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Simulation of multicomponent reactive solute transport in saturated/unsaturated flow by mixed finite elements

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Pollution of soil by organic contaminants is nowadays a serious and widespread problem. A comprehensive active remediation often is not feasible from technical or financial reasons. Alternatively, in situ bioremediation (natural attenuation) has been recognized as a promising approach to restore sites contaminated with organic pollutants because it is less costly than active remediation strategies, the contaminants can ultimately be transformed to innoucous by-products with the help of microorganisms (not just transferred to another phase or place) and it can operate in situ. However, the decision to apply natural attenuation at a specific site depends essentially on the reliable prediction of the fate of the contaminant plume. Together with laboratory and field experiments, mathematical models can be used to predict the evolution of a site over long time periods.

We present a general model to describe the simultaneous reactive transport in porous media of an arbitrary number of organic substances in the presence of some microbial populations. The model includes the effects of advection, dispersion, sorption and degradation. The groundwater movement, taking into account the unsaturated subregions near the surface, is described by the Richards equation.

The interaction of the relevant components (species) via sensitive, highly nonlinear reactive processes stresses the need for very accurate numerical schemes. Artificial numerical diffusion leads to erroneous reactive processes and thus to false predictions

of the contaminant fate by overestimating the availability of the reactants [1]. The need of an adequate approximation of the fluid flow by mixed finite element methods (MFEM) has been recognized in the water resources literature since several decades, see, e.g., [2]. These methods offer the advantage of local mass conservation and continuous flux approximations over the element faces. However, for associated solute transport problems normally conventional methods are applied, e.g. conforming finite element methods or finite volume schemes.

Consequently, to seize the aforementioned advantages, the MFEM is used also for the multicomponent transport equations. This novel formulation of a coupled reactive multicomponent transport model together with a description of water flow in the vadose and saturated zone in the mixed hybrid finite element setting was detailed described in [3]. Here, besides some algorithmic aspects, also new results regarding the accuracy of the scheme are presented. At the end illustrative numerical studies are shown.

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