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Coupling of geochemical and multiphase flow processes for validation of the MUFITS reservoir simulator against TOUGHREACT

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Coupled reactive transport simulations, especially in heterogeneous settings considering multiphase flow, are extremely time consuming and suffer from significant numerical issues compared to purely hydrodynamic simulations. This represents a major hurdle in the assessment of geological subsurface utilization, since it constrains the practical application of reactive transport modelling to coarse spatial discretization or oversimplified geological settings. In order to overcome such limitations, De Lucia et al. [1] developed and validated a one-way coupling approach between geochemistry and hydrodynamics, which is particularly well suited for CO_2 storage simulations, while being of general validity.

In the present study, the models used for the validation of the one-way coupling approach introduced by De Lucia et al. (2015), and originally performed with the TOUGHREACT simulator, are transferred to and benchmarked against the multiphase reservoir simulator MUFITS [2]. The geological model is loosely inspired by an existing CO_2 storage site. Its grid comprises 2,950 elements enclosed in a single layer, but reflecting a realistic three-dimensional anticline geometry. For the purpose of this comparison, homogeneous and heterogeneous scenarios in terms of porosity and permeability were investigated. In both cases, the results of the MUFITS simulator are in excellent agreement with those produced with the fully-coupled TOUGHREACT simulator, while profiting from significantly higher computational performance. This study demonstrates how a computationally efficient simulator such as MUFITS can be successfully included in a coupled process simulation framework, and also suggests ameliorations and specific strategies for the coupling of chemical processes with hydrodynamics and heat transport, aiming at tackling geoscientific problems beyond the storage of CO_2.

References

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