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Transport in heterogeneous flow fields with depth-dependent sorption and decay parameters

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A vertical gradient in chemical and biological properties is prominent in most soils together with an increase in dispersivity with travel distance. Simulations with different 1-D transport models making opposite assumptions about the correlation of solute particle velocities across boundaries of soil layers with different sorption and decay parameters demonstrated the importance of these correlations. The 1-D models either assume perfect (stream tube model, STM) or zero (convective dispersive equation, CDE) correlation of particle velocities. To investigate leaching in layered soils for the more realistic case of imperfect velocity correlation, 2-dimensional flow and transport simulations were carried out in heterogeneous hydraulic conductivity fields. In one set of conductivity fields, the variance and spatial correlation of the hydraulic conductivity was constant and the structure of the conductivity field was continuous across the layer boundaries. In the other set, the spatial structures of the hydraulic conductivity in the top soil layer were different in statistical terms and disconnected from those in the deeper soil layers. A STM, which was calibrated to the averaged inert tracer BTC at 1-m depth in the heterogeneous conductivity field, underestimated the leached mass fraction since it underestimated the dispersive flux through the upper layer. Also a 1-D CDE with different dispersivity parameters in different soil layers to predict the same inert BTCs at the soil layer boundaries as in the 2-D simulations, underestimated the leached mass fraction since the correlation of particle velocities was not considered. A 1-D CDE model with a constant dispersivity always predicted the highest leached mass fraction, since it overestimated the dispersive flux and leached mass fraction through the first layer. Simulations in heterogeneous fields with disconnected structures of hydraulic conductivity in the top and sub-soil showed that the correlation of particle velocities was hardly influenced because the water flow is divergence free.