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# A Second Order Accurate in Time, Energy Stable Finite Element Scheme for a Liquid Thin Film Coarsening Model

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**Abstract.** In this paper, we propose and analyze a second order accurate (in time) mass lumped mixed finite element numerical scheme for the liquid thin film coarsening model with a singular Leonard-Jones energy potential. The backward differentiation formula (BDF) stencil is applied in the temporal discretization, and a convex-concave decomposition is derived, so that the concave part corresponds to a quadratic energy. In turn, the Leonard-Jones potential term is treated implicitly and the concave part is approximated by a second order Adams-Bashforth explicit extrapolation. An artificial Douglas-Dupont regularization term is added to ensure the energy stability. Furthermore, we provide a theoretical justification that this numerical algorithm has a unique solution, such that the positivity property is always preserved for the phase variable at a point-wise level, so that a singularity is avoided in the scheme. In fact, the singular nature of the Leonard-Jones potential term around the value of $0$ and the mass lumped FEM approach play an essential role in the positivity-preserving property in the discrete level. In addition, an optimal rate convergence estimate in the $\ell^\infty(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$ norm is presented. Finally, two numerical experiments are carried out to verify the theoretical properties.

**AMS subject classifications**: 60F10, 60J75, 62P10, 92C37

**Key words**: Liquid thin film model, second order accuracy, mass lumped mixed FEM, positivity preserving, energy stability, optimal rate convergence analysis.

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## 1. Introduction

Certain liquids on a solid, chemo-attractive substrate spontaneously form a droplet structure connected by a very thin precursor (or wetting) layer. After the droplets appear, coarsening will occur, whereby smaller droplets will shrink and larger droplets will grow. The coarsening behavior, especially the rate of coarsening, of droplets has been of great scientific interest [38]. The average droplet size increases with the decrease of the number of droplets and the increase of the characteristic distance. The droplet coarsening model with a singular Lennard-Jones energy potential involved mainly describes the coarsening phenomenon of droplets. The related content of liquid thin film coarsening phenomenon and some numerical simulation results can be found in [7, 8, 14, 20, 24, 30].

Under the assumption that the liquid film does not evaporates, lubrication theory leads to a single equation for the height function, $\phi = \phi(\mathbf{x}, t) > 0$, of a time-dependent film [20], in the form of an $H^{-1}$ gradient flow

$$\partial_t \phi = \nabla \cdot \big(\mathcal{M}(\phi)\nabla \delta_\phi F\big).$$

Here $F$ is the free energy of the film/substrate system and is given by

$$F(\phi) = \int_\Omega \left(\mathcal{U}(\phi) + \frac{\varepsilon^2}{2}|\nabla\phi|^2\right) d\mathbf{x}, \tag{1.1}$$

where $\phi : \Omega \to \mathbb{R}$ is a periodic height function, $\varepsilon > 0$ is the surface diffusion coefficient, and

$$\mathcal{U}(\phi) = \frac{1}{3}\phi^{-8} - \frac{4}{3}\phi^{-2}$$

is the well-known Lennard-Jones-type potential [12]. The $H^{-1}$ gradient flow associated with the given free energy functional (1.1) with constant mobility $\mathcal{M}(\phi) \equiv 1$ (non-constant mobility case could be handled in a similar way) is

$$\partial_t \phi = \Delta\mu, \quad \mu := \delta_\phi F = -\frac{8}{3}(\phi^{-9} - \phi^{-3}) - \varepsilon^2\Delta\phi. \tag{1.2}$$

Obviously, this problem is mass conservation. Due to the gradient structure, the following energy dissipation law is formally available:

$$\frac{d}{dt}F\big(\phi(t)\big) = -\int_\Omega |\nabla\mu|^2\, d\mathbf{x} \le 0.$$

In addition, from the mathematical expression, the structure of the potential function requires that the phase variable has to maintain a fixed sign, that is, being either positive or negative, to avoid a singularity. A positivity-preserving structure is required for the numerical scheme and for physical reality [38]. For simplicity of presentation, we assume periodic boundary conditions hold over the rectangular domain $\Omega$. Other types of boundary conditions, such as homogeneous Neumann, can also be handled.