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Reaction rates in randomly heterogeneous stratified formations

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A multicomponent reactive transport problem is generally addressed through a system of coupled non-linear partial differential equations. Chemical substances are advected by water and mix by local diffusion or dispersion. Mixing causes desequilibrium, forcing reactions to take place in order to locally reequilibrate the system. In the particular case of chemical equilibrium, the problem can be greatly simplified by fully defining the system in terms of conservative (i.e., not influenced by reactions) quantities, termed components, and the space-time distribution of reaction rates. We investigate the parameters controlling reaction rates in a heterogeneous aquifer at short distances from the source. At this scale, the hydraulic conductivity is modeled as a random process with anisotropic correlation structure (large correlation lengths in the flow direction). Closed-form analytical solutions for statistical moments of reaction rates are derived for the particular case of negligible transverse dispersivity. This allows obtaining an expression for an effective hydraulic conductivity, K^R_{eff}, as a representative parameter describing the mean behavior of the reactive system. The resulting K^R_{eff} is significantly smaller than the one representative of the flow problem. Finally, we analyze numerically the effect of accounting for transverse local dispersion. We show that transverse dispersion causes no variation in the distribution of (ensemble) moments of reaction rates at very short travel times, while it becomes the dominant effect on reactions for intermediate to large travel times.