A Study of Behavior for Magnetic Nanoparticles in Vascular System Through LAMMPS

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Nanoparticles have been developed for various biomedical applications. Magnetic nanoparticles have earned significant interest in research in recent years due to their magnetic properties, which can respond and be manipulated by external magnetic field, enabling a variety of prospects for biomedical applications, for example, specific targeting for therapeutic applications. However, when magnetic nanoparticles form a cluster, which can form in different shapes and differently correspond to external magnetic field, leading to difficulty in controlling the particles and application. Here, we present a model of magnetic nanoparticles in blood flow built by LAMMPS, a highly utilized program for molecular dynamics simulations of nanoparticles, to enable studies of the behavior of magnetics nanoparticles in blood flow, in aspect of cluster shape forming and margination of the clusters. Clusters are categorized into four types: linear, dispersed, ring, and lumpy. We consider three factors for simulation condition: the properties of the particles, interface between particles and fluid, and fluid interactions. The simulation shows that an increase in the pairwise potential tends to destabilize the former linear pattern and resulted in the formation of more lumpy patterns. In the margination regime, fluid flow leads to higher portion of lumpy clusters and shorter clusters. Moreover, clusters response differently to an external magnetic field. By finding effects of these factors to shape magnetic particle clusters and their response to external magnetic field to an external magnetic field, this research can give us an insight in development of design of more efficient drug delivery that implements magnetic nanoparticles for targeting desired site in biomedical uses.

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