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An approximate analytical solution for multicomponent cation exchange reactive transport in groundwater

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Cation exchange in groundwater is one of the dominant surface reactions. Mass transfer of cation-exchanging pollutants in groundwater is highly nonlinear. This makes extremely difficult to derive analytical solutions for transport equations (van Genuchten and Cleary, 1982). Bolt (1982) developed analytical solutions for nonlinear cation exchange and transport in steady saturated flow. Bond and Philips (1990) extended his approach to obtain approximate quasi-analytical solutions for transport with nonlinear adsorption during unsteady flow in unsaturated soils. Dou and Jin (1996) used the method of characteristics with a special treatment of shock waves and worked out a closed-form formulation for 1-D transport coupled to binary homovalent ion exchange. Jin and Ye (1999) extended this approach and developed an approximate analytical solution to binary monovalent-divalent ion exchange transport. Due to the complexity of isotherms, most of previous studies to derive analytical solutions are suitable only for 1D transport with binary cation exchange. Here we present an approximate analytical solution for the general case of multi-component reactive transport involving any arbitrary number of cation exchange reactions in steady groundwater flow. The nonlinear mass-action-law equations of cation exchange are linearized by means of a first order Taylor expansion of log-activities of exchanged cations. Approximated chemical equations are substituted back into transport equations to get a set of coupled partial differential equations (PDE). These coupled PDE are uncoupled by means of a similarity transformation. The transformation matrix can be obtained by well-known matrix properties. After application of such transformation to boundary and initial concentrations, uncoupled PDE's can be solved by standard analytical solutions. Finally the concentrations in the original domain can be obtained by trans-

forming the solutions in the new domain. Our analytical solution has been tested with the solutions obtained with CORE^{2D}, a reactive transport code. The analytical solution not only agrees well with numerical results, but provides also additional insight into the nature of the retardation factor caused by multicomponent cation exchange.