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Time-domain random walk modeling of heterogeneous diffusion and trapping in porous media

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Diffusion in heterogeneous media is a ubiquitous process in nature that describes a range of different physical phenomena including chemical transport in low permeability media such as clays and granites and in general in immobile regions of a heterogeneous porous medium, Darcian fluid flow through heterogeneous media, heat transport and electric current through a conductor, as well as diffusion in biological systems. We consider the efficient random walk modeling of diffusion in a heterogeneous medium that is characterized by spatially varying diffusion and trapping properties. We show that a continuous time random walk (CTRW) with a spatially variable exponential transition time distribution solves the spatially discretized heterogeneous diffusion equation. This demonstrates the equivalence of the widely used time-domain random walk (TDRW) scheme and spatially inhomogeneous CTRW and thus also the formal equivalence of the TDRW particle formulation and the heterogeneous diffusion equation. Based on the constructive nature of this demonstration, we develop a TDRW method for heterogeneous diffusion under spatially variable multirate mass transfer properties (TDRW-MRMT).