Accelerated reactive pore-scale model at the cement claystone interface

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Introduction

Background

Reactive transport models (RTM) at the pore scale simulate the solute transport through a porous media coupled with geochemical reactions (using geochemical solvers like PHREEQC or GEMS). However, they are slow. In traditional RTM geochemical solvers may take up to 99% of computational time. Under conditions of fast reaction kinetics, the transport takes place at temporal steady state conditions. The efficiency of RTM can be improved by replacing geochemical solvers with fast surrogate modes (Prasianakis, 2020) and taking advantage of steady state transport conditions. Both methos are applied on a the cement-claystone interface. They are highly reactive due to the strong differences in geochemistry of pore water. Interaction of these materials leads to dissolution of portlandite in cement and precipitation of C-S-H phases in the macropores of the claysone (Nagra, 2022).

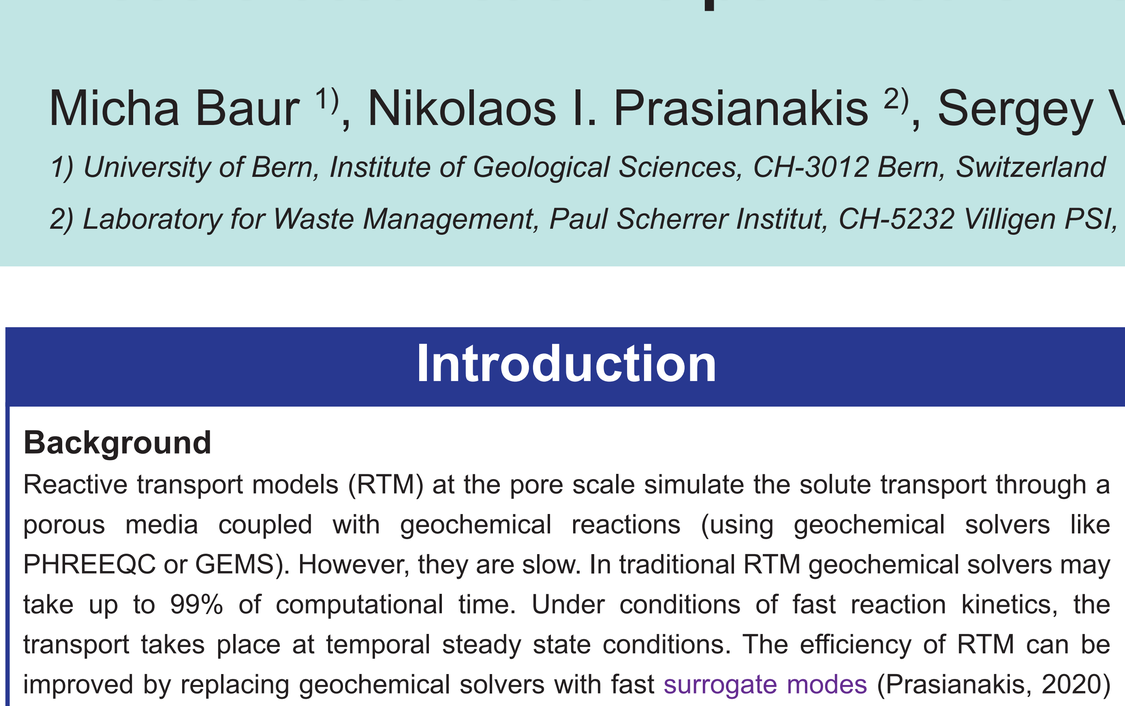


Figure 1: Illustration of a RTM that simulates C-S-H precipitation in a claystone (Top) with a zoom into a pore (down left) and an illustration of an idealized C-S-H structure (down right, from Pinson, 2015)).

C-S-H is the major solid phase of hydrated cement and consists of CaO, SiO and H_2O with a gel porosity

Aims

- Development and training of a neural network based surrogate model for a simplified RTM of the interaction between cement and claystone.
- Development and accuracy testing of an algorithm (adaptive time-stepping) that further accelerates pore scale RTM by taking advantage of steady state transport conditions.

Methodology

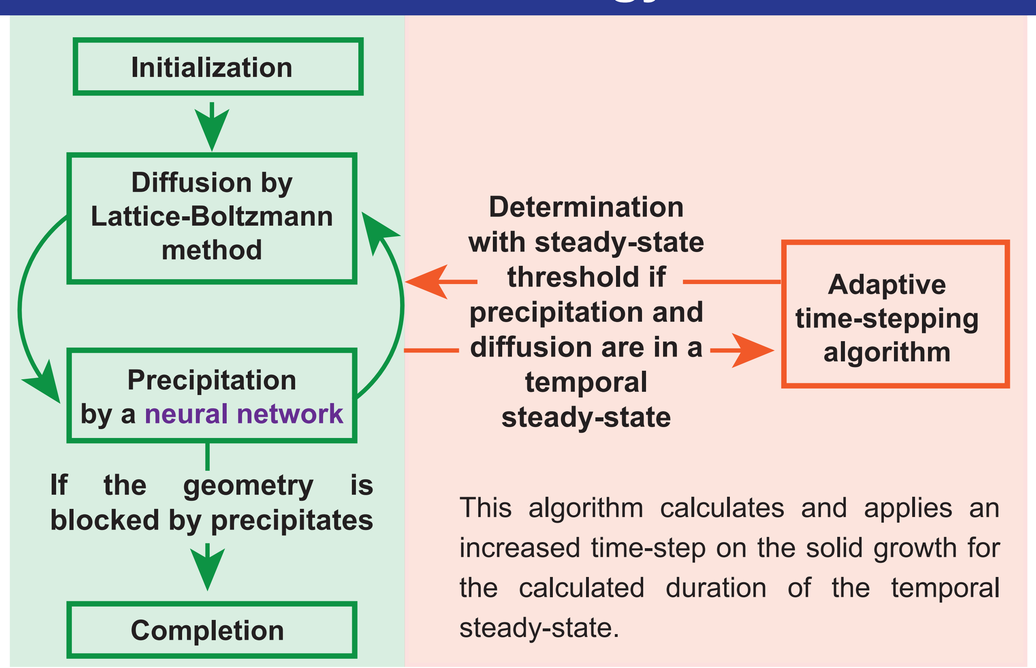


Figure 2: Flow chart of the RTM in green with the adaptive time-stepping as an additional algorithm (orange) when a temporal steady-state is determined.

The precipitation of C-S-H changes the porosity and pore connectivity. Values of the effective diffusivity are computed on snapshots during the simulation. It is a value that compares the diffusivity of solutes in the porous media (D_e) and bulk water (D_0). It is changing due to pore space evolution. The temporal evolution of diffusivity can be used to compare simulations done with different steady-state thresholds on the same geometry.

Results

1 µm x 2 µm geometry

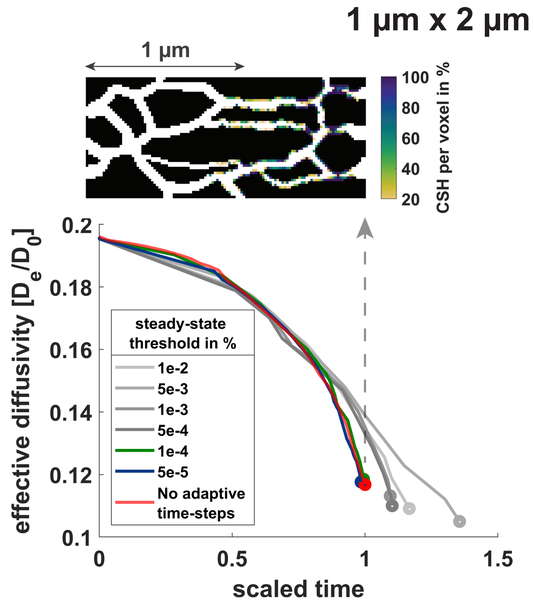


Figure 3: Evolution plots of the effective diffusivity for the 1 µm x 2 µm geometry(down) with different steady-state thresholds and a snapshot of the geometry at completion of the RTM (top).

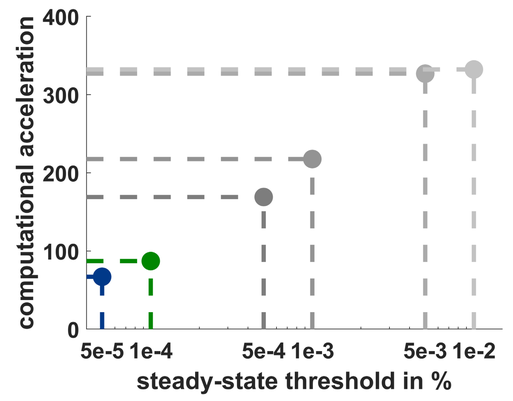
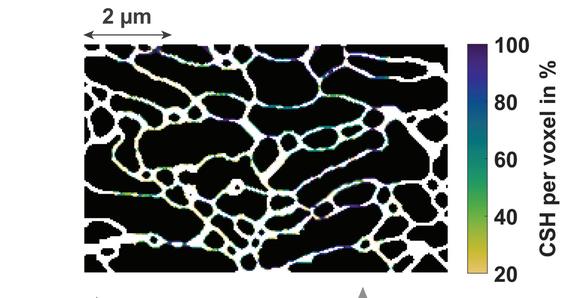


Figure 4: Acceleration by the adaptive time-stepping on the simulations with different steady-state thresholds for the 1 µm x 2 µm

The classical RTM would take 1’500 years to complete this simulation. The RTM with the neural network takes 14 days. The adaptive time-stepping with an additional accelerations of 80 to 330 times finishs it in 1 to 4 hours.

7 µm x 10 µm geometry



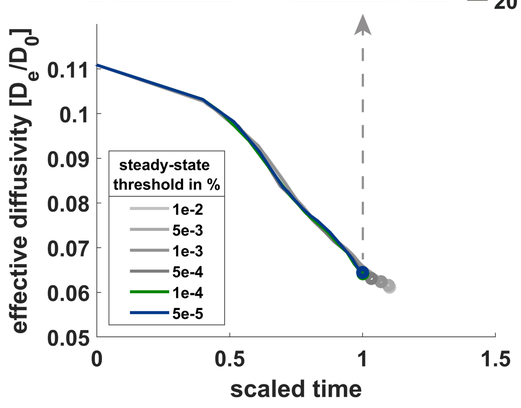


Figure 5: Evolution plots of the effective diffusivity for the 7 µm x 10 µm geometry (down) with different steady-state thresholds and a snapshot of the geometry at completion of the RTM (top).

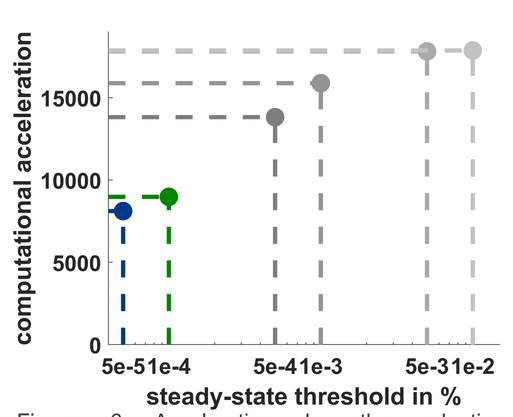


Figure 6: Acceleration by the adaptive time-stepping on the simulations with different steady-state thresholds for the 7 µm x 10 µm geometry.

The classical RTM would take 1’500 years to complete this simulation. The RTM with the neural network would take 15 years. The adaptive time-stepping with an additional acceleration of 8’000 to 19’000 times finishs it in 7 to 16 hours.

Conclusion

The adaptive time-stepping algorithm achieves a high accuracy when the steady-state threshold is set properly. Other parameters that influence the accuracy and acceleration are tested in another stage of this work. The acceleration by this algorithm comes to several magnitudes depending on the RTM model.

References

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