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Discontinuous Finite Element mechanistic water quality model for the simulation of adsorptive pollutants transport in river systems.

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Abstract

The close interaction between humans, animals and the river system requires to have control about the concentration of different pollutants in the water column in order to avoid damage to the environment. Due to the fact that the measurements are time consuming, expensive and in most of the cases very local, it is required to develop tools in order to predict the spatial and temporal distribution of the pollutants in the system.

Once pollutant effluents are discharged in waters, part of them is transported in liquid phase and the rest is attached to the suspended sediments and to the bed sediments. The magnitude of each fraction is determined classically by the partition coefficient $K_d$ that is a function of several environmental parameters such as the pH.

Adsorptive pollutant effluents interact with the sediments present in the water column (adsorption/desorption on suspended matter and bed sediment) being carried downstream by the water flow. Depending on the flow conditions, settling of the suspended particles may occur while during storm events, resuspension takes place influencing the pollutant distribution and transport.

In this research a water quality model focused on the transport of radionuclides/heavy metals in river networks is developed. The model is constituted by sub models for the representation of tracers, non-cohesive/cohesive sediment transport, radionuclides and heavy metals.

The model engine solves the 1D Advection–Diffusion–Reaction equation by means of the Discontinuous Galerkin Finite element Method. The model can be linked to any hydrodynamic model in order to obtain information about the topological description of the river system and the water flow. The model structure includes several tools such as numerical solution stabilization techniques, spatial interpolation of additional computation nodes and individual discretization of specific branches. These tools allows the user to modify the conceptualization of the river system structure in order to increase the accuracy or reduce the computation time depending of the characteristics of the problem to be solved. The model represents the water column sorption/desorption process by a fully kinetic approach. It also takes into account the changes in time of the key processes parameters such as the $K_d$ and the rate reactions. These features provide a more realistic approach during the modelling in comparison with the traditional models for sorption/desorption processes representation.

The first application of the model takes place at the Molse Nete-Grote Nete river system. The main objective is to study radionuclide dispersion. Therefore the model was coupled with the MIKE 11 river model and the hourly version of the SWAT model to feed the model with the required flow variables. The model was verified in four stages. First, the accuracy of the advection dispersion component was evaluated by comparing the numerical solution provided by the model with the
analytical available solution of the advection dispersion equation. Secondly the sediment transport component was verified by comparing the model prediction with the observations at Geel-Zammel. In a third stage, the mathematical formulation of the sorption-desorption kinetics component was validated by comparing the solution provided by the mathematical equations with the results of the experimental in vitro experiments. Finally the complete model was verified comparing the radionuclide concentration measured in the river bed sediments with the model prediction.

In all the stages the model outputs resemble nearly the in stream observed conditions. The main outcome of this research is an accurate and a more mechanistic open source tool to model the transport of adsorptive pollutants in river systems able to be linked with any hydrodynamic river model.

**Keywords**

Finite elements, water quality modelling, adsorptive pollutants, sediment transport.