Multiscale Particulate and Continuum Model for Nanoparticle Targeted Delivery

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Nanomedicine poses a new frontier in medical technology with the advantages of targeted delivery and patient specific medicine. Current advances in nanomedicine are aiding the discovery and rationale design of many new classes of nanoparticles as drug delivery vectors for cancer treatment and image enhancing. In applications of nanoparticle targeted drug delivery, the delivery efficiency is controlled by the physical properties of the nanoparticle such as its size, shape, coating density as well as external environmental conditions such as flow rate and blood vessel diameter. Proper drug dosage choice relies on determination of the attachment and detachment rates of nanoparticles and understanding the complex process of targeted drug delivery. Computational modeling of the nanoparticle delivery process is either limited to a single nanoparticle description, or a continuum concentration description. To correlate the nanoparticle design to its delivery efficiency, it is important to link the particulate nature of the particle to the macroscopic convection-diffusion transport process. In this work, a combined particulate and continuum model is developed to understand the binding dynamics of nanoparticles under vascular conditions. The ligand-receptor binding kinetics is coupled with Brownian dynamics to study the dynamic delivery process of a single nanoparticle under various vascular flow conditions. The effective binding and debinding rates of a particulate nanoparticle design are determined from the particulate model and then coupled into a continuum convection-diffusion-reaction model. The effect of shear rate, particle size, and vascular geometry on bound density of nanoparticles is explored using the coupled multiscale model. The developed multiscale model is expected to give insights into the complex drug delivery process and contribute to the fundamental understanding and knowledge on how particle design affects the transport and targeting efficiency of nanocarriers.