Field-scale modeling of microbially induced calcite precipitation

GRS 2016

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What is microbially induced calcite precipitation (MICP)?

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Microbes change the chemistry in a way that promotes the precipitation of calcite.

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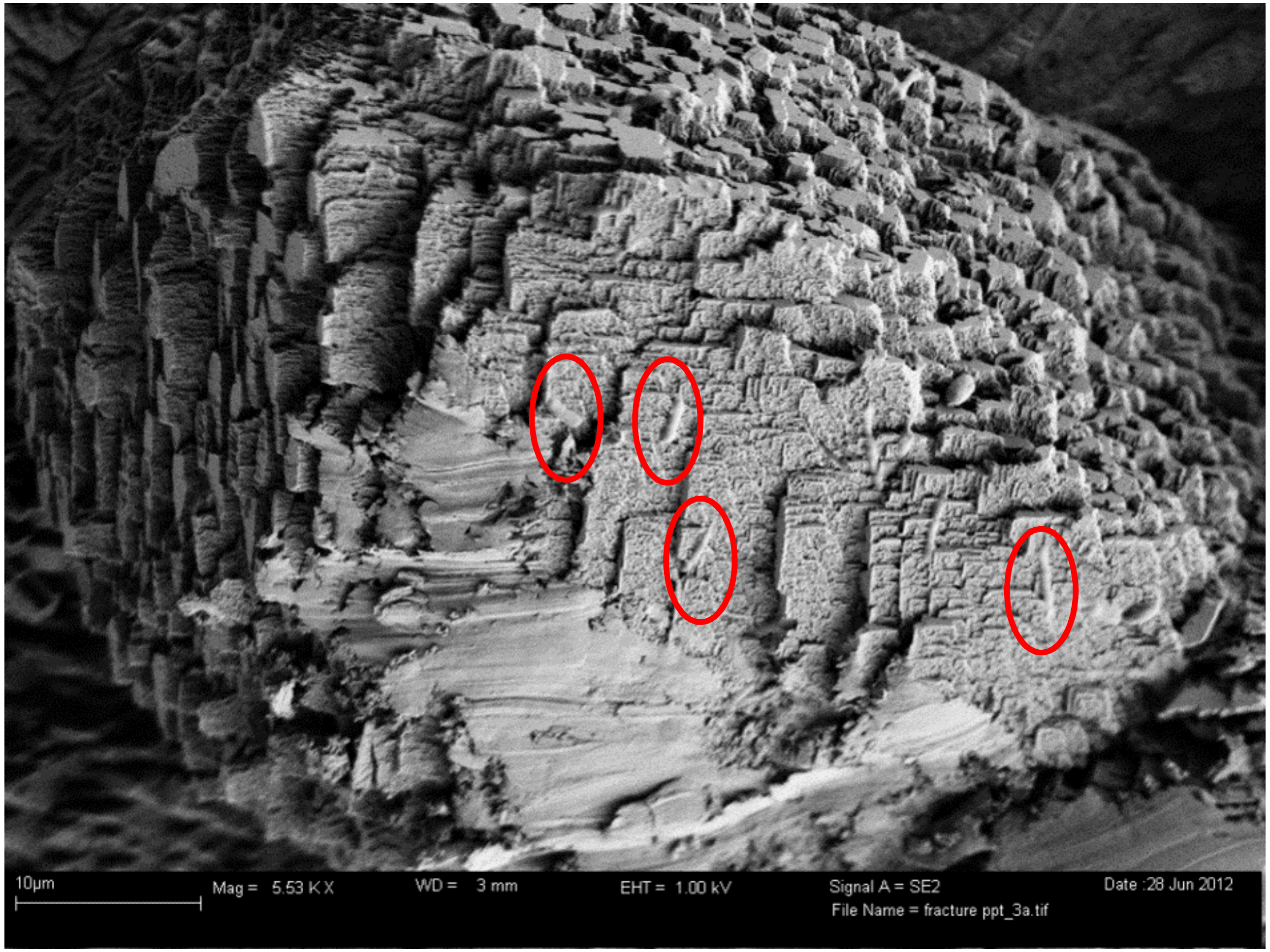

from Phillips et al. 2013 Potential CO_2 leakage reduction through biofilm-induced calcium carbonate precipitation

Why investigate MICP?

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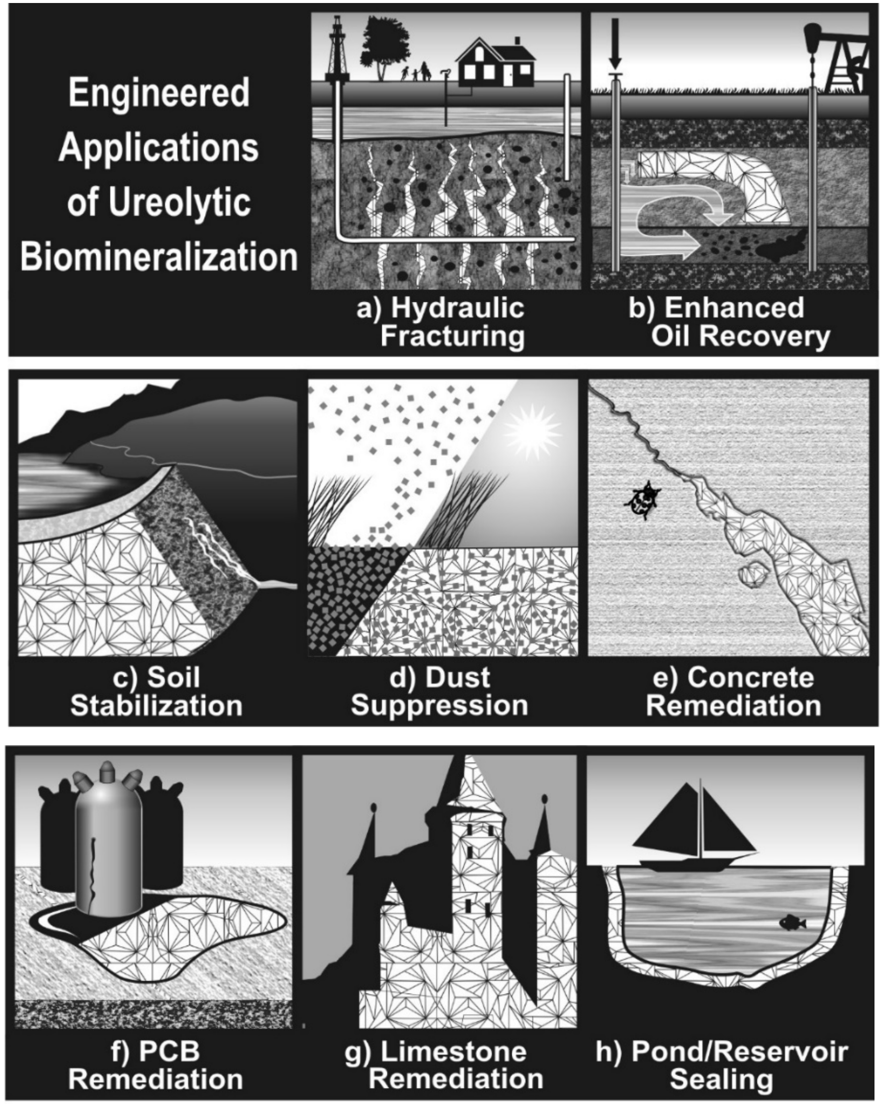
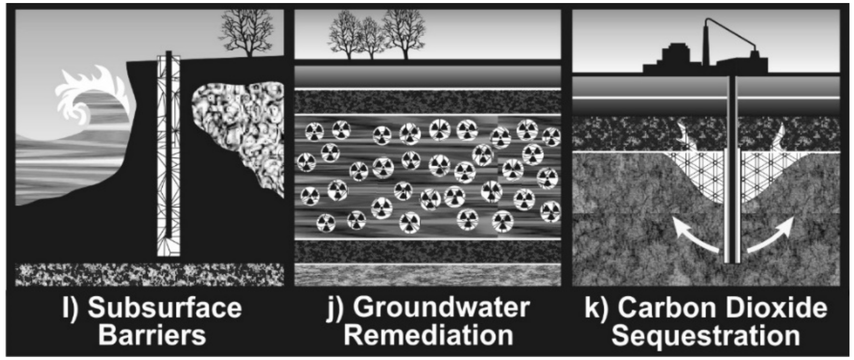
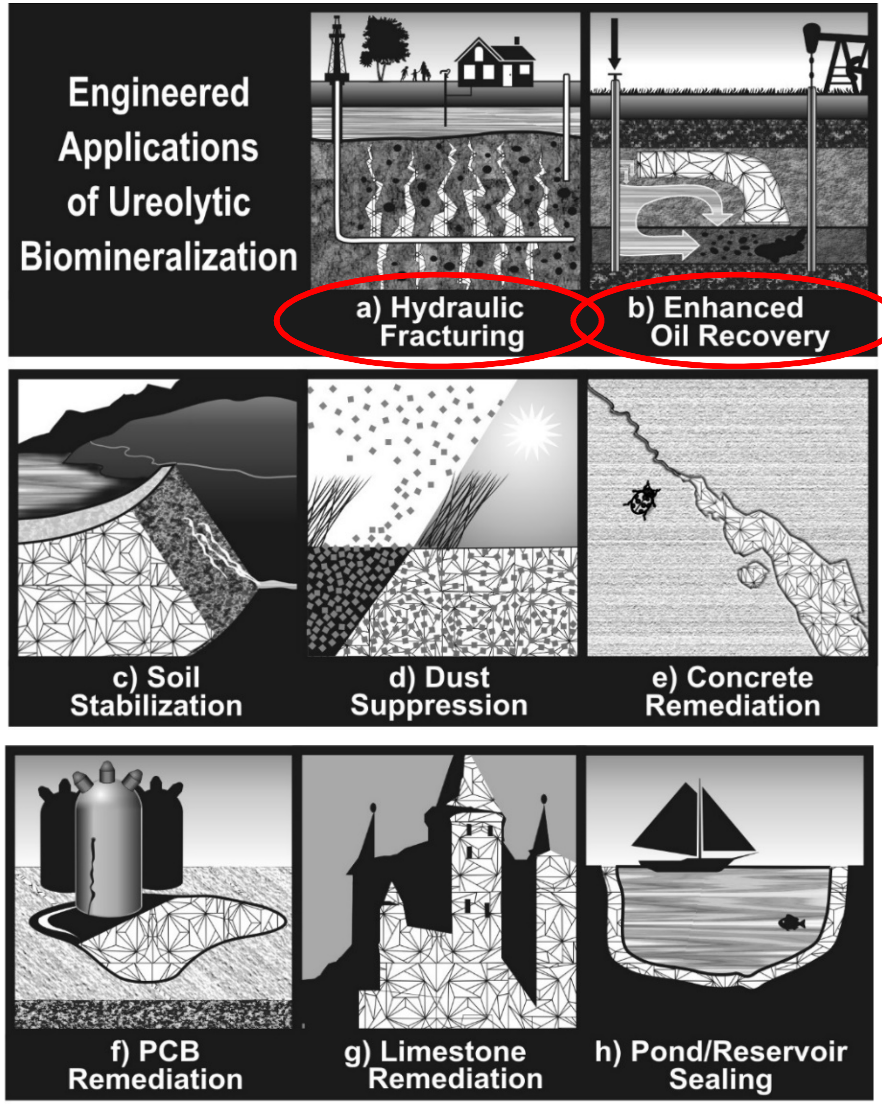
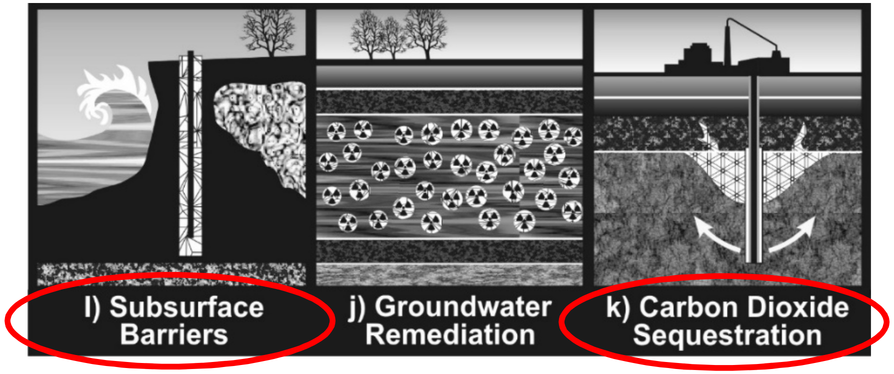




from Phillips et al. 2013
Engineered applications of ureolytic biomineralization: A review.

Why investigate MICP?





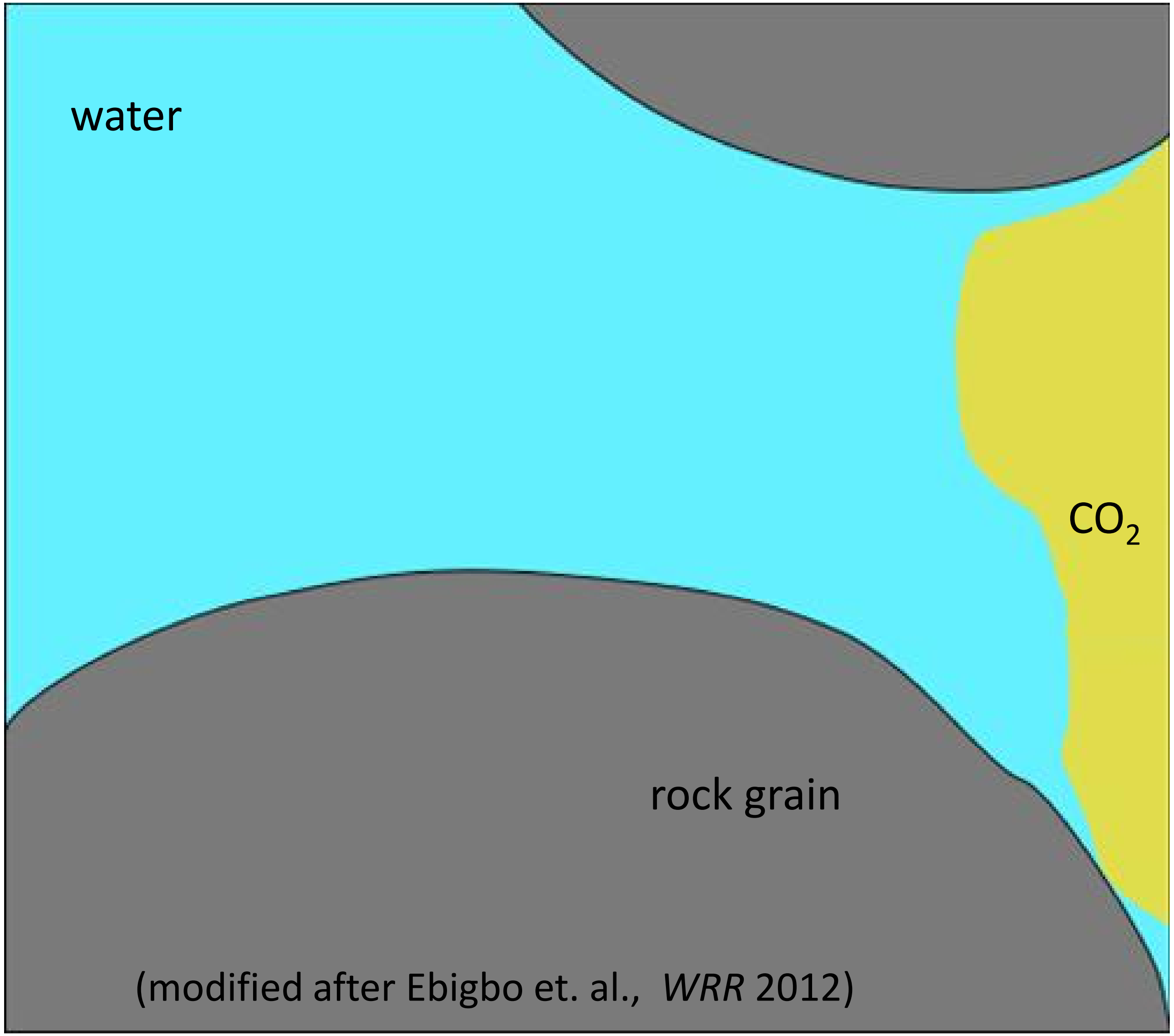
In the context of this presentation mainly:
wellbore integrity remediation in gas storage, oil production, hydraulic fracking

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

Outline

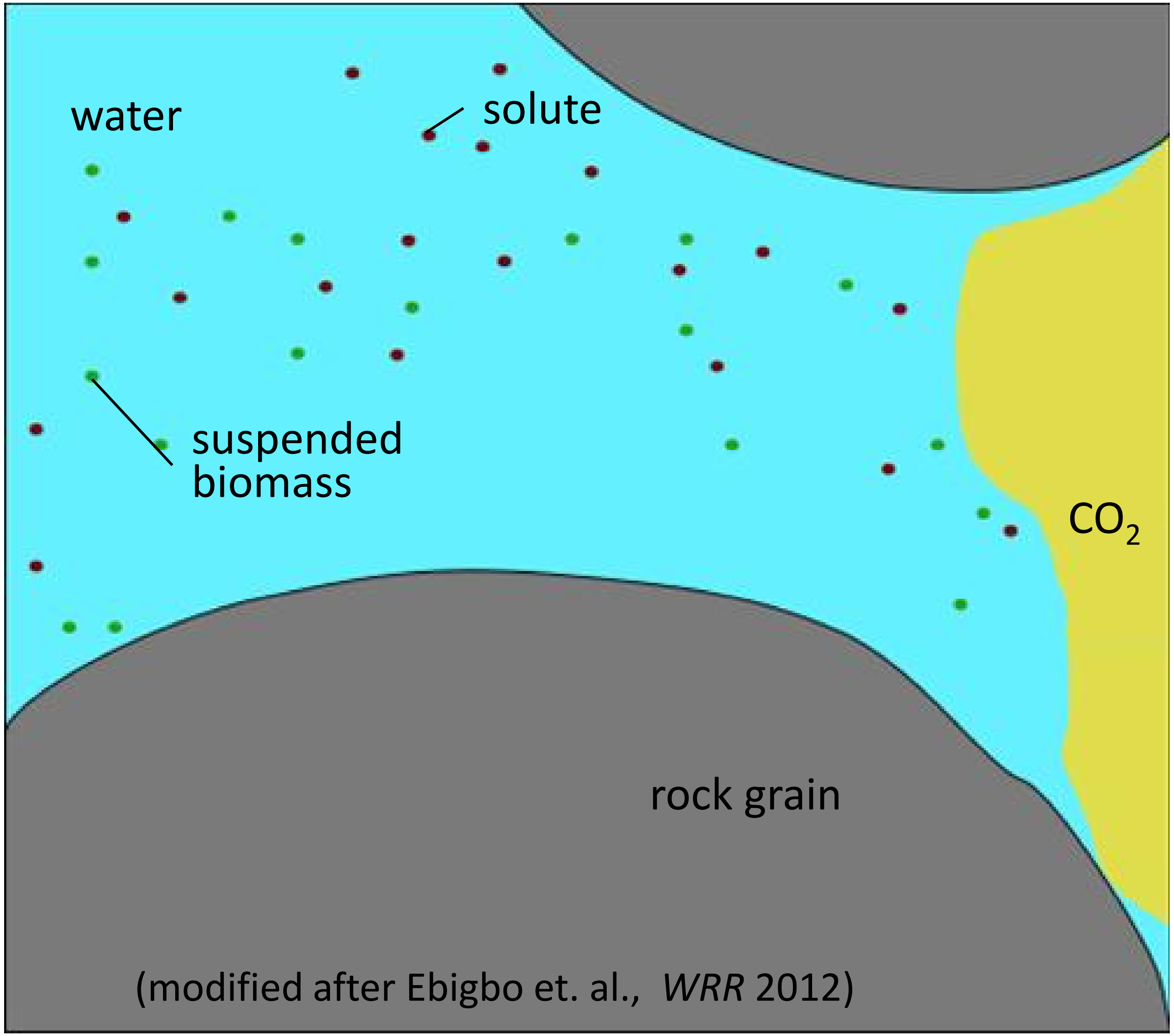
- Introduction and motivation
- **Model concept**
- Application of (MICP and) the model at field scale
- Investigation of efficient solution strategies
- Summary

Model concept: Relevant processes



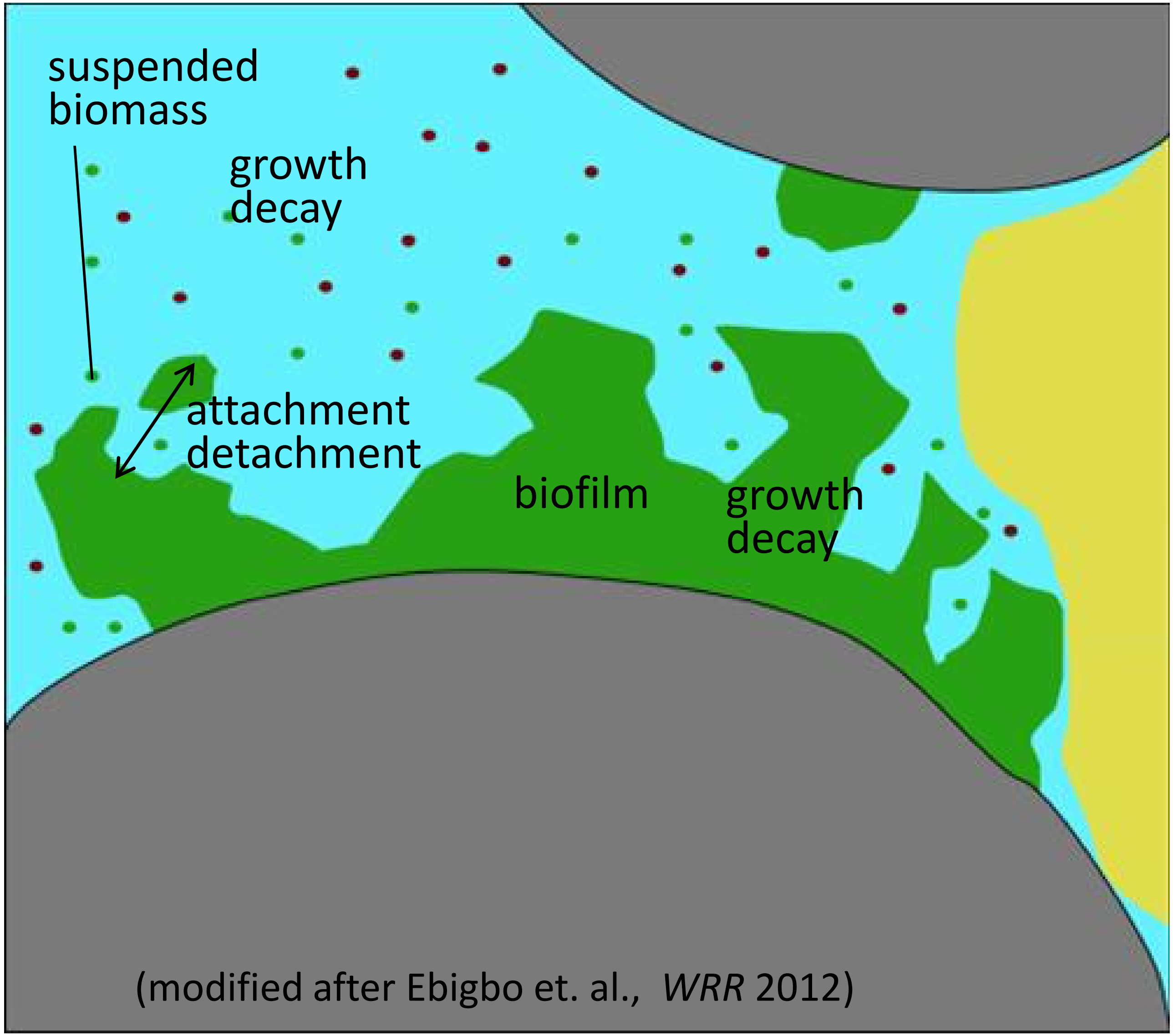
- Two-phase transport

Model concept: Relevant processes



- Two-phase, multi-component transport

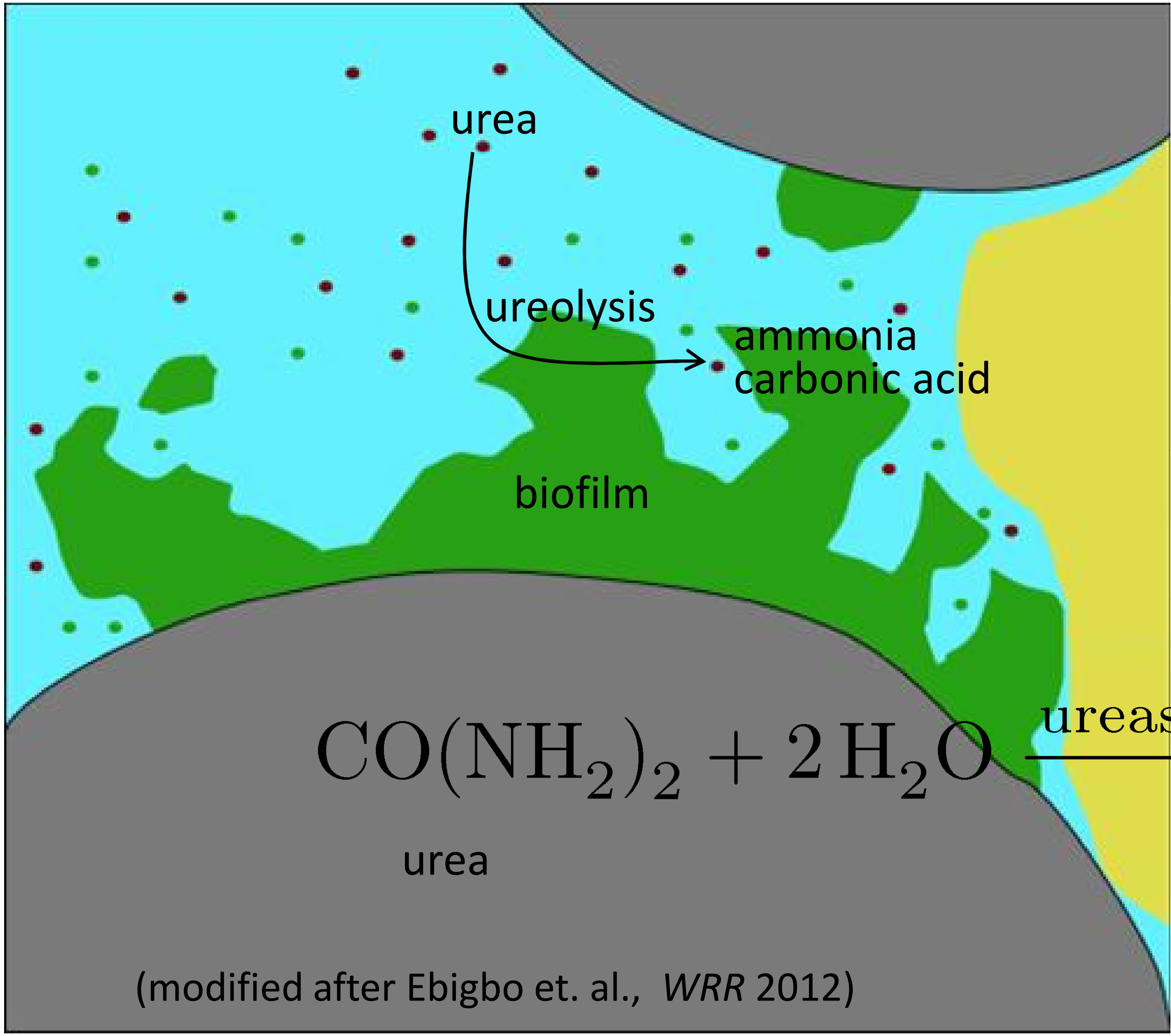
Model concept: Relevant processes



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

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

Model concept: Relevant processes



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

urea — ammonia — carbonic acid

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

- Urea hydrolysis

Model concept: Ureolysis and other reactions

The bacterium *Sporosarcina pasteurii* produces the enzyme urease.

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

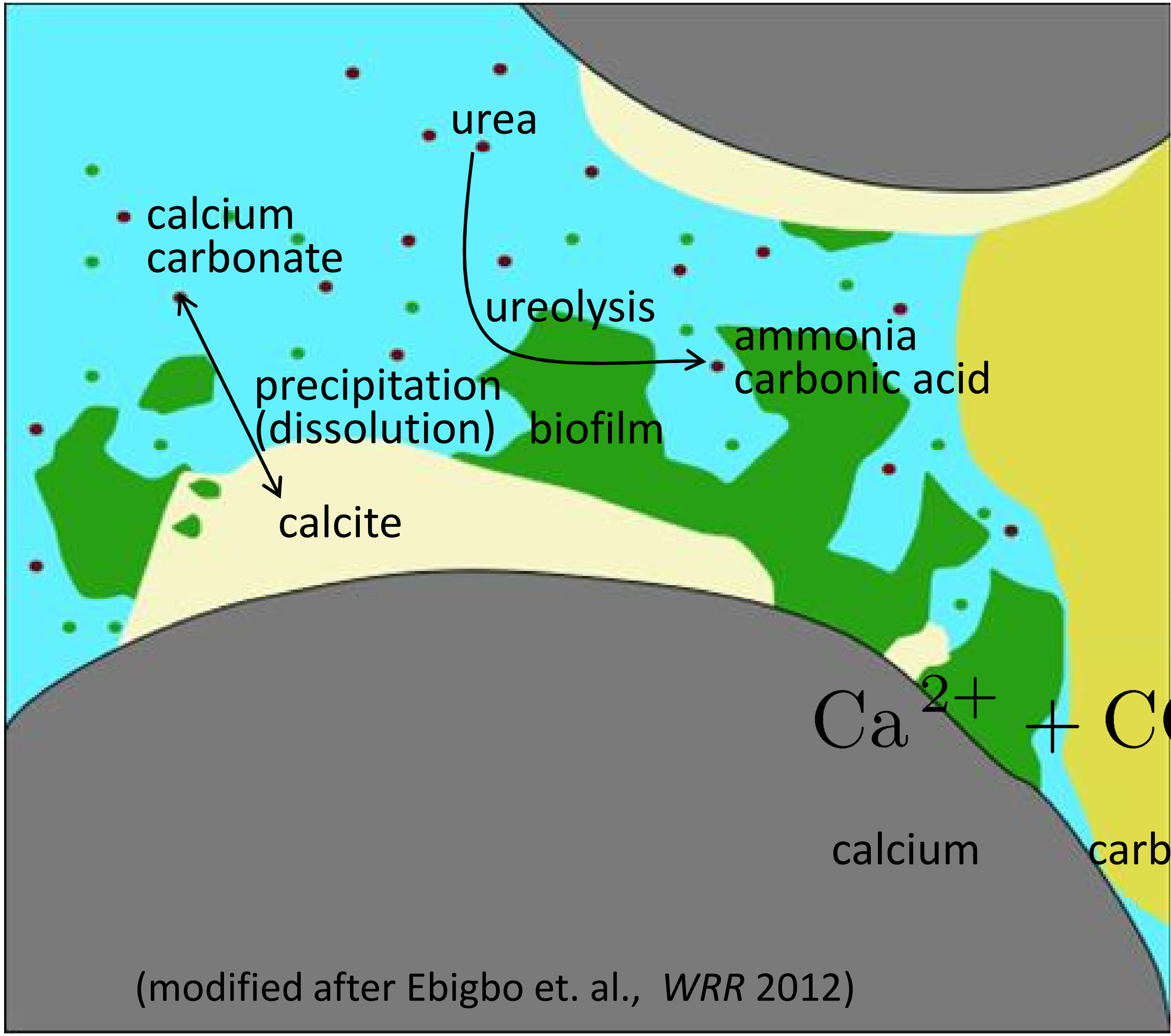
$$H_2CO_3 \longleftrightarrow HCO_3^- + H^+$$ dissociation of carbonic acid

$$HCO_3^- \longleftrightarrow CO_3^{2-} + H^+$$ 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



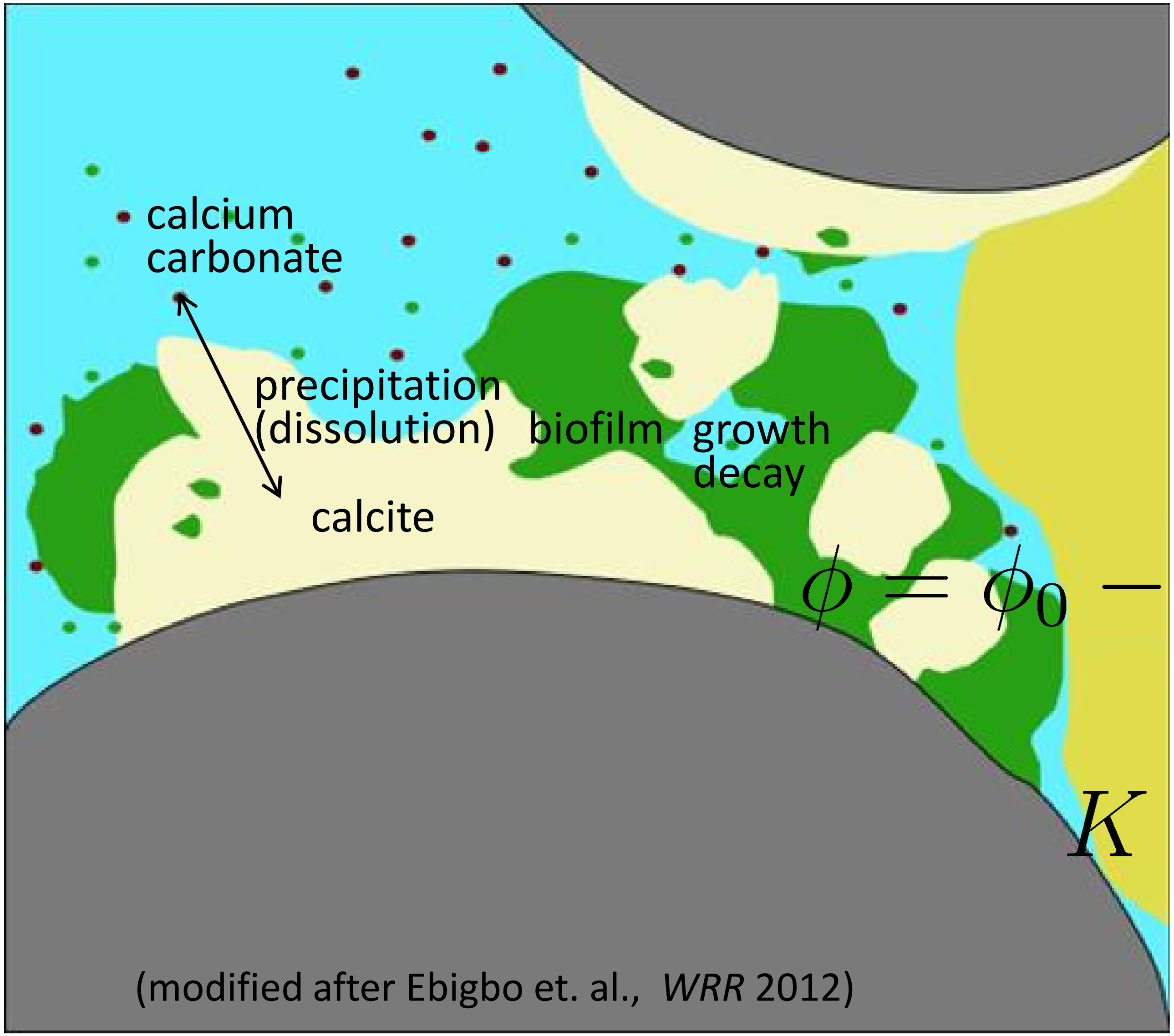
(modified after Ebigbo et. al., *WRR* 2012)

- Precipitation and dissolution of calcite

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

calcium carbonate calcite

Model concept: Relevant processes



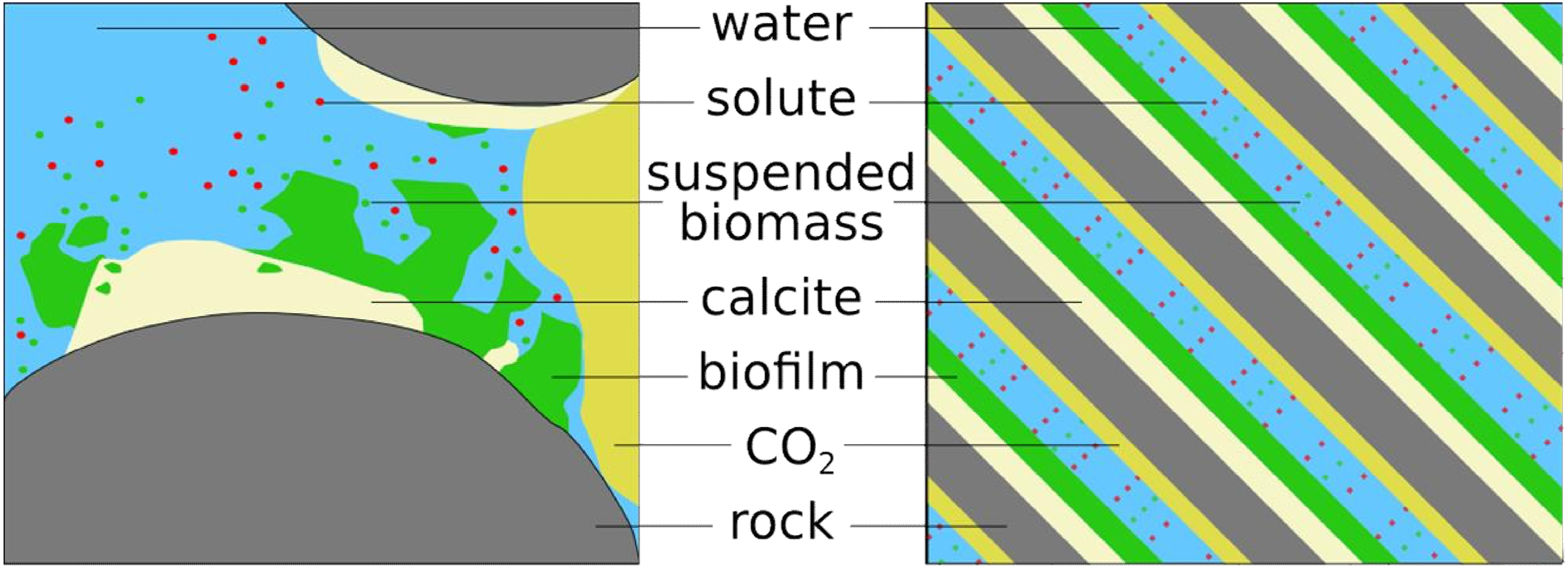
(modified after Ebigbo et. al., *WRR* 2012)

- Clogging: Reduction of porosity and permeability

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

$$K = K_0 \left(\frac{\phi - \phi_{\text{crit}}}{\phi_0 - \phi_{\text{crit}}} \right)^3$$

Model concept: Scale



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

averaging

Pore scale → REV scale

Mass balance equations

Mass balance equation for components in both phases:

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

$$\kappa \in \{\mathrm{water},\ \mathrm{C_{tot}},\ \mathrm{O_2}\};\ \alpha \in \{\mathrm{w},\ \mathrm{n}\}$$

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Mass balance equation of components exclusively in the water phase:

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

$$\kappa \in \{\mathrm{Na},\ \mathrm{Cl},\ \mathrm{Ca},\ \mathrm{susp.\ biomass},\ \mathrm{substrate},\ \mathrm{urea},\ \mathrm{NH_{tot}}\}$$

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$$\kappa \in \{\mathrm{Na},\ \mathrm{Cl},\ \mathrm{Ca},\ \mathrm{susp.\ biomass},\ \mathrm{substrate},\ \mathrm{urea},\ \mathrm{NH_{tot}}\}$$

Mass balance for the immobile components / solid phases:

$$\frac{\partial}{\partial t}\left(\rho_\lambda \phi_\lambda\right) = q^\lambda \qquad \lambda \in \{\mathrm{biofilm},\ \mathrm{calcite}\}$$

Sources & sinks: Solutes and Calcite

Urea: $q^{\text{urea}} = -r_{\text{urea}}$

Total nitrogen: $q^{\text{NH}_{\text{tot}}} = 2r_{\text{urea}}$

Calcium: $q^{\text{Ca}^{2+}} = r_{\text{diss}} - r_{\text{precip}}$

Total carbon: $q^{\text{C}_{\text{tot}}} = r_{\text{urea}} + r_{\text{diss}} - r_{\text{precip}}$

Calcite: $q^{\text{c}} = r_{\text{precip}} - r_{\text{diss}}$

Substrate: $q^{\text{substrate}} = -\left(r^{\text{bio}}_{\text{growth}} + r^{\text{biofilm}}_{\text{growth}}\right)/Yield$

Oxygen: $q^{\text{O}_2} = -\left(r^{\text{bio}}_{\text{growth}} + r^{\text{biofilm}}_{\text{growth}}\right) \cdot 0.5/Yield$

Sources & sinks: Solutes and Calcite

$$
\begin{aligned}
&\text{Urea:} & q^{\text{urea}} &= -r_{\text{urea}}\\
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&\text{Calcium:} & q^{\text{Ca}^{2+}} &= r_{\text{diss}} - r_{\text{precip}}\\
&\text{Total carbon:} & q^{\text{C}_{\text{tot}}} &= r_{\text{urea}} + r_{\text{diss}} - r_{\text{precip}}\\
&\text{Calcite:} & q^{\text{c}} &= r_{\text{precip}} - r_{\text{diss}}\\
&\text{Substrate:} & q^{\text{substrate}} &= -\left(r^{\text{bio}}_{\text{growth}} + r^{\text{biofilm}}_{\text{growth}}\right)/Yield\\
&\text{Oxygen:} & q^{\text{O}_2} &= -\left(r^{\text{bio}}_{\text{growth}} + r^{\text{biofilm}}_{\text{growth}}\right)\cdot 0.5/Yield\\
&\text{Ureolysis rate} & r_{\text{urea}} &= f\left(\phi_{\text{biofilm}},\ \text{pH},\ C^{\text{urea}}_{\text{w}};\ C^{\text{NH}_4^+}_{\text{w}}\right)\\
&\text{Precipitation rate} & r_{\text{precip}} &= f\left(A_{\text{interface}},\ \Omega = \frac{[\text{Ca}^{2+}][\text{CO}_3^{2-}]}{K_{\text{sp}}}\right)\\
&\text{Dissolution rate} & r_{\text{diss}} &= f\left(A_{\text{interface}},\ \Omega = \frac{[\text{Ca}^{2+}][\text{CO}_3^{2-}]}{K_{\text{sp}}},\ \text{pH}\right)
\end{aligned}
$$

Sources & sinks: Biomass

$$\text{Susp. biomass:} \quad q^{\text{bio}} = r^{\text{bio}}_{\text{growth}} - r^{\text{bio}}_{\text{decay}} - r^{\text{bio}}_{\text{attach}} + r^{\text{bio}}_{\text{detach}}$$

$$\text{Biofilm:} \quad q^{\text{biofilm}} = r^{\text{biofilm}}_{\text{growth}} - r^{\text{biofilm}}_{\text{decay}} + r^{\text{biofilm}}_{\text{attach}} - r^{\text{biofilm}}_{\text{detach}}$$

Sources & sinks: Biomass

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Biofilm: $$q^{\text{biofilm}} = r_{\text{growth}}^{\text{biofilm}} - r_{\text{decay}}^{\text{biofilm}} + r_{\text{attach}}^{\text{biofilm}} - r_{\text{detach}}^{\text{biofilm}}$$

Growth:
$$r_{\text{growth}}^{\text{bio}} = \mu \cdot \phi S_{\text{w}} C_{\text{w}}^{\text{bio}}$$
$$r_{\text{growth}}^{\text{biofilm}} = \mu \cdot \phi_{\text{biofilm}} \rho_{\text{biofilm}}$$
$$\mu = \mu_{\max} \cdot \frac{C_{\text{w}}^{\text{substrate}}}{K_{\text{substrate}} C_{\text{w}}^{\text{substrate}}} \cdot \frac{C_{\text{w}}^{\text{O}_2}}{K_{\text{O}_2} C_{\text{w}}^{\text{O}_2}}$$

Decay:
$$r_{\text{decay}}^{\text{bio}} = k_{\text{decay}}^{\text{bio}} \cdot \phi S_{\text{w}} C_{\text{w}}^{\text{bio}}; \; k_{\text{decay}}^{\text{bio}} = f(\text{pH})$$
$$r_{\text{decay}}^{\text{biofilm}} = k_{\text{decay}}^{\text{biofilm}} \cdot \phi_{\text{biofilm}} \rho_{\text{biofilm}}; \; k_{\text{decay}}^{\text{biofilm}} = f(r_{\text{precip}})$$

Attachment: $$r_{\text{attach}} = (c_{\text{a},1} \phi_{\text{biofilm}} + c_{\text{a},1}) \cdot \phi S_{\text{w}} C_{\text{w}}^{\text{bio}}$$

Detachment: $$r_{\text{detach}} = \left(c_{\text{d},1} \left(|\nabla p_{\text{w}}| \phi S_{\text{w}} \right)^{0.58} + \mu \frac{\phi_{\text{biofilm}}}{\phi_0 - \phi_{\text{calcite}}} \right) \cdot \phi_{\text{biofilm}} \rho_{\text{biofilm}}$$

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Field-scale applications of MICP

Main characteristics of field-scale applications of MICP:

- Expensive
- Limited site-specific information
- Limited possibilities for measurements and surveillance due the depth and the restricted access only through the well used for the application
- Limited experience with field-scale applications of MICP

Field-scale modeling

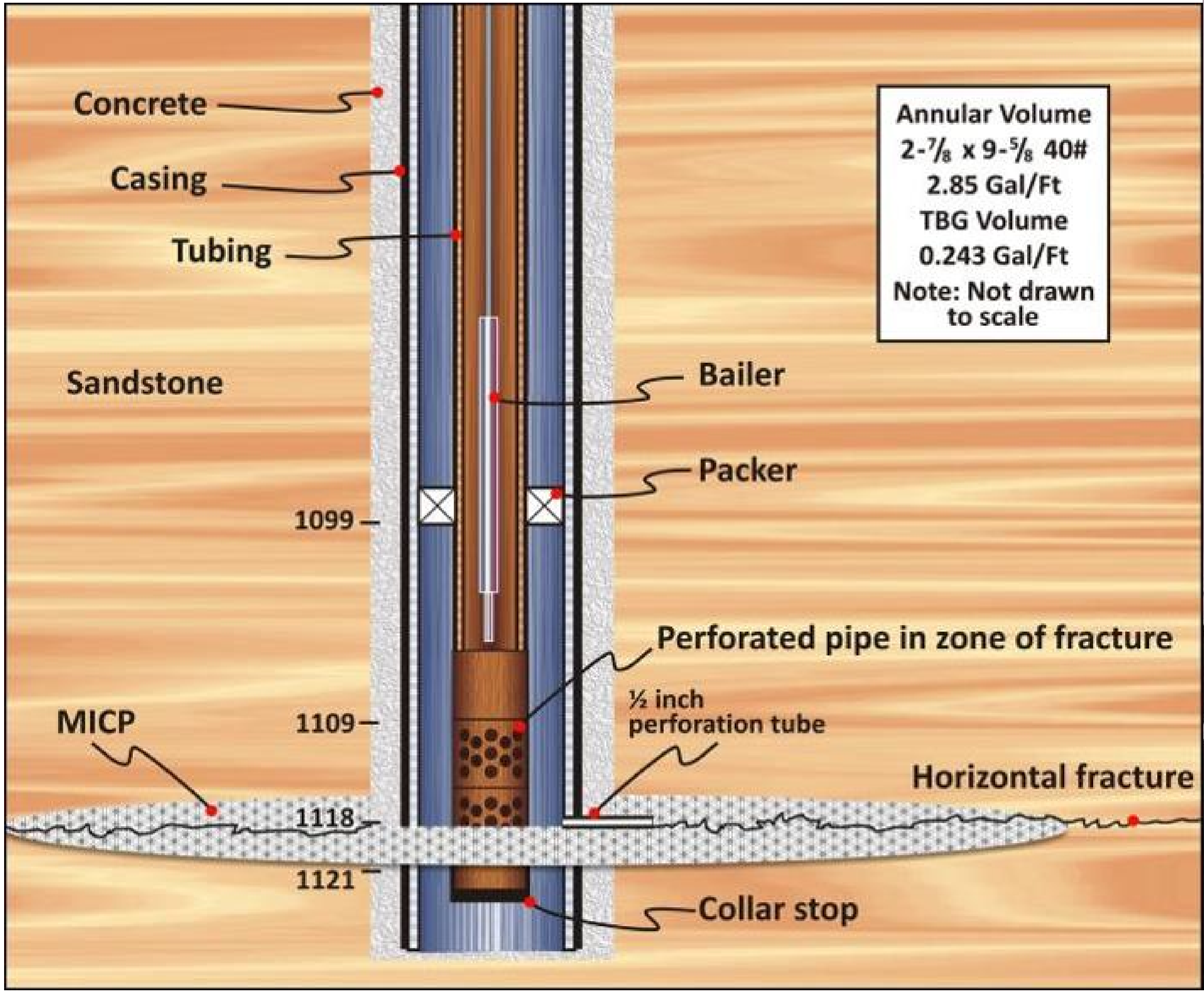
Modeling used to give estimate answers to design questions such as:

- How much reactants (urea, calcium, cells) are necessary?
- What is the best injection strategy?
- What is the time necessary for sealing?

And also post-application question such as:

- What happened underground during the MICP application?
- What is the expected behavior in the future?

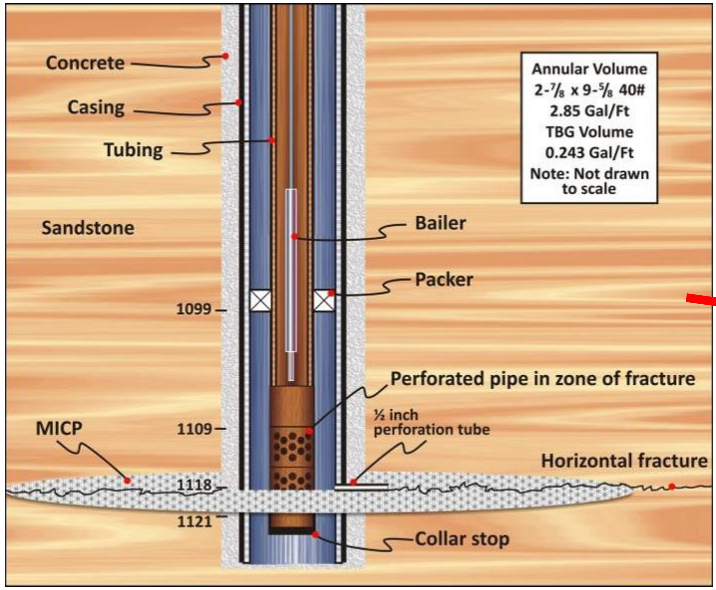
Field-scale applications of MICP



Peggy Dirckx, MSU

Adrienne Phillips, Al Cunningham, MSU

Field-scale modeling



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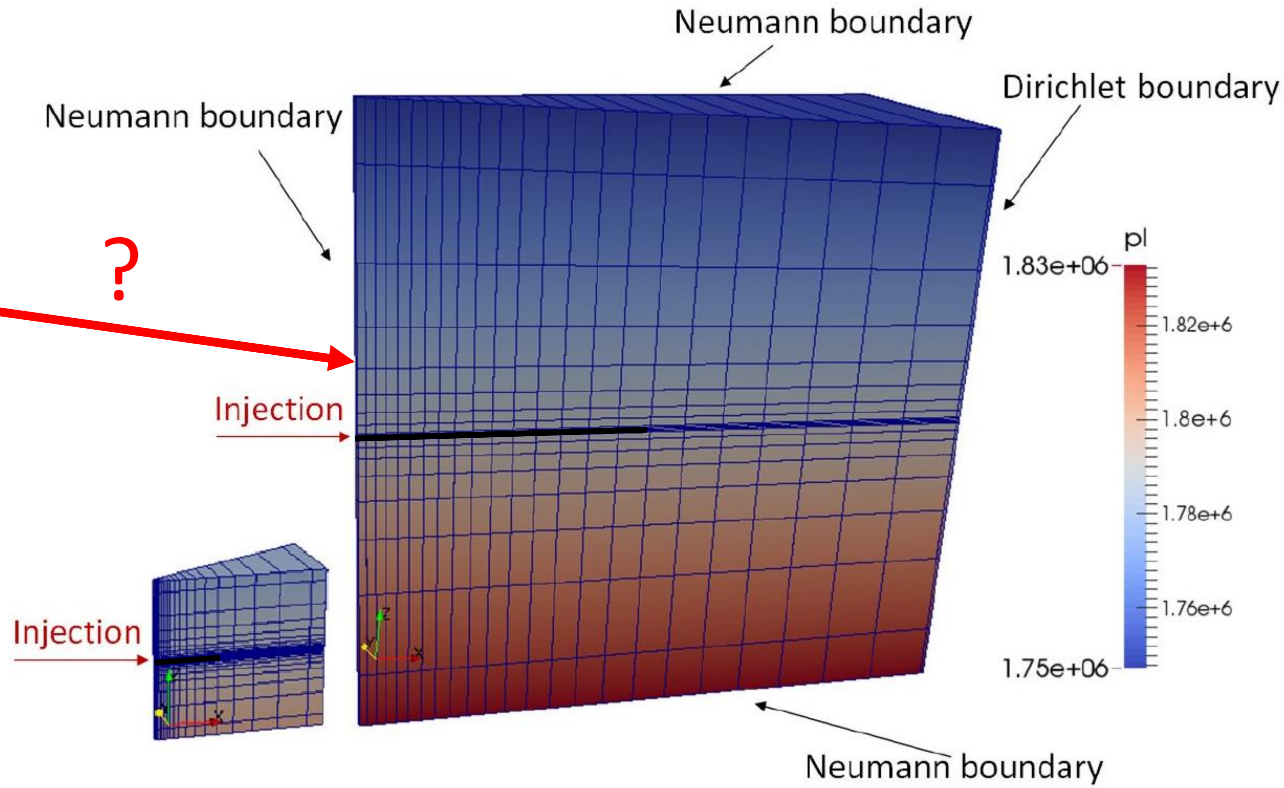
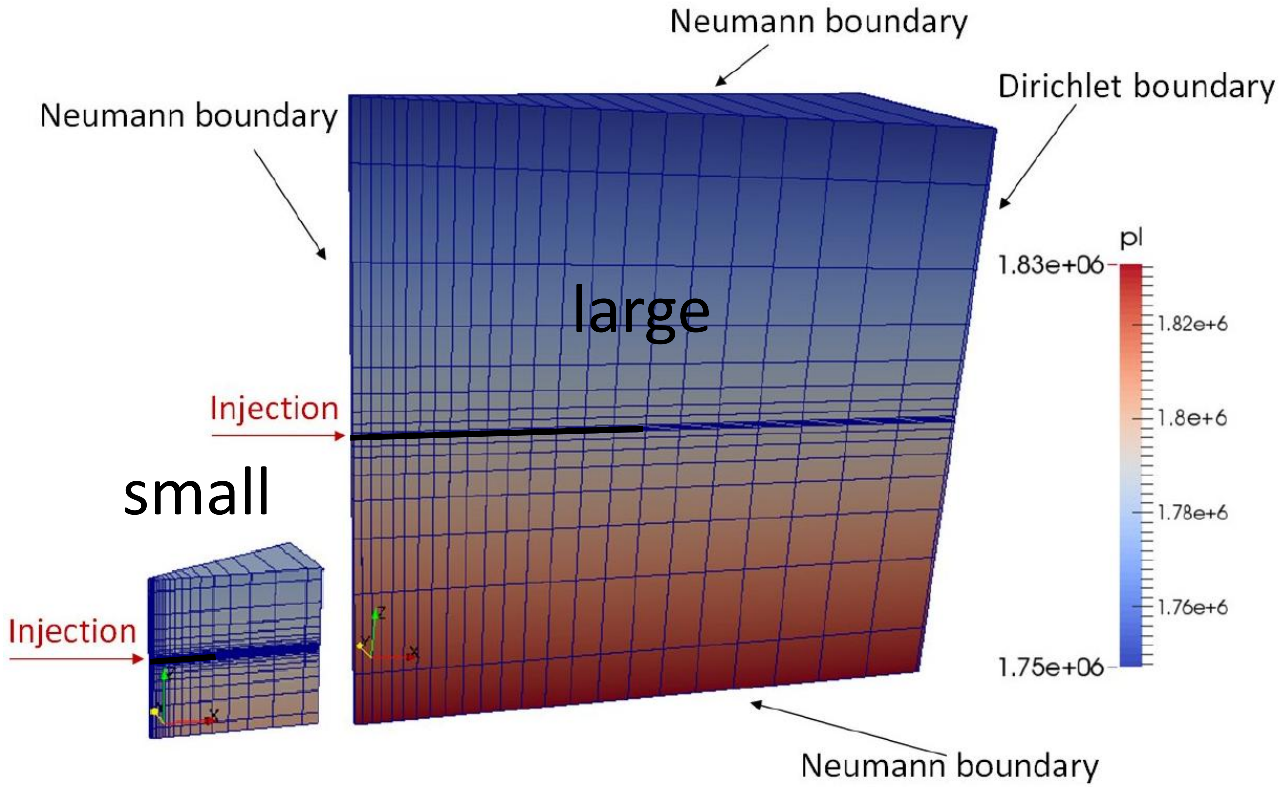


First challenge:

Use the limited information to set up a simplified but still realistic simulation domain.

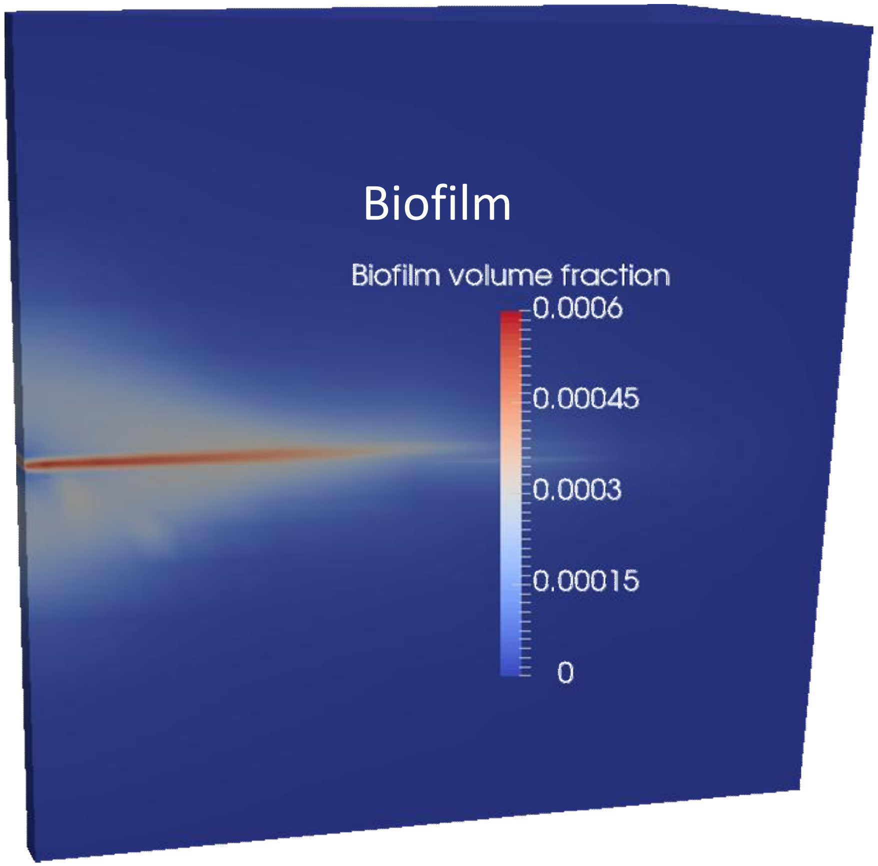
Field-scale modeling

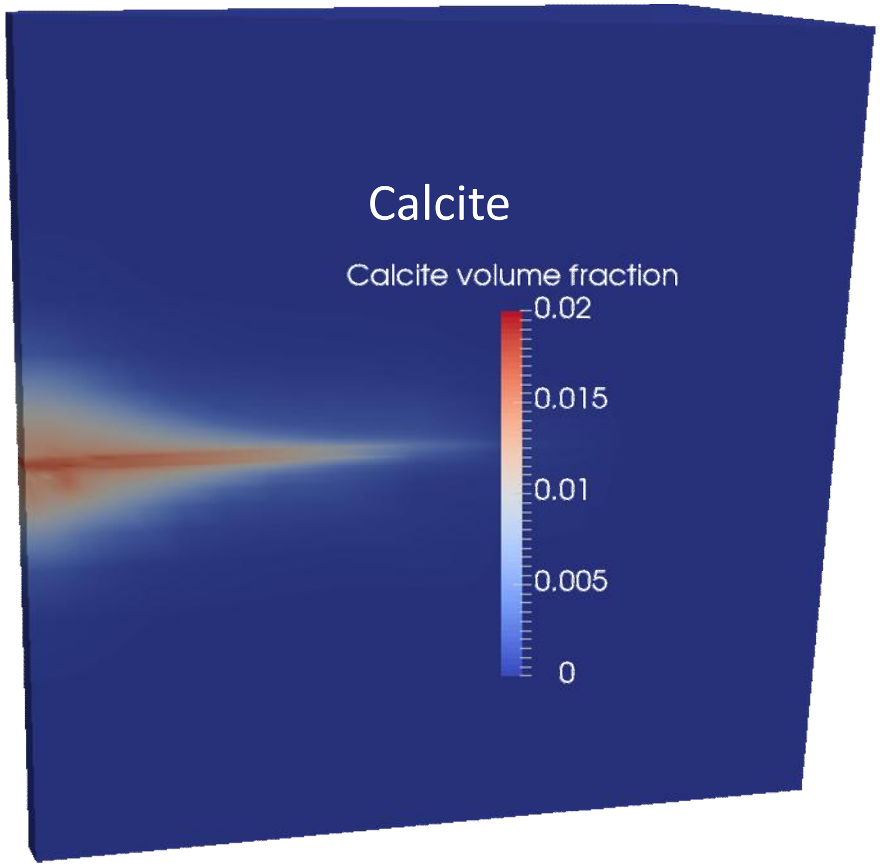


- 2 simulation domains:
  - small
  - large

- 3 different injection strategies:
  - simple: few but long injections
  - ideal: many short injections, proved to be the „best“ injection strategy
  - real: the actual injection strategy from the field test

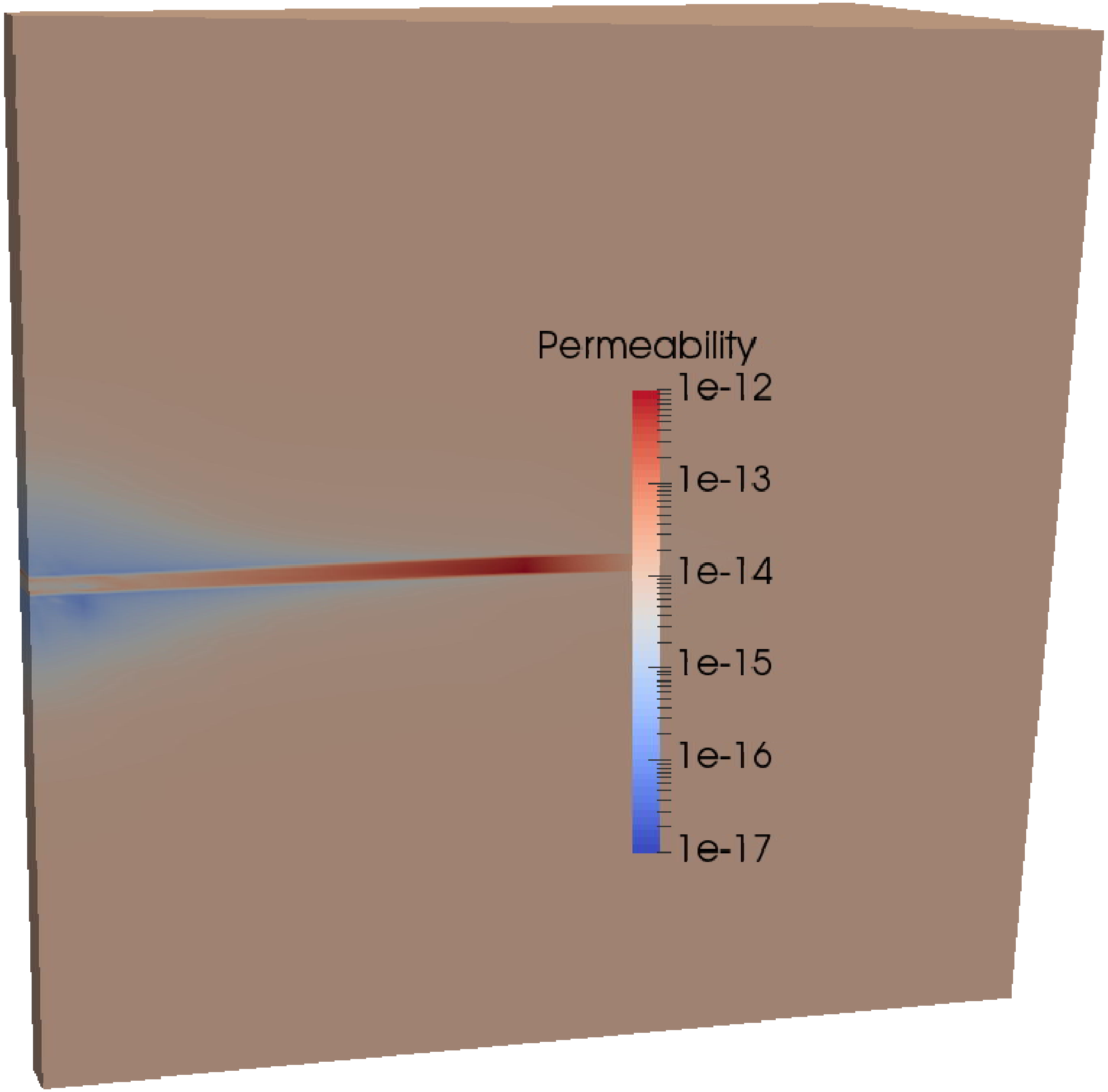
Field-scale modeling: Results



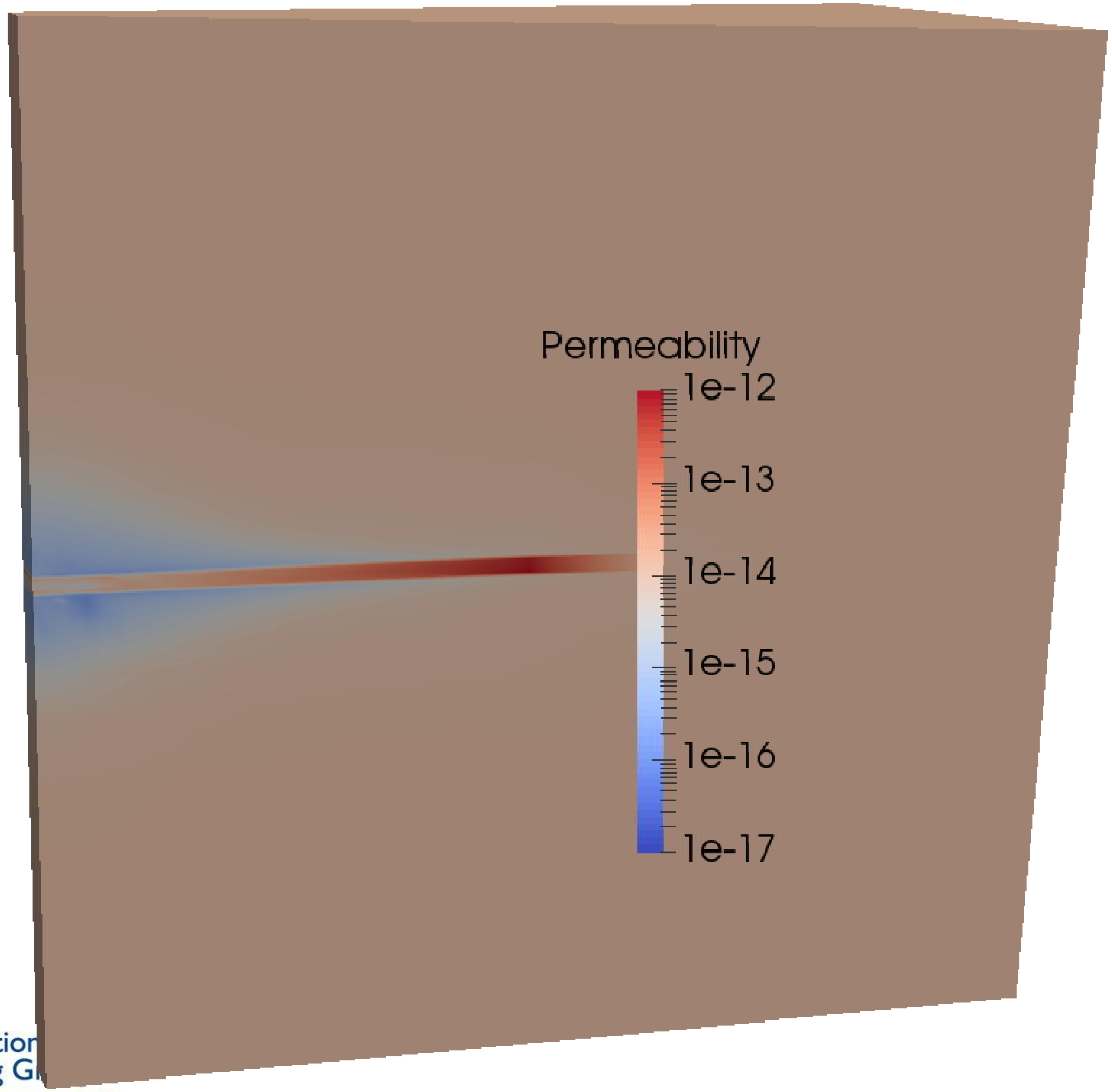


Exemplary results for the ideal scenario on the small domain.

Field-scale modeling: Results



Field-scale modeling: Results



The ideal injection strategy predicted plugging after 24 Calcium rich injections,

25 were done in the field.

The real injection strategy was slightly less efficient.

Field-scale modeling: Results and outlook

The uncertainties in the subsurface properties and the geometry require a statistical analysis of the results for a huge range of scenarios.

But:

Injection strategy	Simulation time [h] small domain	Simulation time [h] large domain
Simple	1.3	96.8
Ideal	1.0	26.1
Real	93.5	38.6

Simulation times of up to a few days limit the simulations to few scenarios

→ Need for more efficient solution strategies

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Efficient solution strategies

Strategies:

- Model simplifications:
  - For realistic applications, the input parameter uncertainty leads to large errors. The model does not need to be more accurate.
  - → Remove model complexity, especially if it is relevant for the model performance.

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- More sophisticated numerical solution schemes:
  - The full model is solved in a more efficient way.

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→ see the poster 18 (GRS) or 67 (GRC, Wednesday)

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Efficient solution strategies: Simplified models

Model simplifications investigated:

- Full complexity model (FC)

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→ less non-linearity, faster convergence

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Setup	FC, N 10^{-6}	IB, N 10^{-6}	SC, N 10^{-6}
Computational time [s]	32110	28089	5758
Newton iterations	4971	5053	1094
Linear solver iter./ Newton iteration	15.15	14.91	14.90
Error (ϕc calcite) *	0.0025	0.0040	0.0070

* Error: $\sqrt{\Sigma_{i=1}^{\text{nodes}} \left(\phi_{c,i} - \phi_{c,\text{ref},i}\right)^2}$

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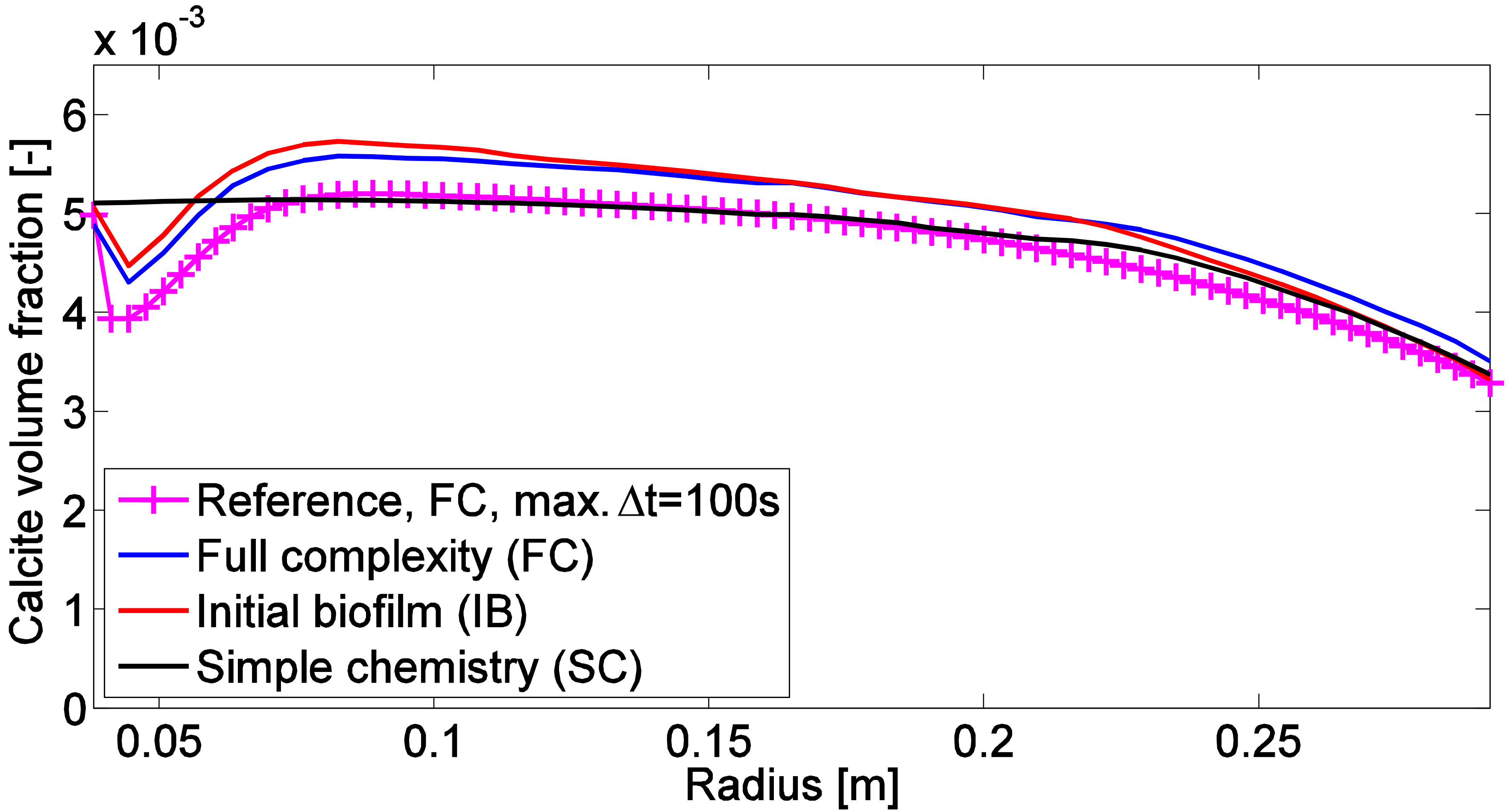
Efficient solution strategies: Simplified models



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Summary

- The developed model for MICP is very complex

- MICP and the model can be successfully applied at field scale

- The full complexity model is too time consuming for field-scale simulations

- Model simplification is useful to reduce the computational time.
  - Especially, if non-linear couplings are reduced
  - It can be used as a “process sensitivity analysis”
  - But each simplification may only be valid for a certain set of initial and boundary conditions
  - → see the poster 18 (GRS) or 67 (GRC, Wednesday)

- Relaxing the convergence criterion of the Newton solver can also be a “first aid” choice to reduce computational time

Thank you for your attention!

All simulations were done using

DuMu^x

Key papers / further information

A. Ebigbo, A.J. Phillips, R. Gerlach, R. Helmig, A.B. Cunningham, H. Class, L.H. Spangler: **Darcy-scale modeling of microbially induced carbonate mineral precipitation in sand columns**. *Water Resources Research*, 2012 (48) WO7519, doi:10.1029/2011WR011714

E.G. Lauchnor, D.M. Topp, A.E. Parker, R. Gerlach: **Whole cell kinetics of ureolysis by *Sporosarcina pasteurii***. *Journal of Applied Microbiology*, 2015 (118) 1321-1332, doi:10.1111/jam.12804

A.J. Phillips, E.G. Lauchnor, J. Eldring, R. Espositos, A.C. Mitchell, R. Gerlach, A.B. Cunningham, L.H. Spangler: **Potential CO_2 leakage leduction through biofilm-induced calcium carbonate precipitation**. *Environmental Science & Technology*, 2013 (47) 142-149, doi:10.1021/es301294q

A.J. Phillips, R. Gerlach, E.G. Lauchnor, A.C. Mitchell, A.B. Cunningham, L.H. Spangler: **Engineered applications of ureolytic biomineralization: a review**. *Biofouling*, 2013 (29) 715-733, doi:10.1080/08927014.2013.796550

Papers / further information

J. Hommel: **Modeling biogeochemical and mass transport processes in the subsurface: Investigation of microbially induced calcite precipitation**. *PhD Thesis*, University of Stuttgart, 2016, doi:0.18419/opus-8770

J. Hommel, E.G. Lauchnor, R. Gerlach, A.B. Cunningham, A. Ebigbo, R. Helmig, H. Class: **Investigating the influence of the initial biomass distribution and the injection strategies on biofilm-mediated calcite precipitation in porous media**. *Transport in Porous Media*, 2015, doi:10.1007/s11242-015-0617-3

J. Hommel, E.G. Lauchnor, A.J. Phillips, R. Gerlach, A.B. Cunningham, R. Helmig, A. Ebigbo, H. Class: **A revised model for microbially induced calcite precipitation: Improvements and new insights based on recent experiments**. *Water Resources Research*, 2015 (51) 3695-3715, doi:10.1002/2014WR016503

J. Hommel, A.B. Cunningham, R. Helmig, A. Ebigbo, H. Class: **Numerical investigation of microbially induced calcite precipitation as a leakage mitigation technology**. *Energy Procedia*, 2013 (40C) 392-397, doi:10.1016/j.egypro.2013.08.045