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MD Simulation of Colloidal Particles Transportation in a Fiber Matrix

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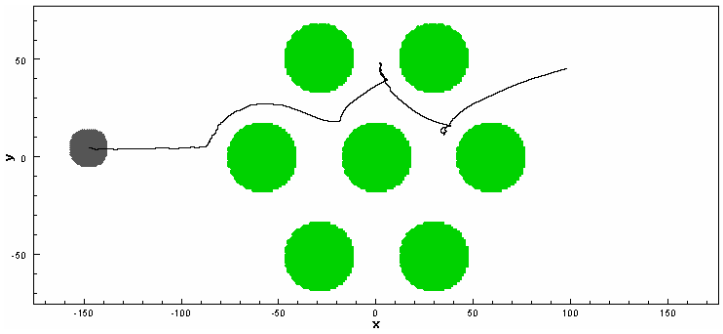
Summary

Surface glycocalyx, as a barrier to material exchange between circulating blood and body tissues, was always treated as a periodic square array of cylindrical fibers. Previous study treated the glycocalyx as porous media and simulated by continuum theory. However, it has recently been found that a relatively hexagonal fibre-matrix structure may be responsible for the ultrafiltration properties of microvascular walls. The fibre-matrix is an underlaying three-dimensional meshwork with a fibre diameter of 10∼12 nm and characteristic spacing of about 20 nm. To study the permeable characteristics of nanosize particle in such fibre-matrix structure, the porous medium assumption may not be appropriate. Molecular dynamics (MD) simulation is a powerful method to simulate the fluid flow at the molecular level, it has been applied successfully in many fields including hydrodynamics and demonstrated surprising results at the nanoscales different from their macroscopic counterparts. Here we use MD to investigate the permeable characteristics of nanoparticle in the new quasi-periodic ultra-structure of the endothelial glycocalyx. As a first attempt, fibre-matrix is simplified as a two dimensional periodic system in which the colloidal particles, fluid solvent, fibers are all treated as atomic systems, and the study is focused on the effect of particle size on transport properties.



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