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AGGREGATION OF HYDROXYPROPYL CELLULOSE IN DILUTE SOLUTIONS WITH SALT IONS

The kinetics of the phase transition in an aqueous solution of hydroxypropyl cellulose with salt ions have been studied using mathematical modeling. Based on the nonlinear Cahn–Hilliard equation with a stochastic term, the hydrophobicity parameter, and the mobility parameter depending on the polymer concentration, the phase separation on a simple one-dimensional Flory lattice was simulated. Data on changes in the average sizes and masses of aggregates were obtained for a set of hydrophobicity parameter values. The simulation results allowed the distinction of three stages of spinodal decomposition: early, intermediate, and final. It was found that the kinetics of cluster mass growth at the intermediate and final stages are described by scaling dependencies, with the power exponents and the crossover time determining the transition from the mode of aggregate mass accumulation driven by surface tension effects to the diffusion mode. It was shown that the variation of the average cluster size can be approximated by a scaling function with a power exponent close to 1/3, which is typical of systems with a conservative scalar order parameter. From the results of computer simulation, it follows that the growth of the interfacial energy density (the enhancement of hydrophobic interactions) makes the size of polymer aggregates larger.

Keywords: hydroxypropyl cellulose, salt ions, aggregation, Cahn–Hilliard equation.

1. Introduction

A characteristic feature of many water-soluble cellulose ethers is their thermoreversible behavior [1], which consists in their ability to change their solubility and consistency as the temperature changes. Solutions of such polymers, when heated, undergo a transition from a liquid state to a gel, and when cooled back, they become liquid again. This phenomenon is called the "sol-gel" phase transition and depends on the structure and degree of modification of cellulose derivatives, the macromolecules of which contain hydrated hydroxyl groups that form hydrogen bonds with water molecules and thus ensure the solubility of the polymer. When the temperature increases, the hydrogen bonds between the polymer and water weaken. In addition, new bonds can form between the molecules of the ester itself. This leads to a reduction in the hydration of the polymer, its aggregation, and the formation of a three-dimensional gel-like structure. If the temperature decreases, the hydrogen bonds are restored, the gel dehydrates and dissolves, and the solution returns to its original liquid state.

The sol-gel transition temperature depends on a number of factors, such as the polymer concentration, the type and degree of substitution [2–4], the pH value [5–8], and the presence of electrolytes in the

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solution [9–13]. A number of works are devoted to the study of the thermosensitive behavior of aqueous solutions of cellulose derivatives with salt ions [9–11,14–19]. In those articles, the mechanisms of phase transition were studied mainly as functions of the type of salt additives and their concentration. In particular, it was shown that the thermosensitive behavior of the polymer solution is governed by the competition between polymer chains and salt ions for interaction with water molecules, which leads to the formation of hydrophobic aggregates [9–12].

Aggregation and precipitation of polymer clusters from dilute solutions have an important practical significance for the development of promising technologies, such as catalysts with controlled activity, nanocomposite film materials [20, 21], and bactericidal polymer films applied to treat wounds [22, 23]. Note that the targeted control of the aggregation process can be achieved by introducing ionic additives into polymer solutions [24], which makes it possible to directly change the structure of microgels and obtain the desired film structure by precipitation. This is important for achieving predictable and stable material characteristics.

In our recent publications [25, 26], the microstructural properties of dilute solutions of hydroxypropyl cellulose with salt ions were studied using the method of static and dynamic light scattering. It was found [25] that at temperatures higher than the phase transition temperature and in the presence of ions in the researched systems, substantial supramolecular associates emerge (clusters), the size of which exceeds the wavelength of visible light by several times. The precipitation of the polymer was observed. In Ref. [26], the conditions for the formation of precipitating microgels were formulated. In this work, as a continuation of Refs. [25, 26], a mathematical model is proposed for the hydrophobic association of polymer molecules in solutions with salt ions.

2. Aggregation of Polymer Molecules in Solutions: the Role of Hydrophobic Interactions

The structural and rheological properties of polymer gels based on cellulose derivatives are intensively studied. All experimental data accumulated to date testify that spinodal decomposition is the mechanism of phase separation in such systems [27–30]. Spinodal decomposition is the initial stage of phase transformation if the system is preliminarily brought into a thermodynamically unstable state. This instability at a given temperature corresponds to the region where the free energy depends on concentration, and its second derivative is negative. During spinodal decomposition, solution regions with an increased or decreased concentration with respect to its average value (clusters), which arise as a result of thermal fluctuations, become stable and begin to grow. This process is supported by upward diffusion [31], when the mutual attraction of particles of the same type makes their concentration in the cluster even higher and the neighboring solution zone more depleted.

When describing the features of phase formation in the spinodal decomposition region, one of the most successful approaches is the Cahn–Hilliard model [32–34], developed on the basis of the free energy density functional method [35, 36]. The Cahn–Hilliard equation does not contain any microscopic data on the described system, but it includes such macroscopic characteristics as the diffusion coefficient, free energy, and interfacial energy. The free energy density functional method allows the coagulation of clusters during the growth of a new phase to be described in a natural way without any approximations [36].

The Ginzburg–Landau type functional for the total energy of the polymer-solvent system has the form [37]

$$U[\phi] = \int d\mathbf{r}\Big\{F(\phi) + \kappa(\phi)|\nabla\phi|^2\Big\}, \quad \phi = \phi(\mathbf{r}, t), \quad (1)$$

where ϕ is an order parameter, whose meaning is the polymer concentration in the solution, and $F(\phi)$ is the free energy density. The second term in the integrand describes the contribution of spatial correlation effects to the free energy with the gradient coefficient [38]

$$\kappa(\phi) = \frac{a^2}{36\phi(1-\phi)}, \quad (2)$$

where a is the size of a polymer chain segment, which is equal to unity in the Flory model [39].

Let us introduce an additional parameter γ into relation (1):

$$U[\phi] = \int d\mathbf{r}\,\Big\{F(\phi) + \gamma\kappa(\phi)|\nabla\phi|^2\Big\}. \quad (3)$$

The physical meaning of γ is as follows. In the works of Cahn and Hilliard [32, 33], it was shown that the coefficient of interfacial surface tension equals

$$\sigma_{\mathrm{i}} \sim \int d\mathbf{r}\, \kappa(\phi)|\nabla\phi|^2. \tag{4}$$

Macromolecules of cellulose derivatives are amphiphilic, i.e., their structure contains both nonpolar and polar hydrophilic regions. In electrolyte solutions, the latter compete with salt ions for interaction with water molecules [9–11, 16]. As a result, the number of hydrophilic water-polymer bonds decreases, and the interfacial energy density, accordingly, increases. In other words, the enhancement of hydrophobic interactions at the polymer-solvent interface leads to an increase in σ_{i}. Therefore, by changing the value of the parameter γ in formula (3), it is possible to "control" the degree of polymer hydrophobicity.

The Cahn–Hilliard equation, which describes the evolution of polymer concentration at a point $\mathbf{r}$ in space and at the time t, looks as follows [37]

$$\frac{\partial\phi}{\partial t} = \nabla\left\{M\nabla\frac{\delta U[\phi]}{\delta\phi}\right\} + \xi, \tag{5}$$

where M is the mobility, and $\xi = \xi(\mathbf{r}, t)$ is a stochastic function (thermal noise) satisfying the fluctuation–dissipation theorem [40]. To solve Eq. (5) with functional (3), we use the Flory–Huggins free energy in the form [39, 41]

$$F(\phi) = N^{-1}\phi\ln\phi + (1-\phi)\ln(1-\phi) + \chi\phi(1-\phi), \tag{6}$$

where N is the degree of polymerization of the molecular chain, and χ is the Flory–Huggins parameter describing the pairwise interaction of monomers. Calculating the variational derivative of the total energy in Eq. (5) gives

$$\frac{\delta U[\phi]}{\delta\phi} = f(\phi) - \gamma\big(\lambda(\phi)|\nabla\phi|^2 + 2\kappa(\phi)\Delta\phi\big), \tag{7}$$

where

$$f(\phi) = N^{-1}(1 + \ln\phi) - \ln(1-\phi) - \\ - \chi(2\phi - 1) - 1, \tag{8}$$

$$\lambda(\phi) = \frac{2\phi - 1}{36\phi^2(1-\phi)^2}. \tag{9}$$

Let us assume that the mobility of polymer molecules depends on their concentration

$$M = M_0\phi(1-\phi). \tag{10}$$

Then, the Cahn–Hilliard equation acquires the final form

$$\frac{\partial\phi}{\partial t} = M_0\nabla\Big\{\phi(1-\phi)\nabla(f(\phi) - \gamma(\lambda(\phi)|\nabla\phi|^2 + \\ + 2\kappa(\phi)\Delta\phi))\Big\} + \xi. \tag{11}$$

This is a nonlinear parabolic fourth-order differential equation with a stochastic term. To ensure the conservation of mass and the decrease in the total energy over time, Eq. (11) must also be supplemented with homogeneous Neumann boundary conditions [35].

Without loss of generality, let us consider solutions $\phi(x, t)$ of the one-dimensional Eq. (11). Let us introduce a space-time grid for x and t with periodic boundary conditions. To solve Eq. (11), we used a semi-implicit differential scheme [37]; the parameters of the polymer-solvent system under study were taken from Refs. [42, 43]. We assumed that the initial phase is homogeneous, and the polymer concentration in the 0.2 wt% solution is $\phi_{\mathrm{in}} = 2 \times 10^{-3}\rho$, where $\rho = 1.3\ \mathrm{g/cm^3}$ is the density of hydroxypropyl cellulose [44]. The growth of the phase structure was simulated on a lattice with $L = 128$.

In Fig. 1, as an example, the result of the phase separation simulation obtained for $\gamma = 0.04$ is shown. One can see how the total polymer concentration $\overline{\phi} = \phi/\phi_{\mathrm{in}}$ changes as functions of the dimensionless distance x and time t. On the basis of the initial random distribution (at $t = 0.001$), there arises an unstable regime, which leads to the appearance of the primary structure of a new phase (at $t = 0.2$) and, afterward, to its further coarsening and final formation (at $t = 1\div5$).

In Fig. 2, the time dependencies of the average cluster mass, $m(t) = \langle S/N_c\rangle$, are shown, where S is the area of the phase structure formed at time t above the level $\overline{\phi} = 1$, and N_c is the number of clusters at the level $\overline{\phi} = 1$. From the analysis of the dependencies presented in Fig. 2, it follows that the self-organization of the phase structure occurs in two stages. At the first stage (the primary structure formation, $t = 0.04\div0.8$), the accumulation of cluster mass is approximated by the scaling function $m(t) \sim t^{\alpha}$, with the power exponent $\alpha = 0.929 \pm 0.074$. This value is close to unity, which corresponds to the mass growth due to surface tension forces at the "polymer-solvent" interface [45]. At the second stage ($t = 0.8\div5$), the dependence $m(t)$

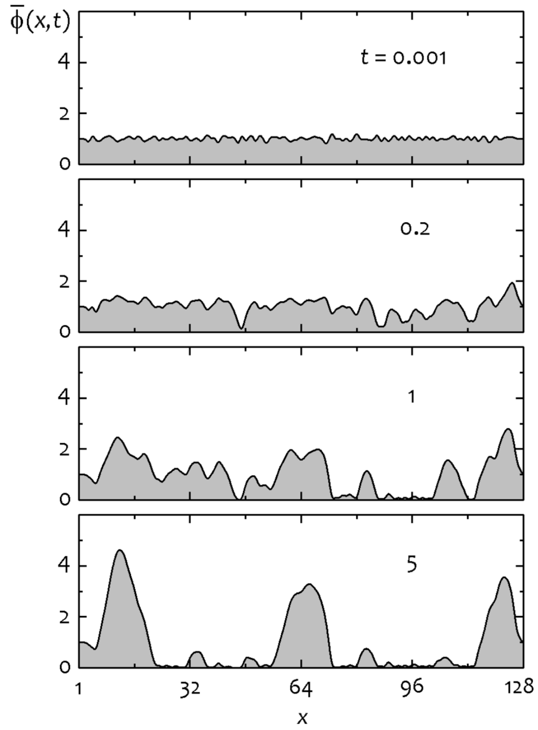

Fig. 1. Distributions of the reduced concentration $\overline{\phi}(x,t)$ on a one-dimensional lattice during spinodal decomposition in the hydroxypropyl cellulose-water system for various times t. $\gamma = 0.04$

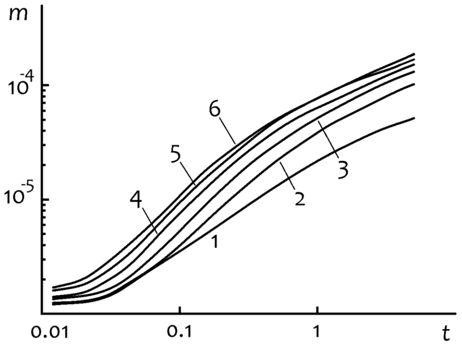

Fig. 2. Time dependencies of the average cluster mass m for various $\gamma = 0.01$ (*1*), 0.02 (*2*), 0.03 (*3*), 0.04 (*4*), 0.05 (*5*), and 0.06 (*6*). The averaging was performed over 100 calculation runs of the program simulating the phase structure

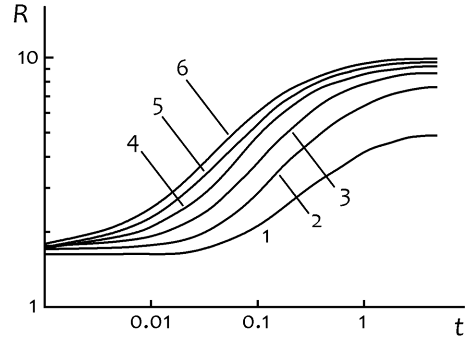

Fig. 3. The same as in Fig. 2, but for the average cluster radius R

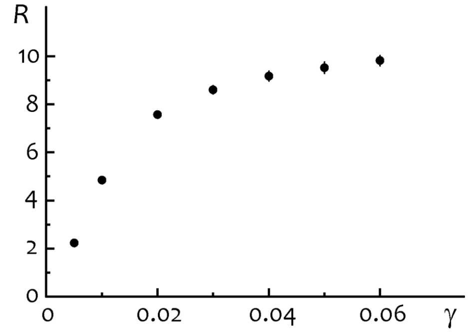

Fig. 4. Dependence of the average cluster radius R on the parameter γ. Simulation time $t = 5$

is approximated by the function t^{β} with the power exponent $\beta = 0.535 \pm 0.024$. This value is close to 1/2, which corresponds to the square-root law for the diffusive mass transfer (see Ref. [46] and references therein). In general, the accumulation kinetics of the average cluster mass is described by the scaling dependencies $(t/t_c)^{\alpha}$ and $(t/t_c)^{\beta}$, where $t_c = 0.8$ is the crossover time, which determines the transition from the cluster mass accumulation regime driven by surface tension effects to the diffusion regime.

One of the features in the asymptotic behavior of the examined system at large simulation times is dynamic scaling. It is determined by the characteristic length $L(t)$ of separate ordered regions of the phase structure [47]. By choosing the average cluster radius $R(t)$ at the level $\overline{\phi} = 1$ as the characteristic length, we find the scaling exponent for the growth law $R(t) \sim t^{\delta}$. An analysis of the time dependencies $R(t)$ in the longest linear sections in Fig. 3 gives $\delta = 0.324 \pm 0.026$. This value is close to $\delta = 1/3$, which is typical of the growth laws for phase structures in systems with a conservative scalar order parameter [48, 49].

In Fig. 4, the dependence of the average cluster radius R on the parameter γ for the formed phase structure (at $t = 5$) is shown. As follows from this figure, the enhancement of hydrophobic interactions at the interfacial boundary (an increase in the parameter γ) leads to the growth of the size of polymer aggregates.

3. Conclusions

To summarize, the following conclusions can be drawn.

1) The kinetics of hydroxypropyl cellulose aggregation in dilute solutions with salt ions have been studied by means of computer simulation.

2) It was shown that there are two aggregation stages. At the first stage (the primary structure formation), the growth of the average cluster mass $m(t)$ is approximated by a scaling function with the power exponent $\alpha = 0.929 \pm 0.074$. This value is close to unity, which corresponds to the mass accumulation driven by surface tension forces at the "polymer-solvent" interface. At the second stage, the dependence $m(t)$ is described by a power function with the power exponent $\beta = 0.535 \pm 0.024$. This value is close to 1/2, which corresponds to the square-root law for the diffusive mass transfer. Thus, the growth kinetics of $m(t)$ is described by two scaling dependencies, $(t/t_{\mathrm{c}})^{\alpha}$ and $(t/t_{\mathrm{c}})^{\beta}$, where $t_{\mathrm{c}} = 0.8$ is the crossover time, which determines the transition from the cluster mass accumulation regime driven by surface tension effects to the diffusion regime.

3) The growth of the average size of the phase structure elements is described by the power function $R(t) \sim t^{\delta}$, with the power exponent $\delta = 0.324 \pm \pm 0.026$. This value is close to 1/3, which is typical of systems with a conservative scalar order parameter.

4) The enhancement of hydrophobic interactions at the "polymer-solvent" interface (for example, the introduction of salt ions into the solution) leads to the growth of the average size of polymer aggregates.

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АГРЕГАЦІЯ ГІДРОКСИПРОПІЛЦЕЛЮЛОЗИ В РОЗБАВЛЕНИХ РОЗЧИНАХ З ІОНАМИ СОЛЕЙ

Методом математичного моделювання досліджено кінетику фазового переходу водного розчину гідроксипропілцелюлози з іонами солей. На основі нелінійного рівняння Кана–Гілліярда зі стохастичним членом, параметром гідрофобності та рухливістю, що залежить від концентрації полімера, виконано симуляцію фазового розділення на простій одновимірній ґратці Флорі. Для набору значень параметра гідрофобності отримано дані про зміну середніх значень розмірів агрегатів та їх маси. За результатами моделювання можна виділити три стадії спінодального розпаду: ранню, проміжну й кінцеву. Встановлено, що для проміжної й кінцевої стадій кінетика зростання маси кластерів описується скейлінговими залежностями з показниками та часом кросовера, які визначають перехід від режиму накопичення маси агрегатів внаслідок ефектів поверхневого натягу до дифузійного режиму. Показано, що зміну середнього розміру кластерів можна представити скейлінговою функцією з показником, близьким до 1/3, типовим для систем із консервативним скалярним параметром порядку. Із результатів комп’ютерної симуляції випливає, що збільшення густини міжфазної енергії (підсилення гідрофобних взаємодій) приводить до зростання розмірів полімерних агрегатів.

Ключові слова: гідроксипропілцелюлоза, іони солей, агрегація, рівняння Кана–Гілліярда.