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Which numerical model is suitable for the simulation of hyporheic residence times and metabolic activity? FE model vs. FV model

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Numerical models have experienced a steady increase in popularity in the scientific community, especially where historically isolated disciplines more and more acknowledge their need for interdisciplinarity. A frequently mentioned example is the interstitial between surface water and ground water in lotic systems, referred to as hyporheic zone. Due to its temporal and spatial heterogeneity, the prediction of hydraulic properties e.g. the residence time remains a challenge in science. Moreover, the hyporheic zone is often described as a reaction chamber due to its repertoire of chemical reactivity, which in turn is highly influenced by the residence times. Ecologically, this habitat is populated by a microbial community that has the potential to alter the chemical characteristics of their environment under the right hydraulic conditions. This small example illustrates the complexity of interdisciplinary research and elucidates the growing requirements concerning numerical models. While the number of numerical models offering to bridge some of these gaps is growing, the decision-making process for the modeler becomes increasingly difficult. It is the objective of this study to identify a suitable model for reproducing measured data from a laboratory flume experiment, in which oxygen was measured as a proxy for metabolic activity under changing dissolved organic carbon inflow in a hyporheic zone with varying residence times. The decision-making process for a suitable numerical model was hereby exemplified by comparing the two numerical models FEFLOW, based on the finite element method (FEM), and MIN3P, based on the finite volume method (FVM). Various aspects of both models are taken into account and evaluated from software technological, numerical or end-user point of view. These include among others the mass balance, meshing algorithm, computational effort and coupling interfaces to surface water models.

Key words: FEFLOW, MIN3P, finite volume method, finite element method, flume experiment