

Abstract Submitted
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Using permeable microcapsules to deliver nanoparticles on substrates ROLF VERBERG, ALEXANDER ALEXEEV, ANNA BALAZS, University of Pittsburgh — We present a novel algorithm to simulate nanoparticles in the presence of a substrate, microcapsules and an externally driven flow. Here, the microcapsules consist of an elastic shell that encloses a fluid with either a dissolved chemical component or a suspension of nanoparticles that are small enough to be treated as so-called tracer particles (mutually non-interacting particles without excluded volume). The model couples a lattice-Boltzmann model for the fluid flow, a lattice-spring model for the elastic shell, and a Brownian dynamics model to simulate tracer trajectories. We then apply the model to simulate the release of nanoparticles from a microcapsule as it rolls along a substrate, as well as the subsequent particle adsorption on the wall. We study the effect of flow conditions, reaction kinetics, capsule elasticity, and capsules-substrate interaction on the rate of deposition and the size of the area of deposition at the substrate. The results provide guidelines for designing effective micro-scale delivery systems.

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