Journal of Computational Mathematics
Vol.35, No.1, 2017, 37–51.

http://www.global-sci.org/jcm
doi:10.4208/jcm.1607-m2014-0109

ENERGY STABLE NUMERICAL METHOD FOR THE TDGL EQUATION WITH THE RETICULAR FREE ENERGY IN HYDROGEL*

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Abstract

Here we focus on the numerical simulation of the phase separation about macromolecule microsphere composite (MMC) hydrogel. The model is based on time-dependent Ginzburg-Landau (TDGL) equation with the reticular free energy. An unconditionally energy stable difference scheme is proposed based on the convex splitting of the corresponding energy functional. In the numerical experiments, we observe that simulating the whole process of the phase separation requires a considerably long time. We also notice that the total free energy changes significantly in initial stage and varies slightly in the following time. Based on these properties, we apply the adaptive time stepping strategy to improve the computational efficiency. It is found that the application of time step adaptivity can not only resolve the dynamical changes of the solution accurately but also significantly save CPU time for the long time simulation.

Mathematics subject classification: 65M06, 65M12, 65Z05.
Key words: TDGL equation, Unconditionally energy stable scheme, Adaptive time-stepping method, Phase transition.

1. Introduction

Hydrogels, which are polymer with 3-D crosslinked hydrophilic network structure, have increasingly extensive applications in industrial and biomedical fields [9,10,26]. Therefore, hydrogels have recently received tremendous attention in scientific communities due to their enhanced properties [1, 16]. Comparing with traditional hydrogels with poor mechanism, recently there has been a lot of novel methods to improve the structure of hydrogels and thus significantly enhancing their mechanical properties [9,10,12], e.g., topological (TP) gels [3,4], nanocomposite (NC) hydrogels [8], double-network (DN) gels [4, 7], MMC hydrogels and so on [9, 10]. MMC hydrogels, which were synthesized by Ting Huang in 2007 [9], have a unique well-defined microstructure and very high mechanical strength. MMC hydrogels are environmentally sensitive and mainly possible to use in drug delivery and other biomedical applications [22]. Many works in chemical structure and dynamics simulation have been done about TP gels, NC hydrogels, and DN gels and much progress has been made [5,11,12,25]. But there are relatively less results about MMC hydrogels [23,24]. Why the MMC hydrogels have such high mechanical strengths?

* Received October 24, 2014 / Revised version received June 13, 2016 / Accepted July 5, 2016 / Published online January 18, 2017 /

What are relation between the structure and property? The structural factors: nanoparticle size, grafting density, polymer chain length, chain conformation, entanglement, how to influent the phase transition? These problems are very important. Now we have investigated the microscopic structures in [24] and large deformation of the MMC hydrogels in [23]. The MMC-TDGL model have been given to get the phase transition of the MMC hydrogels [26]. But it is very large for the computational cost of the MMC-TDGL model. In the following we will introduce the model in details.

Meanwhile, many computational methods have been developed and applied in modeling and simulation of phase separation of hydrogels. They range from molecular scale (e.g., molecular dynamics, Monte Carlo), microscale (e.g., Brownian dynamics, dissipative particle dynamics, lattice Boltzmann, TDGL method, dynamic density functional theory method) to mesoscale and macroscale (e.g., micromechanics, equivalent-continuum and self-similar approaches, finite element method) [25]. These methods are foundation to simulate phase separation of hydrogels. However, observing the whole process of phase separation is computationally expensive and costs a large amount of time when these methods are used. Therefore, seeking for algorithms to decrease computation cost is an urgent task. The adaptive time-stepping method is introduced here. Adaptive time stepping method has been well studied for solving initial value problems in ODEs. The review work [18, 19] summarizes several step control methods for local time adaptivity based on linear feedback theory. A locally varying time step method is developed for solving hyperbolic conservative PDEs where large time step is adopted on region with smooth solution while small time step is taken in domain with nearly singular solution within same time level [20]. In [17], the adaptive time-stepping technique has been developed based on energy variation which is an important physical quantity in the molecular beam epitaxy growth model. Following [17], we improve the choice of adaptive time step according to properties of TDGL equation.

In this work, considering the MMC hydrogels have microstructure with network crosslinking points, we exploit the TDGL method to simulate phase evolution of MMC hydrogels based on reticular free energy deduced in [26], called as the MMC-TDGL model. TDGL method is an accurate and robust method to simulate structural evolution of phase separation in polymer blends and copolymers and many nice results have been gotten in numerical experiments [1, 14, 25]. The main objective of this work is to develop an unconditional energy stable method for the MMC-TDGL model and apply adaptive time step strategy to the algorithm. Our numerical approach is based on the convex splitting of the discrete energy functional. The convex part is discretized using implicit scheme, while the concave part is handled by using explicit scheme. The mass conservation and energy law in discrete sense are proved theoretically. The unique solvability is obtained by minimizing an equivalent convex discrete functional. A couple of numerical experiments are implemented to observe the phase evolution of the model. And also the effectiveness of the adaptive time step method is shown clearly by comparing the CPU time. During the time period with rapid free energy decay, small adaptive time steps are chosen adaptively, while large time steps are used when free energy varies slowly.

This paper is organized as follows. In Section 2, the MMC-TDGL equation is introduced in detail with the reticular free energy. The model is derived based on the variational derivative of the corresponding energy functional. In Section 3, the unconditional energy stable scheme is proposed and some numerical analysis are given. In Section 5, some numerical experiments are performed to observe the phase evolution of the model. In Section 6, based on observations, we propose a suitable adaptive time-stepping strategy and show the effectiveness numerically.