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Failure of the Ogston Model: Systems with Anisotropic Obstacles and Inhomogeneous Diffusivity

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Diffusion plays a critical role in many biological processes, but also in a wide range of experimental devices such as gel electrophoresis and sieving. The well-known Ogston model predicts that the diffusivity of a migrating particle through a random network of fibers (e.g., a gel matrix) is proportional to the fractional volume available to the migrating particle in the given medium. As such, the Ogston model is essentially a mean-field model. Despite wide acceptance of this model in the biological sciences and many studies that investigated the diffusion of various particle shapes, a comprehensive understanding of how the gel architecture and the shape of the obstacles impact the overall diffusion constant of a free particle is still lacking. In this talk, we will present computational studies of 2D systems consisting in anisotropic rod-shape obstacles with various correlated and uncorrelated orientations, a toy model that allows us to examine the impact of microscopic details on the global diffusivity of particles in structured and random porous systems. First, we show that how the diffusivity of particle in systems with identical free volume fractions would vary as a function of the obstacles orientation when the latter is controlled using an \textit{Ising}-like phase transition. We then explore systems containing zones with different obstacle orientations and therefore, different diffusivities. Having calculated the exact diffusivity for individual zone and the overall system, we show how these individual diffusivities contribute to the overall diffusivity of a particle in the system.

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