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A Kinetic Monte Carlo Algorithm for Swelling Drug Delivery Systems

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Due to their highly tunable physical properties and their biocompatibility, hydrogels-based drug delivery systems have sparked huge interests over the past twenty years. One of the reasons of this interest lies to the ability to encapsulate drug particles inside the porous hydrogel structure. In addition, by adjusting the density of cross-links in the gel matrix, it is possible to modify the diffusion coefficient of the drug particles and thus to control the drug release in order to maintain the dose of drugs delivered within a therapeutic window. Furthermore, the hydrogel structure can swell during the drug release process when surrounded by an aqueous environment due to their hydrophilic affinity. Consequently, it leads to a non trivial competition between the diffusion and the swelling processes; and therefore can strongly affect the release dynamics.

Mathematically, even for simple geometries, finding an analytical solution for the drug concentration evolution remains very complicated or even impossible. For this reason, it is necessary to tackle this problem numerically. Therefore, we have developed a Lattice Kinetic Monte Carlo (LKMC) method which allows to simulate the release dynamics from swelling delivery systems.

Our results show that our LKMC method perfectly reproduces the expected release properties and can be used over a large variety of swelling systems. Finally, we compare our numerical result to the rare existing analytical solution: the adiabatic release.

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