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Verification of TRANsport Simulation Environment coupling with PHREEQC for reactive transport modelling

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Many types of geological subsurface utilisation are associated with fluid and heat flow as well as simultaneously occurring chemical reactions. For that reason, reactive transport models are required to understand and reproduce the governing processes. In this regard, reactive transport codes must be highly flexible to cover a wide range of applications, while being applicable by users without extensive programming skills at the same time. In this context, the TRANsport Simulation Environment (Kempka, 2020) was coupled with the geochemical reaction module PHREEQC (Parkhurst & Appelo, 2013), providing multiple features that make it applicable to complex reactive transport problems in various fields. Code readability is ensured by the applied high-level programming language Python which is relatively easy to learn compared to low-level programming languages. In the present study, common geochemical benchmarks are used to verify the numerical code implementation.

Currently, the coupled simulator can be used to investigate 3D single-phase fluid and heat flow as well as multicomponent solute transport in porous media. In addition to that, a wide range of equilibrium and nonequilibrium reactions can be considered. Chemical feedback on fluid flow is provided by adapting porosity and permeability of the porous media as well as fluid properties. Thereby, users are in full control of the underlying functions and equations of state. Both, the solution of the system of the partial differential equations and PHREEQC module, can be easily parallelised to increase computational efficiency.

The benchmarks used in the present study include density-driven flow as well as advective and diffusive reactive transport of solutes. Furthermore, porosity, permeability and diffusivity changes caused by kinetically controlled dissolution-precipitation reactions are considered to verify the main features of our reactive transport code. In future, the code implementation may be used to quantify processes encountered in different types of subsurface utilisation, such as geothermal energy production, geological energy, CO_2 and nuclear waste storage.

References:

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