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A process-based reactive hybrid transport model for coupled discrete conduit–continuum systems

Sabine M. Spiessl [a,b,*], Henning Prommer [c], Tobias Licha [a], Martin Sauter [a], Chunmiao Zheng [d]

[a] *Applied Geology, Geoscience Center, University of Goettingen, Goldschmidtstr. 3, 37077 Goettingen, Germany*
[b] *Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Theodor-Heuss-Str. 4, 38122 Braunschweig, Germany*
[c] *CSIRO Land and Water, Private Bag No. 5, Wembley, WA 6913, Australia*
[d] *Department of Geological Sciences, University of Alabama, 202 Bevill Building, Tuscaloosa, AL 35487-0338, USA*

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Summary A process-based reactive hybrid transport model, RUMT3D, was developed to quantify the fate of dissolved contaminants and their interaction with solid phases in domains where discrete conduit networks are embedded in a permeable matrix. Such hybrid systems can be found, for example, in flooded underground mines, discrete karstic and fractured systems as well as in aquifers with intersecting boreholes. RUMT3D specifically takes into account the two distinctly different transport regimes within such hybrid systems: (i) rapid transport within the network of the highly conductive conduits, shafts, drifts, ventilation raises or roadways and (ii) the low velocity regime within the considerably less permeable matrix. RUMT3D is an extension of the existing reactive transport model PHT3D. Compared to the original model, which combines the multi-species transport simulator MT3DMS with the geochemical model PHREEQC-2, RUMT3D additionally incorporates a conduit transport model. A benchmark problem simulating the principal processes occurring at contaminated sites affected by acid mine drainage (AMD) was used to evaluate the model. The results suggest that for the simulation of contaminant transport in a hybrid system the consideration of rapid transport pathways is necessary. Conduits can strongly affect groundwater hydraulics and therefore become responsible for rapid hydrochemical changes.

* Corresponding author. Address: Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Theodor-Heuss-Str. 4, 38122 Braunschweig, Germany. Tel.: +49 531 8012 272; fax: +49 531 8012 200.
E-mail address: sabine.spiessl@grs.de (S.M. Spiessl).

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Introduction

Groundwater contamination by acidic drainage from mines and from mine wastes is one of the main environmental problems faced by many countries (Nordstrom and Alpers, 1998; Mayer, 1999). In many cases the oxidation of naturally abundant pyrite was identified to be the key process that causes acidic geochemical environments and the subsequent mobilisation of metals (Singer and Stumm, 1970; Wisotzky, 1996; Wunderly et al., 1996; Bain et al., 2000; Blowes et al., 2004).

Flooded underground mines, where these types of problems mainly occur, are typically composed of networks of highly conductive 'pipes' or 'conduits', i.e., shafts, drifts, ventilation raises, or roadways (Younger, 2002) within an otherwise considerably less permeable ore material. These highly conductive conduits are often sparsely distributed and likely possess no characteristic size limits in the porous rock matrix. The discrete conduit network, imbedded in a less permeable ore matrix, implies two distinct flow and transport regimes: (i) rapid, even sometimes turbulent flow in the discrete conduits and (ii) laminar flow with comparably low velocities within the surrounding continuum flow system.

The understanding and quantification of such dual flow aquifer systems becomes particularly important when abandoned, previously dewatered underground mines are flooded and predictions of the future development of the chemical composition of mine discharge is required. Flooding of mines aims to re-establish reducing (redox) conditions to prevent further pyrite oxidation and its associated adverse effects such as acid production and high concentrations of dissolved iron and sulphate (Singer and Stumm, 1970). Through the presence of conduits, geochemical constituents, including toxic substances, will generally spread out much more rapidly in mine-affected aquifers than in comparable porous aquifers. Since the characteristic properties of the conduits cannot be expressed with uniform continuous variables, the representative elementary volume concept (REV, Bear and Verruijt, 1987) is not applicable for the discrete conduit networks at the scale of interest and reactive transport models based on continuum approaches (i.e., single, double and multiple continuum models) generally fail to reproduce the characteristic behaviour of mining-affected aquifers containing conduits. Furthermore, mass fluxes from the solid mineral phase into the mobile water phase and chemical reactions are potentially controlled by the actual surface area between rock matrix and mobile conduit water. Continuum models might not be well suited to capture the resulting physico-chemical effects. Therefore, simulation of reactive transport in such domains might best be accomplished by so-called ''hybrid'' models, which combine aspects of discrete and continuum models (Berkowitz, 2002).

Currently, only a few existing reactive hybrid transport models are capable of taking into account a more comprehensive range of geochemical reactions. Early studies were limited to adsorption—desorption or precipitation—dissolution reactions — all within a single fracture, along the fracture walls and/or within the adjacent porous host rock (Berkowitz, 2002). These early studies investigated simple geometries and aimed at gaining a principal understanding of the governing processes in such systems.

Initial studies on dissolution/precipitation reactions in hybrid systems were carried out by Steefel and Lichtner (1994), Novak (1996) and Steefel and Lichtner (1998a,b). The main motivation for those studies was to understand the controls on reactive contaminant transport near waste repositories and to determine the mineral distribution within fractured systems (see also Ghogomu and Therrien, 2000). Transport within the aquifer matrix and mass transfer between the conduit and the matrix were both assumed to be solely driven by molecular diffusion. Emrén (1998) developed the model CRACKER, which allowed the simulation of reactive transport in single conduits in combination with heterogeneous mineral compositions in the matrix. Dijk and Berkowitz (1998) investigated the precipitation—dissolution in a single fracture and the changing fracture openings that resulted from this process.

More recently, Ghogomu and Therrien (2000) presented a new hybrid transport model for reactive multi-species problems in saturated discretely-fractured porous media. They used the model presented by Therrien and Sudicky (1996) to simulate physical transport within aquifers consisting of both a porous matrix and a set of discrete fractures and embedded an existing equation solver for chemical reactions (Schäfer et al., 1998) through a sequential iterative operator-splitting algorithm (SIA). The chemical species in both the fractures and the porous matrix can undergo either equilibrium-based or kinetically controlled chemical reactions. To eliminate direct calculation of the matrix/fracture exchange terms, Ghogomu and Therrien (2000) assumed similar hydraulic head and concentration values for both the conduit nodes and the corresponding matrix cells. This limits the model's application to systems where exchange between the continuum cells and the conduit nodes is not locally controlled by a concentration gradient. The hydraulic conductivity of the conduits or the fractures is computed on the basis of the cubic law, which generally leads to much higher conductivities compared to the ones in the matrix cells. Viswanathan and Sauter (2001) developed a hybrid model, coupling a discrete pipe-flow model to a continuum model for the simulation of the long-term release of dissolved uranium. The model assumes instantaneous mixing within the conduit system and includes aqueous speciation calculations, but no reactions with solid phases were considered.

Other reactive hybrid transport models, or more specifically compartment models, are the simulators KAFKA (Colenco, 2001; Wilhelm et al., 2002) and EMOS (Buhmann, 1999). Both were developed for fluid flow and contaminant transport in converging underground waste repositories. Apart from flow and reactive transport, they also consider porosity variations caused by convergence/creeping. Furthermore, they calculate time-dependent gas generation induced by corrosion and microbial degradation. Reactive processes considered KAFKA and EMOS include sorption of radionuclides, radioactive decay, and simplified dissolution/precipitation reactions.

The major objective of this paper is to present the development and evaluation of the new MODFLOW/MT3DMS-based numerical model RUMT3D (three-dimensional reactive underground mine transport model), which combines a comprehensive range of key features that allow