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Evaluation of model approaches to couple transient aerobic zonation and removal of redox-dependent trace organic compounds in porous media: Results from a meter - scale experimental flow-through sand tank

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The presence of a well-developed aerobic zonation in the adjacent subsurface media of river and lake water bodies is one of the most relevant processes to enhance the removal efficiency of trace organic compounds in the receiving water by the natural attenuation along the soil passage. However, such natural remediation processes depend on daily and seasonal variations of dissolved oxygen concentration in the surface water when infiltrates into the aquifer; with the subsequence modification of the extension of the aerobic zonation, mostly hardly measurable. From a model perspective, coupling transient dissolved oxygen concentration and nonlinear redox processes in hydraulic subsurface models may transfer significant uncertainty to the simulated outcomes, as well as to increase considerably the computation effort. To cope such challenges, among other numerical strategies, there is a demand of probed hypothesis to figure out simplified assumptions in the setup of key parameters and variables describing the fundamental equations of groundwater flow and reactive transport. In this study, a two-dimensional model is performed according to three different approaches to characterize the established aerobic zonation in a highly monitored pilot experiment, known as the SMARTplus tank. The tank media mimics a bank filtration site fed by pre-treated wastewater outflow, but rich in pharmaceutical and personal care products at remaining concentrations. After the continuous performance for 4-5 months, the pilot-scale experiment provides enough information to model the aerobic biodegradation of trace organic compounds by two simplified assumptions of the transient dissolved oxygen inlet boundary: case A considers the whole tank as aerobic zone, and estimate first-order degradation rate according to inlet-outlet trace organic concentration; case B assumes stable first meters from the inlet of aerobic zonation, stablished based on a previous simulation of dissolved oxygen penetration plume into the subsurface media. Both approaches are compared with the case C, a fully-coupled transient aerobic zonation, therefore computationally expensive. The comparison of the model results with the long-term observed concentrations of trace organic compounds along the tank experiment provides excellent fitting in certain trace organic compounds for the simplified approaches. Additional information about the estimated bio-reactive parameters (first and second Monod reactions) at the three approaches provides valuable range of values at the meter-scale, commonly analyzed in column experiments or at field site.