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A multiscale model for nanoparticle binding dynamics under shear flow YALING LIU, JIFU TAN, Lehigh University, KYTAI NGUYEN, University of Texas at Arlington — Nanomedicine poses a new frontier in medical technology with the advantages of targeted delivery and patient specific design. In applications of nanoparticle targeted drug delivery, the delivery efficiency is controlled by the physical properties of the nanoparticle such as its size, shape, ligand density, as well as external environmental conditions such as blood flow rate, blood vessel diameter. Proper drug dosage choice relies on determination of the attachment and detachment rates of the nanoparticles at the active region and the understanding of the complex process of targeted drug delivery. A few particulate models have been proposed to study the adhesion probability of individual spherical or non-spherical nanoparticles. Meanwhile, continuum convection-diffusion-reaction models have been widely used to calculate the drug concentration, which usually assumes specific binding and de-binding constants. However, there has not been any study that links the particulate level nanoparticle size and shape information to the system level bounded particle concentration. A hybrid particle binding dynamics and continuum convection-diffusion-reaction model is presented to study the effect of shear flow rate and particle size on binding efficiency. The simulated concentration of bounded nanoparticles agrees well with experimental results in flow chamber studies.

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