SCS: Specific Chemical Simulators dedicated to chemistry-transport coupled modelling: Part III. Coupling of SCS with the hydro-transport modelling software MARTHE

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We detailed in part I of the present abstract (Kervévan and Baranger) the reasons why BRGM decided to develop its own Specific Chemical Simulators (SCS) and then, to use these SCS as subroutines embedded in general 3D Hydro-Transport Modelling Softwares (HTMS) in order to perform coupled modelling. We present here the general methodolodgy and some characteristic examples of coupled simulations carried out with various Specific Coupled Codes (SCC) constructed by associating MARTHE (a BRGM HTMS; Thiéry, 1990) and various SCS.

BRGM general methodology in chemistry-transport coupled modelling

Yeh and Tripathi (1989) identified three different general methods for coupling chemistry and transport: (1) simultaneous solving of Differential and Algebraic Equations (DAE), (2) the Direct Substitution Approach (DSA) and (3) the Sequential Iterative Approach (SIA). They concluded that, although more accurate, DAE and DSA cannot be used for complex 2D and 3D simulations for reasons of CPU and memory requirements far beyond the capacities of actual supercomputers. SIA was therefore the recommanded method to be used for realistic simulations.

Following these recommendations, BRGM based its coupled approach on a sequential calculation, at each time step, of hydrodynamics, transport and then chemistry. One of the key points highlighted by Yeh and Tripathi (1989) was the choice of the Primary Dependant Variables (PDV) used in both chemical and transport equations. In order to decrease the number of transport equations to be solved, BRGM decided to chose the total amounts of the chemical elements (i.e. H, O, C, ...) as chemical PDV instead of the aqueous species (i.e. H^+, OH^-, HCO_3^-, CO_3^{2-}, H_2CO_3, ...).

Because of both the particular chemical PDV used and the way the equations of a SCS are structured, we did not implement any iterative algorithm in our SCC

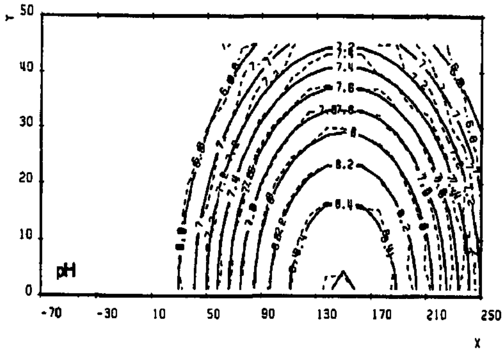

FIG. 1. Comparison between calculated (dashed line) and analytical (solid line) pH 150 days after injection in (0,0). Only half of the domain is displayed.

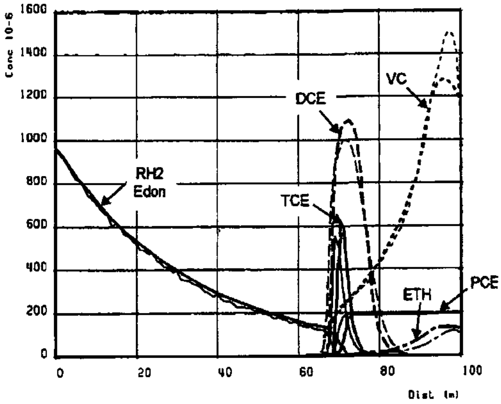

FIG. 2. Concentration distributions 30 days after initial injection of RH2. Comparison between Cirpka's results (bold line) and MARTHE + SCS results.

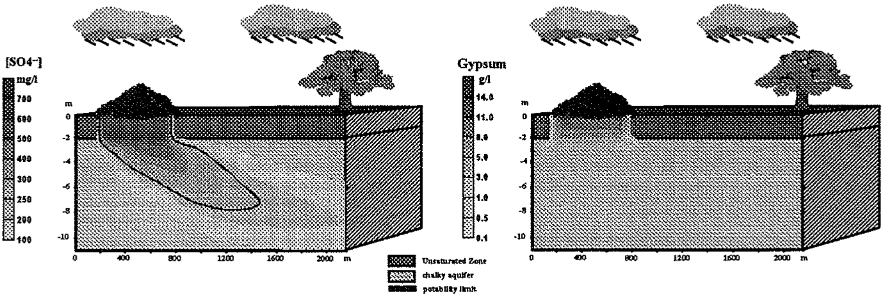

FIG. 3. Sulphate (SO_4^{2-}) and gypsum distributions after 25 days.

so that our calculations are purely sequential. This relies on the assumption that chemical source/sink terms can be applied only after the transport calculations. This approximation is perfectly valid when no exchange between aqueous and other phases occurs. In other cases, it is necessary to adapt the time step duration so that this assumption becomes reasonable.

Examples of coupled simulations

This very general coupling approach allows us to easily construct a SCC on the basis of a SCS embedded (as a subroutine) in any of general HTMS available at BRGM. The following simulations were all performed using MARTHE + SCS.

The first case study presented here is one of the CHEMVAL validation exercises (Read *et al.*, 1991). This test was based on the instantaneous injection of NaOH into a 2D siliceous aquifer. It was designed in order to find an analytical solution. 5 aqueous species, 3 aqueous reactions, and 1 mineral phase are considered. The corresponding SCS is then relatively simple. The velocity is 1D along x axis but dispersion is 2D. Fig. 1 shows a good agreement between simulation and analytical solution:

The second example simulates reductive dechlorination of tetrachloroethene (PCE) in a 1D aquifer. The global process successively transforms PCE into TCE, cis-DCE, VC and, finally, ETH and is controlled by initial injection of an electron donor (RH2) and competitive biotransformation processes. The SCS constructed for handling this problem typically shows the great interest of our approach since none of the classical general-purpose geochemical codes described in the literature is capable of simulating such bio-processes. For his calculations, Cirpka used a specific finite element coupled code based on a two-step iterative coupling algorithm (Cirpka and Helmig, 1994). Figure 2 shows that our results can be favourably compared to those of Cirpka (pers. com., 1995).

The third example is based on real field data. BRGM was asked to simulate various scenarios of percolation of a sulphate-rich waste disposal leachate through an unsaturated zone underlying an aquifer. Dealing with a natural sytem, the corresponding SCS is thus relatively complex. It takes into account 25 aqueous species, 1 gas phase and 5 mineral phases. As an example among various scenarios tested, the results obtained for 2D sulphate (SO_4^{2-}) and gypsum deposit distributions are illustrated in Fig. 3.

References

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