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Coupled Rapid Cell and Lattice Boltzmann Models to Simulate Hydrodynamics of Bacterial Transport in Response to Chemoattractant Gradients in Confined Domains CAMERON MCKAY, HOA NGUYEN, Trinity University, HAKAN BASAGAOGLU, ALEXANDER CARPENTER, Southwest Research Institute, SAURO SUCCI, Southwest Research Institute', FRANK HEALY, Trinity University — The Rapid Cell (RC) model was developed to simulate motility and adaptation dynamics of flagellar bacterial chemotaxis in environments with spatiotemporal variations in chemoattractant gradients. RC is best suited to motility studies in unbounded domains within non-fluid environments; this limits its use as a simulation tool. In this study, we eliminate these constraints by dynamically coupling RC with the colloidal lattice-Boltzmann (LB) model, a versatile tool for simulating transport of particles (e.g., surrogate bacteria) of distinct shapes and finite sizes in transient flow fields in geometrically complex microchannels. This was accomplished by tracking positions of chemoreceptor clusters on the particle surface that vary with particle angular and translational velocities, and by including additional forces and torques due to particles tumbling and to running motions in particle force-balance and torque-balance equations. The coupled RC-LB model successfully simulated transport of multiple particles in confined domains with single- or multi-attractant sources in a variety of settings. The coupled RC-LB model represents a first step toward development of a new modeling capability to simulate chemotaxis-driven bacterial transport in a network of geometrically irregular flow channels typically observed in tumor vasculature in the context of targeted drug delivery.

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