Multiscale modeling of mechanosensing channels on vesicles and cell membranes in 3D constricted flows and shear flows

ZHANGLI PENG, University of Notre Dame, ON SHUN PAK, Santa Clara University, YUAN-NAN YOUNG, New Jersey Institute of Technology, ALLEN LIU, University of Michigan, HOWARD STONE, Princeton University — We investigate the gating of mechanosensing channels (Mscls) on vesicles and cell membranes under different flow conditions using a multiscale approach. At the cell level (microns), the membrane tension is calculated using a 3D two-component whole-cell membrane model based on dissipative particle dynamics (DPD), including the cortex cytoskeleton and its interactions with the lipid bilayer. At the Mscl level (nanometers), we predict the relation between channel gating and the membrane tension obtained from a cell-level model using a semi-analytical model based on the bilayer hydrophobic mismatch energy. We systematically study the gating of Mscls of vesicles and cell membranes in constricted channel flows and shear flows, and explore the dependence of the gating on flow rate, cell shape and size. The results provide guidance for future experiments in inducing Mscl opening for various purposes such as drug delivery.