Universität Stuttgart
DuMu^X Course 2018

Modeling porous medium modification through induced calcite precipitation

SFB Project Area C
Biomineralization

DuMu^X

What is induced calcite precipitation?

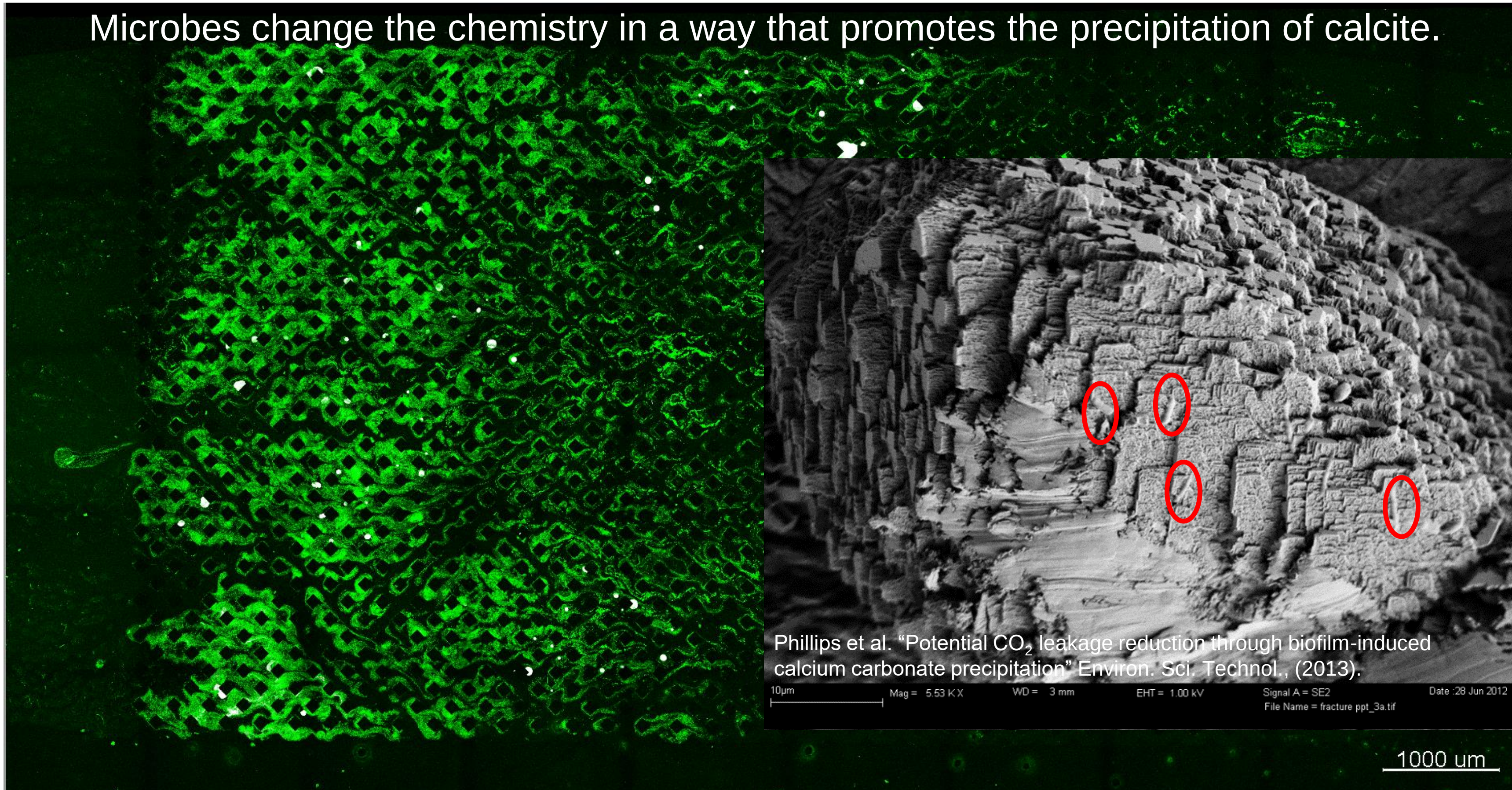


Image: James Connolly, Montana State University

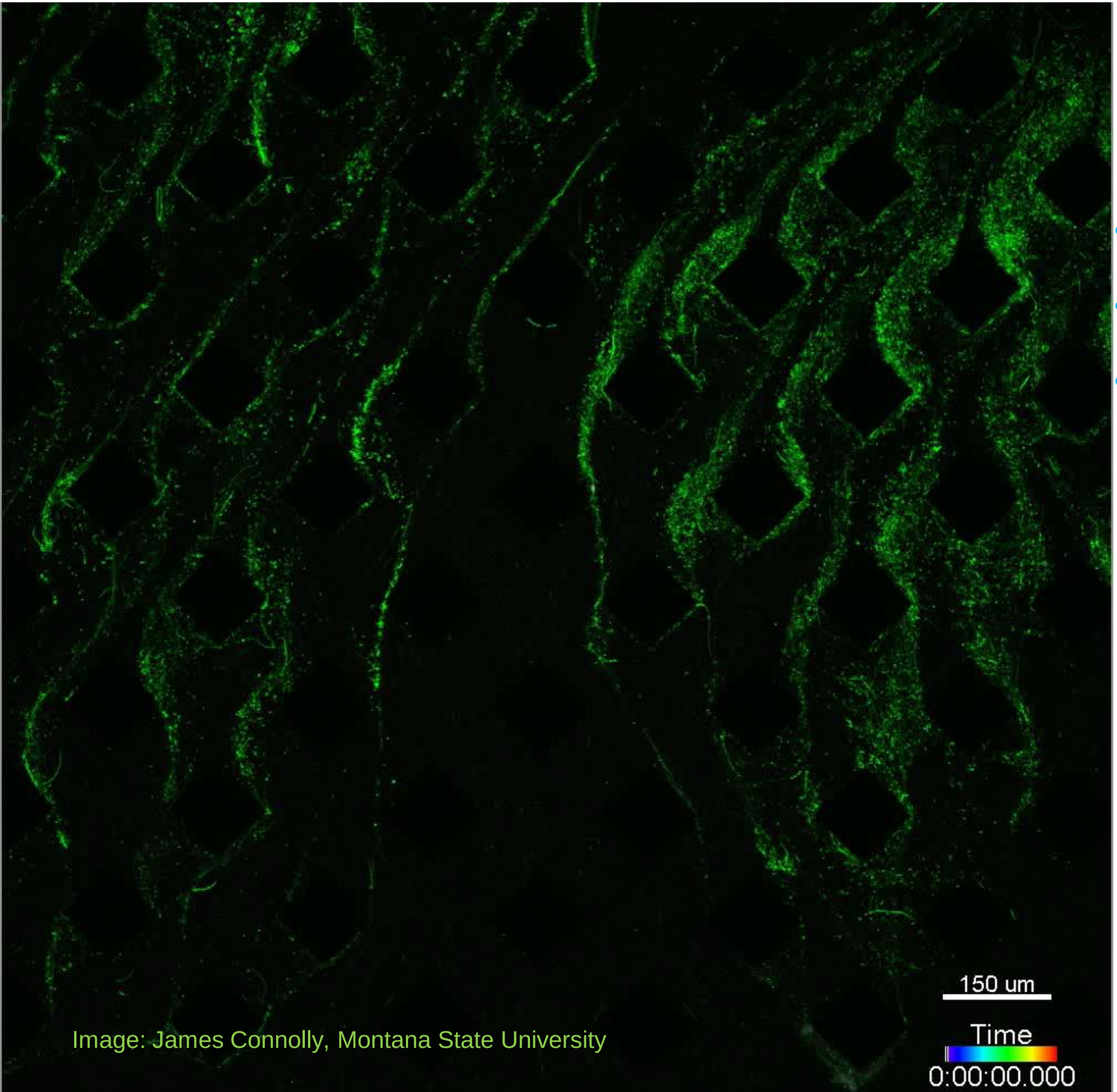


Image: James Connolly, Montana State University

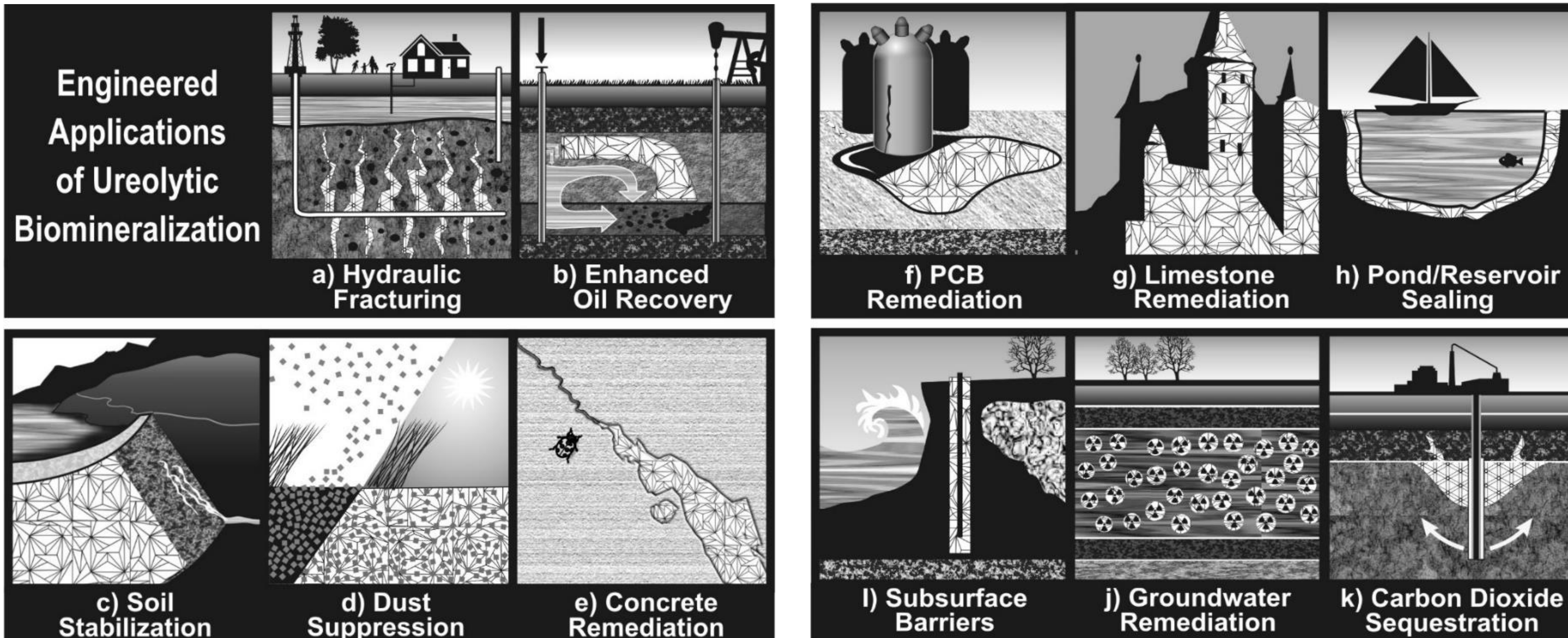
- Biofilm (green) is alive
- Flow is induced, biofilm moves
- Reactions occur
  → Calcite precipitates (white)
  → Biofilm dies slowly

What is induced calcite precipitation?

Van Paassen et. al. “Quantifying Biomediated Ground Improvement by Ureolysis: Large-Scale Biogrout Experiment”. JGGE (2010)

Why investigate Induced Calcite Precipitation (ICP)?

Phillips et al. 2013 Engineered applications of ureolytic biomineralization: A review.



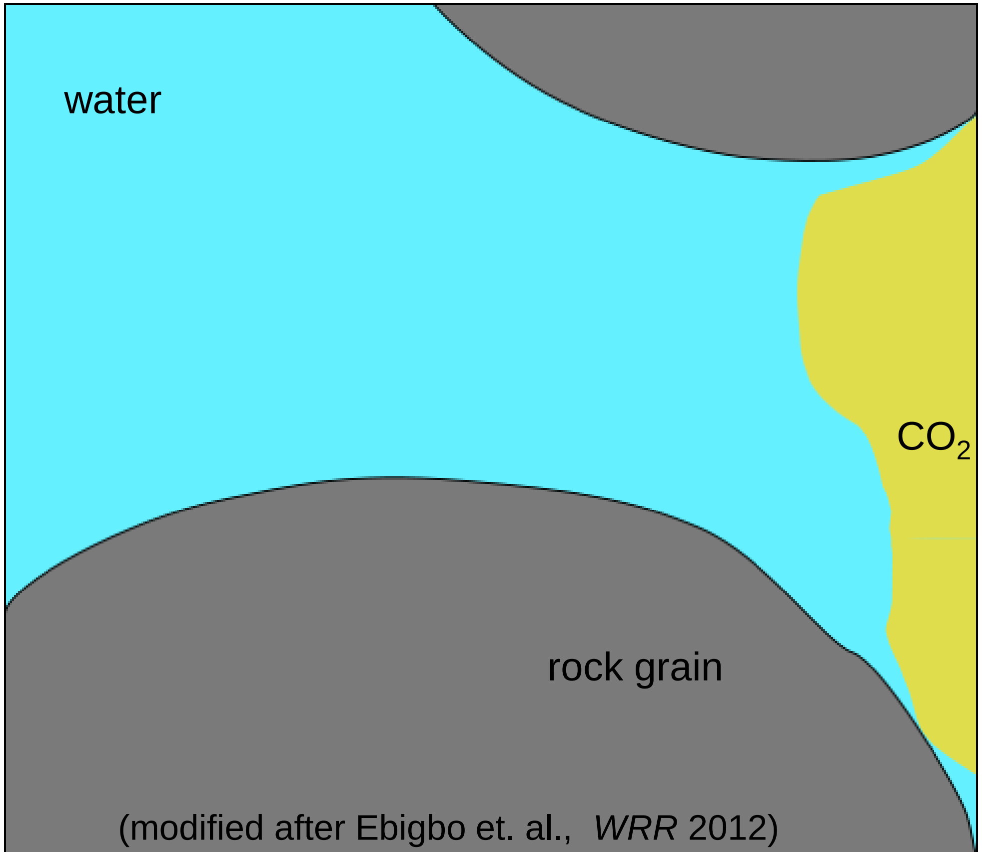
In the context of this presentation mainly: wellbore integrity, remediation in gas storage, oil production and hydraulic fracking

→ reduce flow (reduce K and k_r, increase p_c)

→ increase mechanical strength

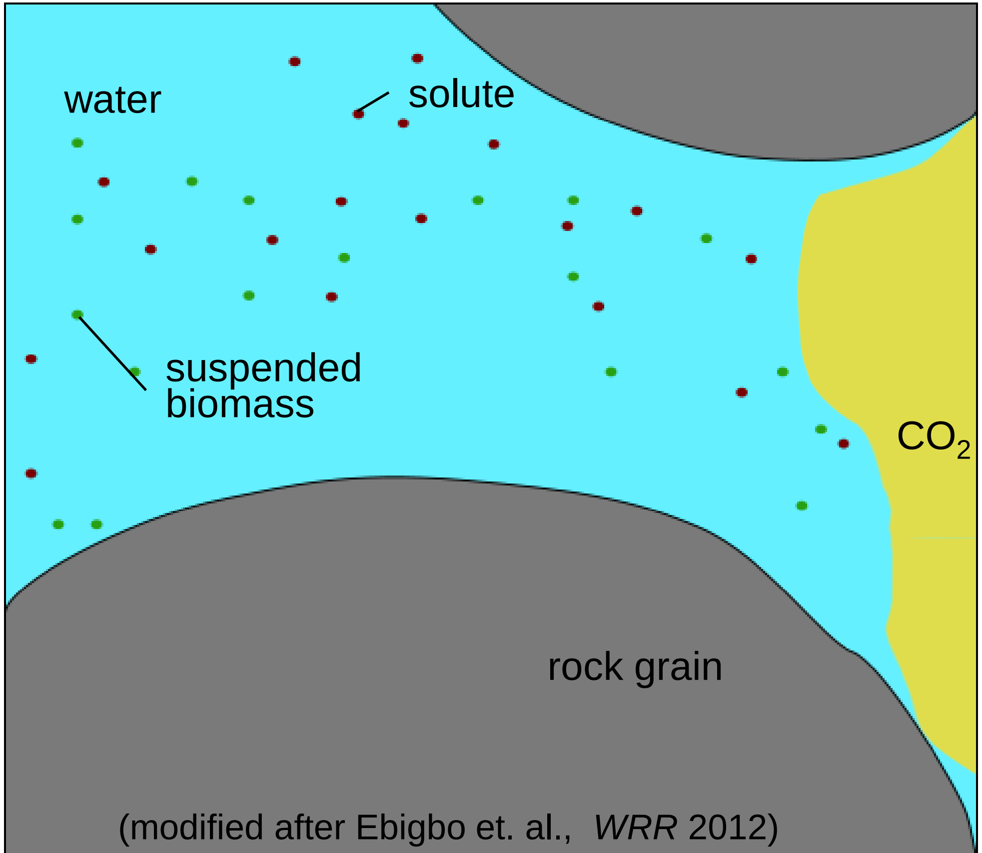
Model concept

Model concept: Relevant processes



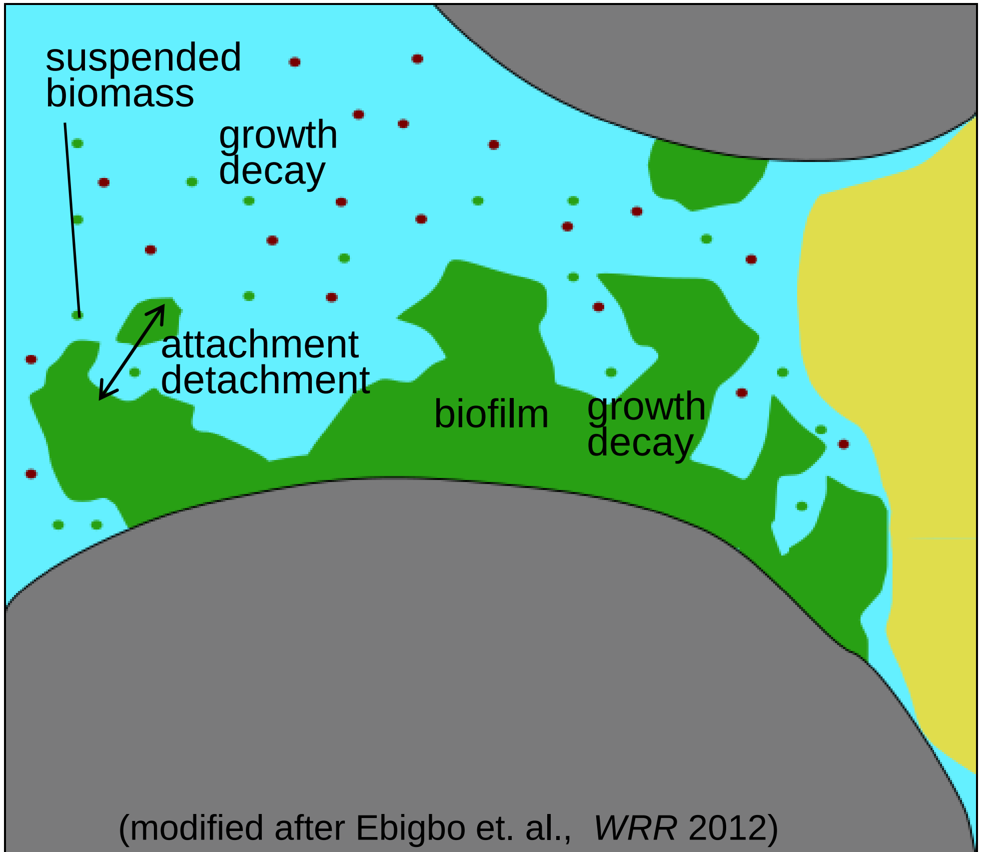
- Two-phase transport

Model concept: Relevant processes



- Two-phase, multi-component transport

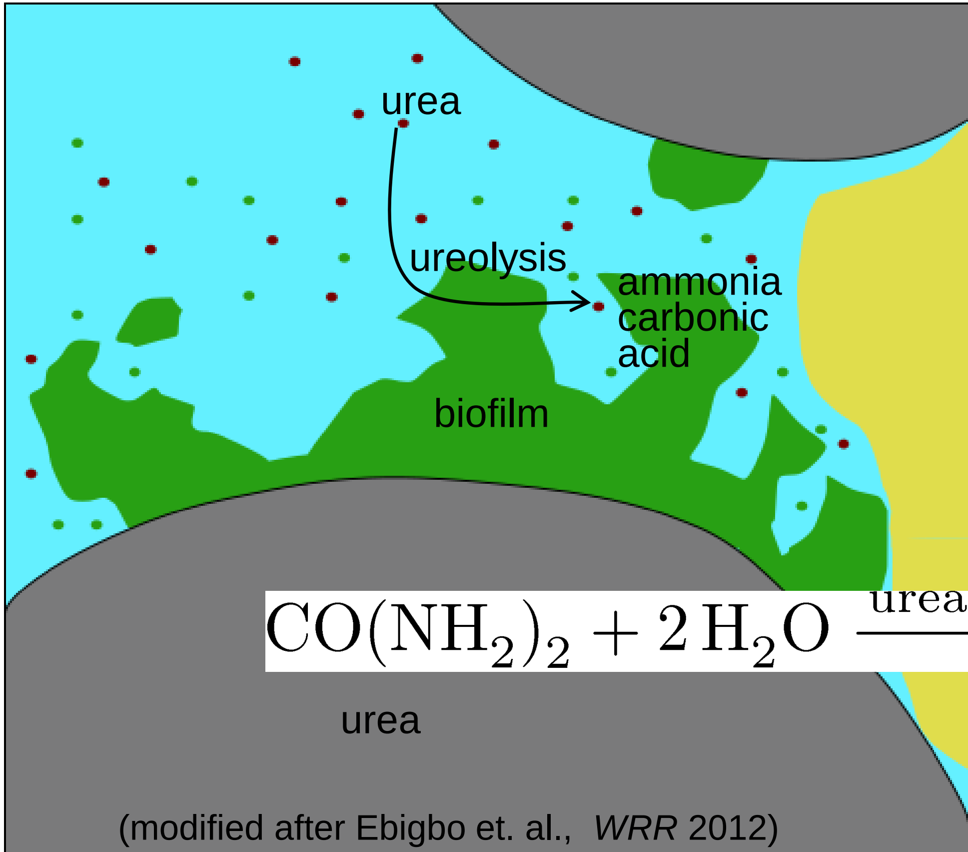
Model concept: Relevant processes



For this exercise:
Neglecting microbial growth and decay, attachment and detachment!

- Biomass (*S. pasteurii*)
  - growth / decay
  - attachment / detachment

Model concept: Relevant processes



- **Urea** hydrolysis

$$CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$$

urea | ammonia | carbonic acid

(modified after Ebigbo et. al., *WRR* 2012)

MICP: Main reactions

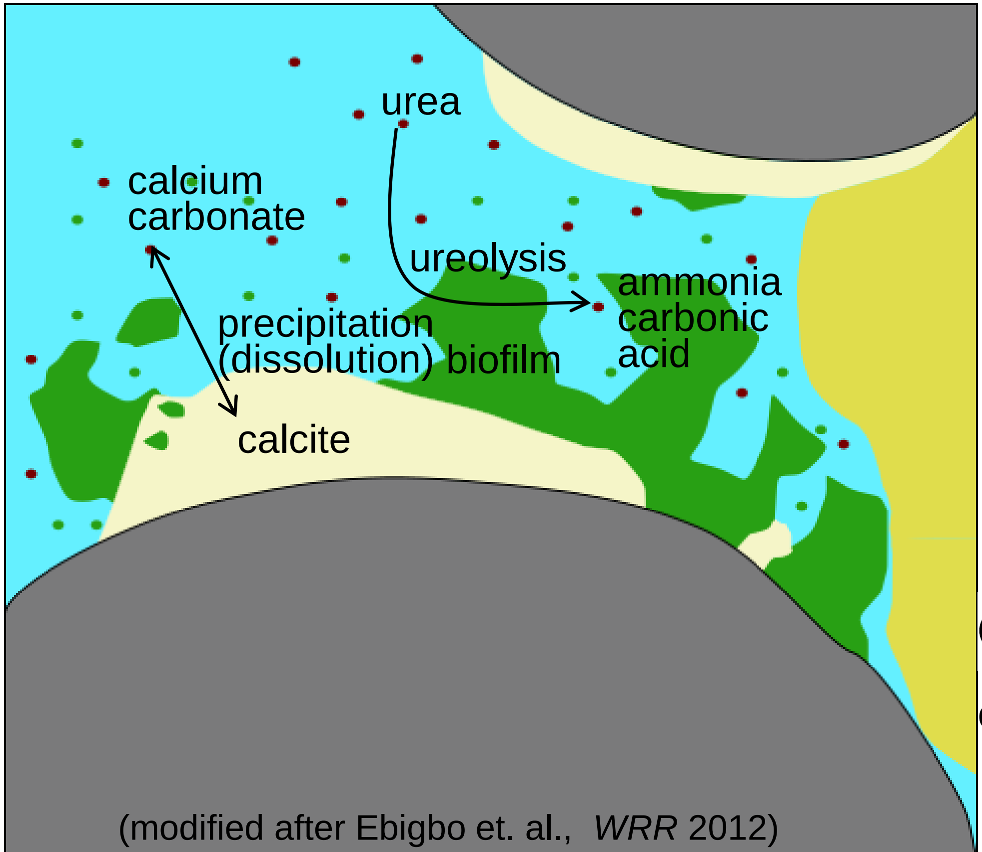
Here: Ureolytic microbes produce the enzyme urease (MICP)

$$CO(NH_2)_2 + 2H_2O + Ca^{2+} \rightarrow 2NH_4^+ + CaCO_3$$

Different reactions in detail:

$CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$	ureolysis
$H_2CO_3 \longleftrightarrow HCO_3^- + H^+$	dissociation of carbonic acid
$HCO_3^- \longleftrightarrow CO_3^{2-} + H^+$	dissociation of bicarbonate ion
$2\,NH_4^+ \longleftrightarrow 2\,NH_3 + 2\,H^+$	dissociation of ammonia
$Ca^{2+} + CO_3^{2-} \longleftrightarrow CaCO_3 \downarrow$	calcite precipitation/dissolution

Model concept: Relevant processes

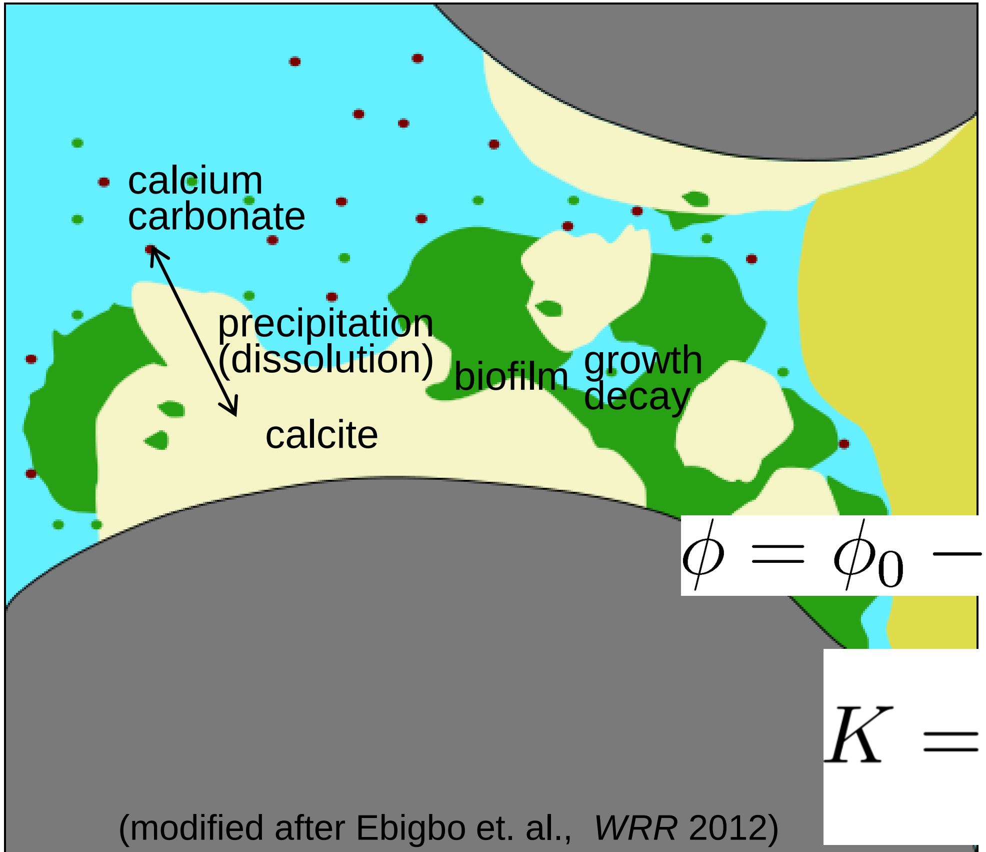


- Precipitation and dissolution of calcite

$$Ca^{2+} + CO_3^{2-} \longleftrightarrow CaCO_3 \downarrow$$

calcium carbonate calcite

Model concept: Relevant processes



- Clogging: Reduction of porosity and permeability

$$\phi = \phi_0 - \phi_{\mathrm{biofilm}} - \phi_{\mathrm{calcite}}$$

$$K = K_0 \left(\frac{1-\phi_0}{1-\phi}\right)^2 \left(\frac{\phi}{\phi_0}\right)^3$$

Equations

Balance Equations

- Mass balance equation of components

$$\sum_{\alpha} \frac{\partial}{\partial t} \left(\phi \rho_\alpha x_\alpha^\kappa S_\alpha \right) + \nabla \cdot \left(\rho_\alpha x_\alpha^\kappa \mathbf{v}_\alpha \right) - \nabla \cdot \left(\rho_\alpha \mathbf{D}_{\alpha,\mathrm{pm}}^\kappa \nabla x_\alpha^\kappa \right) = q^\kappa$$

- Mass balance for the immobile components / solid phases: $\frac{\partial}{\partial t} \left(\rho_\varphi \phi_\varphi \right) = q^\varphi$

Overall procedure of implementing chemical reactions in DuMu^X:

1. Chemical equation → calculate equilibrium/kinetic reaction rate e.g. r_{urea}
2. Reaction rate → set component source/sink term e.g. q^φ depending on and chemical reaction

Sources & Sinks:

For this exercise:
Neglecting microbial growth and decay, attachment and detachment!

$$\begin{aligned}
\text{Urea:} \quad & q^{\mathrm{urea}} &=& -r_{\mathrm{urea}} \\
\text{Calcium:} \quad & q^{\mathrm{Ca}^{2+}} &=& -r_{\mathrm{precip}} \\
\text{Total carbon:} \quad & q^{\mathrm{C_{tot}}} &=& r_{\mathrm{urea}} - r_{\mathrm{precip}} \\
\text{Calcite:} \quad & q^{\mathrm{c}} &=& r_{\mathrm{precip}}
\end{aligned}$$

$$\text{Precipitation rate} \quad r_{\mathrm{precip}} = f\left(A_{\mathrm{interface}},\ \Omega = \frac{[\mathrm{Ca}^{2+}][\mathrm{CO}_3^{2-}]}{K_{\mathrm{sp}}},\ T\right)$$

$$\text{For this exercise:} \quad r_{\mathrm{precip}} = r_{\mathrm{urea}}$$

$$\text{Ureolysis rate} \quad r_{\mathrm{urea}} = k_{\mathrm{u}}^{\mathrm{m}}\, k_{\mathrm{u,biofilm}} \left(\rho_{\mathrm{biofilm}} \phi_{\mathrm{biofilm}}\right) \frac{m_{\mathrm{urea}}}{K_{\mathrm{u}} + m_{\mathrm{urea}}}$$

Supplementary Equation:

- Updating permeability and porosity

$$K = K_0 \left(\frac{1-\phi_0}{1-\phi}\right)^2 \left(\frac{\phi}{\phi_0}\right)^3, \; \phi = \phi_0 - \sum_{\varphi} \phi_{\varphi}$$

Specific Implementations

- Implement reactive sources and sinks, calling a seperate chemistry file

```
#include "chemistry/simplebiocarbonicacid.hh"   // chemical reactions
…
using Chemistry = typename Dumux::BioCarbonicAcidChemistry<TypeTag>;
…
NumEqVector source(const Element &element, const FVElementGeometry& fvGeometry, const
ElementVolumeVariables& elemVolVars, const SubControlVolume &scv) const
{
        NumEqVector source(0.0);
        Chemistry chemistry;

        const auto& volVars = elemVolVars[scv];
        chemistry.reactionSource(source, volVars);

        return source;
}
…
```

Specific Implementations

- Update **porosity** in dumux/material/fluidmatrixinteractions/porosityprecipitation.hh

```
…
auto priVars = evalSolution(element, element.geometry(), elemSol, scv.center());
Scalar sumPrecipitates = 0.0;

for (unsigned int solidPhaseIdx = 0; solidPhaseIdx < numSolidPhases; ++solidPhaseIdx)
    sumPrecipitates += priVars[numComp + solidPhaseIdx];

using std::max;
return max(minPoro, refPoro - sumPrecipitates);
…
```

- Update **permeability** in /material/fluidmatrixinteractions/permeabilitykozenycarman.hh

```
template<class Scalar>
PermeabilityType evaluatePermeability(PermeabilityType refPerm, Scalar refPoro, Scalar
poro) const
{
       using std::pow;
       auto factor = pow((1.0 - refPoro)/(1.0 - poro), 2) * pow(poro/refPoro, 3);
       refPerm *= factor;
       return refPerm;
}
```

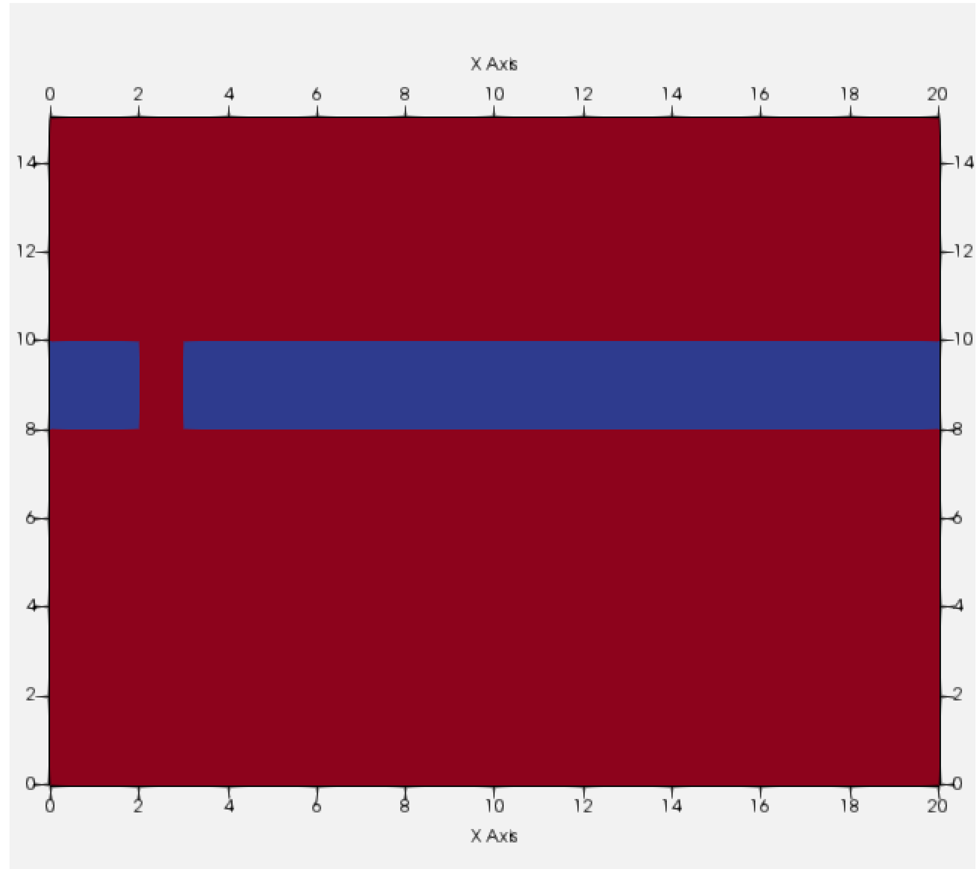
Biomineralization exercise

Exercise

Academic problem setup

- 2 aquifers with sealing aquitard
  - upper aquifer: “drinking water”
  - Lower aquifer: “CO_2 storage”
- Problem:
  - Leakage pathway

  → stored CO_2 would migrate to drinking water aquifer!
- Biomineralization injection could “seal” the leakage pathway



Exercise

Tasks:

1. Get familiar with the code
2. Implement chemical reaction
   - Add kinetic reaction to chemistry-file
   - Use source()-function to link chemistry-file to problem
3. Vary parameters, so that leakage pathway is „sealed“ (porosity < 0.07)
4. Implement new boundary condition for CO_2-injection in lower aquifer

First step: Go to https://git.iws.uni-stuttgart.de/dumux-repositories/dumux-course/tree/master/exercises/exercise-biomineralizationand and check out the README

University of Stuttgart
Institute for Modelling Hydraulic and Environmental Systems

Thank you!

DuMu^x

http://dumux.org/
https://dune-project.org/

Dune
Distributed and Unified Numerics Environment

e-mail simon.scholz@iws.uni-stuttgart.de
phone +49 (0) 711 685-67015
fax +49 (0) 711 685-60430

University of Stuttgart
Institute for Modelling Hydraulic and Environmental Systems
Pfaffenwaldring 61, 70569 Stuttgart