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Generic reactive transport codes as flexible tools to integrate soil organic matter degradation models with water, transport and geochemistry in soils

Diederik Jacques (1), Fréderic Gérard (2), Uli Mayer (3), Jirka Simunek (4), and Bertrand Leterme (1)

(1) SCK-CEN, Belgium (djacques@sckcen.be), (2) INRA, UMR Eco&Sols, Montpellier, France, (3) Earth, Ocean and Atmospheric Sciences, University of British Columbia, Vancouver, BC, Canada, (4) Department of Environmental Sciences, University of California Riverside, CA, USA

A large number of organic matter degradation, CO_2 transport and dissolved organic matter models have been developed during the last decades. However, organic matter degradation models are in many cases strictly hard-coded in terms of organic pools, degradation kinetics and dependency on environmental variables. The scientific input of the model user is typically limited to the adjustment of input parameters. In addition, the coupling with geochemical soil processes including aqueous speciation, pH-dependent sorption and colloid-facilitated transport are not incorporated in many of these models, strongly limiting the scope of their application. Furthermore, the most comprehensive organic matter degradation models are combined with simplified representations of flow and transport processes in the soil system. We illustrate the capability of generic reactive transport codes to overcome these shortcomings. The formulations of reactive transport codes include a physics-based continuum representation of flow and transport processes, while biogeochemical reactions can be described as equilibrium processes constrained by thermodynamic principles and/or kinetic reaction networks. The flexibility of these type of codes allows for straight-forward extension of reaction networks, permits the inclusion of new model components (e.g.: organic matter pools, rate equations, parameter dependency on environmental conditions) and in such a way facilitates an application-tailored implementation of organic matter degradation models and related processes. A numerical benchmark involving two reactive transport codes (HPx and MIN3P) demonstrates how the process-based simulation of transient variably saturated water flow (Richards equation), solute transport (advection-dispersion equation), heat transfer and diffusion in the gas phase can be combined with a flexible implementation of a soil organic matter degradation model. The benchmark includes the production of leachable organic matter and inorganic carbon in the aqueous and gaseous phases, as well as different decomposition functions with first-order, linear dependence or nonlinear dependence on a biomass pool. In addition, we show how processes such as local bioturbation (biodiffusion) can be included implicitly through a Fickian formulation of transport of soil organic matter. Coupling soil organic matter models with generic and flexible reactive transport codes offers a valuable tool to enhance insights into coupled physico-chemical processes at different scales within the scope of C-biogeochemical cycles, possibly linked with other chemical elements such as plant nutrients and pollutants.