

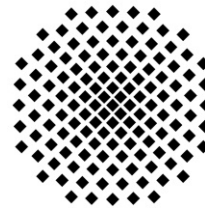


A balance between accuracy and effort for modeling biomineralization

NUPUS Meeting, September 2015

Johannes Hommel,

Anozie Ebigbo, Robin Gerlach, Alfred B. Cunningham, Rainer Helmig, Holger Class



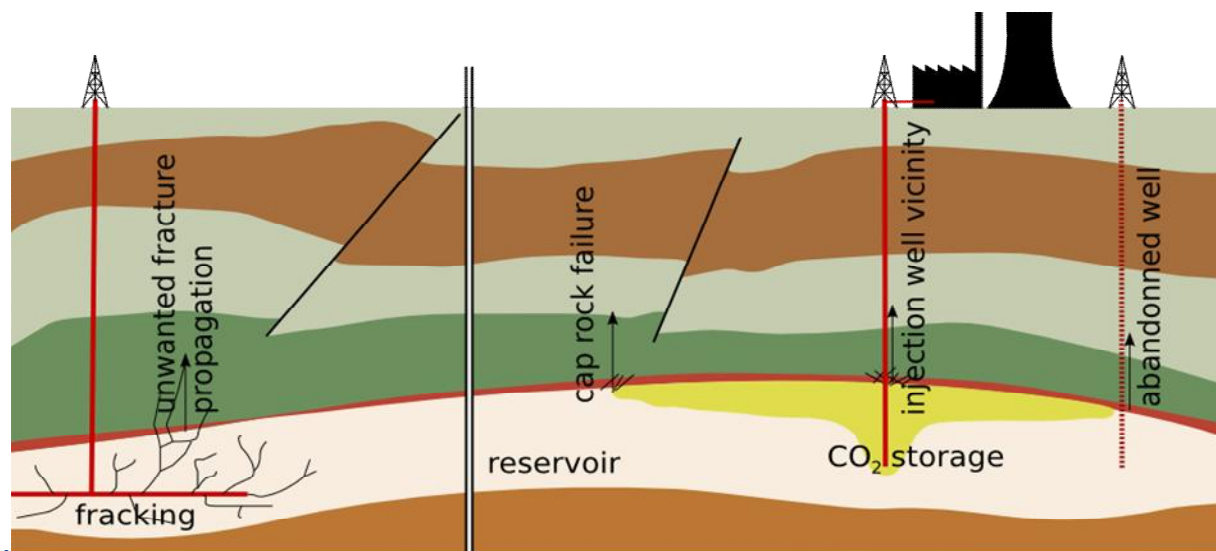
University of Stuttgart

Germany

Motivation

- Increased use of the subsurface injecting or extracting fluids.
- Exclusive and storage uses require separation.
→ sealing of leakage pathways is important
- Reactive transport models are needed to optimize the sealing.

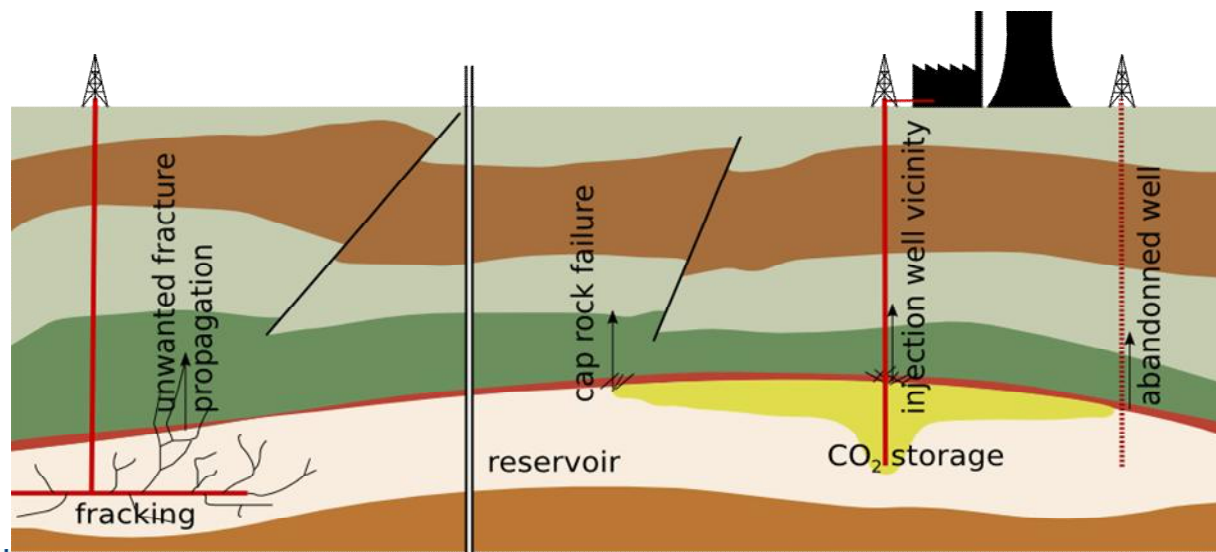
- But on the relevant field scale, reactive transport models quickly become prohibitively expensive in terms of the computational effort!



Motivation

- On the relevant field scale, reactive transport models quickly become prohibitively expensive in terms of the computational effort!

→ Models should be as simple and as fast as possible, but at the same time as accurate as possible!



Outline

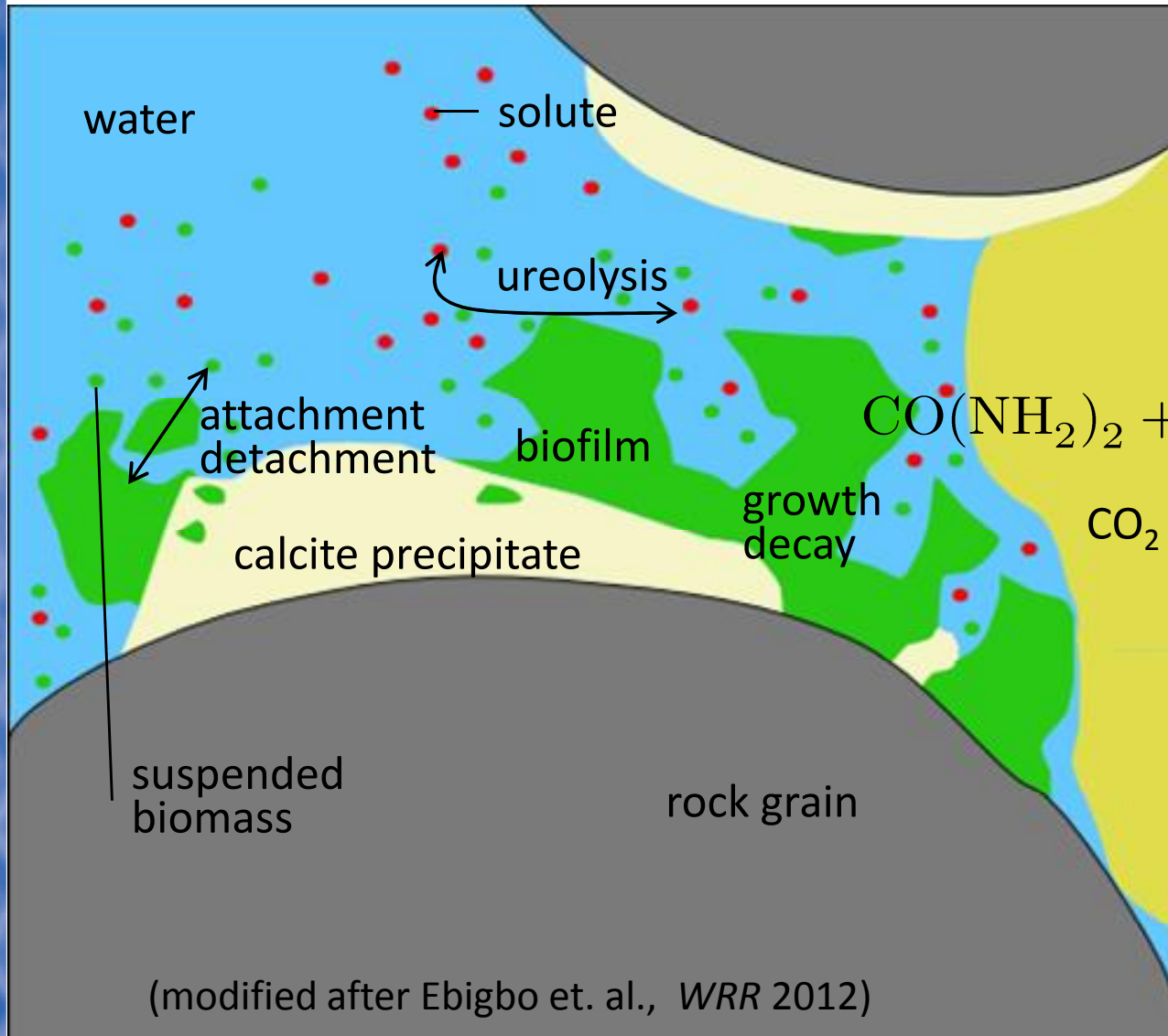
Model concept

Methods to reduce computational effort:

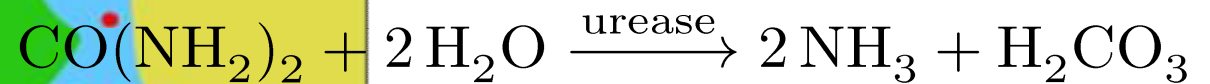
- Model simplifications
- Sequential approach

Results

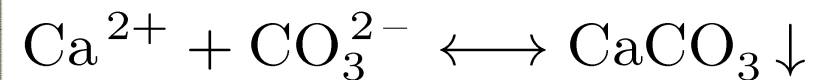
Model concept: Relevant processes



- Two-phase multi-component transport
- Biomass
 - growth / decay
 - attachment / detachment
- Urea hydrolysis



- Precipitation / dissolution of calcite



- Clogging

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

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

Mass balance equations

Mass balance equation for components in both phases:

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

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

Mass balance equation of components exclusively in the water phase:

$$\frac{\partial}{\partial t} (\phi \rho_w x_w^{\kappa} S_w) + \nabla \cdot (\rho_w x_w^{\kappa} \mathbf{v}_w) - \nabla \cdot (\rho_w \mathbf{D}_w \nabla x_w^{\kappa}) = q^{\kappa}$$

$$\kappa \in \{Na, Cl, Ca, \text{bio}, \text{substrate}, N_{\text{tot}}, \text{urea}\}$$

Mass balance for the immobile components / solid phases:

$$\rho_{\lambda} \frac{\partial \phi_{\lambda}}{\partial t} = q^{\lambda} \quad \lambda \in \{\text{biofilm}, \text{calcite}\}$$

Sources and sinks q^{κ} and q^{λ} are due to reactions or microbial processes.

Outline

Model concept

Methods to reduce computational effort:

- Model simplifications
- Sequential approach

Results

Model simplifications

For the globally implicit approach, the **full complexity model (FC)** and two simplifications are investigated:

Initial biofilm (IB): Instead of an inoculation period, the model is started at a later time with a pre-established biofilm. The component „suspended biomass“ is neglected, as suggested in [1], resulting in a reduced number of unknowns.

Simple chemistry (SC): Activities and saturation index are neglected, the precipitation rate is assumed to be equal to the ureolysis rate as in e.g. [2]. This model has the full set of unknowns.

[1] J. Hommel, E. Lauchnor, R. Gerlach, A. B. Cunningham, A. Ebigbo, R. Helmig, H. Class: Investigating the influence of the initial biomass distribution and injection strategies on biofilm-mediated calcite precipitation in porous media, submitted to *Transp. Porous Med.*, 2015

[2] W. K. van Wijngaarden, F. J. Vermolen, G. A. M. Meurs, and C. Vuijk: A mathematical model for Biogrout, *Comput. Geosci.*, 2013, 17(3), 463–478, doi:10.1007/s10596-012-9316-0.

Sequential approach: mass balances split into transport and reaction

- Mass balance, fully implicit:

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

- Mass balance, transport only:

$$\sum_{\alpha} \frac{\partial}{\partial t} (\phi \rho_{\alpha} x_{\alpha}^{\kappa} S_{\alpha}) + \nabla \cdot (\rho_{\alpha} x_{\alpha}^{\kappa} \mathbf{v}_{\alpha}) - \nabla \cdot (\rho_{\alpha} \mathbf{D}_{\alpha} \nabla x_{\alpha}^{\kappa}) = 0$$

→ No reactive sources in the
transport subproblem

- Mass balance, reaction only:

$$\sum_{\alpha} \frac{\partial}{\partial t} (\phi \rho_{\alpha} x_{\alpha}^{\kappa} S_{\alpha}) = q^{\kappa}$$

→ Only local information is needed in the
reaction subproblem

Sequential approach: mass balances split into transport and reaction

- Mass balance of solid phases, fully implicit:

$$\rho_{\lambda} \frac{\partial \phi_{\lambda}}{\partial t} = q^{\lambda} \quad \lambda \in \{\text{biofilm, calcite}\}$$

- Mass balance of solid phases, transport only:

$$\rho_{\lambda} \frac{\partial \phi_{\lambda}}{\partial t} = 0 \quad \rightarrow \text{Solid phases disappear in the transport subproblem}$$

- Mass balance of solid phases, reaction only:

$$\rho_{\lambda} \frac{\partial \phi_{\lambda}}{\partial t} = q^{\lambda}$$

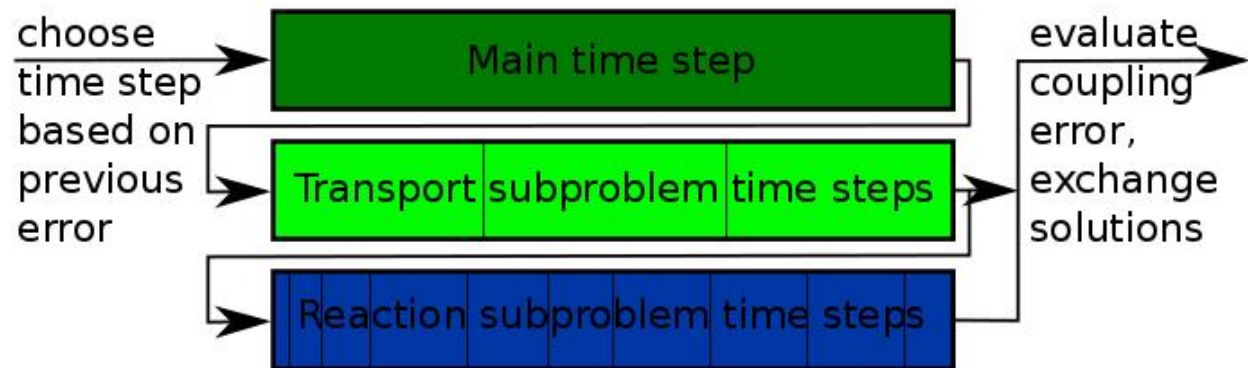
Sequential approach used

- Sequential non-iterative coupling scheme.

$$CE = \max \left(\frac{2 |p_{w,transp} - p_{w,chem}|}{p_{w,transp} + p_{w,chem}}, |x_{w,transp}^{\kappa} - x_{w,chem}^{\kappa}| \right)$$

(Based on literature)

- Advantages:
 - easy to implement
 - suitable for large scale
 - suitable for advection dominated systems like the vicinity of an injection well
- Disadvantages:
 - time step size constraints or increasing error due to the sequential calculation
- Other sequential schemes are yet to be tested



Outline

Model concept

Methods to reduce computational effort:

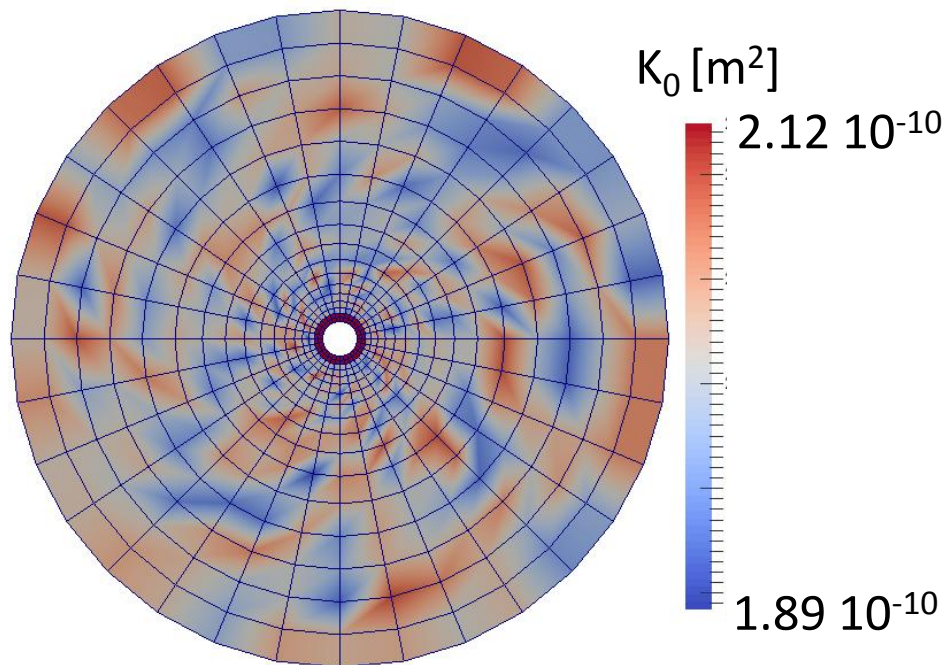
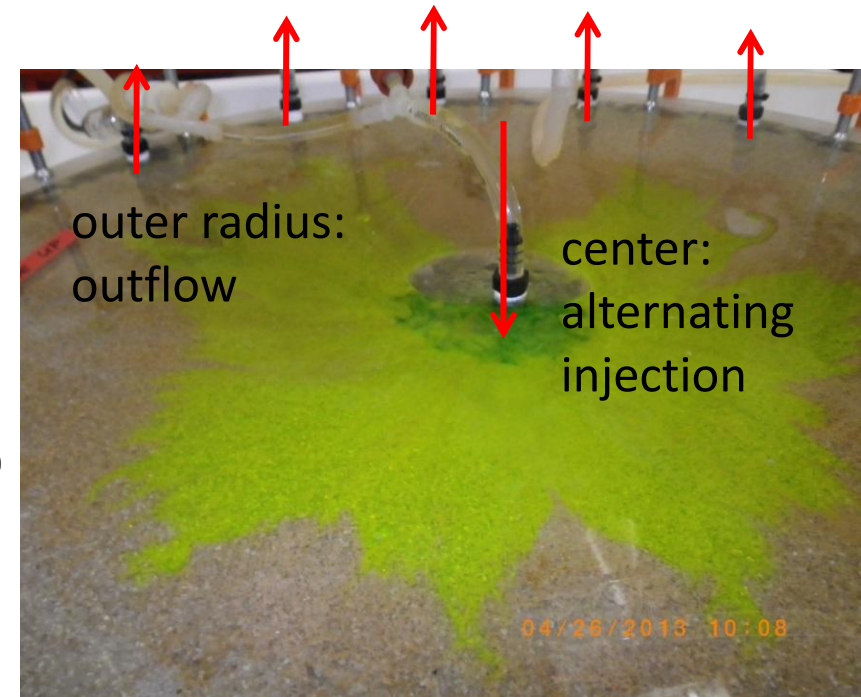
- Model simplifications
- Sequential approach

Results

Test setup: Radial Flow

Original experiment shows heterogeneities

→ Using the comparison of homogeneous and heterogeneous case (estimated using [3]) as a base error.



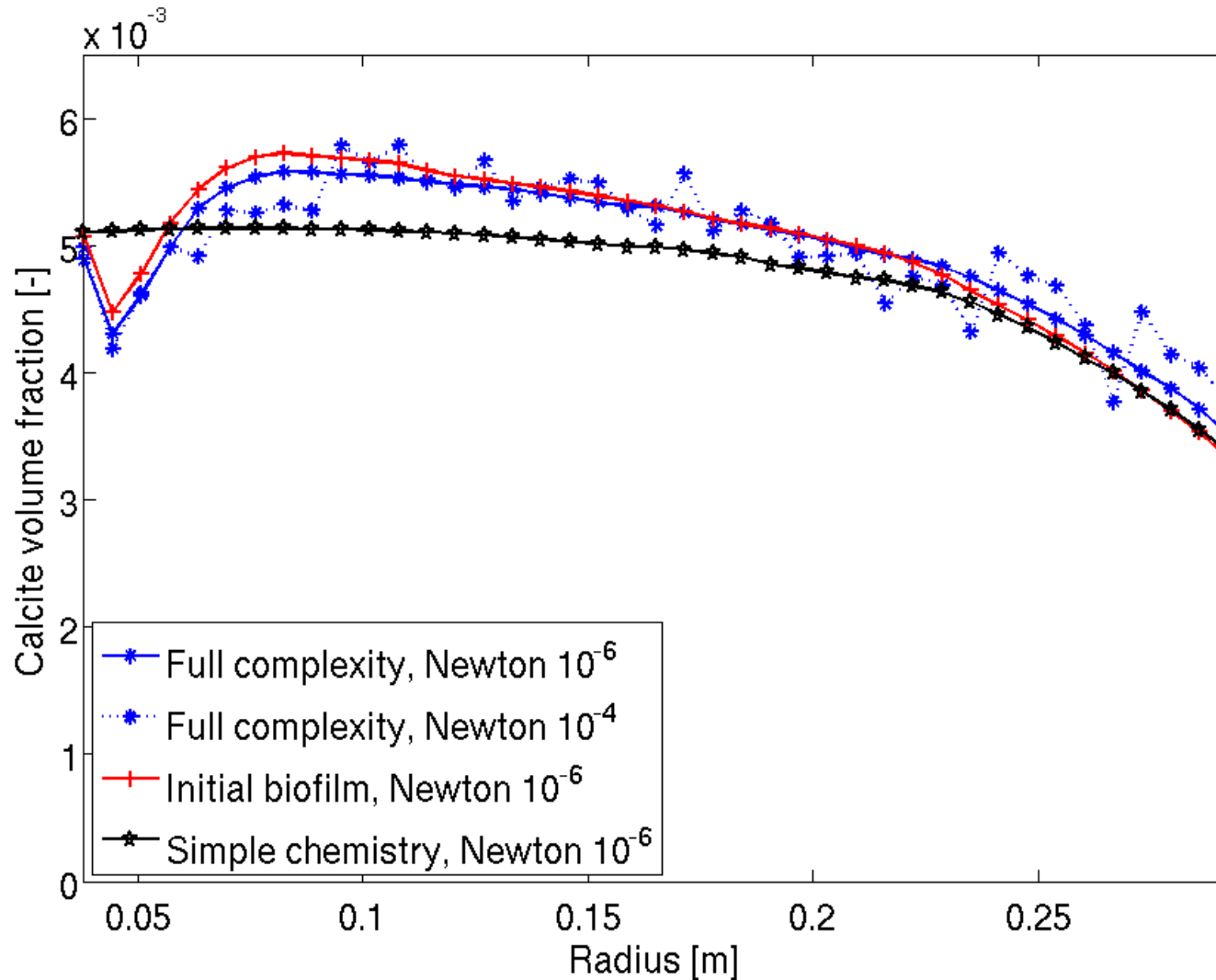
Error:

$$\sqrt{\sum_{i=1}^{\text{nodes}} (\phi_{c,\text{homo},i} - \phi_{c,\text{hetero},i})^2}$$

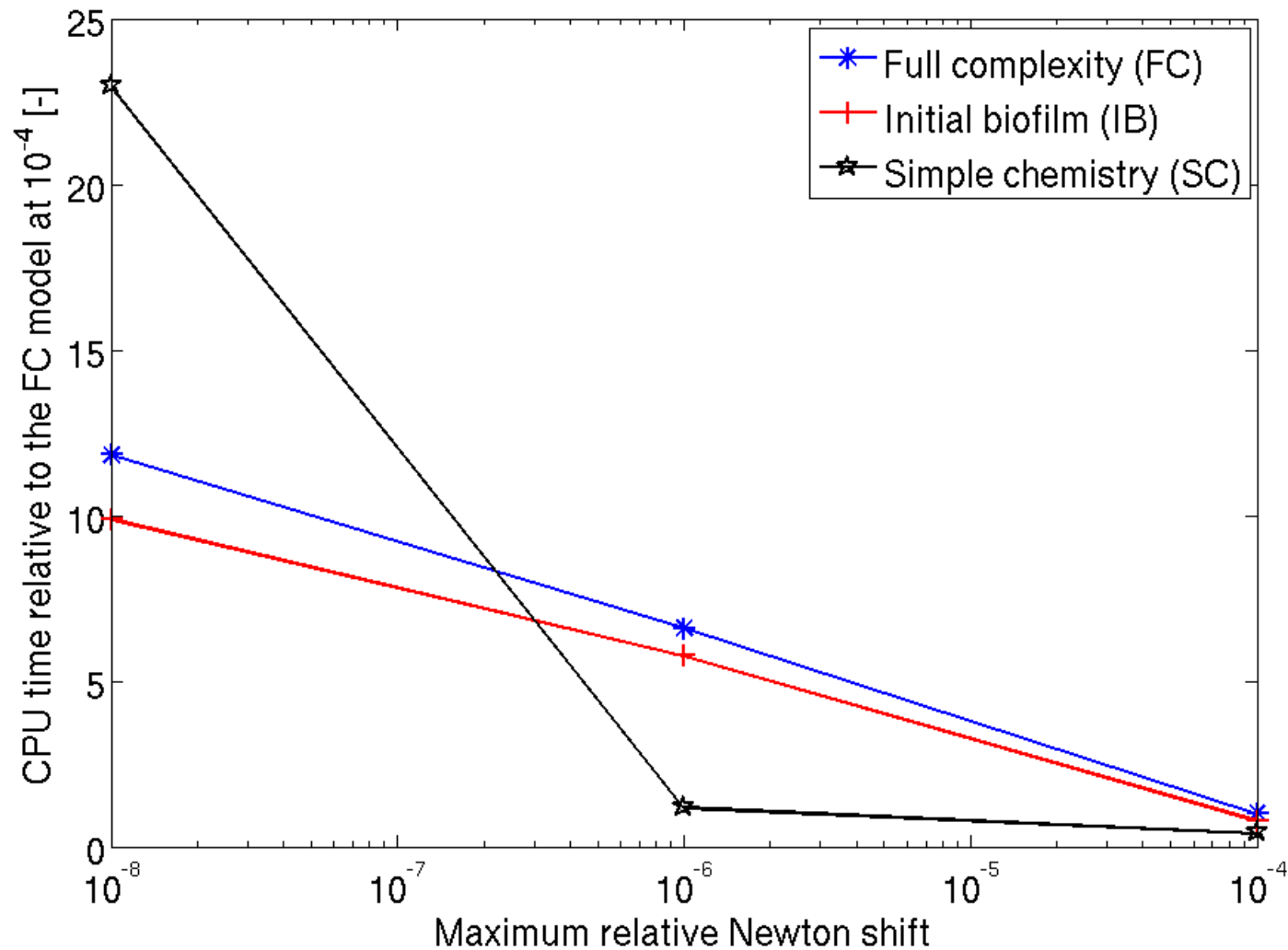
→ Error hetero-homo = 0.0033

[3] R. F. Carsel, R. S. Parrish: Developing joint probability distributions of soil water retention characteristics, Water Resour. Res., 1988, 24(5), 755-769.

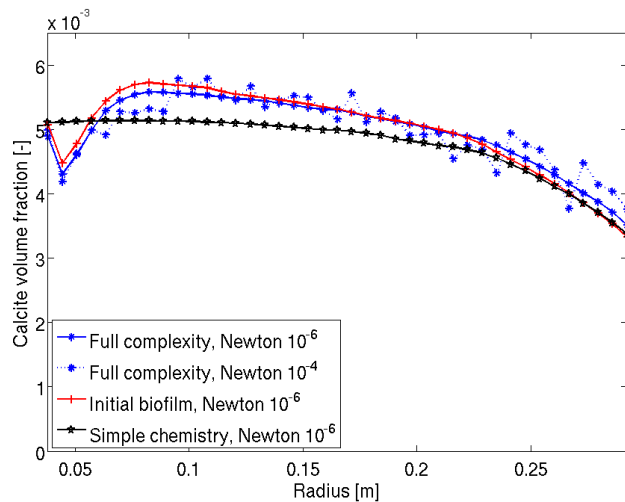
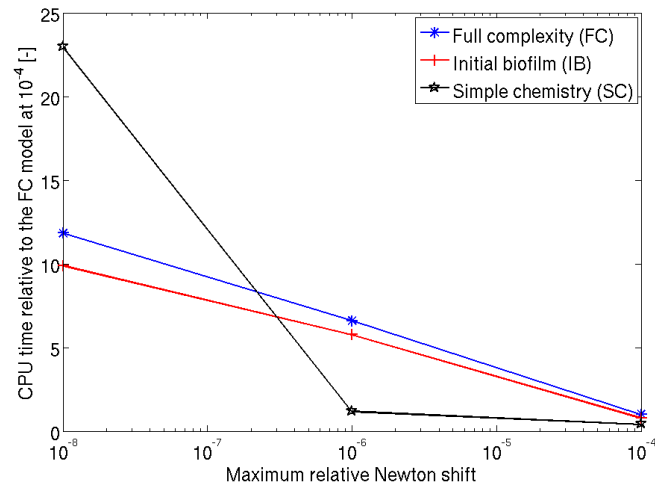
Results: model simplification



Results: model simplification



Results: model simplification



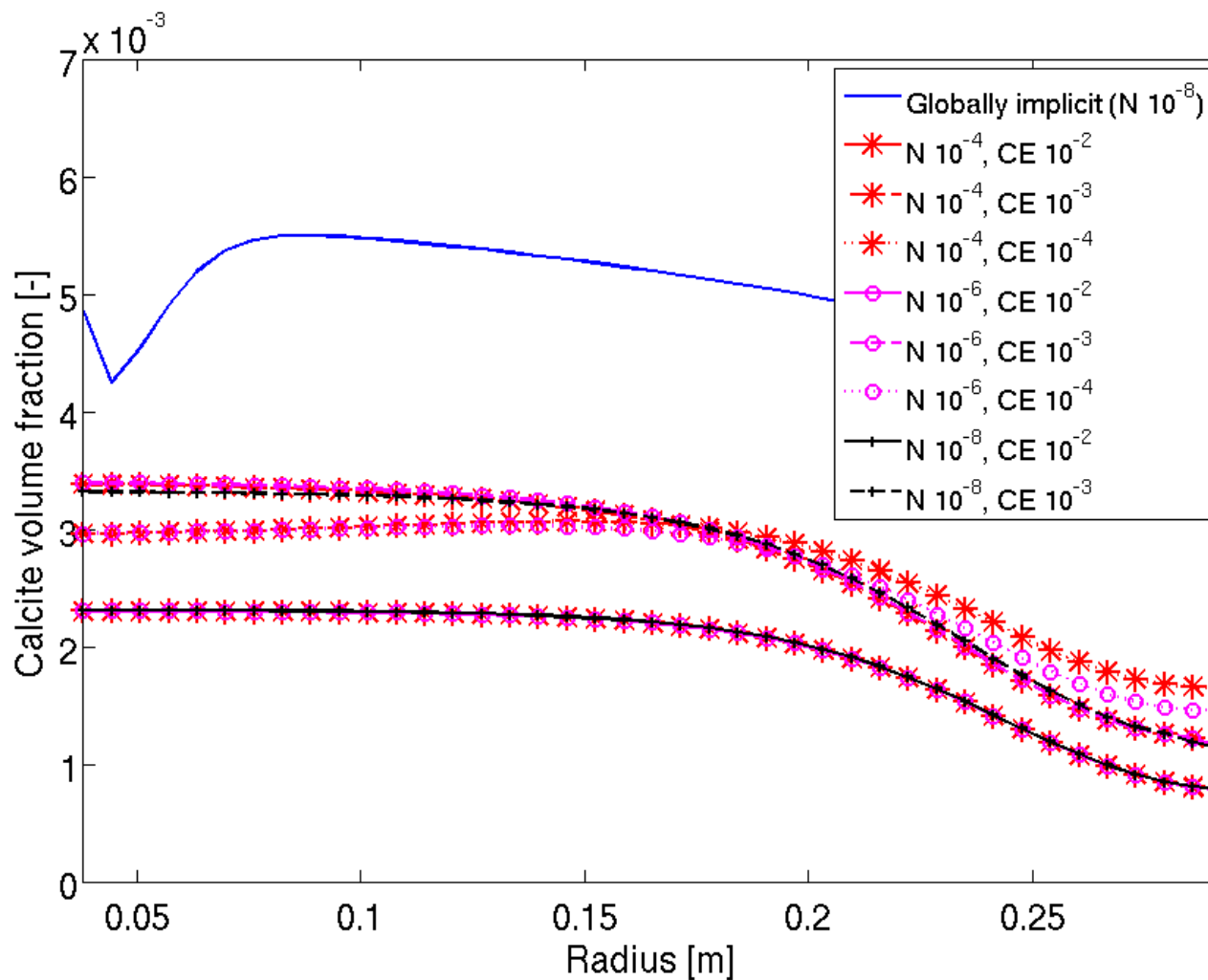
Setup	FC, N 10 ⁻⁶	FC, N 10 ⁻⁴	IB, N 10 ⁻⁶	SC, N 10 ⁻⁶
CPU time [s]	32110	4861	28089	5758
Newton iterations	4971	776	5053	1094
Linear solver iter./ Newton iteration	15.15	6.57	14.91	14.90
Error (ϕ_c calcite) *	0.0025	0.0065	0.0039	0.0070

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

Reference: homogeneous, full complexity, Newton 10⁻⁸, fine discretization (dt and dx)

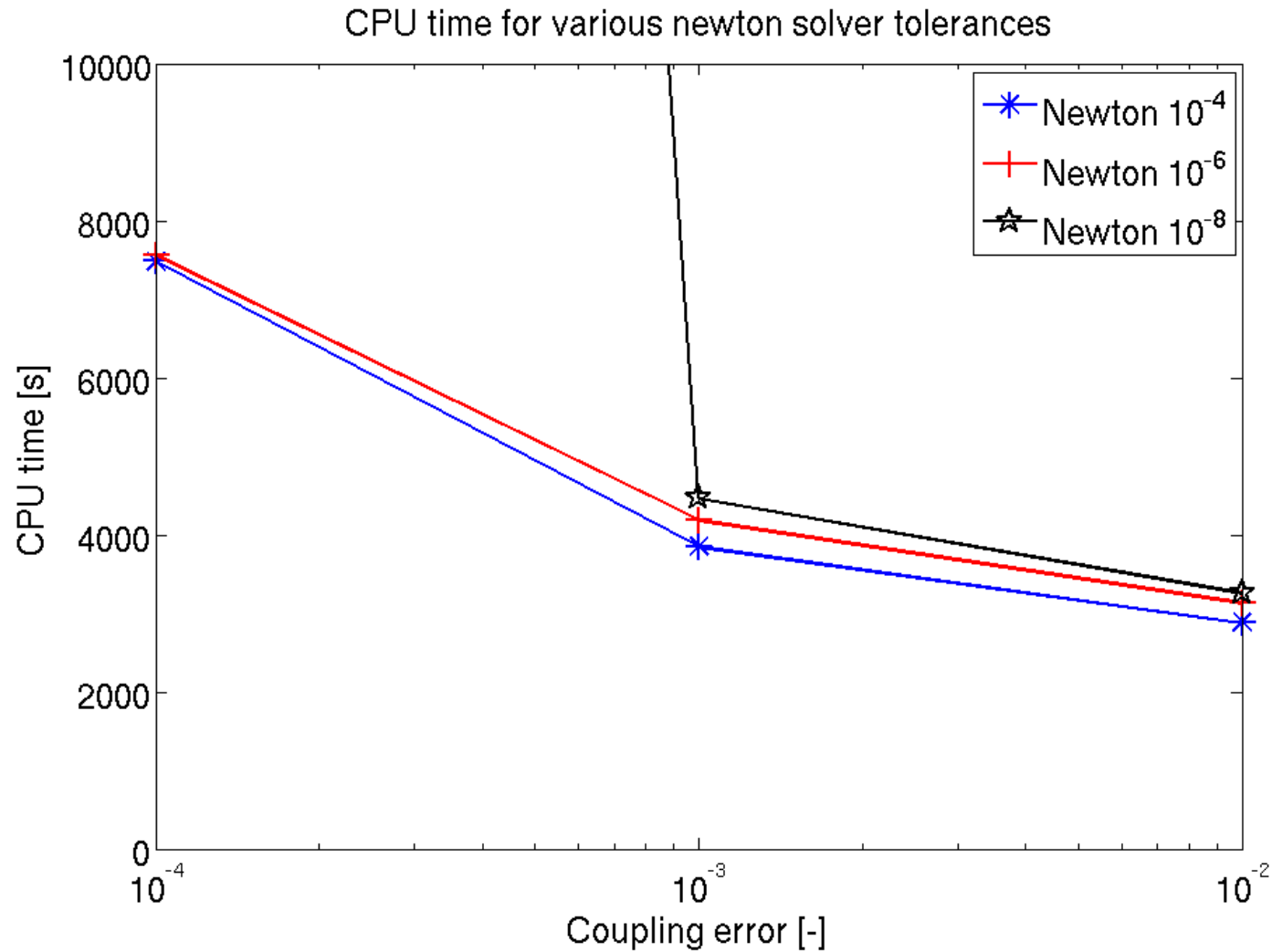
Error hetero-homo = 0.0033

Results: sequential approach

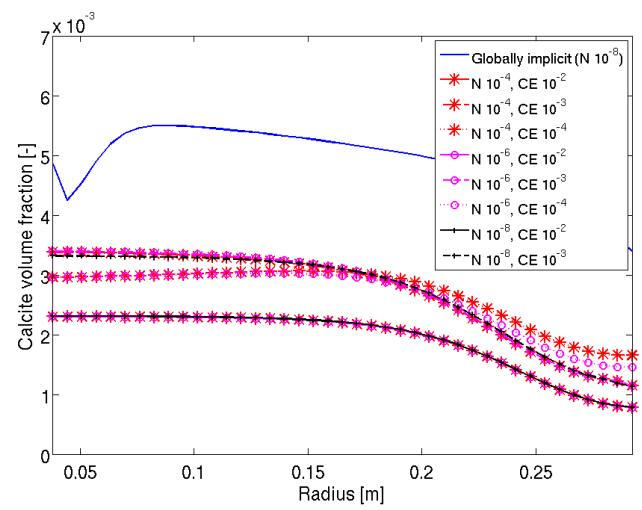
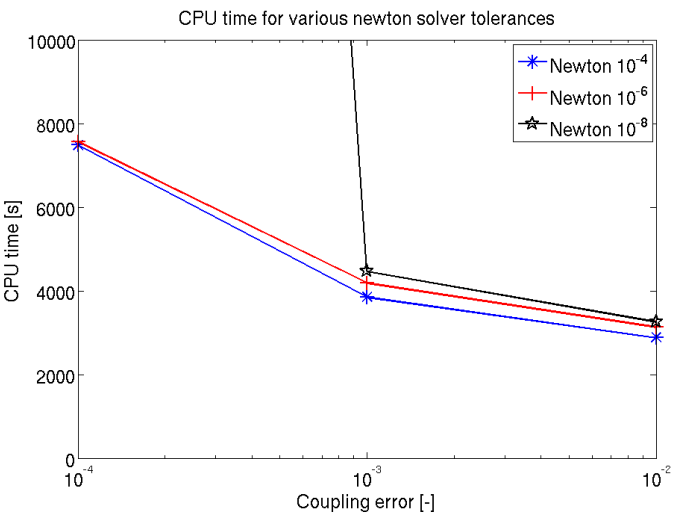


Results: sequential approach

www.hydrosys.uni-stuttgart.de



Results: sequential approach



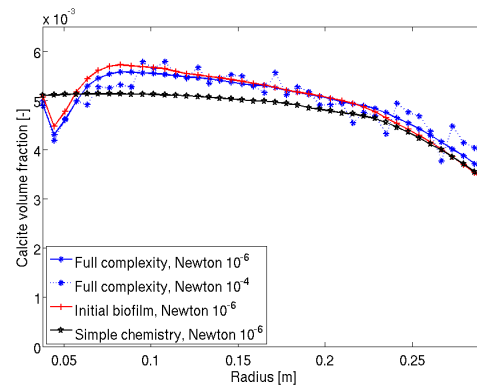
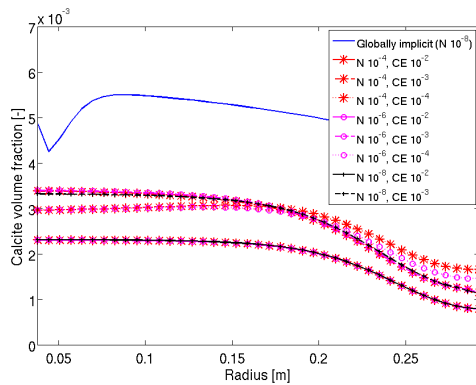
Setup	FC, N 10 ⁻⁶	CE 10 ⁻² N 10 ⁻⁶	CE 10 ⁻² N 10 ⁻⁴	CE 10 ⁻³ N 10 ⁻⁴	CE 10 ⁻⁴ N 10 ⁻⁴
CPU time [s]	32110	3135.6	2882.8	3856.6	7486.4
Main Δt	580	18	18	30	138
transport Δt		171	159	172	439
Newton iter. (transport)	4971	409	327	352	893
Linear solver iter./ Newton iter. (transp.)	15.15	12.33	12.28	12.21	11.21
Error (φ _c calcite) *	0.0025	0.0770	0.0770	0.0575	0.0568

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

Reference: homogeneous, globally implicit, full complexity, Newton 10⁻⁸, fine discretization

Summary

- Sequential (non-iterative) approach:
 - large errors and underestimation of the precipitated calcite

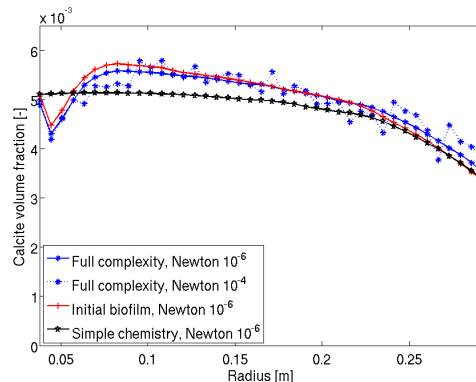
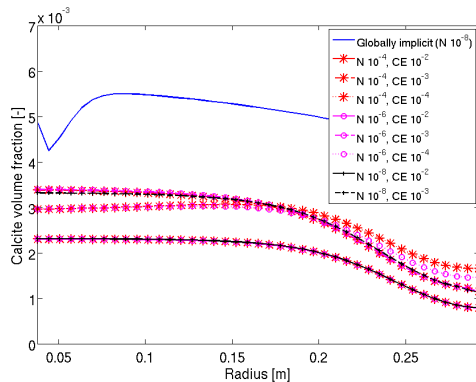


	CE 10 ⁻² N 10 ⁻⁴	SC, N 10 ⁻⁶	FC, N 10 ⁻⁴
CPU time	2882.8	5758	4861
Error	0.0770	0.0070	0.0065

- Simplification of the globally implicit model:
 - Simple chemistry leads to a significant reduction of CPU time, but it is not generally applicable. (e.g. less calcium than urea)
 - Relaxing the Newton's convergence criteria has similar effects as SC, the results getting „noisy“ compared to the reference.
 - Initial biofilm model does not reduce the CPU time significantly.

Summary

- Sequential (non-iterative) approach:
 - large errors and underestimation of the precipitated calcite



	CE 10 ⁻² N 10 ⁻⁴	SC, N 10 ⁻⁶	FC, N 10 ⁻⁴
CPU time	2882.8	5758	4861
Error	0.0770	0.0070	0.0065

Error hetero-homo = 0.0033

- Simplification of the globally implicit model:
 - Simple chemistry leads to a significant reduction of CPU time, **but it is not generally applicable.** (e.g. less calcium than urea)
 - Relaxing the Newton's convergence criteria** has similar effects as SC, the results getting „noisy“ compared to the reference.
 - Initial biofilm model does not reduce the CPU time significantly.
- To do:
 - Test other sequential approaches and a one-phase biomineralization model.

Key papers / further information

A. Ebigbo, A.J. Philipps, 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

A.J. Philipps, R. Gerlach, E. Lauchnor, A.C. Mitchell, A.B. Cunningham, L.H. Spangler: **Engineered applications of ureolytic biomineralization: a review**. Biofouling, 2013, 29(6) 715-733, doi:10.1080/08927014.2013.796550

J. Hommel, E. Lauchnor, A.J. Philipps, 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(5) 3695-3715, doi:10.1002/2014WR016503

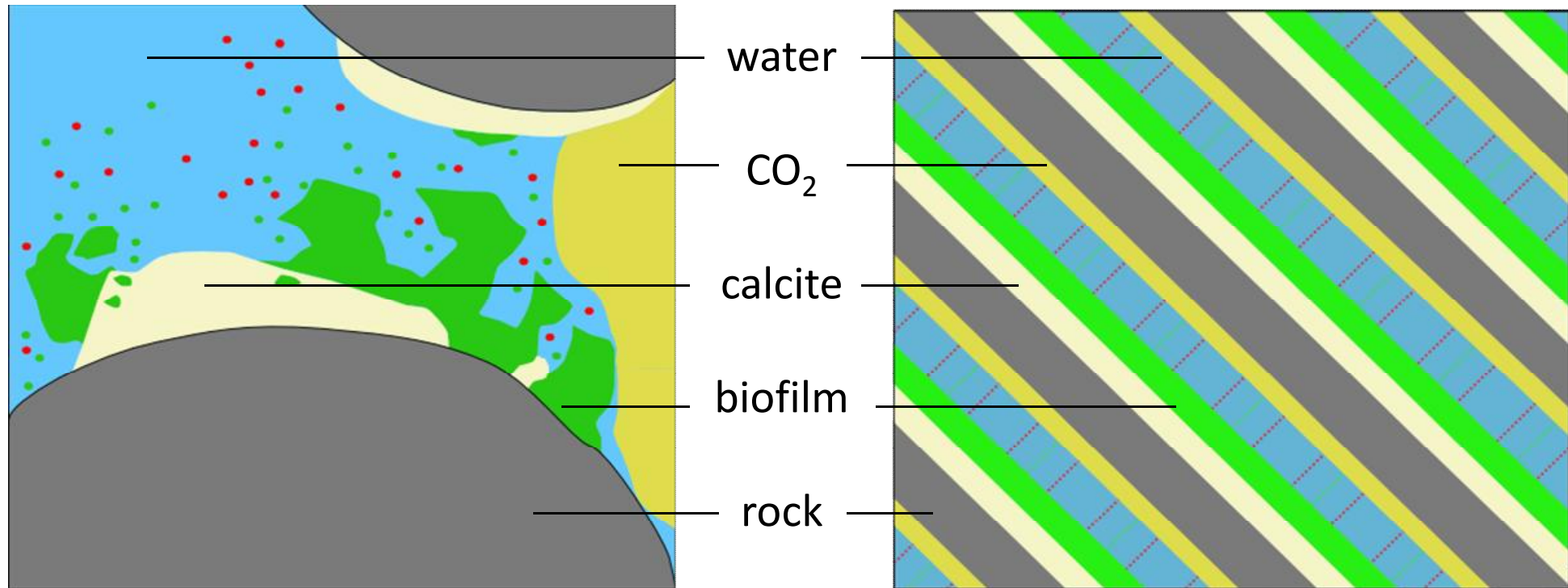
Thank you for your attention!

NUPUS and DFG are acknowledged for funding

***All simulations were
done using DuMu^X***

***For further information on DuMu^X, see:
<http://dumux.org/>***

Model concept: Scale



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

Pore scale

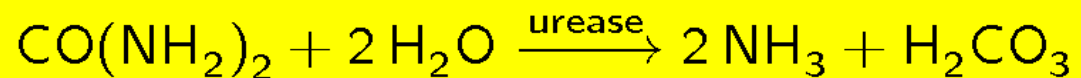
averaging



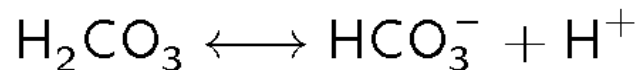
REV scale

Model concept: Important reactions

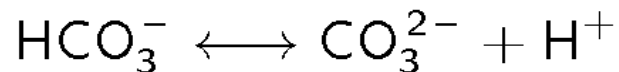
The bacterium *Sporosarcina pasteurii* produces the enzyme urease. Urease catalyzes the hydrolysis of urea, which produces ammonia and leads to an increase in pH.



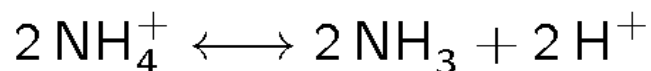
ureolysis



dissociation of carbonic acid



dissociation of bicarbonate ion



dissociation of ammonia



calcite precipitation/dissolution

→ in the presence of calcium ions, the rise in pH due to ureolysis will drive the precipitation of calcite.

Sources & sinks: Biomass

Suspended biomass: $q^{\text{bio}} = r_{\text{growth}}^{\text{bio}} - r_{\text{decay}}^{\text{bio}} - r_{\text{attach}} + r_{\text{detach}}$

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

Growth: $r_{\text{growth}}^{\text{bio}} = \mu \phi S_w C_w^{\text{bio}}$
 $r_{\text{growth}}^{\text{biofilm}} = \mu \phi_{\text{biofilm}} \rho_{\text{biofilm}}$

Growth coefficient: $\mu = \mu_{\text{max}} \text{Yield} \frac{C_{\text{substrate}}}{K_{\text{substrate}} + C_{\text{substrate}}} \cdot \frac{C_w^{\text{O}_2}}{K_{\text{O}_2} + C_w^{\text{O}_2}}$

Decay: $r_{\text{decay}}^{\text{bio}} = k_{\text{decay}}^{\text{bio}} \phi S_w C_w^{\text{bio}}$
 $r_{\text{decay}}^{\text{biofilm}} = k_{\text{decay}}^{\text{biofilm}} \phi_{\text{biofilm}} \rho_{\text{biofilm}}$

Attachment: $r_{\text{attach}} = (c_{a,1} \phi_{\text{biofilm}} + c_{a,2}) C_w^{\text{bio}} \phi S_w$

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

Sources & sinks: Solutes and Calcite

Substrate: $q^{\text{substrate}} = -(r_{\text{growth}}^{\text{bio}} + r_{\text{growth}}^{\text{biofilm}}) / \textit{Yield}$

Oxygen: $q^{\text{O}_2} = -(r_{\text{growth}}^{\text{bio}} + r_{\text{growth}}^{\text{biofilm}}) \cdot (0.5 / \textit{Yield})$

Urea: $q^{\text{urea}} = -r^{\text{urea}} = f(\phi_{\text{biofilm}}, C_{\text{w}}^{\text{urea}}, \text{pH}, C_{\text{w}}^{\text{NH}_4})$

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

Calcium: $q^{\text{Ca}} = r_{\text{diss}} - r_{\text{precip}} = f(\textit{area}, \textit{saturation state}, \text{pH})$

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

Calcite: $q^{\text{calcite}} = r_{\text{precip}} - r_{\text{diss}} = f(\textit{area}, \textit{saturation state}, \text{pH})$