INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 20, Number 4, Pages 459–477

doi: 10.4208/ijnam2023-1019

UNCONDITIONAL ENERGY STABILITY AND SOLVABILITY FOR A C0 INTERIOR PENALTY METHOD FOR A SIXTH-ORDER EQUATION MODELING MICROEMULSIONS

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Abstract. We consider a C0 interior penalty finite element approximation of a sixth-order Cahn-Hilliard type equation that models the dynamics of phase transitions in ternary oil-water-surfactant systems. The nonlinear sixth-order parabolic equation is expressed in a mixed form whereby a second-order (in space) parabolic equation and an algebraic fourth-order (in space) nonlinear equation are considered. The temporal discretization is chosen so that a discrete energy law can be established leading to unconditional energy stability. Additionally, we show that the numerical method is unconditionally uniquely solvable. We conclude with several numerical experiments demonstrating the unconditional stability and first-order accuracy of the proposed method.

Key words. Finite element, Cahn-Hilliard, unconditional energy stability, microemulsions and unique solvability.

1. Introduction

Microemulsion systems are of great interest across many different fields due to the flexibility of these models to adapt to a variety of applications such as oil recovery [2], development of environment-friendly solvents [1], consumer and commercial cleaning product formulations [3], and drug delivery systems [4]. One such model, which is outlined below, can be described as a sixth-order conserved evolution system that models the dynamics of phase transitions in ternary oil-water-surfactant systems. This model was introduced and studied by Gompper and co-authors in [5, 6, 7, 8, 9] and has demonstrated great ability in capturing many essential static properties of the ternary oil-water-surfactant systems. The existence and uniqueness of strong and weak solutions have been analyzed by Pawlow et al. in [10, 11].

Assume that $\Omega \subset \mathbb{R}^2$ is a bounded polygonal domain occupied by the oil-water-surfactant mixture with boundary $\partial\Omega$. Then, according to Gompper [9], the free energy functional assumes the form

$$E(\phi) = \int_\Omega f_0(\phi)\ dx + \frac{1}{2}\int_\Omega \left\{(\phi^2 - a_0)|\nabla\phi|^2 + \lambda(\Delta\phi)^2\right\}\ dx, \tag{1}$$

where ϕ is the scalar order parameter representing the local difference between oil and water concentrations and a_0 and λ are positive constants. Here, $f_0(\phi)$ denotes the volumetric nonlinear free energy functional which has the form

$$f_0(\phi) = \frac{\beta}{2}(\phi-1)^2(\phi^2+0.5)(\phi+1)^2 = \frac{\beta}{2}\Big(\phi^6 - 1.5\phi^4 + 0.5\Big),$$

and possesses three extrema at $\phi = \pm 1,\ 0$ which correspond to the water-rich (-1), oil-rich (+1), and microemulsion (0) phases. We note that while this model

Received by the editors on September 7, 2022 and, accepted on March 7, 2023.
2000 *Mathematics Subject Classification.* 65M60, 74N20, 74S05.
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is defined for an arbitrary choice of a_0, in this paper, we limit the range of a_0 to positive numbers. The impact of a_0 can be explained as follows. When the surfactant is added to the system, a minimum develops in the microemulsion phase which is represented by $\phi = 0$. The minimum is of value $-a_0$. When surfactant concentration is increased, the phase field ϕ satisfies $\phi^2 < a_0$. For a detailed discussion, we direct the interested reader to [10] and references therein.

To construct a system of equations representing the dynamics of phase transitions in ternary oil-water-surfactant systems, we follow Pawlow and Zajaczkowski [10] and assume the initial value condition

$$\phi(0) = \phi_0 \in H^4(\Omega) \text{ such that } \mathbf{n} \cdot \nabla\phi_0 = \mathbf{n} \cdot \nabla\Delta\phi_0 = 0 \text{ on } \partial\Omega, \tag{2}$$

and homogeneous Neumann-type boundary conditions

$$\mathbf{n} \cdot \nabla\phi = \mathbf{n} \cdot \nabla\Delta\phi = \mathbf{n} \cdot \nabla\mu = 0. \tag{3}$$

Additionally, we consider the following conservation law

$$\partial_t\phi - \nabla \cdot (\mathcal{M}\nabla\mu) = 0, \tag{4}$$

where $\mathcal{M} > 0$ is a constant mobility and μ is the chemical potential given by $\delta_\phi E$, i.e. the variational derivative of the energy functional E with respect to ϕ:

$$\mu := \delta_\phi E = 3\beta(\phi^5 - \phi^3) + \phi|\nabla\phi|^2 - \nabla \cdot ((\phi^2 - a_0)\nabla\phi) + \lambda\Delta^2\phi. \tag{5}$$

Therefore, we consider the following system of equations for which the well-posedness was established in [10]:

$$\partial_t\phi - \nabla \cdot (\mathcal{M}\nabla\mu) = 0, \tag{6a}$$

$$3\beta(\phi^5 - \phi^3) + \phi|\nabla\phi|^2 - \nabla \cdot ((\phi^2 - a_0)\nabla\phi) + \lambda\Delta^2\phi - \mu = 0. \tag{6b}$$

The following theorem establishes the energy stability of the above system.

Theorem 1.1. *Let ϕ be a sufficiently regular solution to the system* (6)*. Then, for $t \geq 0$, the following equality holds.*

$$\frac{d}{dt}\Big(\int_\Omega f_0(\phi)\ dx + \frac{1}{2}\int_\Omega \left\{(\phi^2 - a_0)|\nabla\phi|^2 + \lambda(\Delta\phi)^2\right\}\ dx\Big) + \ \mathcal{M}\int_\Omega |\nabla\mu|^2\, dx = 0.$$

Proof. The proof can be found in Lemma 3.1 from [10]. □

Despite its popularity, there has been a lack of available numerical schemes solving these systems. Indeed, the only established numerical method developed for the model (6) known to the authors was introduced by Hoppe and Linsenmann in [12] in which a C^0 interior penalty (C0-IP) method was utilized for spacial discretization but where a fully implicit backward Euler time discretization strategy was adopted for the error analysis. As such, the work presented in that paper focuses on establishing quasi-optimal error estimates but no discrete energy law is obtained.

Similar to the work presented in [12], we propose a spacial discretization based on the C0-IP method. These methods are characterized by the use of C^0 Lagrange finite elements where C^1 continuity requirements imposed by utilizing a conforming mesh are replaced with interior penalty techniques. C0-IP methods were first introduced by G. Engel et.al. in [13] and revisited and analyzed by Brenner et.al. in [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24] and further investigated by others in [25] and [26] to solve the fourth-order biharmonic problem. However, in contrast to the work presented by Hoppe and Linsenmann, we propose a time discretization strategy from which a discrete energy law closely related to (1) is satisfied by solutions to