a reduction in porosity. Propose a simple model for bio-film production and its effect on porosity.



Main question (3)

- Couple



Derive the equations for the transport of microbes, nutrients. Include in the model the production of bio-films and accumulation of microbes which modifies the porosity and the permeability.

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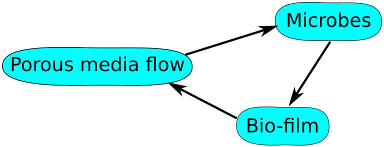

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- Relation between porosity and permeability: The Kozeny-Carman equation

$$K = \frac{\Phi_s^2 D_p^2}{180} \frac{\phi^3}{(1-\phi)^2}$$

where Φ_s is the sphericity and D_p the diameter of the rock particles.

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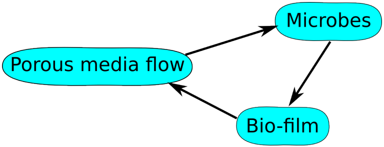

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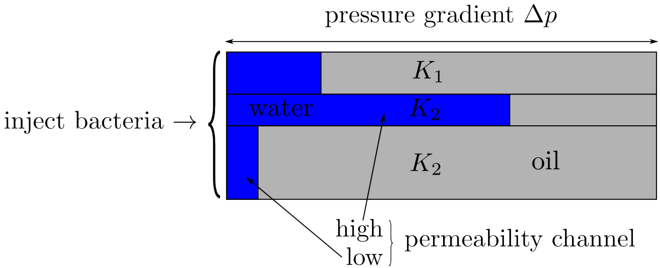
- *Derive a numerical scheme for the equations and implement it.*

Main question (4) : Application

We add microbes to the water. The largest amount of microbes will then be found in the region with highest water flow. Then, the microbes will start producing bio-films which will reduce the permeability, favoring the flow in the other regions of the reservoir. Check the feasibility of this scenario.



Two-phases flow

- Water/oil volume fraction is the saturation s_α ($\alpha = \{w, o\}$),

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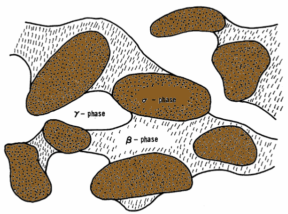
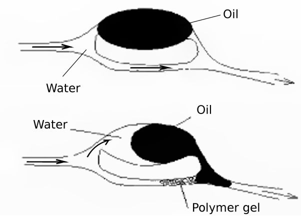
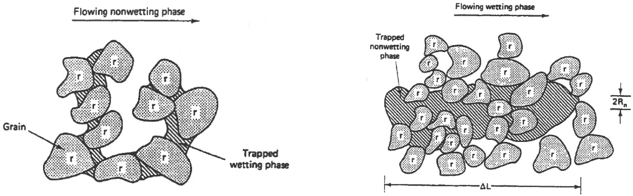
- Pore scale effects due to wettability and interfacial surface tension



Capillary forces

- Oil remains trapped due to capillary forces.

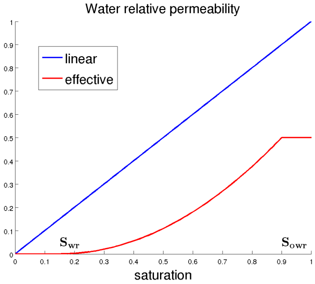




(a) Trapped wetting phase

(b) Trapped nonwetting phase

Relative permeability



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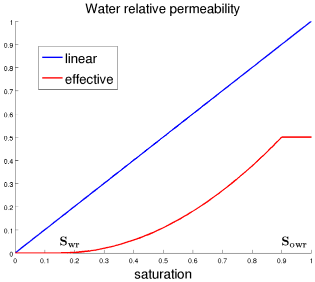
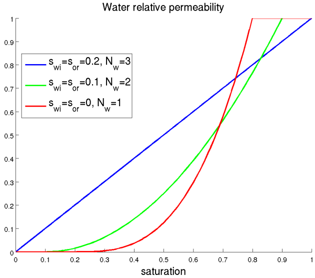


Corey relative permeability

$$k_{rw}(S_w) = k_{rw}^0 s_{wn}^{N_w},$$
$$k_{ro}(S_w) = (1 - S_{wn})^{N_o},$$

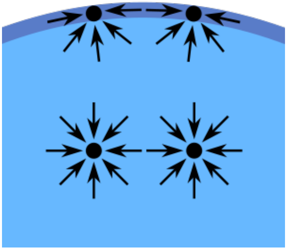
N_w, N_o, k_{rw}^0: parameters,
s_{wn}: normalized saturation,

$$S_{wn}(S_w) = \frac{S_w - S_{wi}}{1 - S_{wi} - S_{or}},$$



Surfactants

- Surfactants reduce interfacial surface tension, change wettability



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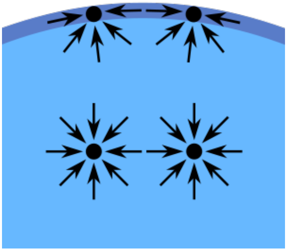

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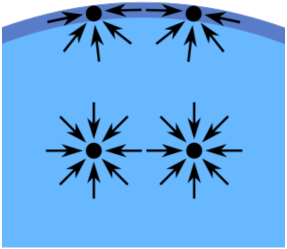
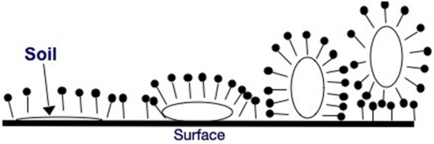
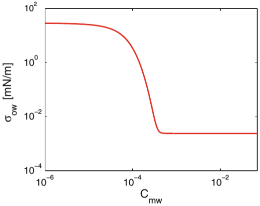




Surfactants

- Nonlinear effect of surfactants on surface tension



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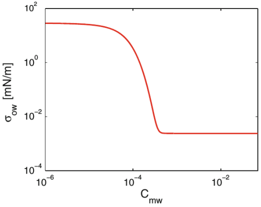
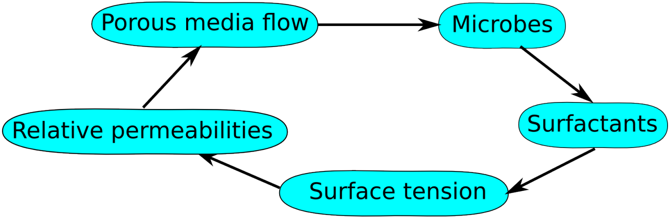


- Couplings



Questions

Consider a simple reservoir model with and quantify the effect of the following parameters,

- *concentration of nutrient injection,*
- *surfactant production rate of the microbes,*
- *surfactant parameters,*

on the increase in oil recovery.

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- Complex environment
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- *Introduce in your model a parasite microbe*

  Application: Introduce two types of nutrients, type A and type B. The nutrient A is used by both species and they compete for it. The nutrient B is only used by the beneficial specie. By injecting nutrient B, we favor the beneficial microbe. Quantify the benefit in increased oil recovery.

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