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Diffusion-controlled drug delivery: Avoiding pitfalls when using Lattice Monte Carlo (LMC) simulations

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Lattice Monte Carlo (LMC) methods are frequently used to model drug delivery systems. In a typical case, the drug, initially encapsulated in a porous material (e.g., a hydrogel), is released via two processes: (i) disintegration of the material and (ii) diffusive escape. One way to control diffusive release is to design layered materials with regions that have different porosities. However, modelling inhomogeneous systems where both the porosity and the diffusivity are space-dependent is ambiguous in LMC simulations. In this talk, we examine two fundamental issues: 1) how to replace connected regions with different porosities by free-solution regions of different effective viscosities; 2) how to treat the LMC jumps between regions with different effective viscosities. We present computational and theoretical studies of 2D systems consisting in two different sets of immobile obstacles that create two media with different effective viscosities, as well as their equivalent obstacle-free 1D systems with effective diffusion coefficients. Using this toy model, we examine how interfacial diffusion is treated by the various flavours of stochastic calculi, and we demonstrate that Isothermal calculus is the correct choice as opposed to the generally employed Ito calculus. We then explore the corrections that must be considered to simplify such inhomogeneous systems while conserving the proper static and dynamic properties of the original system.

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