Modeling of Membranes with Complex Rheology: Computational Aspects

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October 13, 2016

The mathematical and computational modeling of the equilibrium and dynamic behavior of membranes is a general problem in mechanics and biomechanics with a wide application to the medicine, pharmacy, foam and emulsion technologies, etc. The protein adsorption layers, phospholipid mono- and multilayers (biomembranes), floating thin polymer films, layers of nanoparticles on oil/water interfaces, monolayers of metal-organic complexes, etc. are modeled as 2D elastic membranes, which interact with the surrounding bulk phases.

We developed a theoretical model for 2D elastic continuum, which accounts for the complex rheology of interfaces. The parameters of the model are the surface (membrane) stretching and shear elasticity, Helfrich curvature elastic moduli. It is a special case of the general concept of Cosserat continuum with bending elasticity. The final result is a system of six strongly nonlinear partial differential equations, which expresses:

1. The surface balance of the linear momentum written for the pressure difference and surface stress tensor;

2. The surface balance of the angular momentum written for the surface torque and stress tensors.

To close the system of equations we use surface rheological constitutive relationships - the dependencies of the stress and torque tensors on the metric and curvature tensors of membrane surface. When one defines the necessary boundary conditions one should solve numerically the respective boundary value problem. For known physical constants the boundary value problem has many solutions and the criterion for the physical one is the minimization of the free energy of the system. For that reason original numerical methods are developed.

The model is applied to and verified with experimental data for different systems. In the case of biomembranes it is used to determine the membrane tension and adhesion energy of erythrocytes and the mechanism of stomatocyte-echinocyte transformations of red blood cells [1,2]. For elastic Langmuir layers and membranes the model is applied to calculate various shapes (nonharmonic oscillations, toothed profiles, and profiles with two characteristic wavelengths) and the bending elasticity [3]. Different numerical schemes for real time data processing of rotating axisymmetric drops are compared in Ref. [4]. The numerical procedures for calculation of experimental values of the components of stress tensors and energy of adhesion of drops and bubbles at different interfaces become a basis of the capillary meniscus dynamometry (CMD) realized on commercial apparatuses.

References:

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