Supplementary Material – Overview of some coupled reactive transport codes

1 Core^{2D} V5

CORE^{2D} V5 (Fernández, 2017) is a code for transient saturated and unsaturated water flow, heat transport and multicomponent reactive solute transport under both local chemical equilibrium and kinetic conditions in heterogeneous and anisotropic media. The flow and transport equations are solved with Galerkin finite elements and an Euler scheme for time discretization. The solute transport equation accounts for advection, molecular diffusion and mechanical dispersion. The chemical formulation is based on the ion association theory and uses an extended version of the Debye-Hückel equation (B-dot) for the activity coefficients of aqueous species. The following chemical reactions are considered: aqueous complexation, acid-base, redox, mineral dissolution/precipitation, cation exchange, surface complexation and gas dissolution/exsolution. CORE^{2D} V5 relies on the "com" thermodynamic database of EQ3/6 (Wollery, 1992). The code also allows the use of other thermodynamic databases. CORE^{2D} V5 is based on the sequential iteration approach to solve for chemical reactive solute transport. Iterations are repeated until some prescribed convergence criteria are attained (Samper et al., 2009). The concentrations of secondary species are computed from the concentrations of primary species through appropriate mass action laws (Xu et al., 1999). The concentrations of precipitated, exchanged and adsorbed species are computed using similar equations. The Gaines-Thomas convention is used for cation exchange. Surface complexation is modelled by using three types of protonation/deprotonation sites, S^{S}-OH, S^{W1}-OH and S^{W2}-OH, as proposed by (Bradbury and Baeyens, 1997). A detailed description of calculations of chemical reactions can be found in (Xu et al., 1999). CORE^{2D} V5 takes into account the changes in porosity due to mineral dissolution/precipitation reactions and their feedback effect on the flow and transport parameters under isothermal and nonisothermal conditions (Águila et al., 2020, Fernández, 2017).

The code has been extensively verified against analytical solutions and other reactive transport codes. In addition, the code has been widely used to model laboratory and in situ experiments (Dai et al., 2008, Samper et al., 2008b, Samper et al., 2008c, Yang et al., 2008, Zhang et al., 2008), the interactions of corrosion products and bentonite (Lu et al., 2011, Samper et al., 2008a), to evaluate the long-term geochemical evolution of repositories in granite and clay (Mon et al., 2017, Samper et al., 2016, Yang et al., 2008), and model the impact of CO_2(g) leakage on groundwater quality (Yang et al., 2015, Yang et al., 2013).

Fernández (2017) updated and improved the THCM conceptual and numerical models and the flow and reactive transport codes of the CORE series. These activities included: (1) Improvements in the code CORE^{2D}V5 dealing with porosity changes due to mineral dissolution/precipitation and the feedback effect on flow, transport and chemical parameters; (2) Update of CORE^{2D}V5 to use available public-domain post-processing tools; (3) Improve the convergence criteria to solve flow in variably saturated porous media in CORE^{2D}V5; and (4) Update of INVERSE-CORE2D to estimate large sets of variables. Particularly noteworthy were the improvements implemented by Fernández (2017) in CORE^{2D}V5 dealing with porosity changes and its verification. The reactive transport code was extended to take into account the porosity changes due to mineral dissolution/precipitation and their feedback effect on transport properties. The changes of the porosity in a porous medium due to mineral alteration processes, and the associated change of transport parameters are important processes which influence the evolution of the engineered barrier systems. If porosity increases substantially, preferential fluid migration pathways may be developed, accelerating solute transport. On the other hand, a significant porosity decrease may inhibit fluid and solute transport. Clogging occurs when the porosity is close to zero and the aqueous phase may completely vanish.

2 Crunchflow

CrunchFlow[1] is a multidimensional reactive transport code in porous media developed by C. Steefel and coworkers at LBL (Steefel et al., 2015a). It allows for the simulation of advective, dispersive, and diffusive transport in 1D and 2D with a global implicit method and up to 3D using the "operator splitting" mode. Of particular interest in the project, diffusive transport and reactions can be treated in non-isothermal conditions including exchanges at equilibrium between the gas and aqueous phases (simulations with partially saturated flow requires a separate software).

The chemical processes taken into account in Crunchflow include:

- multicomponent aqueous complexation and redox reactions,
- ion exchange on multiple sites,
- surface complexation on multiple sites with or without electrostatic correction based on the double layer model (site densities may be linked to mineral amounts),
- kinetically controlled precipitation and dissolution of minerals based on the Transition State Theory, and microbially mediated reactions based on the Monod type formulation,
- kinetic isotope fractionation associated with mineral reactions.

For the diffusive transport, the user can also provide different diffusion coefficients for each aqueous species. The diffusive flux is then calculated accounting for the electrochemical migration of the ions and corrected for electroneutrality using the Nernst-Planck equation. Feedback induced by reactions on porosity, permeability, and diffusion can also be treated. Porosity is updated using the volume balance of dissolved and precipitated minerals. Diffusion coefficients can be updated using Archie's law with a user defined formation factor or cementation coefficient.

Crunchflow has been extensively used in a variety of contexts (Steefel et al., 2015b) and, in particular, in studies concerning the physicochemical evolution of disposal cells in deep geological repositories (e.g. Bildstein et al. (2016), Bildstein et al. (2006), Marty et al. (2015), Wersin and Birgersson (2014), Wersin et al. (2008). Two specific features of the code are useful for simulating the chemical evolution at interfaces between materials and at the disposal cell scale. The first one is the capability of the code to treat the alteration of glass with a specific kinetic model, where the dissolution rate is controlled by the diffusion of water and ions in a passivating layer (the GRAAL model, Frugier et al. (2018)). The second one is the coupling of the code with the electrochemical corrosion model Calipso (Bataillon et al., 2010).

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[1] https://bitbucket.org/crunchflow/crunchtope-dev/wiki/Home

3 HPx

HPx (Jacques et al., 2018, Jacques et al., 2008a, Jacques et al., 2008b, Jacques et al., 2006)) couples the flow and transport codes HYDRUS-1D[2] and HYDRUS(2D/3D)[3] (Šimůnek et al., 2024, Šimůnek et al., 2016) with PHREEQC (Parkhurst and Appelo, 2013) using a sequential non-iterative coupling approach as described in Jacques et al. (2006). The HYDRUS-codes act as the transport solver solving equations for variable-saturated water flow, advective-dispersive transport of solutes, diffusive transport in the gas phase and heat transport. The current version includes the latest PHREEQC version (version 3.6.2, see paragraph 8). The coupling between HYDRUS and PHREEQC is done using hard-coupling and HPx is fully integrated in the graphical user interfaces of HYDRUS (see https://www.pc-progress.com/en/default.aspx). Geochemical calculations are calculated in parallel using the OpenMP (www.openmp.org) shared memory approach.

Using the flow and transport capabilities of HYDRUS, flow and transport can be simulated for both large scale (different materials) and small scale heterogeneity (spatial-variable hydraulic parameters, mobile-immobile transport models, dual porosity models) (Šimůnek and van Genuchten, 2008). From a geochemical point of view, virtually all geochemical models from PHREEQC can be used within HPx. The possibility to have scripts in the input file (similar to PHREEQC) increases the flexibility of the code to handle kinetic rate equations. This functionality is enhanced in HPx by introducing a more flexible variant of BASIC scripting (https://github.com/paladin-t/my_basic) or more recently including python (version 3.7) as a scripting language. Scripts within an input file can be defined with different functionalities for preprocessing and initialization, specific calculations during the transport simulation or post-processing.

HPx allows for dynamically altering flow and transport properties during the transport simulations. The functional form of e.g. the relation between permeability and porosity is not hard-coded but the user supplies the relations between the geochemical state variables and the transport properties. To model the spatial-temporal evolution of flow parameters, the concept of linear scaling of hydraulic properties (Vogel et al., 1991) is used. The user thus defines the values of the scaling factors for the porosity, pressure head or hydraulic conductivity for each node at each time step using any model ranging from e.g. the Kozeny-Carman relation to models given in e.g. (Wissmeier and Barry, 2009) or Freedman et al. (2004). A similar flexibility exists for tortuosity in the aqueous or gaseous phase, dispersivity and parameters related to the heat transport equations.

4 HYTEC

The reactive transport code HYTEC (van der Lee et al., 2003) accounts for many commonly encountered chemical processes, including interface reactions (surface complexation with electrostatic correction and cation exchange), precipitation and dissolution of solid phases (minerals and colloids), organic complexation, and redox and microbial reactions. All reactions can be modelled using a full equilibrium or a mixed equilibrium–kinetic approach. Thermodynamic data are taken from international databases, such as Thermoddem and ThermoChimie.

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[2] https://www.pc-progress.com/en/Default.aspx?h1d-hp1

[3] https://www.pc-progress.com/en/Default.aspx?h3d2-hp2

The hydrodynamic module of HYTEC is adapted for hydrodynamic conditions commonly encountered in the laboratory or in the field. The code allows for dual porosity, saturated, unsaturated or two-phase flow, variable boundary conditions, sinks, and sources. HYTEC searches for an accurate solution to the multicomponent transport problem using an iterative, sequential, so-called strong coupling scheme. Strong coupling permits variable hydrodynamic parameters as a function of the local chemistry. For example, the porosity of a porous medium decreases after massive precipitation of newly formed mineral phases, which modifies the water flow paths and transport parameters, e.g., diffusion coefficients.

HYTEC solves this interdependency accurately, which makes the tool particularly useful for, e.g., cement alteration at long timescales. Heat-transfer by conduction and convection can also be modelled, with chemical and flow/transport parameters that are temperature-dependent. HYTEC has been widely used for the long-term safety assessment of nuclear waste disposal, from the waste form and engineered barrier to the host-rock (De Windt and Spycher, 2019).

5 INVERSE-FADES-CORE-V2

INVERSE-FADES-CORE V2 (Mon, 2017) is a finite element code for modelling non-isothermal multiphase flow, heat transport and multicomponent reactive solute transport under both chemical equilibrium and kinetic conditions in deformable media. The code takes into account the mass balance of water, air, solid and enthalpy, the transport of solids and the mechanical equilibrium. The solute transport equation accounts for advection, molecular diffusion and mechanical dispersion.

INVERSE-FADES-CORE V2 solves both forward and inverse multiphase flow and multicomponent reactive transport problems in 1-, 2- and 3-D axisymmetric porous and fractured media. The code is the result of integrating the capabilities of the THM code FADES (Navarro, 1997); the reactive transport code CORE^{2D} (Samper et al., 2011), the THMC code FADES-CORE (Enresa, 2000) and the inverse methodology of INVERSE-CORE (Dai and Samper, 2004). The state variables of the forward model include the liquid and the gas pressures and temperature, which are solved with a Newton-Raphson method. Similar to CORE^{2D} V5, the concentrations of secondary species are computed from the concentrations of primary species. The Gaines-Thomas convention is used for cation exchange. Surface complexation is modelled by using three types of protonation/deprotonation sites, S^{S}-OH, S^{W1}-OH and S^{W2}-OH. INVERSE-FADES-CORE V2 uses also a sequential iteration approach.

The equilibrium constants for aqueous complexes and minerals change with temperature under non-isothermal conditions. They are calculated with an analytical expression, which is valid for temperatures ranging from 0 to 300 ºC. The “com” thermodynamic database of EQ3/6 (Wollery, 1992) is used for aqueous complexes and minerals. INVERSE-FADES-CORE V2 also allows the use of other thermodynamic databases.

The inverse problem is solved by minimizing a generalized least-squares criterion with a Gauss-Newton-Levenberg-Marquardt method (Dai and Samper, 2004). The forward routines of INVERSE-FADES-CORE have been widely verified with analytical solutions and other reactive transport codes. The main applications of INVERSE-FADES-CORE include: the THC and THCM models of the FEBEX in situ test (Samper et al., 2018, Zheng et al., 2011, Samper et al., 2008a, Zhang et al., 2008); the THCM model of the FEBEX mock up test (Zheng and Samper, 2008); the THCM model of a heating and hydration lab experiment performed on compacted FEBEX bentonite (Samper et al., 2018, Zheng et al., 2010); and the THC model of the Ventilation Experiment on the Opalinus Clay (Zheng et al., 2008).

Mon (2017) implemented the reactive gas transport in the reactive transport code INVERSE-FADES-CORE V2 by including additional mass balance equations for the reactive gaseous species in the gaseous phase. The mass balance equation for a given gas accounts for: a) Advection; b) Molecular diffusion; c) Mechanical dispersion; and d) Exchange with the liquid phase. The implementation of the reactive gas transport was verified by comparing the numerical results of INVERSE-FADES-CORE V2 with the results computed with TOUGHREACT (Xu et al., 2006) with four test cases. In addition, INVERSE-FADES-CORE V2 was benchmarked with other codes for the following two benchmarking problems: 1) Modeling the chemical interactions of the concrete liner with the compacted bentonite of the engineered barrier and the host clay rock; and 2) Modelling the carbonation of concrete in unsaturated conditions during the operational period of a repository.

6 OPENGEOSYS

OpenGeoSys[4] (OGS) is a scientific open-source initiative for the numerical simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media. The basic concept of OGS consists of providing a flexible numerical framework, using primarily the Finite Element Method (FEM) for solving multi-field coupled processes with application in different scientific and technical disciplines. For example, OGS has been successfully applied in the fields of regional, contaminant and coastal hydrology (Nixdorf et al., 2017, Walther et al., 2017, Jing et al., 2019, Jing et al., 2018), fundamental and geothermal energy systems (Chen et al., 2019, Parisio et al., 2019b, Parisio et al., 2019a, Meng et al., 2018, Hein et al., 2016), geotechnical engineering (Zhu et al., 2020), energy storage (Lehmann et al., 2019, Miao et al., 2019, Nagel et al., 2017, Böttcher et al., 2017, Pfeiffer et al., 2016), CO_2 sequestration/storage (Li et al., 2014, Beyer et al., 2012); and nuclear waste management and disposal (Shao et al., 2019a, Shao et al., 2019b).

Since the mid-eighties (kolditz, 1990, Wollrath, 1990, Kroehn, 1991, Helmig, 1993) OpenGeoSys is in continuous development evolving through Fortran, C, and C++ implementation with the current released version being OpenGeoSys 6.5.1 (Bilke et al., 2024). OpenGeoSys-6 (Bilke et al., 2019, Naumov et al., 2018) is a complete re-implementation of OpenGeoSys 5 (Kolditz et al., 2012b, Wang and Kolditz, 2007, Kolditz and Bauer, 2004) which uses advanced methods in software engineering and architecture with focus on code quality, modularity, performance and comprehensive documentation. Till the present moment, particular emphasis has been placed on the implementation of advanced numerical methods for simulating propagation of discontinuities, such as enriched finite element function spaces (Watanabe et al., 2012), non-local formulations (Parisio et al., 2018) and phase-field models (Yoshioka et al., 2019). As in the previous version, OGS-6 is taking advantage of High Performance Computing (HPC) platforms on both MPI and OpenMP concepts to analyze realistic complex geosystems (Fischer et al., 2019, Wang et al., 2017, Wang et al., 2015).

Regarding reactive transport processes, different approximations have been implemented in OGS along its development in order to consider multicomponent mass transport and bio/geochemical reactions (Chen et al., 2020, Boog et al., 2020, Boog et al., 2019). For example, Ballarini et al. (2014) used an internal OGS library to simulate kinetically controlled

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[4] https://www.opengeosys.org/

biogeochemical reactions. In other cases, OGS has been coupled in a sequential non-iterative approach with well-known external geochemical solvers (i.e. PHREEQC, GEMS, BRNS and ChemApp). The coupling of these codes are referred as OGS-PHREEQC (He et al., 2015, Xie et al., 2006), OGS-GEM (Kosakowski and Watanabe, 2014), OGS-BRNS (Centler et al., 2010) and OGS-ChemApp (Li et al., 2014, Beyer et al., 2012). Very recently, an alternative coupling solution of reactive transport has been developed and implemented by approximating the complex chemical reactions into a quickly calculating look-up table (Águila et al., 2021, Huang et al., 2018). The novel implementation provides fast and efficient simulations, a feature especially relevant for long-term simulations. Reactive transport calculations referred above have been mainly performed with OGS-5, although OGS-6-iPHREEQC version is already released (Bilke et al., 2024). This new version includes a new implementation with direct memory access which allows efficient computational simulations. Application of OGS on reactive transport modelling in the framework of nuclear waste disposal includes long term cementitious materials/clay interactions (Idiart et al., 2020, Kosakowski et al., 2014, Kosakowski and Berner, 2013, Berner et al., 2013, Shao et al., 2013), laboratory scale precipitation/dissolution processes in combination with density driven flow and clogging effects (Maes et al., 2021, Poonoosamy et al., 2021, Poonoosamy et al., 2020, Poonoosamy et al., 2015) and with mechanical processes (Lu et al., 2018), concrete degradation due to reactive aggregates in combination with multi-phase transport of CO_2 (Huang et al., 2018) and radionuclide migration in clays (Águila et al., 2021). Recently, the look up table approach has also been applied to model gas and humidity transport in combination with concrete/ organic matter degradation and corrosion of metals in a waste package during 100 years of intermediate storage (Huang et al., 2018).

Finally, OpenGeoSys is participating in several international model development, validation and benchmarking initiatives, e.g., DEVOVALEX (with applications mainly in the assessment of nuclear waste repositories (Birkholzer et al., 2018), CO2BENCH (Kolditz et al., 2012a), SeS Bench (Steefel et al., 2015b) and HM-Intercomp (Maxwell et al., 2014), providing ongoing series of benchmark books (Lehmann et al., 2018) and tutorials (Jang et al., 2018). For more information please refer to the OpenGeoSys webpage (www.opengeosys.org).

7 PFLOTRAN

PFLOTRAN[5] (Hammond et al., 2014) is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent and multiscale reactive flow and transport in porous materials. The code is designed to run on massively parallel computing architectures as well as workstations and laptops. Parallelization is achieved through domain decomposition using the PETSc (Portable Extensible Toolkit for Scientific Computation) libraries. PFLOTRAN has been developed from the ground up for parallel scalability and has been run on up to 2^{18} processor cores with problem sizes up to 2 billion degrees of freedom. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with experienced domain scientists, without which PFLOTRAN's sophisticated process models would not exist. The reactive transport equations can be solved using either a fully implicit Newton-Raphson algorithm or the less robust operator splitting method.

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[5] https://www.pflotran.org/

8 PHREEQC-3

PHREEQC-3[6] (Parkhurst and Appelo, 2013) is able to perform aqueous geochemical calculations including all typical processes relevant for subsurface reactive transport. It includes several options for (i) aqueous activity correction calculations (Davies, Debye-Hückel association models, Pitzer and specific-ion interaction theory), (ii) exchange models, (iii) surface complexation (diffuse double layer model, constant capacitance model, CD-MUSIC model), and (iv) solid solutions (ideal, binary non-ideal model). The code allows for calculating temperature and pressure dependence of equilibrium constants (Appelo et al., 2014). PHREEQC-3 handles full equilibrium or mixed kinetic-equilibrium reaction networks with kinetic homogeneous and heterogeneous rate equations of arbitrary rate equations defined via the embedded BASIC interpreter.

The native transport possibility of PHREEQC-3 allows for one dimensional advection-dispersive transport, multi-dimensional diffusion calculation (Appelo and Wersin, 2007, Weetjens et al., 2009) or diffusion according the Nerst-Planck equation (Appelo, 2017, Appelo and Wersin, 2007). However, PHREEQC-3 is frequently used as the geochemical solver coupled to flow and transport solvers either directly via the source code (e.g. HPx, Jacques et al. (2018)), or via the modules IPhreeqc (Charlton and Parkhurst, 2011) and PhreeqcRM (Parkhurst and Wissmeier, 2015). Examples of the latter are coupling with OPENGEOSYS (He et al., 2015) or with COMSOL (Nardi et al., 2014, Perko et al., 2015, Wissmeier and Barry, 2011).

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[6] https://www.usgs.gov/software/phreeqc-version-3

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