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Numerical simulation of shear-induced drug encapsulation. MEHDI NIKFAR, MEGHDAD RAZIZADEH, YALING LIU, Lehigh Univ — Recent studies show that shear-induced drug loading methods in the microfluidic device is an efficient intracellular drug loading approach. In this study, a cellular-scale numerical model based on dissipative Lattice Boltzmann Method and spring connected network is utilized for modeling the drug encapsulation into a compound cell after rapid squeezing through microfluidic channels. The radius of the shear-induced pores is computed via a mathematical correlation derived from the results of coarse-grained molecular dynamics. We assume that the drug loading occurs after squeezing as a result of passive diffusion. To calculate the drug concentration inside the cell, a mathematical correlation is proposed for passive diffusion after squeezing. The numerical algorithm is validated by simulation a compound cell under simple shear flow. Upon the validation, the drug concentration inside the cell is quantified for different range of squeezing velocities, constriction lengths and constriction widths. The results show that the drug loading is enhanced by increasing the squeezing velocity, increasing the constriction length and decreasing constriction width. Our results are qualitatively in agreement with experimental observations.

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