

Applicability of Travel- and Exposure-Time Concepts to Nonlinear Bioreactive Transport in Groundwater

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Travel-time based concepts of modeling subsurface transport have been established as computationally efficient alternatives to spatially explicit simulation methods. The spatial coordinates are replaced by travel time, resulting in one-dimensional transport with a constant „velocity“ of unity. The concept is straight forward in linear transport applications, and under these conditions the results are exact provided that the coefficients of linear transport don't vary in space. In nonlinear transport, mixing can jeopardize the validity of the approach. This holds particularly true for transverse mixing, exchanging solute mass between streamtubes. We have performed systematic analyses of nonlinear bioreactive transport, involving oxygen, nitrate, organic carbon, as well as aerobic and denitrifying bacteria to analyzed under which conditions the errors introduced by travel-time and similar formulations are negligible. In steady-state flows with uniform reactive parameters, an excellent agreement between multi-dimensional reactive transport results, affected by transverse dispersion and flow heterogeneity, and one-dimensional travel-time results could be achieved by mapping the reactive-species concentrations to the multi-dimensional domain according to the local mean groundwater age. Aliasing of local transverse dispersion to macroscopically longitudinal mixing can be addressed by using a distance-dependent longitudinal dispersion coefficient. The approach also works for transient flows as long as the direction of flow remains constant and only the magnitude varies. Under these conditions, the groundwater age for the time-averaged velocity field is an adequate mapping variable, provided that flow transients are accounted for in the one- and multi-dimensional simulations. If the reaction takes place only in specific regions, the time of exposure to the according conditions is a better predictor of reactive transport than the overall travel time. Spatially variable intensity of reaction can be accounted for by relative reactivity, resulting in a framework, in which time is replaced by cumulative relative reactivity. Our studies emphasize that the assessment of travel times and relative reactivity is very useful in the assessment of reactive transport. However, if the direction of flow varies and immobile compounds are involved in the reaction, travel and exposure times are inadequate predictors of reactive transport. Likewise, systems in which macroscopic control of the reaction is exerted by transverse mixing, e.g., in quasi steady-state plumes of pollutants reacting with compounds provided by ambient flow, a spatially explicit description appears necessary.