Three-dimensional reactive transport modelling in the vadose zone

A. Brovelli and D.A. Barry

Laboratoire de technologie écologique, Institut des sciences et technologies de l'environnement, Station No. 2, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland (alessandro.brovelli@epfl.ch)

In this work we present a novel numerical model capable of modelling reactive transport in both the saturated and vadose zone. The model is obtained coupling MODFLOW 2000 VZF with MT3DMS and PHREEQC. The version of MODFLOW 2000 we use was extended and improved to allow simulation of flow in the unsaturated zone. An operator-splitting approach is used to couple the different models. Both the iterative and non-iterative splitting operator algorithms have been implemented. The resulting software is extremely flexible and powerful. An arbitrary number of mobile and immobile chemical components can be incorporated in each simulation. Full chemical speciation, pH and redox equilibria and kinetic chemical can be accounted for.

The new code has been tested against a similar numerical model and experimental data, showing a reasonably good agreement in all cases. Advantages and limitations of the model implementation are investigated and discussed.