The MOOSE geochemistry module

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Summary

Geochemical models are used to understand the chemistry of natural waters and other aqueous solutions and their interaction with minerals in many areas of practical interest, for example, geothermal wells and reservoirs, contaminant flow through aquifers, ore creation and mining techniques, petroleum and gas exploitation, and rock diagenesis. The models are frequently extremely complicated, with thousands of interacting chemical species, and often require computer software to find the chemical concentrations.

Reactive transport simulations involve predicting the flow of chemical-species and temperature in a spatial domain (such as an aquifer) in addition to solving a chemical model at each point, at each time, in the domain. Such models are used to explore spatio-temporal dependence of concentration, precipitation, dissolution, sorption, etc, and often require significant computational resources. Deformation of the subsurface in response to the chemistry and flows can be considered as well, greatly increasing the complexity of the models.

The MOOSE geochemistry module enables users to solve such models.

Statement of need

Numerical modeling is essential to solve increasingly complicated problems, where the interplay between different physics, perhaps acting at different scales, is important. For instance, understanding the impact of subsurface CO_2 injection (in carbon sequestration projects) can involve assessing the water-chemistry and rock-mineral changes resulting from temperature changes and the presence of CO_2, how these changes impact the porosity and permeability of the subsurface, and how the subsurface deforms and possibly fractures due to the injection. Another example is understanding ore deposition, which commonly involves assessing how fluid and heat flows interact with geochemistry and tectonic features (e.g. faults) within the Earth's crust. Similar remarks hold for hydraulic fracturing, aquifer thermal energy storage, in-situ leaching, and fossil fuel extraction using enhanced recovery techniques.

In the past, researchers have typically answered such questions using separate models for subsets of the physical processes, or loosely-coupled models solved using multiple software packages. The MOOSE geochemistry module introduced here allows researchers to perform stand-alone geochemical modelling, but also to draw upon the power of other MOOSE modules to solve complicated coupled transport, geomechanical and geochemical models using a single code.

Existing software

A number of commercial and free (open or closed source) packages can solve reactive-transport models. Some of these are: CrunchFlow (Beisman et al., 2015); EQ3/6 (Wolery, 1992); the Geochemist's Workbench (Bethke, 2007); MIN3P (Maher & Mayer, 2019; Su et al., 2020); OpenGeoSys (Bilke et al., 2019; Kolditz et al., 2012); PHREEQC (Pankhurst, 1995; Pankhurst & Appelo, 1999); PHAST (Pankhurst et al., 2010); HP2 (Šimůnek et al., 2012); Reaktoro (Leal, 2020); and TOUGHREACT (T. Xu et al., 2004). Many of these have been developed over decades by teams of researchers, and have sophisticated reaction-modelling capabilities, along with well-established GUIs to assist in model creation and the analysis of results. Many of them have been used in hundreds of studies by thousands of researchers.

Overview and comparisons with other software

The geochemistry module is built upon, and provided as part of, the open-source, massively parallel, fully implicit multiphysics simulation framework MOOSE (Multiphysics Object-Oriented Simulation Environment) (Permann et al., 2020). MOOSE is an open-source library from Idaho National Laboratory that provides a high-level interface to the libMesh finite element library (Kirk et al., 2006) and PETSc nonlinear solvers (Balay et al., 1997, 2019, 2020). MOOSE and the geochemistry module follow strict quality controls. The geochemistry module's test suite contains over 350 tests, ranging from simple unit tests to fully-fledged benchmarks against other codes.

As outlined in this article, the MOOSE geochemistry module can solve models involving aqueous geochemistry, including aqueous equilibrium, kinetics, oxidation-reduction, sorption and surface complexation, dissolution-precipitation and gas buffering. One aspect that makes the geochemistry module different to the codes mentioned above is the ease of coupling additional physics to the geochemical functionality. In particular, when used in conjuction with the MOOSE PorousFlow module (Wilkins, Green, et al., 2020), sophisticated reactive-transport simulations may be performed, including multi-phase and unsaturated fluid flows, high-precision equations of state for fluids, dynamic porosity and permeability distributions, and sophisticated numerical stabilization. Geomechanics may also be incorporated by using MOOSE's TensorMechanics module, to explore the interplay between geomechanical stresses and strains, and fluids, heat and reactions. Fracturing of the skeleton material may also be included using MOOSE's XFEM module (Jiang et al., 2020; Zhang et al., 2018). An additional advantage of MOOSE is that its beautifully-designed APIs allow for easy modification of existing physics, or the addition of new physics.

Harnessing the power of MOOSE means that geochemistry simulations efficiently use multi-processors and automatically utilize threading/OpenMP, without developers or users having to worry about the software technicalities (MOOSE scales well to over 100,000 cores). From the user's perspective, a variety of integration schemes and unstructured meshes may be used. Various time-stepping schemes may be employed. A variety of I/O formats are available, such as Exodus and VTK files as well as CSV plaintext. Users may utilize the "MultiApp" system that allows simulations to be embedded inside other simulations, which enables intuitive coupling of different physics at different spatio-temporal scales. A generic GUI helps users create, run and analyse models.

Having said this, the aforementioned codes offer advantages too. Some offer specialist features not available in the geochemistry module, while some of them include preprocessing and postprocessing capabilities that are far superior to the generic GUI offered by MOOSE. Being focussed on reactive-transport alone, their learning curve is much easier.

The geochemistry module's functionality is a subset of that described in the authoratative, pedagogical textbook by Bethke (2007). It is not possible to describe all geochemical-modelling

85   concepts in this short article, so the reader is referred to Bethke (2007) for further information.

86   For convenience, the source code for the geochemistry module is bundled within the MOOSE
87   framework. Detailed documentation of the module, it's capability, and an extensive suite of
88   examples can be found at https://mooseframework.org/modules/geochemistry/index.html.

Reaction functionality

90   This section describes the types of geochemical reactions that the geochemistry module can
91   solve. Both equilibrium and kinetic reactions may be used in models solved by the geochemistry
92   module.

Database

94   The geochemical database defines the possible scope of geochemical models and includes
95   information about all components and reactions. The geochemistry module uses a database
96   in a specific JSON format. The default database used in all geochemistry module examples and
97   tests is a JSON version of the freely available January 2019 LLNL thermodynamic database.
98   For convenience, a python script is provided to convert the popular Geochemist's Workbench
99   and EQ3/6 (Wolery, 1992) database formats to the required JSON format.

Types of species and reactions

101   The user may select from the database a subset of chemical components and reactions that
102   are relevant for their particular model. These are:

103   - aqueous species in equilibrium;
104   - minerals in equilibrium with the aqueous solution that may precipitate or dissolve (a
105   subset of all possible minerals may be chosen, and a user-supplied list of minerals may
106   be prevented from precipitating);
107   - dissolved gases and gases in equilibrium with an external buffer such as the atmosphere
108   (a subset of all possible gases may be used);
109   - species in alternative oxidation states (redox couples), and the user may set individual
110   couples to be in equilibrium or disequilibrium with the aqueous solution;
111   - sorbed species in equilibrium with the aqueous solution, which are governed by a Lang-
112   muir approach or a surface-complexation approach that accounts for the electrical state
113   of the porous-skeleton surface and how it varies with pH, ionic strength and solution
114   composition;
115   - minerals, redox species and sorbed species whose dynamics are governed by kinetic rates.
116   Rates are sums of terms that may be dependent on the mass of kinetic species, a specific
117   surface area, molality or activity of any promoting species, a temperature-dependent
118   Arrhenius term, and the activity-product and equilibrium constant of the kinetic species.
119   The approach allows acid-neutral-alkali promotion as listed in the correlations prepared
120   by Palandri & Kharaka (2004) to be used in geochemistry models, as well as many other
121   types of rates.

Activity and fugacity models

123   Only the Debye-Huckel B-dot model along with the related formulae for neutral species and
124   water are coded into the geochemistry module. The virial Pitzer/HMW models are not
125   included. The activity of all mineral species is assumed to be unity. The Spycher-Reed

(Spycher & Reed, 1988) fugacity formula (Prausnitz et al., 1998; Tianfu Xu et al., 2014) is used in the geochemistry module.

Constraints

A constraint must be supplied by the user for each member of the equilibrium basis in order that the geochemical system has a unique mathematical solution. The following types of constraints are possible in the geochemistry module:

- For water: the mass of solvent water, or the total bulk mole number, or the activity;
- For aqueous basis species: the free molality, the total bulk number, or the activity (so that pH may be controlled, for instance);
- For precipitated minerals: the free (precipitated) mole number, or the total bulk mole number;
- For gases with fixed fugacity: fugacity
- For sorbing sites: the free molality of unoccupied sites, or the total bulk mole number.

In addition, all kinetic species must be provided with an initial mole number.

Reaction paths

The following reaction paths are available in the geochemistry module:

- Adding reactants at user-defined rates. These reactants may be basis species, secondary species, minerals, etc.
- Controlling temperature with a user-defined function.
- Changing temperature and altering the composition by adding cooler/hotter reactants at user-defined rates.
- Removing activity constraints on one or more species, or removing gas fugacity constraints, at user-supplied times.
- Controlling the activity of species (such as the pH) or gas fugacity with user-supplied functions.
- Discarding masses of any minerals present in the equilibrium solution (called a "dump" by Bethke (2007)).
- Removing mineral masses at the end of each time-step (called "flow-through" by Bethke (2007))
- Adding pure H_2O and removing an equal mass of water components and solutes it contains (called "flush" by Bethke (2007)).

Combinations of these may be used. For instance, changing temperature while controlling the activity of species.

Mathematical solution strategy

At each time-step, the geochemistry module calculates: the mass of solvent water; the molality of all aqueous species and dissolved gases; the mineral activity products and saturation indices; the mole number of precipitated minerals; the molality of unoccupied surface sites; the surface potentials; the molality of sorbed species; the mole number of kinetic species; and all activities and activity coefficients. To achieve this, a fully-implicit, under-relaxed, iterative Newton-Raphson procedure is used.

During this procedure, care is taken to avoid numerical overflows or underflows. Multiple sub-steps may be performed in each time-step to ensure good convergence. Minerals are allowed to precipitate or dissolve during the procedure. Charge neutrality is enforced.

Features not yet implemented

The geochemistry module's functionality allows it to handle most common modelling tasks, but a number of features have not yet been implemented. These include the virial Pitzer/HMW activity models; certain kinetic rate forms used in biogeochemical modelling such as Michaelis–Menten and monod; the K_d and Freundlich approaches to sorption; and isotopic fractionation. The geochemistry module does not include a dedicated GUI to help with model creation and analysis.

Reactive transport

One of the notable features of the MOOSE framework is the ability to couple different physics together. Different types of couplings are available: tight (full) coupling; operator-splitting; etc. To perform reactive-transport simulations using the geochemistry module, we recommend employing MOOSE's PorousFlow module (Wilkins, Green, et al., 2020) in an operator-splitting approach, which means that each time-step involves a two-step process:

1. The PorousFlow module transports the solutes in the aqueous phase, as well as the temperature distribution. This provides the temperature and extra chemical source terms (to be added to the geochemical equations) at each point in the spatial domain.
2. With these sources, the geochemistry module solves for the mole numbers of each species at each point in the spatial domain, using the Newton-Raphson method mentioned in the previous section.

It is easy to use multiple sub-steps within (1) and/or (2), which may be necessary if the time-scales of the transport and chemical reactions are very different. The operator-split approach is also used by other reactive-transport solvers, such as the Geochemist's Workbench. The PorousFlow module is a sophisticated multi-component, multi-phase transport code, and employing it means:

- pressure and temperature are tightly coupled with fluid flows
- densities, viscosities, etc, may depend on solute concentrations, temperature and pressure
- porosity and permeability can change with precipitation and dissolution
- multiphase flows can be used
- coupling with sophisticated geomechanics (including plasticity (Adhikary et al., 2016; Wilkins, Spencer, et al., 2020), fracture and large strains) is straightforward
- sophisticated numerical stabilization is available.

Nevertheless, rudimentary transport capability has been included in the geochemistry module, which models advective-diffusive transport of the mobile concentrations, with hydrodynamic dispersion. It is assumed that precipitated minerals, sorbed species and sorption sites are immobile. The temperature, porosity, Darcy flux vector and dispersion tensor are fixed by the user. All of these may vary spatially and temporally, but the geochemistry module provides them with no dynamics (in contrast with the PorousFlow module, where temperature evolution is governed by an advection-diffusion equation, for instance). An operator-splitting method may be used to provide the mathematical solution, as described above.

Computational aspects

Spatially-varying geochemistry simulations use a large amount of memory since they store information about a complete geochemical system at each finite-element node. On the other

212 hand, ignoring transport, they are almost embarrassingly parallel, and can be solved efficiently
213 using a large number of processors. Even reactive-transport models scale well with multiple
214 processors, since multi-component flow in porous media is essentially multiple coupled diffusion
215 equations. Figure 1 shows an example of scaling in which a model of fixed size is run on
216 multiple processors. Further experiments involving memory usage, solver choices and cpu-
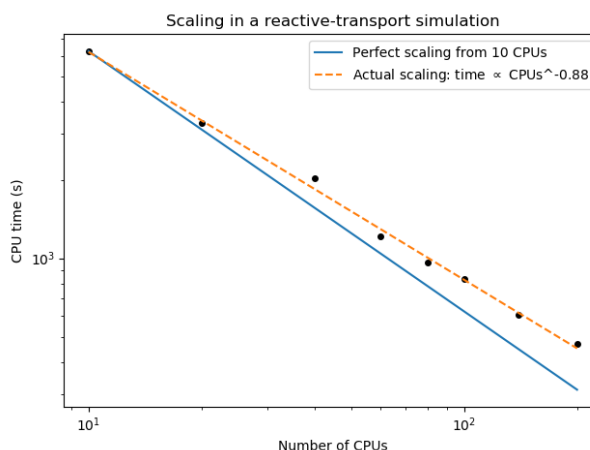217 scaling can be found in the online documentation.

Figure 1: CPU time required to solve a reactive-transport simulation using the PorousFlow and geochemistry modules.

Example: cooling with feldspars

219 One of the geochemistry tests and examples involves slowly cooling an aqueous solution
220 from 300°C to 25°C. The aqueous solution is in equilibrium contact with albite, maximum
221 microcline, muscovite and quartz. This example is documented in Section 14.1 of Bethke
222 (2007). Figure 2 shows the comparison of the results from MOOSE's geochemistry module
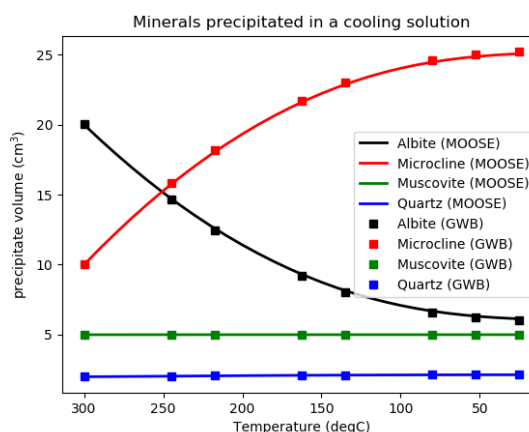223 and the Geochemist's Workbench.

Figure 2: Precipitated volumes as a function of temperature when an aqueous solution in contact with feldspars is cooled.

Example: reactive transport in an aquifer thermal energy storage scenario

The Weber-Tensleep Formation in the USA has been proposed to store renewably-generated, high-temperature water, for later use in electricity generation (McLing et al., 2019; Wendt et al., 2019). During the storage phase, formation water from the reservoir is produced, heated to 160°C under pressure, and re-injected. The cycle is reversed during electricity generation. A 3D reactive transport study assessing potential precipitates in the engineering equipment, and mineralogy changes around the hot-water injection well in the deep reservoir, is provided as one of the geochemistry module examples.

The major ions in the Weber-Tensleep Formation water are Cl^-, Na^+, SO_4^{2-}, HCO_3^-, K^+, Ca^{2+} and HS^-, with a host of additional minor ions. The pH is around 6.5, the ionic strength is around $1.7\,mol.kg^{-1}$ (which is close to the limit of $3\,mol.kg^{-1}$ for the Debye-Huckel activity model (Bethke, 2007)), and the temperature around 90°C. The observed mineralogy involves quartz (80%), K-feldspar (8%), Calcite (5%), Siderite and Dolomite (each 2%), Fe-chlorite and Illite (each 1%) and a host of trace minerals.

The 3D MOOSE model involves coupling 3 models representing: (1) the heat exchanger; (2) injection, production and transport of water through the formation; (3) a geochemical model of the reservoir. These three models are loosely coupled using MOOSE's "multiapp" approach, using the geochemistry and PorousFlow modules. The coupled modelling reveals that anhydrite is the main precipitate in the heat exchanger, that illite and kaolinite dissolve around the injection well, and that K-feldspar and quartz precipitate around the injection well. Figure 3 illustrates the results.
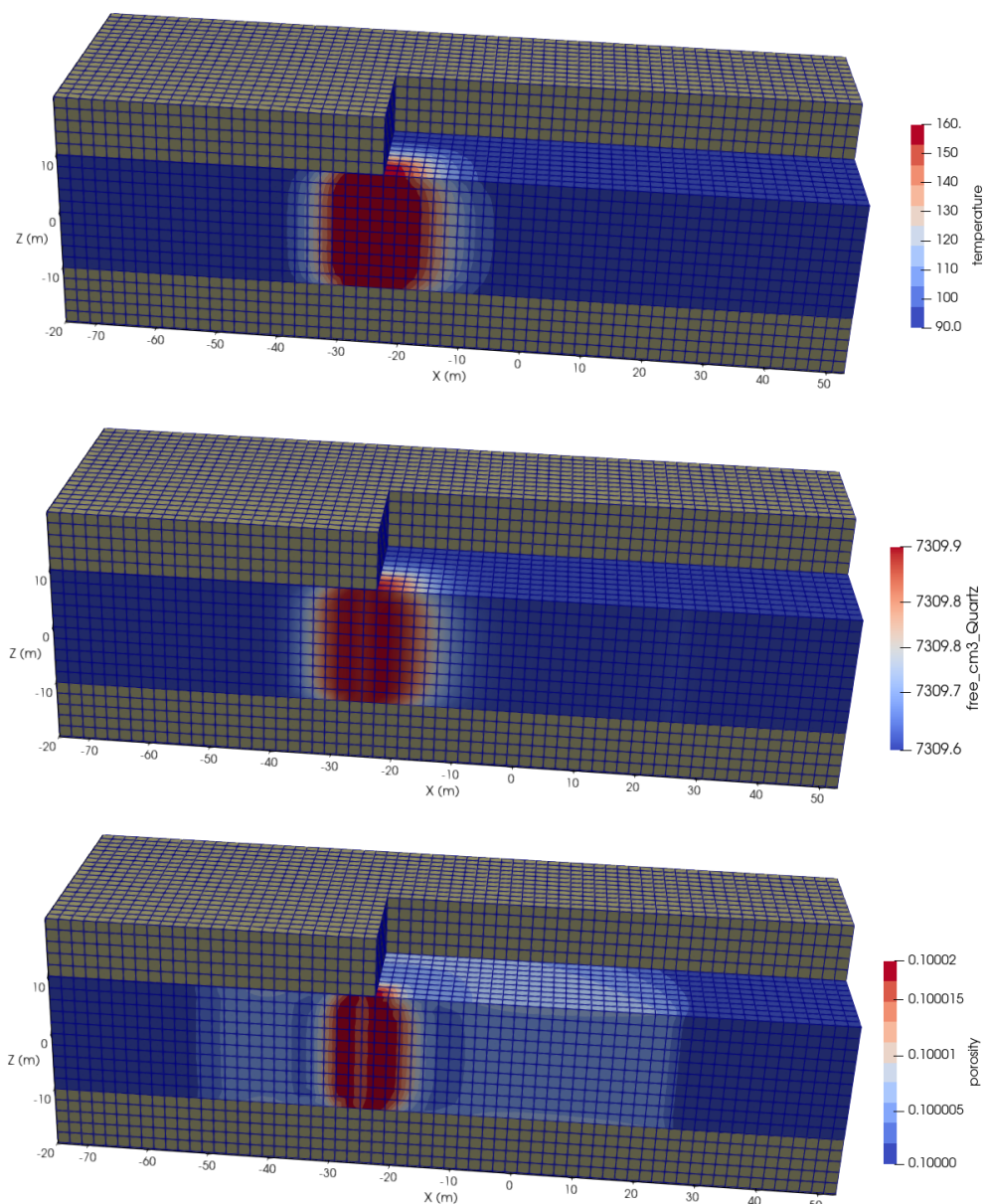
Figure 3: Temperature, free volume of Quartz, and porosity after 90 days of hot water injection in the Weber-Tensleep aquifer. The gray areas represent low-permeability cap rocks above and below the aquifer.

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