

Attachment 1.

CRUNCH **A Computer Program** **for Multicomponent Reactive Transport in Porous Media**

CRUNCH is a computer program for simulating multicomponent multi-dimensional reactive transport in porous media. The code is written entirely in FORTRAN 90 and incorporates into a single code most of the features previously found in the *GIMRT/OS3D* package (Steeffel and Yabusaki, 1996; Steeffel, 2001) along with a large number of new features. The use of the FORTRAN 90 language allows for runtime allocation of memory for arrays, thus minimizing the memory requirements while maximizing the number of options which can be selected at runtime. Using an automatic read of a thermodynamic and kinetic database, the code can be used for reactive transport problems of arbitrary complexity and size (i.e., there is no *a priori* restriction on the number of species or reactions considered).

The main features of the code include:

- simulation of advective, dispersive, and diffusive transport transport in up to two dimension using the global implicit (*GIMRT*) option or three dimensions using time-splitting of transport and reaction (*OS3D*);
- non-isothermal transport and reaction;
- unsaturated transport with gas-aqueous phase exchange;
- multicomponent aqueous complexation;
- kinetically-controlled mineral precipitation and dissolution;
- multicomponent ion exchange on multiple sites;
- multicomponent surface complexation on multiple sites with or without an electrostatic correction based on the double layer model (Dzombak and Morel, 1990). Site densities are linked to mineral concentrations which may evolve;
- biologically-mediated reactions based on Monod-type formulations;
- radioactive decay chains;
- advective transport of solid phases to simulate erosion or burial;
- multicomponent diffusion with an electrochemical migration term to correct for electroneutrality where diffusion coefficients of charged species differ;
- automatic read of a reformatted version of the EQ3/EQ6 database augmented with a kinetic database;
- multiple options (equilibration with a gas or mineral phase, total concentration, fixed activity) for initialization of boundary and initial conditions.

The code uses an integrated finite volume approach currently restricted to orthogonal grids. Advective transport may be simulated with the standard upwind method or with a third order accurate TVD method when using the *OS3D* runtime option.

Example Problems

Upwelling non-isothermal flow on the flanks of the Juan de Fuca Ridge: A one-dimensional multicomponent diffusion-advection-reaction calculation with over 100 equilibrium and kinetic reactions was run to steady-state to match observed pore water profiles.

Cesium ion exchange in Hanford sediments: Matching of column and field results using the multicomponent, multi-site ion exchange capability within *CRUNCH*. A 3D simulation of field results, which included 12 component species, 24 aqueous complexes, and 12 ion exchange reactions, took about 1.5 hours to run on a dual processor 933 MHz Pentium III Xeon-based PC.

Copper leaching benchmark problem from PNNL workshop: A 2D multicomponent benchmark involving copper leaching proposed by P.C. Lichtner (see [description on PNNL WEB site](#)) required about 8 minutes on a dual processor 933 MHz Pentium III Xeon-based PC using *CRUNCH*.

Biodegradation of VOC at the Aberdeen proving ground in Maryland: History matching of anerobic biodegradation of VOC using *CRUNCH*.

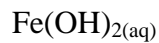
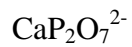
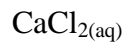
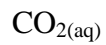
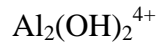
Reactive transport through Opalinus clay from Switzerland: This example shows *CRUNCH* used to model diffusive and advective transport and reaction in column experiments on the Opalinus clay (courtesy M. Adler, Universitat Bern).

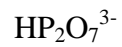
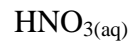
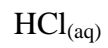
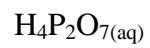
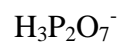
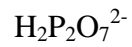
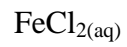
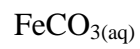
References

- Dzombak D.A. and Morel F.M.M. (1990) *Surface Complexation Modeling: Hydrous Ferric Oxide*. Wiley-Interscience, 393 p.
- Steeffel, C.I. (2001) GIMRT, version 1.2: Software for modeling multicomponent, multidimensional reactive transport. User's Guide, **UCRL-MA-143182**. Livermore, California: Lawrence Livermore National Laboratory.
- Steeffel, C.I., and Yabusaki S.B. (1996) OS3D/GIMRT, Software for multicomponent-multidimensional reactive transport: User's Manual and Programmer's Guide, **PNL-11166**, Pacific Northwest National Laboratory, Richland, Washington.

Attachment 2.

List of secondary species.





HSO_4^-
 HSiO_3^-
 $\text{KCl}_{(\text{aq})}$
 KHPO_4^-
 $\text{KHSO}_{4(\text{aq})}$
 $\text{KOH}_{(\text{aq})}$
 $\text{KP}_2\text{O}_7^{3-}$
 KSO_4^-
 $\text{MgCO}_{3(\text{aq})}$
 MgCl^+
 $\text{MgH}_2\text{PO}_4^+$
 MgHCO_3^+
 $\text{MgHPO}_{4(\text{aq})}$
 $\text{MgP}_2\text{O}_7^{2-}$
 MgPO_4^-
 $\text{MgSO}_{4(\text{aq})}$
 $\text{Mn}(\text{NO}_3)_{2(\text{aq})}$
 $\text{Mn}(\text{OH})_{2(\text{aq})}$
 $\text{Mn}(\text{OH})_3^-$
 $\text{Mn}(\text{OH})_4^{2-}$
 $\text{Mn}_2(\text{OH})_3^+$
 $\text{Mn}_2\text{OH}^{3+}$
 $\text{MnCO}_{3(\text{aq})}$
 MnCl^+
 MnCl_3^-
 $\text{MnH}_2\text{PO}_4^+$
 MnHCO_3^+
 $\text{MnHPO}_{4(\text{aq})}$
 MnNO_3^+
 MnO_4^{2-}
 MnOH^+

