COMSOL CONFERENCE 2017 ROTTERDAM

Reactive transport modeling of CO_2 in carbonate rocks: Single pore model

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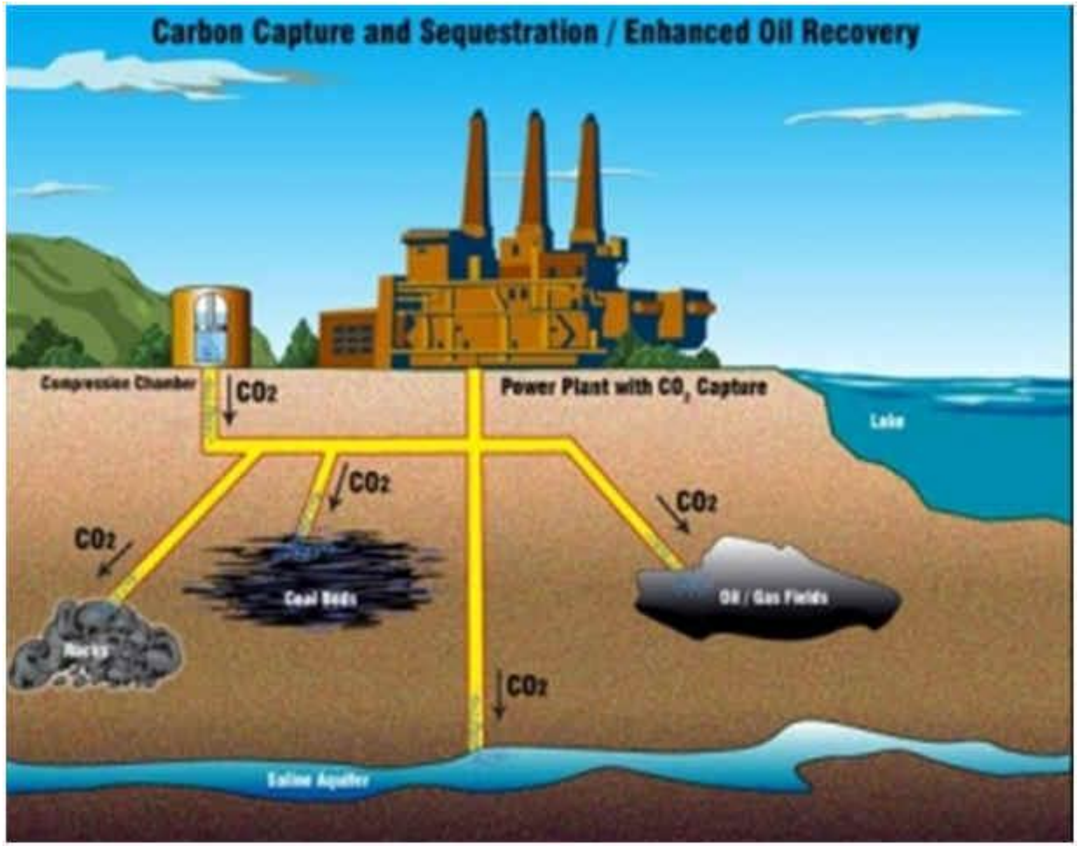
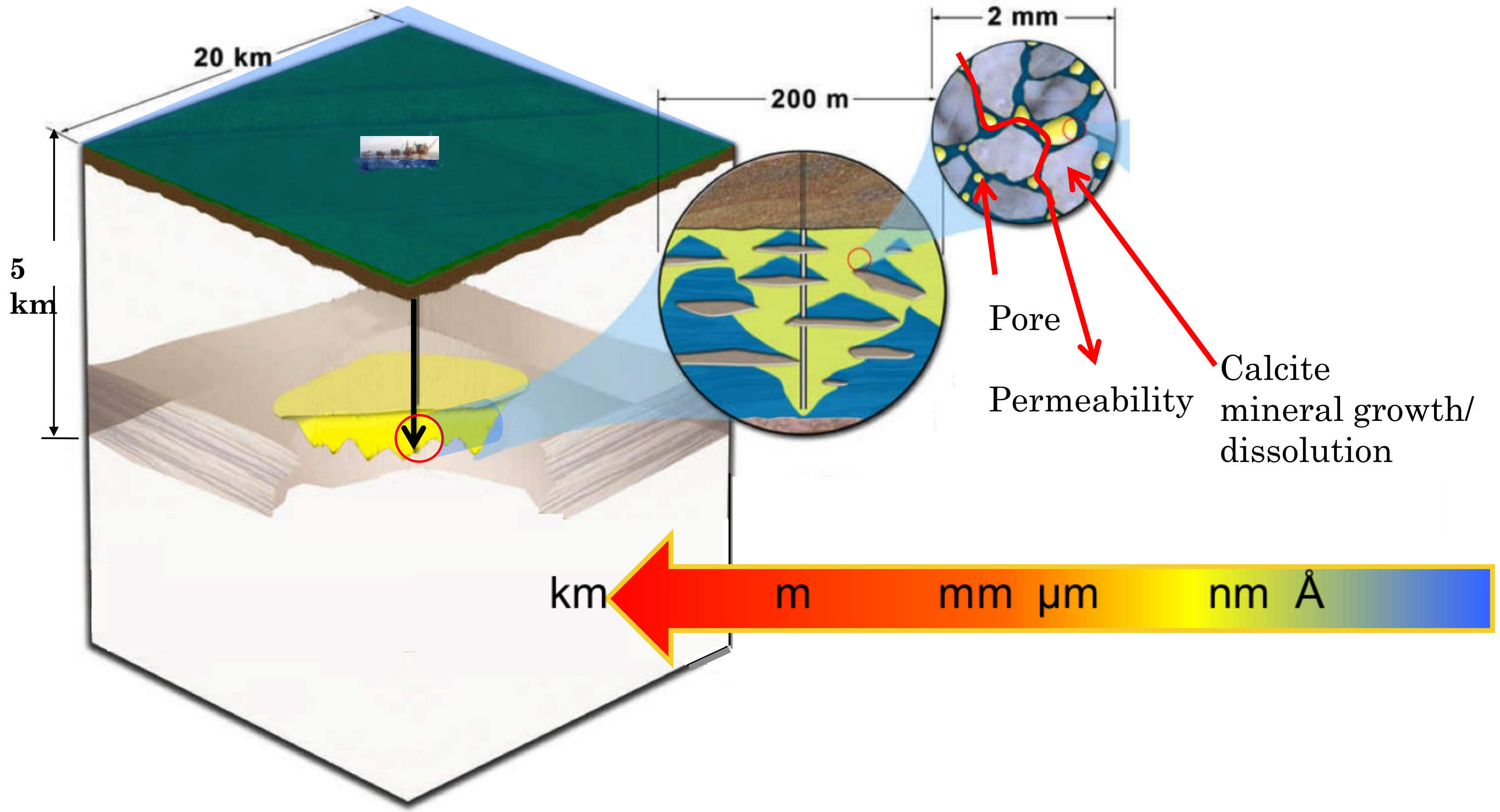
Agenda

- Motivation
- Single pore model
- Results
- Challenges
- Conclusions

MOTIVATION

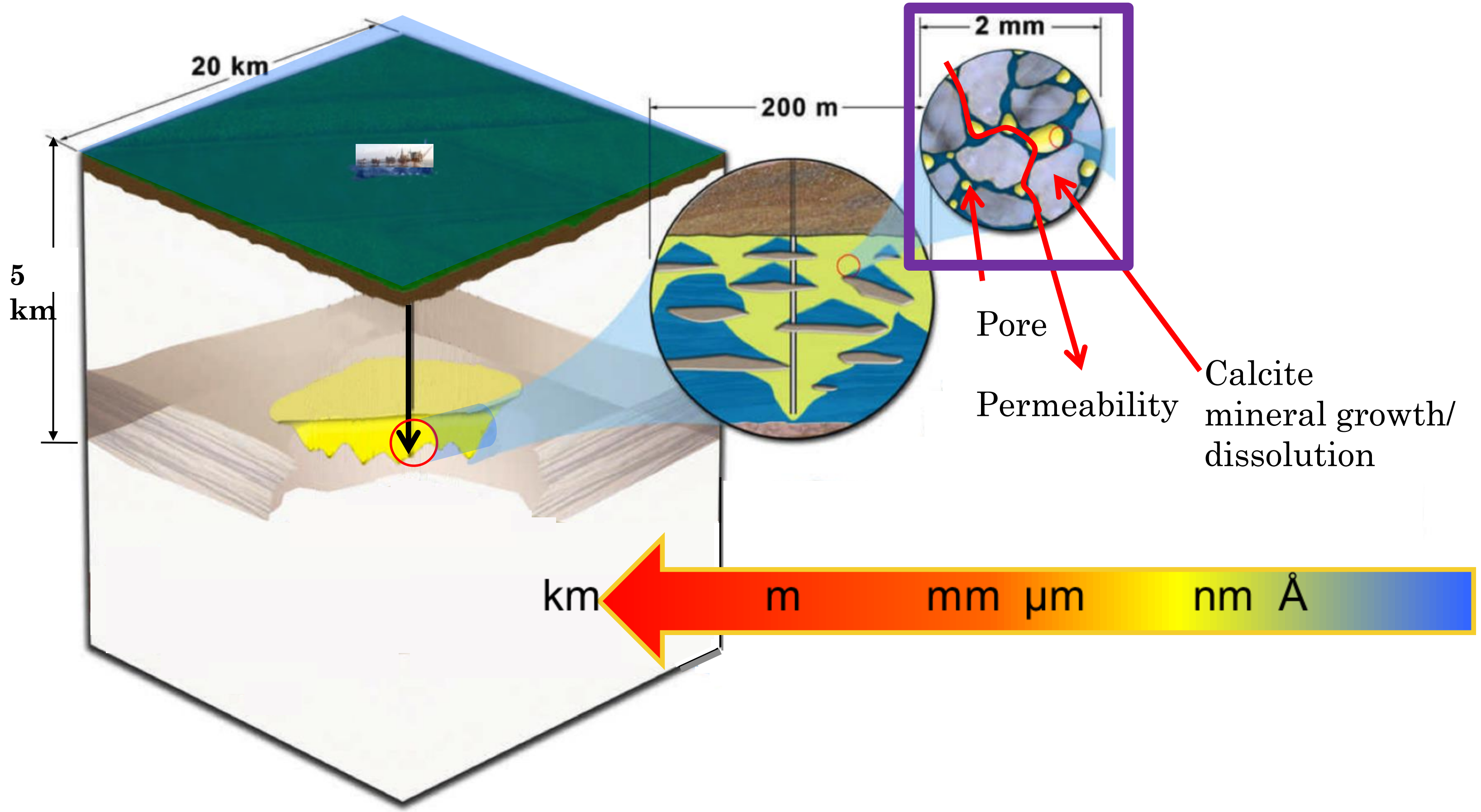

Carbon Capture and Sequestration / Enhanced Oil Recovery
Compression Chamber
CO_2
Power Plant with CO_2 Capture
Lake
CO_2
CO_2
CO_2
Coal Beds
Oil / Gas Fields
CO_2
Saline Aquifer

MOTIVATION



20 km
5 km
200 m
2 mm
Pore
Permeability
Calcite mineral growth/ dissolution
km
m
mm µm
nm Å

MOTIVATION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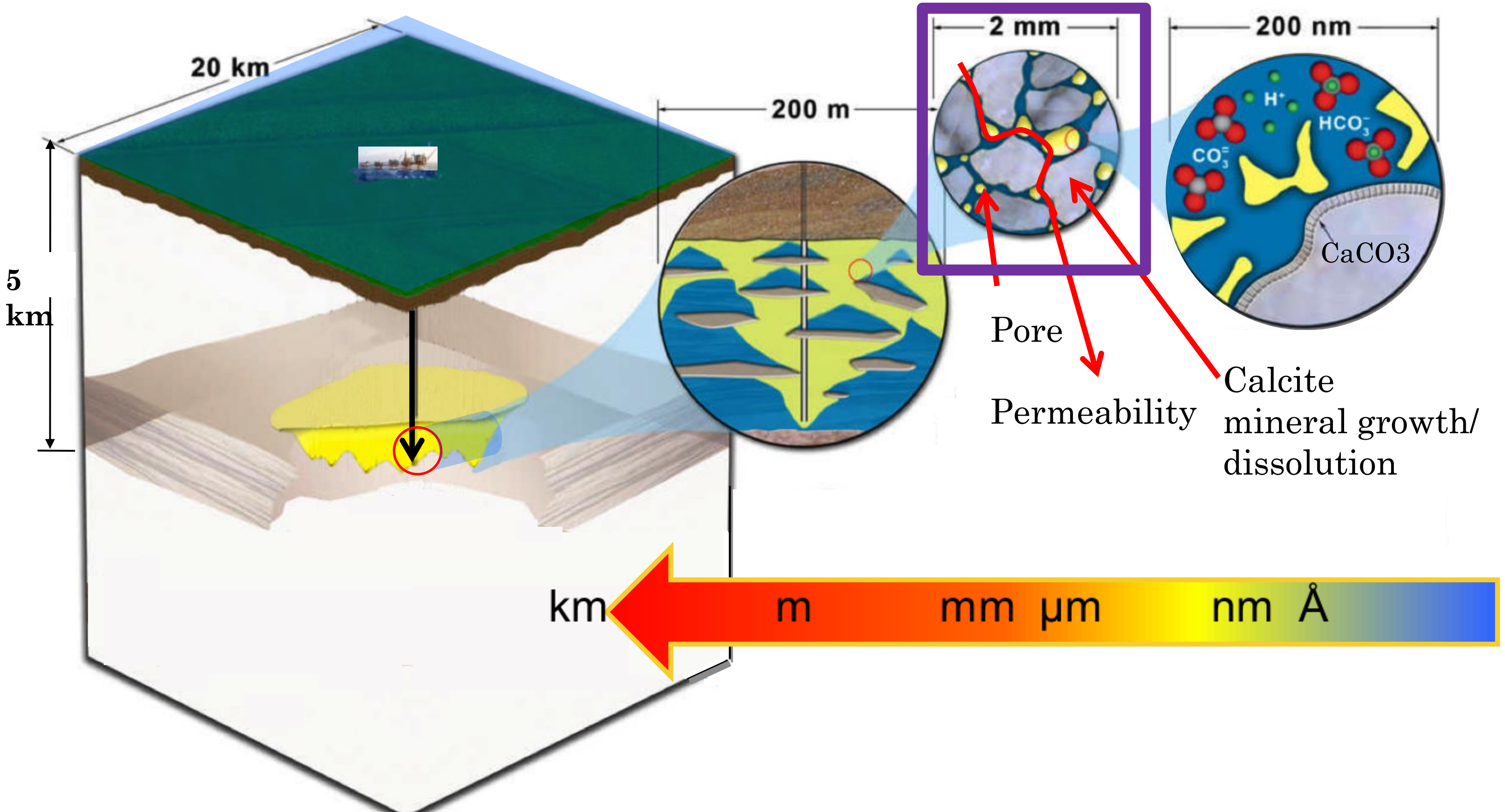
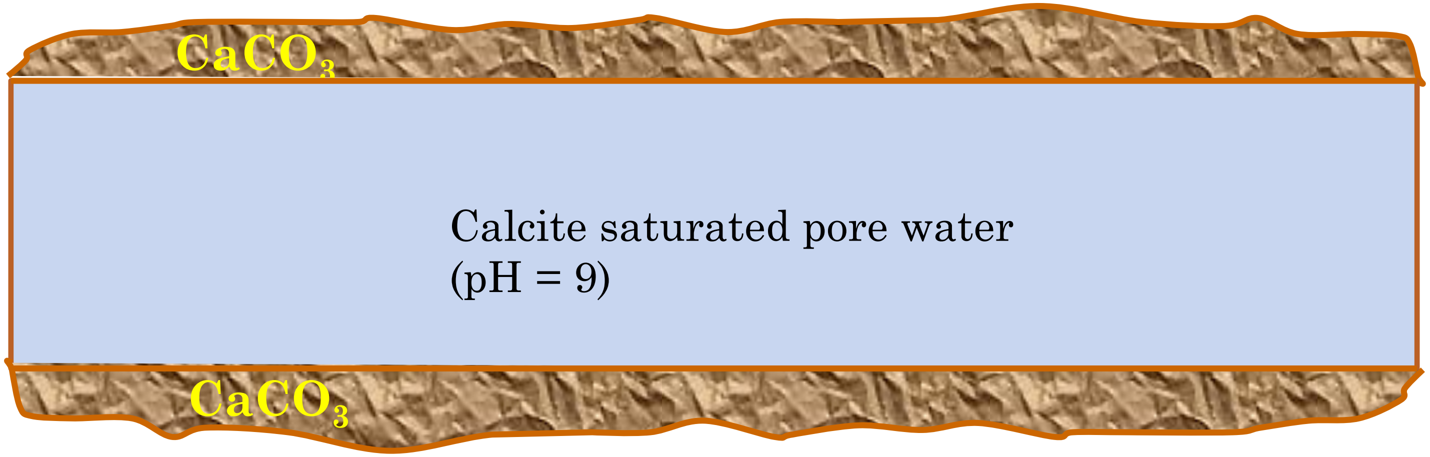


20 km
5 km
200 m
2 mm
200 nm
H+
HCO3-
CO3=
CaCO3
Pore
Permeability
Calcite mineral growth/ dissolution
km
m
mm µm
nm Å

SINGLE PORE MODEL



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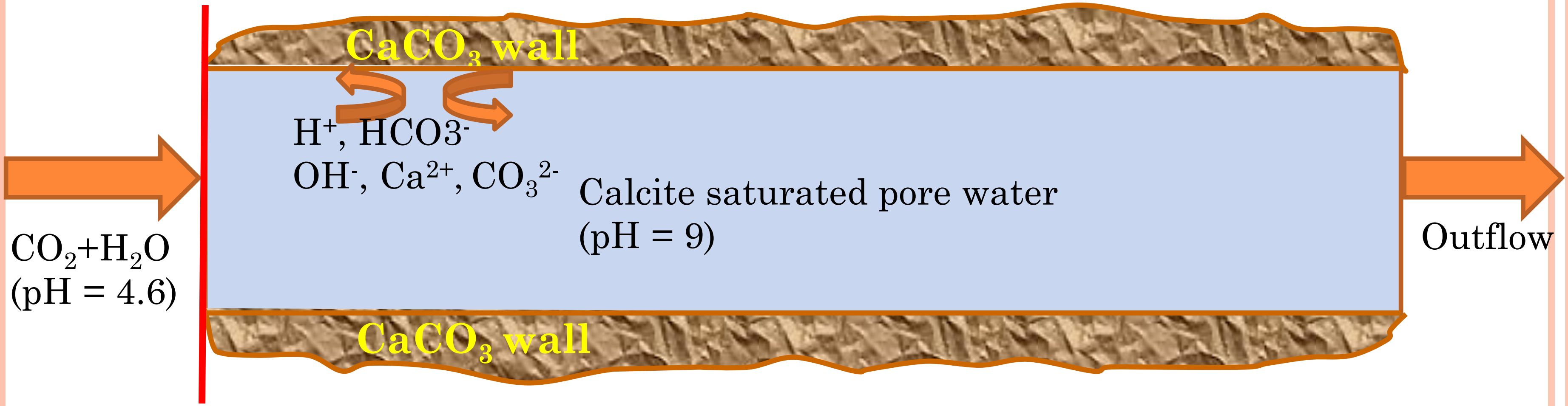

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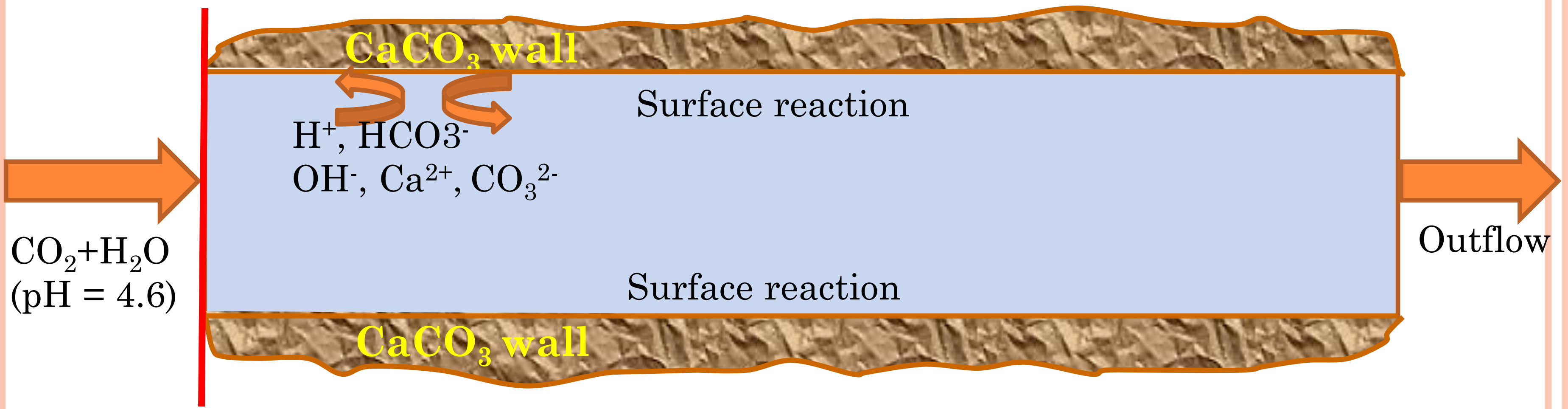

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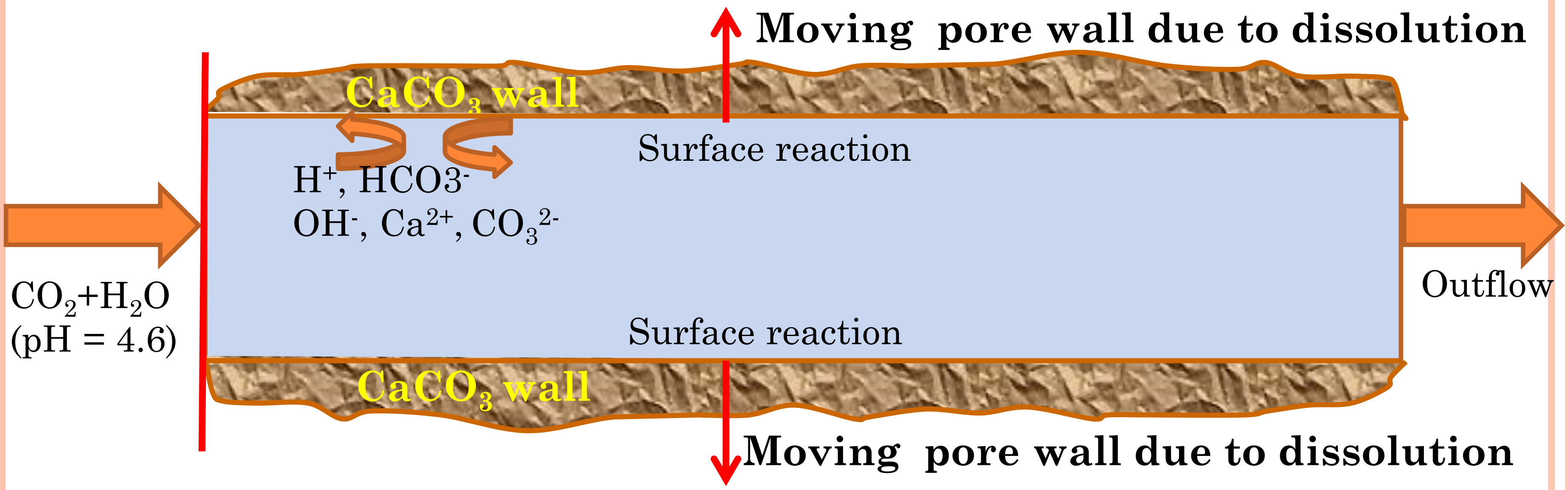

SINGLE PORE MODEL

MULTIPHYSICS MODEL

- Fluid flow
- Chemical Reactions
- Transport of diluted species
- Moving mesh

SINGLE PORE MODEL

MULTIPHYSICS MODEL

- **Fluid flow**
- Chemical Reactions
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FLUID FLOW

Re << 1 → Laminar Flow → Stokes Eq

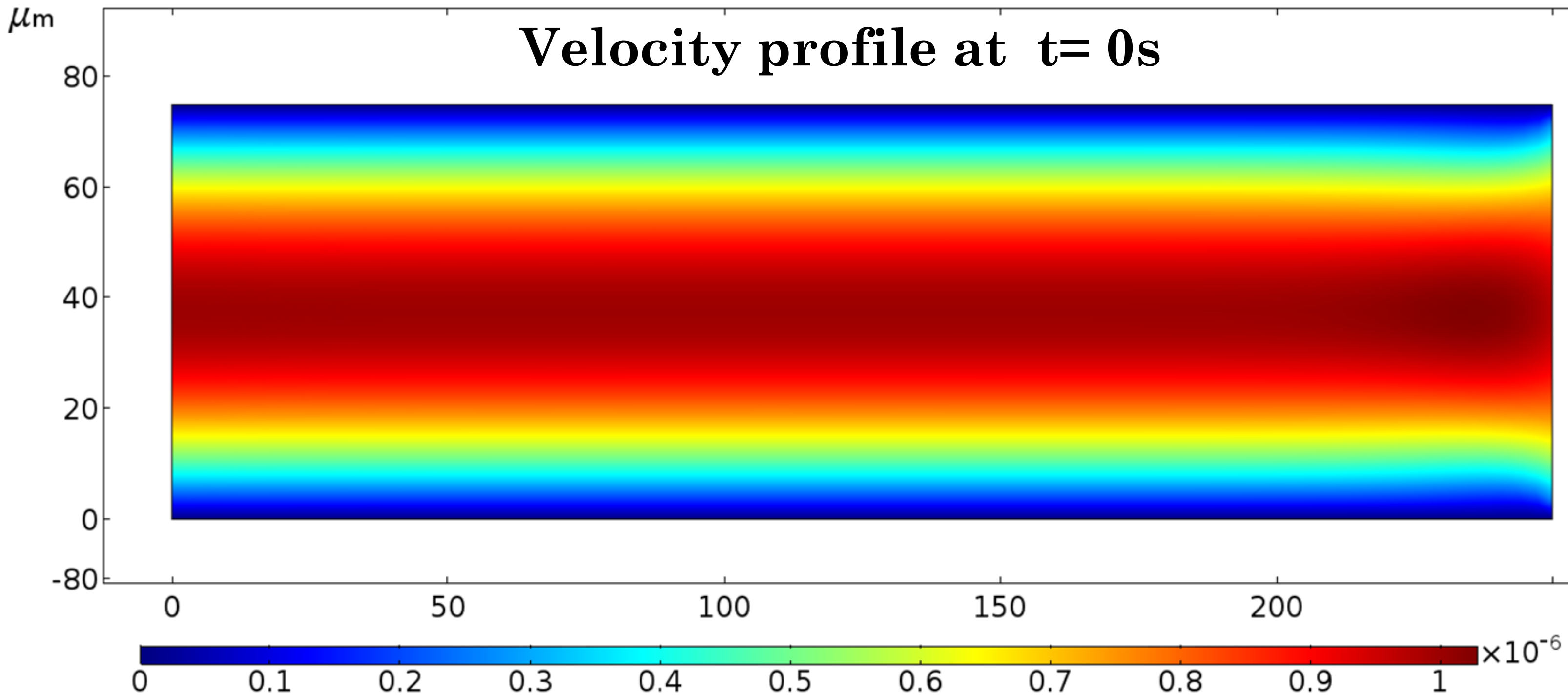
$$\rho \frac{\partial u}{\partial t} + \nabla . p = \mu(\Delta u)$$
$$\nabla . \mathrm{u} = 0$$

- Boundary Conditions:

  Inlet: $V(s) = Vmax * 4 * s * (1 - s)$

  Outlet: Constant pressure

FLUID FLOW


Velocity profile at t= 0s
μm
80
60
40
20
0
-80
0
50
100
150
200
μm
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
×10^-6

SINGLE PORE MODEL

MULTIPHYSICS MODEL

- Fluid flow
- **Chemical Reactions**
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CHEMICAL REACTIONS

Solution Species
$CO_2(g)$
CO_2_aq
H^+
OH^-
CO_3^{-2}
HCO_3^-
Ca^{2+}

Equilibrium Reaction	Keq
$CO_2(g) = CO_2\_aq$	3.38*10^-2
$CO_2\_aq + H_2O = H^+ + HCO_3^-$	10^-6.35
$HCO_3^- = H^+ + CO_3^{-2}$	4.69*10^-11
$H_2O = H^+ + OH^-$	1.023*10^-14

Reversible reaction on the surface of pore boundary

$$CaCO3 \Leftrightarrow Ca^{2+} + CO_3^{-2}$$

$$R_{calcite}=(k_1 a_{H+} + k_2 a_{CO2(aq)} + k_3)*\{1-[(a_{Ca2+}*a_{CO3}{}^{2-})/K_{eq}]\}$$

(Plummer et.al., 1978)

SINGLE PORE MODEL

MULTIPHYSICS MODEL

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Transport of diluted species

Advection-Diffusion-Reaction controlled transport

$$\frac{\partial ci}{\partial t} - \nabla.(D_i.\nabla ci) + u.\nabla ci = Ri$$

- Flux due to surface reaction

$$-n.(-Di.\nabla ci + u.ci) = Rcalcite$$

- Inflow Condition: Danckwerts flux condition

$$-n.(-Di.\nabla ci + u.ci) = u.coi$$

SINGLE PORE MODEL

MULTIPHYSICS MODEL

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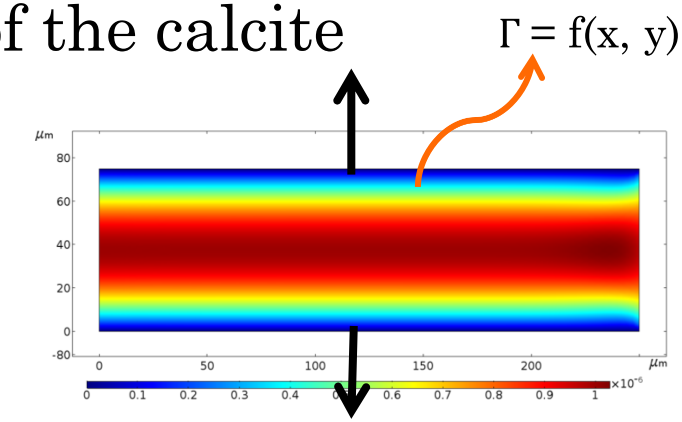
Moving Boundary

Mesh velocity, due to dissolution of the calcite



$$\frac{\partial \Gamma}{\partial t} . n = v_o$$

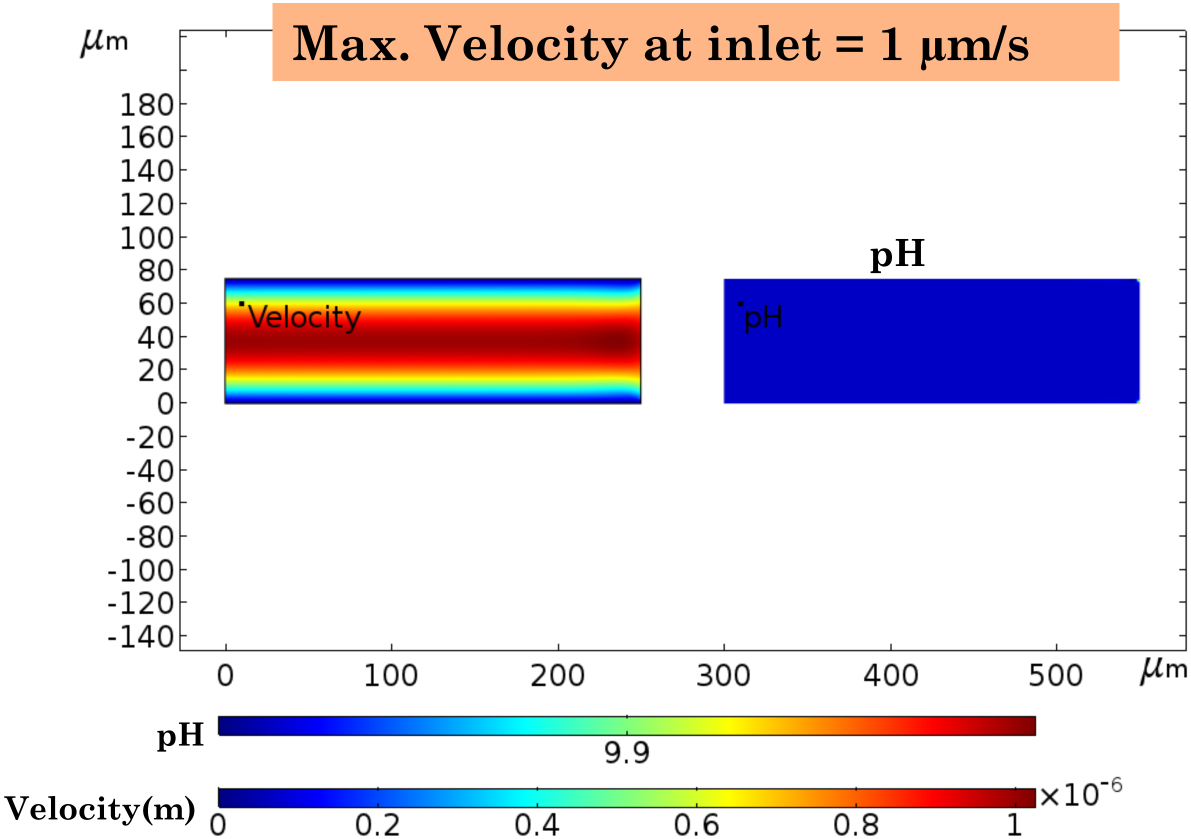
$$v_o = (R_{calcite} * MV)$$

$R_{calcite}$: Rate of calcite dissolution (mol m^{-2} s^{-1})

MV: Molar volume of calcite ($m^3 mol^{-1}$)

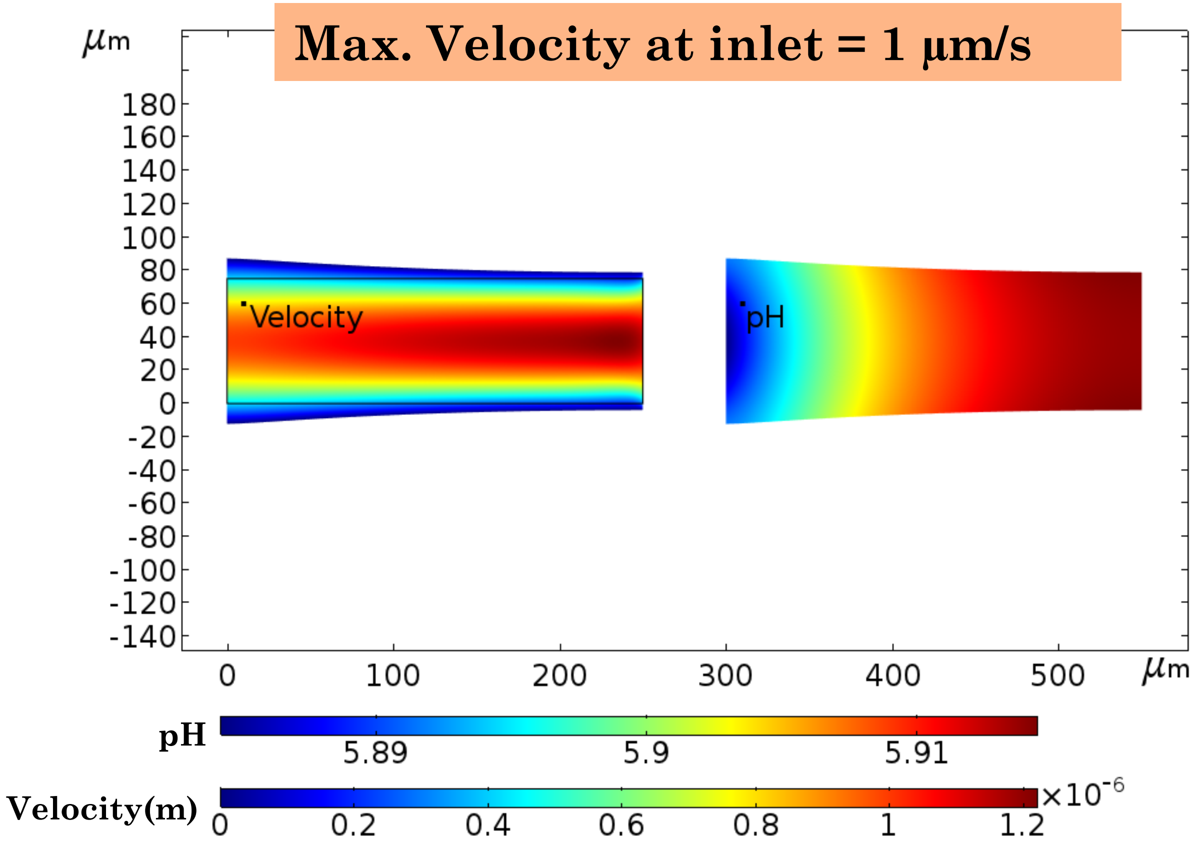
Results

Average flow velocity = 1 µm/s PV = 0



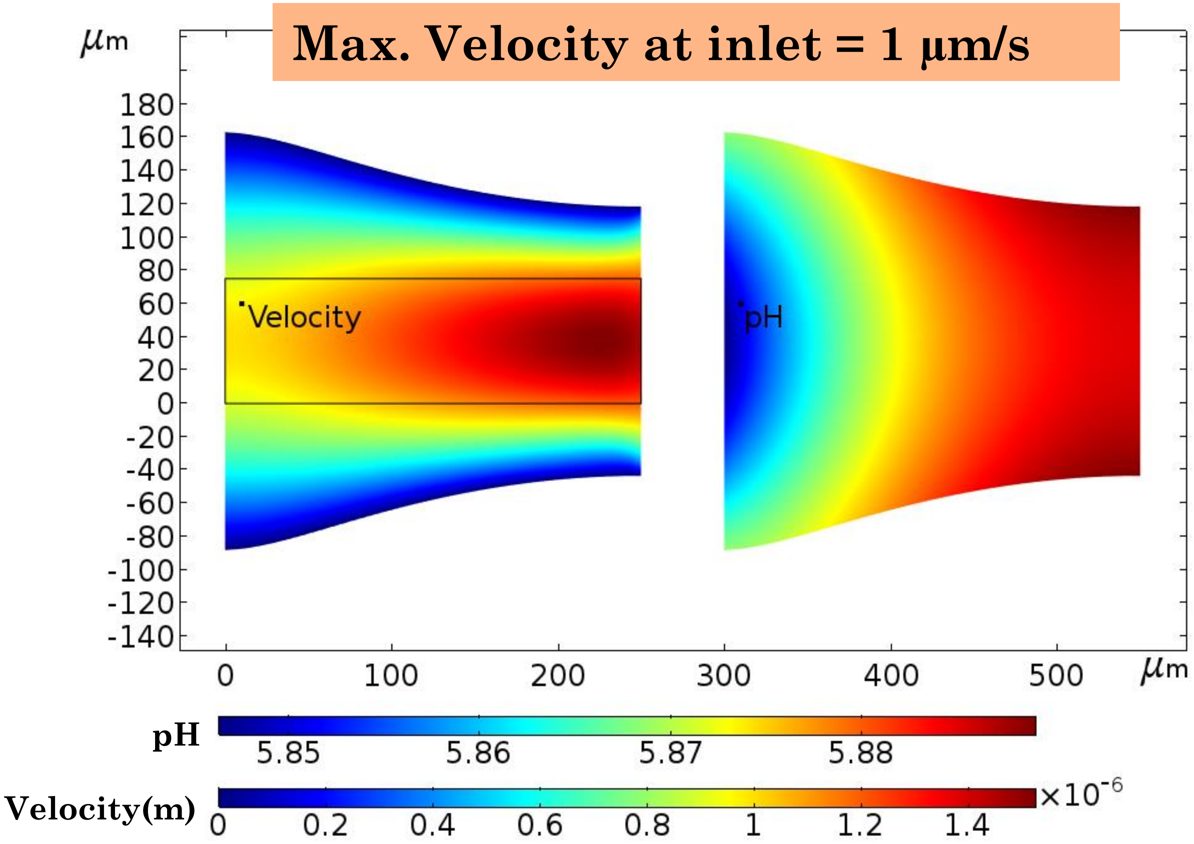
RESULTS

Average flow velocity = 1 μm/s PV = 1620



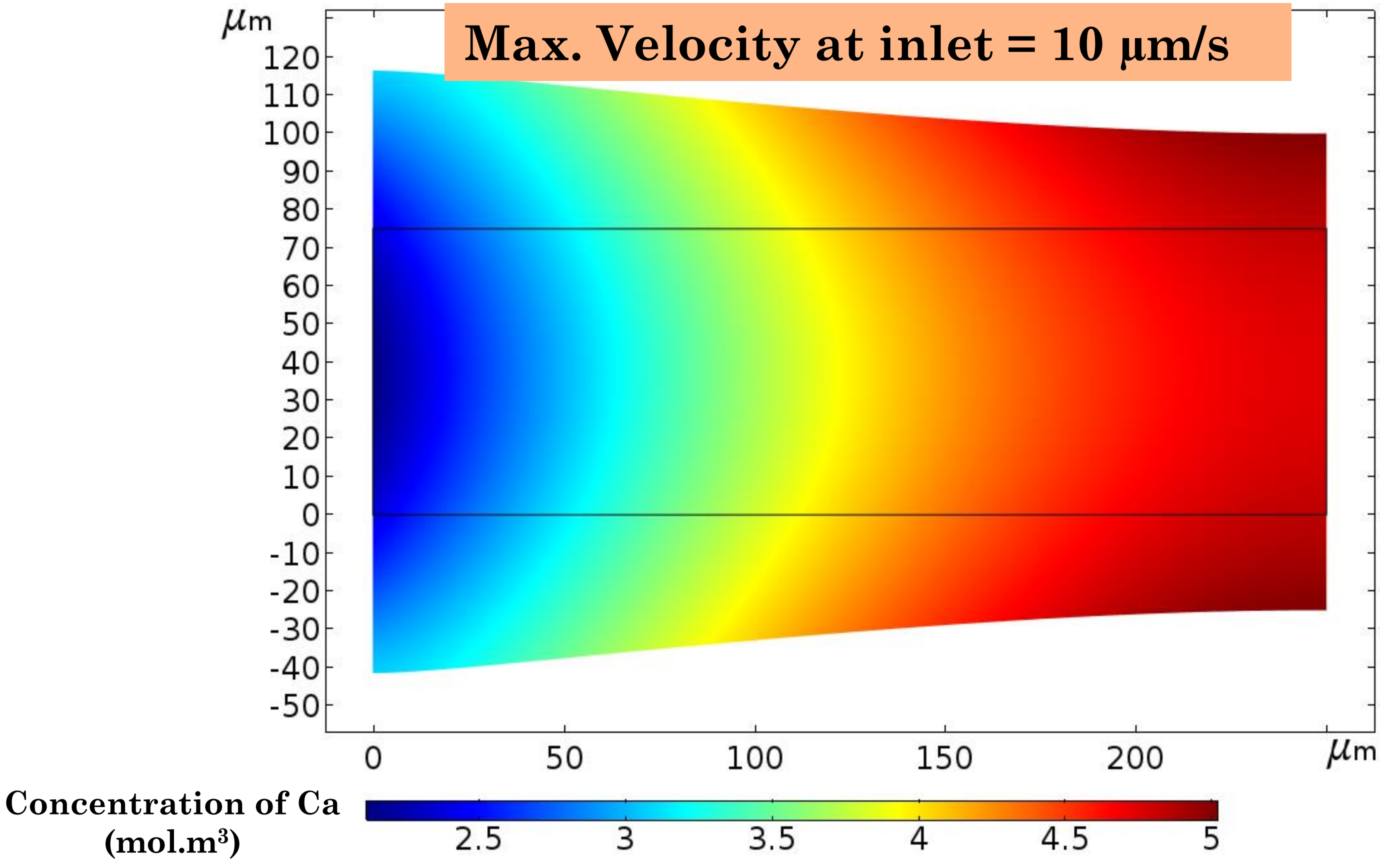
Results

Average flow velocity = 1 μm/s PV = 3300



RESULTS

After injection of same number of PV = 3300



Results

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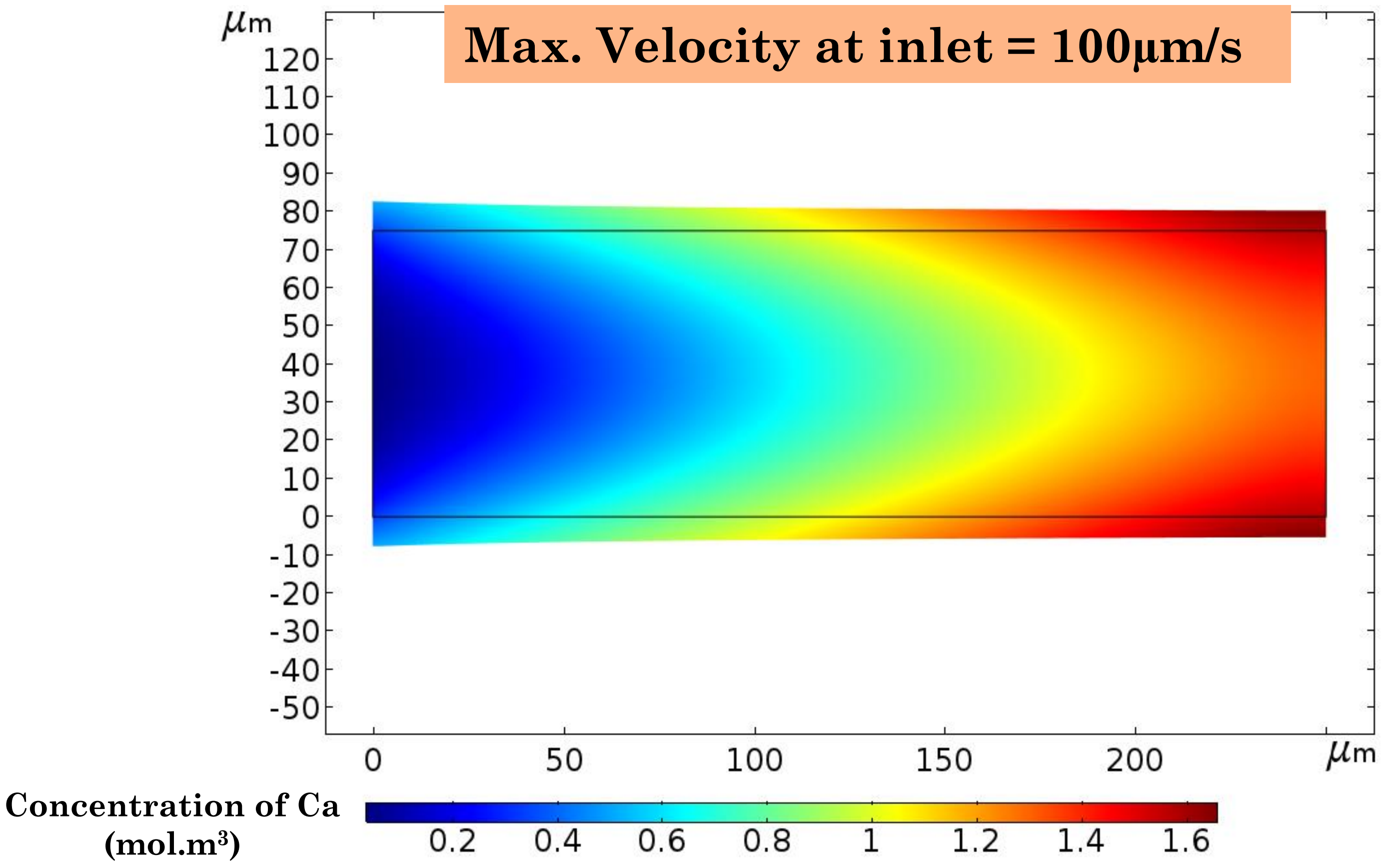
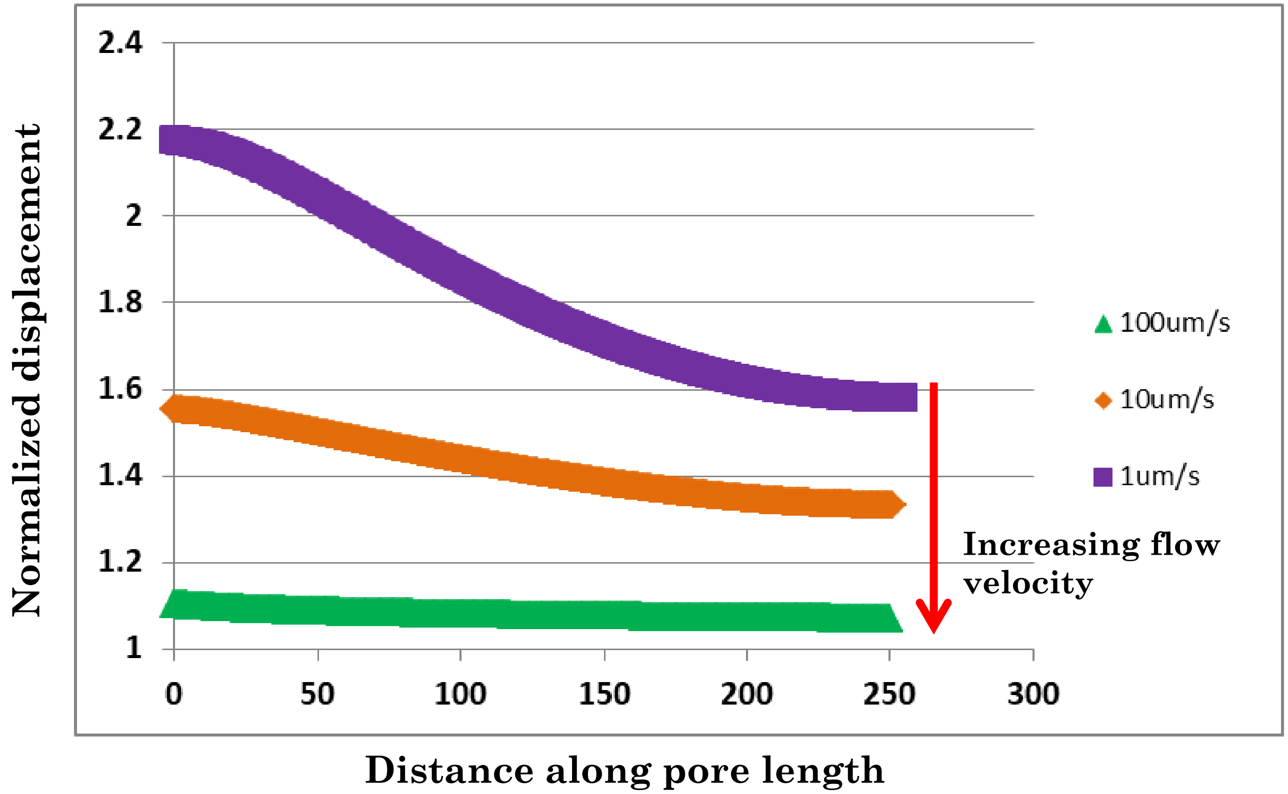


Results:

Normalized displacement profile along pore wall for different flow velocity



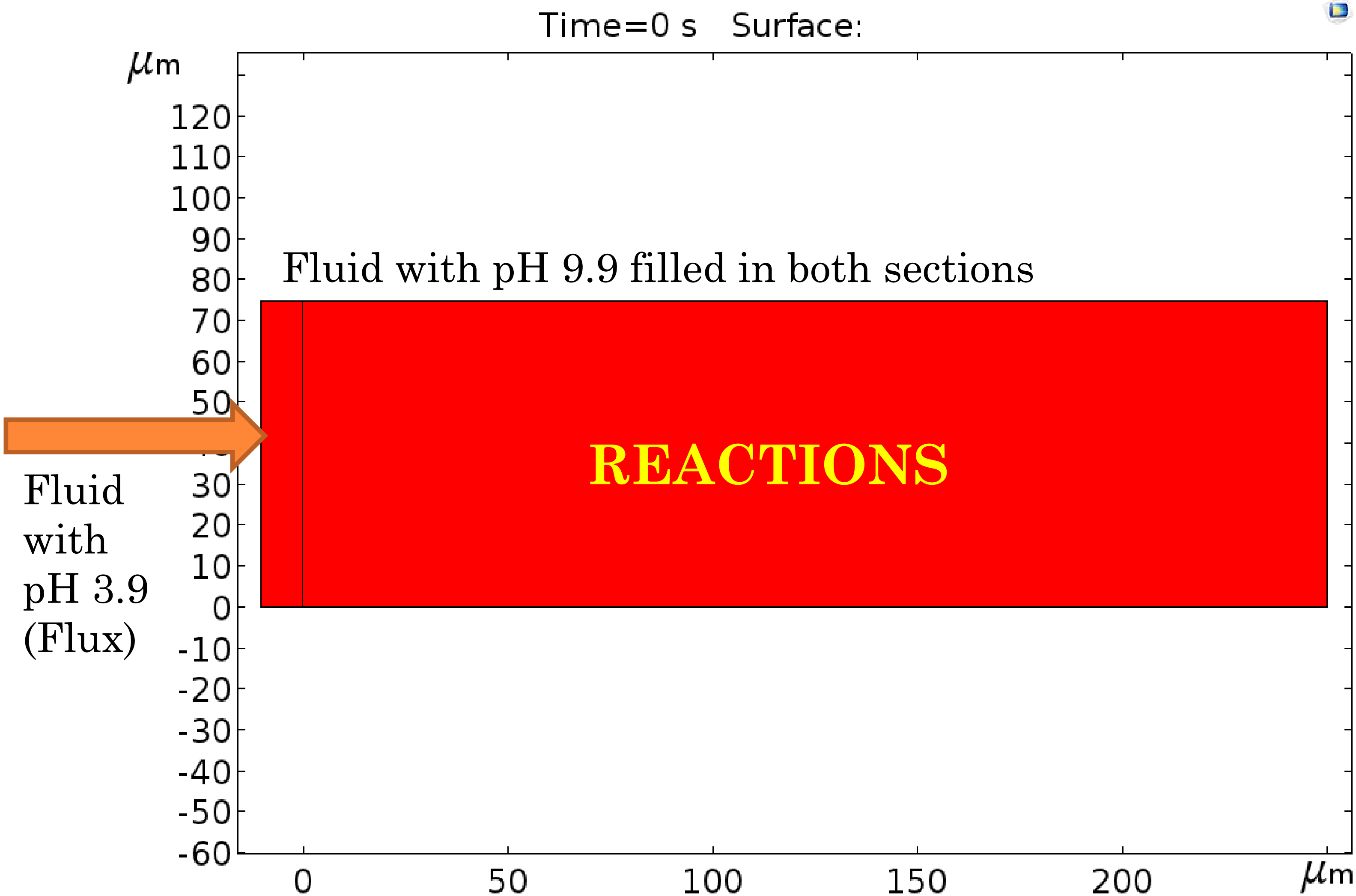
Challenges

- Concentration gradient between pore fluid (pH 9.9) and injecting fluid (pH 4.4)
    - Flux based condition

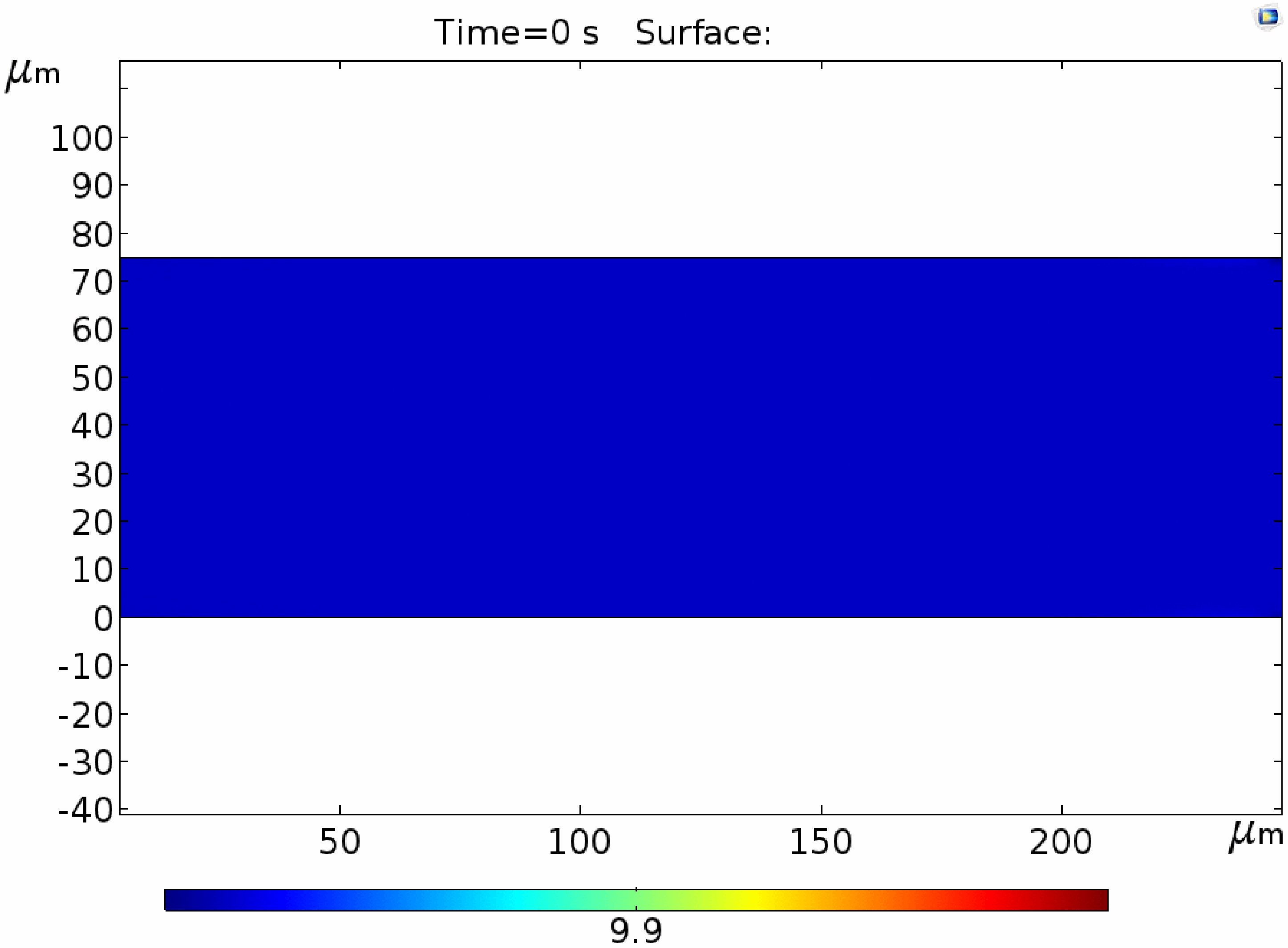
Challenges

- Concentration gradient between pore fluid (pH 9.9) and injecting fluid (pH 3.9)
  - Flux based condition
  - **Concentration constraint condition**

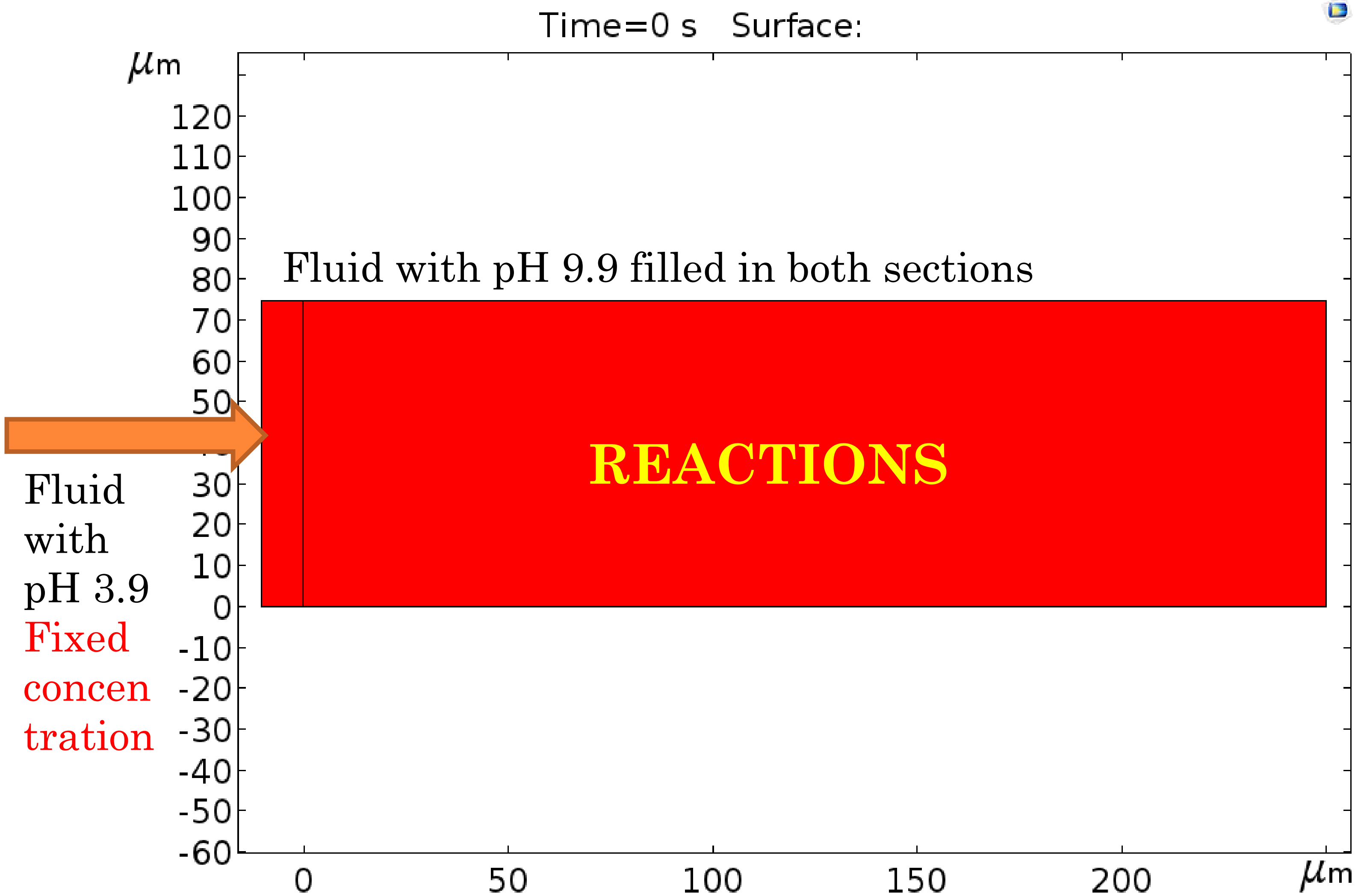
Challenges – Flux based condition



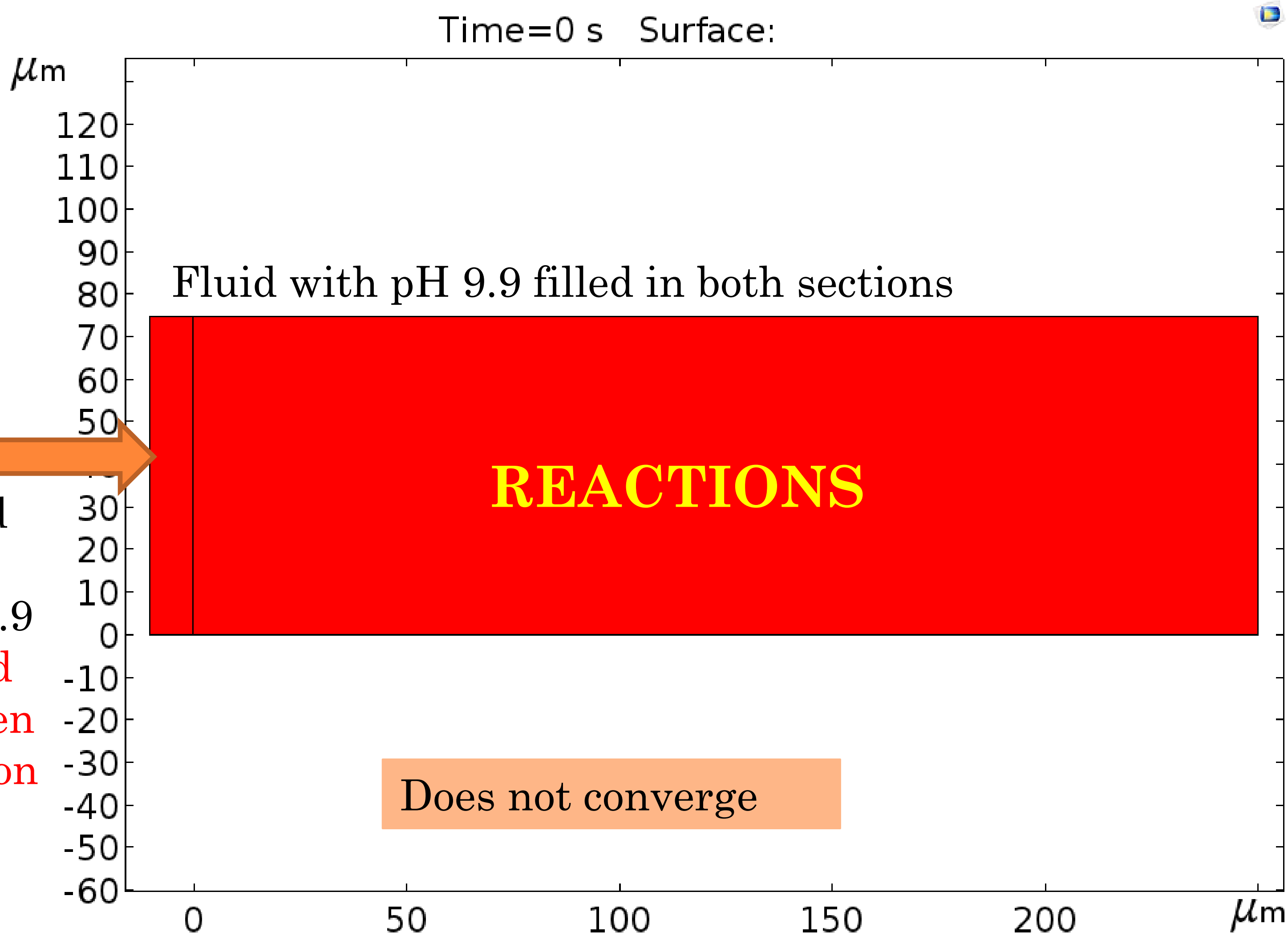
Challenges - Flux based condition



Challenges - Concentration constraint condition

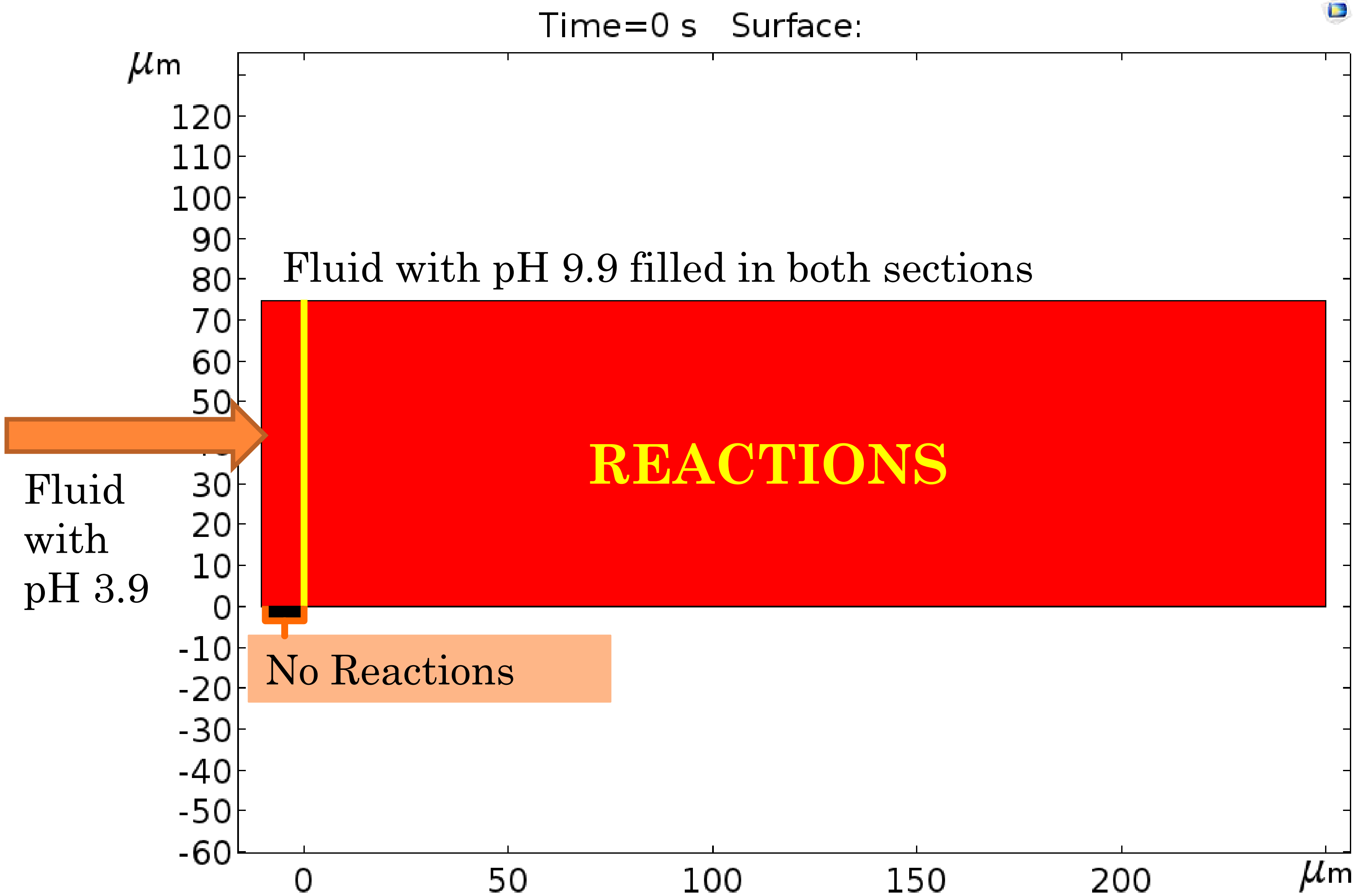


CHALLENGES - CONCENTRATION CONSTRAINT CONDITION

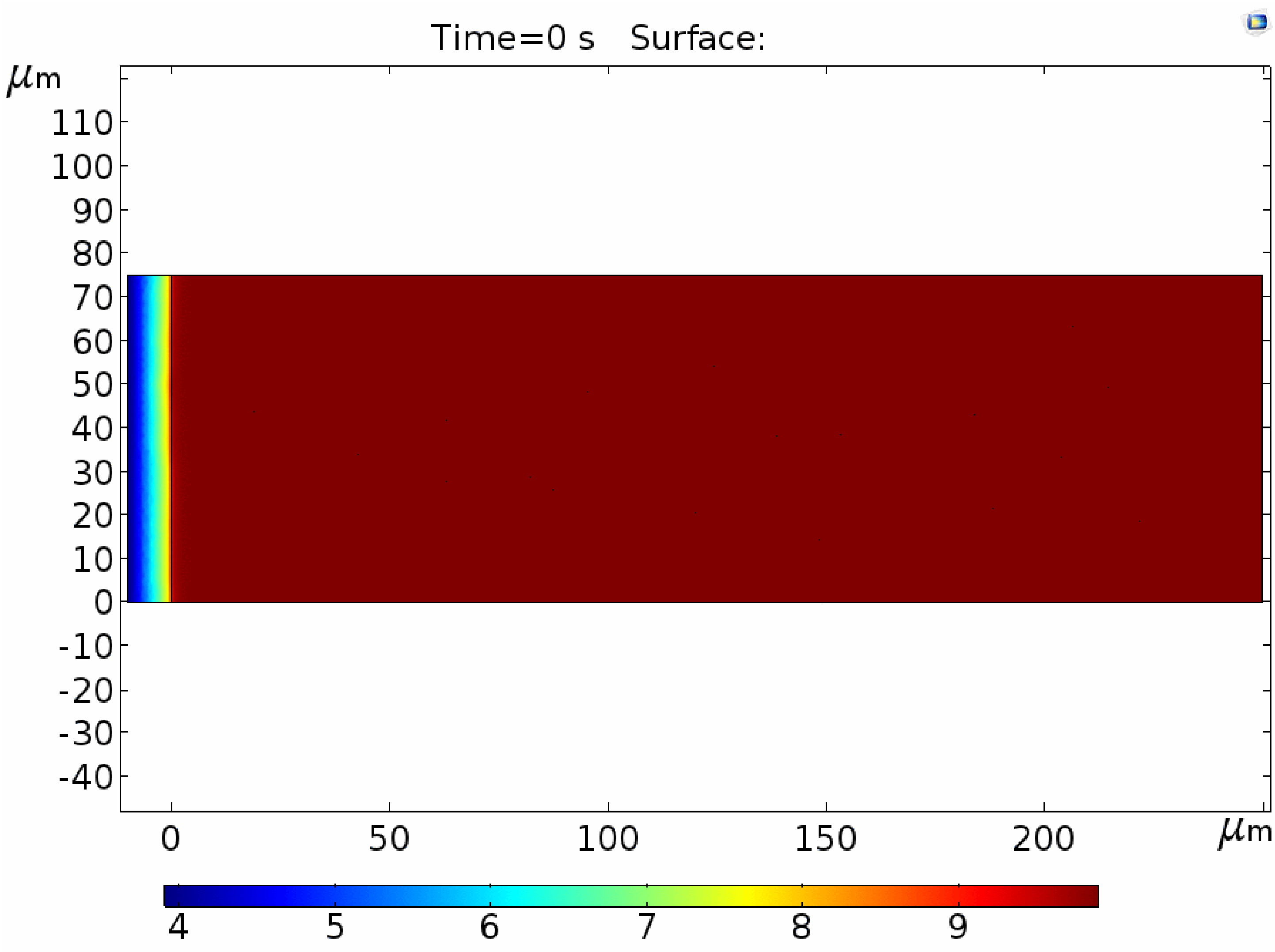


Fluid with pH 3.9 Fixed concentration

Challenges - Concentration constraint condition



Challenges - Concentration constraint condition



Challenges

- Concentration gradient between pore fluid (pH 9.9) and injecting fluid (pH 3.9)

- High velocity impact on numerical stability
  - $Pe = \frac{u*h}{2*D} > 1$
  - Fine Mesh
  - Time dependent step function for concentration of injecting fluid

CONCLUSION

- Uniform dissolution for high flow velocity and non-uniform for low velocity
- Low flow velocity dissolves more for the same number of pore volumes
- High flow velocity dissolves in same duration of time.
- COMSOL – A strong multiphysics solver to couple moving boundary with reactions.

THANK YOU