Coupled Problems Arising in the Design of Drug Carriers

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ABSTRACT

Nano-scale liposomes have proven to be highly effective and versatile drug delivery vehicles. One of the mechanisms they rely on to deliver drugs to cell interiors is membrane fusion. Liposomes that contain cationic lipids are known for their high fusogenicity. However, concerns arise regarding the toxicity of these lipids when used at high concentrations. Therefore, designing delivery liposomes that offer both high fusogenicity and low toxicity is a challenge. This challenge may be overcome by controlling the surface density of cationic lipids on the surface of liposomes using membrane phase separation.

To aid the design of phases-separated liposomes, we created a computational platform that simulates membrane phase-separation coupled to fluid flow and electrostatic interactions. The underlying model is written for tangential flows of fluids constrained to a surface and consists of (surface) Navier-Stokes-Cahn-Hilliard type equations. For its numerical solution, we apply an unfitted finite element method and a scheme that decouples the fluid and phase-field equation solvers at each time step. We provide numerical examples to demonstrate the stability, accuracy, and overall efficiency of our approach and provide validation against experimental data.