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Random walk simulation of solute transport for identifying diffusivity in biomaterial scaffolds for tissue engineering

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Diffusion is an important transport mechanism influencing growth and extracellular matrix regeneration in cell-seeded scaffolds used in tissue engineering applications. In many such systems, relationships between solute diffusivity at the mesoscale and the microscopic structure of the evolving scaffold are not well understood. We directly simulate diffusion via random walks of solute particles in the presence of obstacles modeling the scaffold structure. Simulations are performed within a representative domain with periodic boundary conditions. Many previous studies have analyzed such relationships using analytical and computational approaches on prescribed lattices; however, less is understood in the case of (more realistic) off-lattice models. We investigate off-lattice models, where the particle step size and direction can be varied continuously. Simulations at the microscopic scale are used to analyze and identify mesoscale relationships between diffusivity, solute size and structural features of the scaffold, e.g. scaffold volume fraction.