Abstract Submitted
for the DFD20 Meeting of
The American Physical Society

Coarse-grained Modeling of Liposome Nano-extrusion Using Fluctuating Lattice Boltzmann Method MEGHDAD RAZIZADEH, MEHDI NIKFAR, YALING LIU, Lehigh University — Liposome nano-extrusion is a popular technique to produce small liposomes by squeezing large lipid vesicles through an array of nanochannels. There is little understanding of such a small-scale dynamic process. An implicit solvent, coarse-grained (CG) model is utilized to study nanoscale topological changes of lipid vesicles. The CG model is coupled with a fluctuating Lattice-Boltzmann flow solver that transfers fluid velocities and thermal fluctuations between CG beads and fluid lattice points. We analyzed the effects of liposome size on the pore formation and rupture process by modeling the squeezing of lipid vesicles with the diameter of D=40-100nm through channels with various widths and lengths. The Reynolds number, defined by the vesicle diameter and maximum squeezing velocity, is in the range of 1-100. Results show that initial pore formation is more probable for larger vesicles, narrower constrictions, and higher Reynolds numbers. Moreover, three different regimes of passing without damage, transient hydrophilic pore formation, and complete rupture, are identified by performing a complete parametric study.

Meghdad Razizadeh
Lehigh University

Date submitted: 20 Nov 2020 Electronic form version 1.4