MODELING THE INTERACTION BETWEEN PARTICLE-FILLED CAPSULES AND SUBSTRATES: POTENTIAL FOR HEALING DAMAGED SURFACES

ROLF VERBERG, ALEXANDER ALEXEEV AND ANNA C. BALAZS

Chemical Engineering Department
1233 Benedum Hall, University of Pittsburgh
Pittsburgh, PA 15261, USA
balazs1@engr.pitt.edu

In biological wound healing, specific cells are recruited to the damaged areas and are driven to release components that play an active role in the healing process. Taking our inspiration from this biological system, we examine the behavior of porous microcapsules that contain nanoparticles and are driven by an imposed shear flow to move over a polymeric substrate. Our aim is to design responsive substrates that can cause the microcapsules to become localized at particular sites on the substrate and then, trigger the release of the encapsulated nanoparticles. We consider the case where the particles are attracted to the surface and thus, once the particles are released, they could bind to the underlying layer and effectively provide a protective coating or fill any nanoscale cracks or defects in the surface. In this manner, the particle-filled capsules can be harnessed to diminish the wear and enhance the lifetime of the surface. Using theory and simulation, our challenge is to establish the necessary conditions for realizing these events.

To carry out these studies, we will integrate two new computational models in order to capture the interactions of the fluid-driven microcapsules and the substrates, the release of the nanoparticles from the capsules and the interactions of the particles with the surface. In particular, we will use our recently developed approach for modeling the interactions between fluid-filled capsules and a compliant polymeric substrate [1,2]. In the latter method, we coupled the lattice Boltzmann model (LBM) for fluid dynamics and the lattice spring model (LSM) for the micromechanics of solids. This hybrid LBM/LSM approach allows for a dynamic interaction between the elastic walls and the surrounding fluid. In other words, dynamically and interactively, the moving walls exert a force on the fluids and, in turn, the fluids react back on the walls. The LBM/LSM provides a computationally efficient method for capturing not only the interactions between the polymer shell and the encapsulated fluid, but also the entire microcapsule and complex, heterogeneous surfaces.

We will augment this model by introducing mobile nanoparticles within the system. In a recent study, we developed a hybrid computational method for simulating mixtures of binary fluids and mobile, sub-micron particles [3]. Using this model, we isolated conditions where the flow of a binary fluid/particle mixture past surfaces with well-defined asperities lead to the formation of monodisperse droplets, which encapsulate the nanoparticles [3].

Our new, integrated model will allow us to simulate both the dynamic behavior of nanoparticles that are encased within a fluid-filled capsule and the release of the nanoparticles from the capsule. In addition, we can tailor the interaction between the released particles and the substrate. Consequently, we can isolate optimal conditions for targeting the particles to specific sites on the surface, regulating the release of the particles and thereby delivering a means of repairing damaged surfaces or imparting additional functionality to polymeric substrates.

References

[1] A. Alexeev, R. Verberg, and A. C. Balazs, "Modeling the Motion of Capsules on Compliant Polymeric Surfaces", *Macromolecules* **28**, 10244, 2005.
[2] G. A. Buxton, R. Verberg, D. Jasnow, and A. C. Balazs, "A Newtonian Fluid Meets an Elastic Solid: Coupling Lattice Boltzmann and Lattice Spring Models", *Phys. Rev. E* **71**, 056707, 2005.
[3] R. Verberg, J. M. Yeomans, and A. C. Balazs, "Modeling the Flow of Fluid/Particle Mixtures in Microchannels: Encapsulating Nanoparticles Within Monodisperse Droplets", *J. Chem. Phys.* **123**, 224706, 2005.

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