CSIAM Trans. Appl. Math.
doi: 10.4208/csiam-am.SO-2021-0036

Vol. **3**, No. 3, pp. 480-514
September 2022

An Efficient and Unconditionally Energy Stable Fully Discrete Scheme for the Confined Ternary Blended Polymers Model

Guanghua Ji[1], Zhen Xu[2] and Yuqi Yang[1,*]

[1] *Laboratory of Mathematics and Complex Systems (Ministry of Education), School of Mathematical Sciences, Beijing Normal University, Beijing 100875, P.R. China.*
[2] *Faculty of Science, Beijing University of Technology, Beijing, 100124, P.R. China.*

Received 9 July 2021; Accepted 19 December 2021

Abstract. In this paper, we develop a fully discrete scheme to solve the confined ternary blended polymers (TBP) model with four order parameters based on the stabilized-scalar auxiliary variable (S-SAV) approach in time and the Fourier spectral method in space. Then, theoretical analysis is given for the scheme based on the backward differentiation formula. The unconditional energy stability and mass conservation are derived. Rigorous error analysis is carried out to show that the fully discrete scheme converges with order $\mathcal{O}(\tau^2+h^m)$ in the sense of the L^2 norm, where τ is the time step, h is the spatial step, and m is the regularity of the exact solution. Finally, some numerical results are given to demonstrate the theoretical analysis. Moreover, the phase separation of two kinds of polymer particles, namely, Ashura and Janus core-shell particles, is presented to show the morphological structures.

AMS subject classifications: 65H10, 65M06, 65M22

Key words: Confinement, ternary blended polymers, unconditional energy stability, error estimates, Fourier spectral method.

1 Introduction

Nanostructured polymer particles have attracted some experimental and theoretical studies because they have been widely applied in biological, photonic, mechanical and many other fields, such as drug delivery [6, 32], photonic materials [1, 31, 33, 34], electronic ink [2, 40] and so on [17, 18, 24, 38]. To produce various kinds of polymer blended particles, H. Yabu et al. [39] proposed a simple method called the self-organized precipitation

*Corresponding author. *Email addresses:* ghji@bnu.edu.cn (G. Ji), xuzhenmath@bjut.edu.cn (Z. Xu), 201721130050@mail.bnu.edu.cn (Y. Yang)

(SORP) method. The process is introduced as follows. First, two miscible solvents should be prepared: volatile (good) and nonvolatile (poor). Polymers are dissolved in the good solvent, and then, the poor solvent is mixed into the polymer emulsion. After the good solvent is completely evaporated, uniformly sized polymer blended particles will form in the poor solvent.

Using the SORP method, various kinds of nanostructured polymer particles in binary polymer blended systems can be prepared. Janus-type particles [14] and core-shell-type particles [41] can be formed from polymer blends. Lamellar, onion, screw, wheel, mushroom and tennis structures can be formed from block copolymer blends [15]. Moreover, in [37], ring, helix and multi-pod structures are prepared.

To prepare ternary polymer blended particles, Y. Hirai et al. [16] studied the relationship between the surface tensions of polymers and the phase-separated structures in binary polymer blended systems. They found that when the two polymers both have low surface tensions, Janus-type particles are formed. A combination of low and high surface tension polymers forms core-shell-type particles, in which the polymer with the lower surface tension forms the core and the polymer with the higher surface tension forms the shell. Thus, in ternary polymer blended systems, three polymers with low surface tensions form Ashura particles, and if one of the polymers has a much higher surface tension, they form Janus core-shell particles.

Here, we pay more attention to how to simulate the phase separation of different structures in ternary polymer blended systems. In [16], a model of phase separation based on Cahn-Hilliard equations with four order parameters, namely, confined ternary blended polymers (TBP) model, was constructed to describe the dynamical systems of Ashura and Janus core-shell particles. Moreover, a semi-implicit scheme was implemented to simulate the phase separation process. However, Hirai et al. only focused on the physical experiment and simulation results of the confined TBP model. It lacks of energy stable schemes and numerical analyses, which is what we concern about.

In fact, there are many numerical methods that have been applied for solving coupled Cahn-Hilliard equations, with the aim of developing energy stable schemes. Examples are the convex splitting method [12, 13], the stabilization method [29, 30, 43], the invariant energy quadratization (IEQ) approach [42], the scalar auxiliary variable (SAV) approach [27, 28] and the new Lagrange Multiplier approach [10]. These approaches provide different methods of time discretization. A. Edgar et al. [3, 4] used the linear splitting method to solve two coupled Cahn-Hilliard equations with a nonlocal term. Q. Li et al. [19] used the scalar auxiliary variable (SAV) approach to achieve two second-order, efficient, decoupled, and linear numerical schemes for the block copolymer. Using the new Lagrange Multiplier approach combined with the stabilization method, a second-order and unconditionally energy stable scheme for the coupled nonlocal Cahn-Hilliard system was proposed by Q. Cheng et al. in [10]. C. Chen et al. [7] established a ternary Cahn-Hilliard-type Nakazawa-Ohta phase-field model for the triblock copolymer and solved the model via the stabilized-SAV (S-SAV) approach.

For the confined TBP model, we have two main tasks. The first task is constructing