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MICROEMULSIONS AND POLYMERS COMPLEXES STABILIZED BY CATIONIC SURFACTANT: STRUCTURAL AND THERMODYNAMIC PROPERTIES

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Abstract- The purpose of this work is to model and explain the relationships between very diluted O/W neutral MEs, Φ=2.8%, to which a telechelic polymer PEO-2m has been added in large quantities (r=29.6). In order to form a multi-connected network, the polymeric ends are integrated into the droplets. Once the gel state is established, controlled amounts of cationic surfactant CpCl with distinct rates of charge τ, τ=+0.22%, τ=+0.5%, τ=+0.75%, τ=+1%, are added, the charged polar heads of the CpCl (Cp^+) adsorb to the surface of droplets, introducing a repulsive electrostatic interaction. First, we talk about structural characteristics, regarding the radial distribution function, $g(r)$, we have integrated the hypernetted chain closure relation (HNC) with Ornstein-Zernike integral equations (IEMs) and Simulation of molecular dynamics (MD), to investigate the impact of adding charges on the structure of the mixed system (MEs + PEO-2m). Second, thermodynamic properties (the standard diffusion coefficient, the viscosity) are examined in relation to charge rates τ. Generally, the agreement observed between the numerical spectra and MD simulations is reasonable, indicating the appropriate choice of the adopted potential model.

Keywords: Microemulsions (MEs), Integral Equation Method (IEM), Hypernetted Chain (HNC), Dynamics Simulations (MD), Telechelic Polymer PEO-2m, Ionic Surfactant (CpCl), Fluid.

1. INTRODUCTION

Microemulsions (MEs) are combinations of surfactant, water, and oil, thermodynamically stable, with a transparent appearance [1]. Several recent studies have focused on mixtures of MEs and copolymers, which have the advantage of improving the stability and diffusion of MEs systems, they are widely used as drug delivery systems [2, 3], Because of its excellent interfacial tension reduction and solubilization properties, MEs are used in a wide range of the oil industry, particularly in enhanced oil recovery [4, 5].

Filali et al. have been working for a few years on mixed systems made of decane/water MEs coated in moderate concentrations of PEO polymer that has been hydrophobically modified (PEO-m, PEO-2m) by utilizing a combination of SANS measurements, DLS and rheology [6, 7].

Moderate concentrations of polymers do not influence the size or form of the droplets, according to SANS profiles. Structural characterization has been done by using a combination of SANS measurements and integral-equation methods (IEMs): While the PEO-m results in an unpleasant interaction, the PEO-2m's existence creates an appealing contact between droplets that is effective. Diffusion coefficients were calculated regarding dynamics according to volume fraction, for both concentrated and diluted situations [8-11]. Ahfir, et al. have recently focused on combining molecular dynamics (MD), Integral Equations Method, and Small-Angle Neutron Scattering experiment (SANS), to explore the structure and behavior of networks in oil in water MEs with polymers (PEO-m, PEO-2m), for a range of volume fractions Φ (from 2.8% to 26.5%, and modest concentrations of polymers (r from 4 to 12) [12-14]. In this article, we present a model system consisting of significantly diluted O/W neutral MEs droplets, Φ=2.8%, with biocompatible doubly grafted PEO-2m polymers on their surfaces (r=29.6). We explore the possibility of enhancing the stability and diffusivity of this MEs/PEO-2m mixture system by adding controlled amounts of charged surfactant CpCl. Structural properties are studied by examining the behavior of the RDF, $g(r)$, derived from HNC and MD simulations for different charge rates τ, and then this model is used to describe how viscosity and normal diffusion coefficient behave as a function of τ. The organization of the article is as follows: Section 2 exclusively focuses on the adequate interaction potential between charged particles covered with PEO-2m, with a theoretical reminder on Ornstein-Zernike integral equations (IEMs). In Section 3, the principles of molecular dynamics simulations (MD) are presented. The collected results are provided in Section 4. The article concludes in the final section.

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2. THEORY

2.1. Expression of Pair Potential

2.1.1. Reference Case: Bare Microemulsion

The interaction potential in the bare ME reference situation is the product of two contributions: The van der Waals potential, $U_{vdw}(r)$ and a hard-sphere potential, $U_{HS}(r)$:

$$U(r) = U_{HS}(r) + U_{vdw}(r) \quad (1)$$

Between two hard spheres with diameter $2R$, the pair potential $U_{HS}(r)$ is given by:

$$U_{HS}(r) = \begin{cases} \infty & \text{for } r \le 2R \\ 0 & \text{for } r > 2R \end{cases} \quad (2)$$

The terms "r" and "R" stand for the particle separation and radius. When two spheres are separated, the $U_{vdw}(r)$ potential is roughly [15]:

$$U_{vdw}(r) = -\frac{A_H}{6}\left(\frac{2R^2}{r^2-4R^2} + \frac{2R^2}{r^2} + \ln\left(\frac{r^2-4R^2}{r^2}\right)\right) \text{ for } r > 2R \quad (3)$$

In our case, the effective Hamaker constant A_H, is: A_H=1.1k_BT. This number makes sense for decan nanodroplets interacting with water [16].

2.1.2. Microemulsion with PEO-2m

To the neutral ME, the PEO-2m (r=29.6) is added, it is necessary to consider both a steric repulsive and an additional appealing contribution [17]:

$$V(r) = V_{steric}\left(\frac{2R}{r}\right)\exp\left(-\frac{r-2R}{\lambda_{steric}}\right) \quad \text{(a)}$$

$$W(r) = W_{bridging}\left(\frac{2R}{r}\right)\exp\left(-\frac{r-2R}{\lambda_{bridging}}\right) \quad \text{(b)} \quad (4)$$

The contact potentials for the bridging and steric interactions are $W_{bridging}$ and V_{steric}. The size of the polymers determines the spectrum of their interactions. The parameters have been set to the same range of interactions λ_{steric} of 35 Å and $\lambda_{bridging}$ of 100 Å [8].

2.1.3. Microemulsion with PEO-2m and CpCl

A screened Coulombic repulsive potential [18] is added to the preexisting interaction in the system (MEs/PEO-2m) upon the addition of the cationic surfactant CpCl:

$$U_{Coulomb}(r) = k_BT\frac{Z_{eff}^2 l_B}{(1+KR)^2}\frac{e^{-K(r-2R)}}{r} \quad (5)$$

where, T is the temperature, l_B is a Bjerrum length, the number of effective charges per droplet is denoted by Z_{eff}, K^{-1} is the length of Debye. In this work: T= 298 K, $l_B = 7.18$Å, $K^{-1} = 6.77$Å^{-1}, $Z_{eff} = 130$ [8, 10].

The dimensionless pair potential $U(r)/k_BT$ is:

$$\frac{U(r)}{k_BT} = \begin{cases} \infty & \text{for } r \le 2R \\ -\frac{1.1}{6}\left(\frac{2R^2}{r^2-4R^2} + \frac{2R^2}{r^2} + \ln\left(\frac{r^2-4R^2}{r^2}\right)\right) + \\ +\frac{Z_{eff}^2 l_B}{(1+KR)^2}\frac{e^{-K(r-2R)}}{r} + \frac{2RV_{steric}}{k_BT}\frac{e^{-(r-2R)/\lambda_{steric}}}{r} + \\ +\frac{2R.W_{bridging}}{k_BT}\frac{e^{-(r-2R)/\lambda_{bridging}}}{r} & \text{for } r > 2R \end{cases} \quad (6)$$

The potential $U(r)/k_BT$ versus the distance r/σ is shown in Figure 1. In the first case, bare MEs, τ=0 (Figure 1a), for small distances, $r \le \sigma$, we observe a strong repulsion reflecting the non-overlapping of MEs droplets (Pauli Exclusion Principle). As the distance between nanodroplets increases $r > \sigma$, the attractive effect becomes more important, when the attractive and repulsive contributions are exactly balanced, a potential well with a minimum is observed (~22k_BT). At longer distances, attraction dominates over repulsion.

When the PEO-2m is added, both attractive and repulsive contributions need to be considered; As a result, the depth of the potential well decreases to (~15.65k_BT) and a potential barrier of around (~4k_BT) emerges. Additionally, a second minimum at (~0.57k_BT) is observed, indicating a strong attraction between MEs. In the second case, MEs/PEO-2m/CpCl (Figure 1b); at low values of τ (+0.22%, +0.5%), a second minimum is observed, corresponding to -0.458k$_B$T for τ=+0.22%, and -0.256k_BT, for τ=+0.5%, proving that specific bridges exist between drops, even in the presence of charges; the attractive effect is still present, and an amplification of the potential barrier is noted (from ~4k_BT, at τ=0, to ~4.36k_BT at τ=+0.22%, then to ~5.13k_BT at τ=+0.5%). For larger values of τ (+0.75%, +1%), the steric and electrostatic repulsive effect becomes dominant, this is manifested by a remarkable amplification of the potential barrier (from ~9.28k_BT, at +0.75%, to ~11.5k_BT at +1%). Thus, the second minimum has completely disappeared, meaning that the solution becomes entirely viscoelastic and loses its attracting effect. Generally, the increase in τ led to a monotonic increase in the potential barrier, with a decrease at the potential well. These findings are in line with a related study that looked at how adding PEO-m polymers, which have one hydrophobic end function, affected the potential barrier for interactions between charged MEs droplets; the potential barrier rises in direct proportion to the quantity of PEO-m polymers added per ME [13], and studies the Pickering emulsion structure stabilized by adsorbed charged particles [19, 20]. Indeed, a good understanding of the interaction potential allows for a detailed description of the structure and dynamics of the system under study. The parameters of plot are:

$R = 82\text{Å},\ l_B = 7.18\text{Å},\ K^{-1} = 6.77\text{Å}^{-1},\ \lambda_{steric} = 35\text{Å}$

$\lambda_{bridging} = 100\text{Å},\ V_{steric} = 10.5k_BT$

$\tau = 0.22\%\left(Z_{eff} = 4.8,\ W_{bridging} = -4.02k_BT\right)$

$\tau = 0.5\%\left(Z_{eff} = 8,\ W_{bridging} = -3.9k_BT\right)$

$\tau = 0.75\%\ \left(Z_{eff} = 17,\ W_{bridging} = -2.8k_BT\right)$

$\tau = 1\%\ \left(Z_{eff} = 21,\ W_{bridging} = -2.5k_BT\right)$

2.2. Ornstein-Zernike Equation (OZE)

The characteristics of colloidal systems are determined from the interaction potential and the RDF, $g(r)$. The integral equation method (IEM) provides a fast and efficient approach to access the RDF, $g(r)$ and thermodynamic properties [15]. In this work, we have concentrated on the (OZE), where the $c(r)$ is related to $h(r)$ by [21]:

$$h\left(\vec{r}\right) = \rho\int c\left|\vec{r}-\vec{r'}\right|.h\left(\vec{r'}\right)d\vec{r} + c\left(\vec{r}\right) \tag{7}$$

In other words, it is impossible to solve this equation with two unknowns $h(r)$ and $c(r)$. It requires an additional relationship, which is expressed in a general form [15]:

$$h(r)+1 = \exp\left[B(r)+\gamma(r)-\beta U(r)\right] \tag{8}$$

where, the bridge function is B(r). In this study, we have adopted the hypernetted chain approximation (HNC) [16], which is particularly adapted for mixtures of charged particles with long-range potentials.

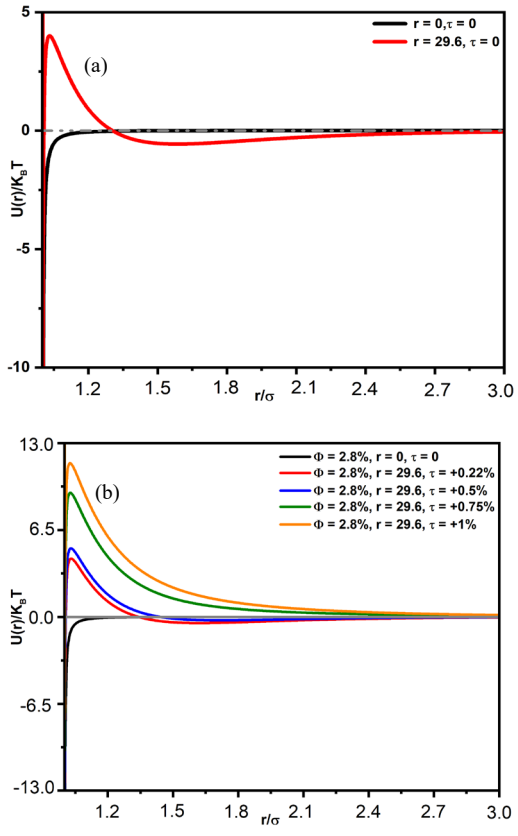


Figure 1. The pair-potential, $U(r)/kBT$ as a function of the distance r/σ

For this approximation, $B(r) = 0$ [15] and the *RDF*, $g(r)$ can be written:

$$g(r) = \exp\left[\gamma(r)-\beta U(r)\right] \tag{9}$$

with:

$$g(r) = h(r)+1 \tag{10}$$

The structure factor [16] is related to the *RDF*, $g(r)$ by:

$$S\left(\vec{q}\right) = 1+\rho\int\left(1-g\left(\vec{r}\right)\right).e^{-i\vec{q}.\vec{r}}d\vec{r} \tag{11}$$

where, r is the number density.

For $q \to 0$, the structure factor can be written:

$$S(0) = \rho k_BT.\chi_T = 1+4\pi\rho\int\left(1-g(r)\right).r^2dr \tag{12}$$

where, the isothermal compressibility χ_T can be expressed as a result of both the osmotic pressure $\prod$ and the volume fraction Φ:

$$\chi_T = \frac{1}{\rho}\left(\frac{\partial\rho}{\partial\Pi}\right)_T \tag{13}$$

We can then write:

$$\chi_T = \frac{I(q\to 0)}{(\Delta\rho)^2 k_BT} \tag{14}$$

The MSD characterizes the equilibrium dynamics given as:

$$\left(\Delta r_{CM}(t)\right)^2 = <\left(r_{CM}(t+t_0)\right)-r_{CM}(t_0))^2> \tag{15}$$

where, r_{CM} is the site of the mass center described as:

$$r_{CM} = \frac{1}{N}\sum_{i=1}^{N} r_i \tag{16}$$

where, r_i is the coordinate of colloid (i). The diffusion coefficient D is related to the mean-square-displacement by the Einstein relation;

$$D = \lim_{t\to\infty}\frac{\left(\Delta r_{CM}(t)\right)^2}{6t} \tag{17}$$

The viscosity η is related to the radius of the MEs and to the diffusion coefficient D by the Stokes-Einstein relation [15]:

$$D = \frac{k_BT}{6\pi\eta R} \tag{18}$$

3. MD SIMULATIONS

An effective tool for examining material properties is MD simulation [22]. This method is based on Newton's second law, which yields the trajectories and velocities of atoms. for a system of N atoms [23]. In this study, we have used molecular dynamics (MD) simulation with the LAMMPS package [24]. We have worked in the NVT statistical ensemble; The Verlet algorithm [23] is utilized to integrate the equations of motion over 10^6 steps, with a time step to $\delta t^* = 0.001$.

In order to remove surface effects and allow for the modeling of an infinite system, periodic boundary conditions are used [12-14]. In order to optimize the calculation time [23], we have adopted dimensionless units; we have used reduced units: temperature is set to $T^* = 1k_BT$, for energy, R for length, $R\sqrt{m/k_BT}$ for time,

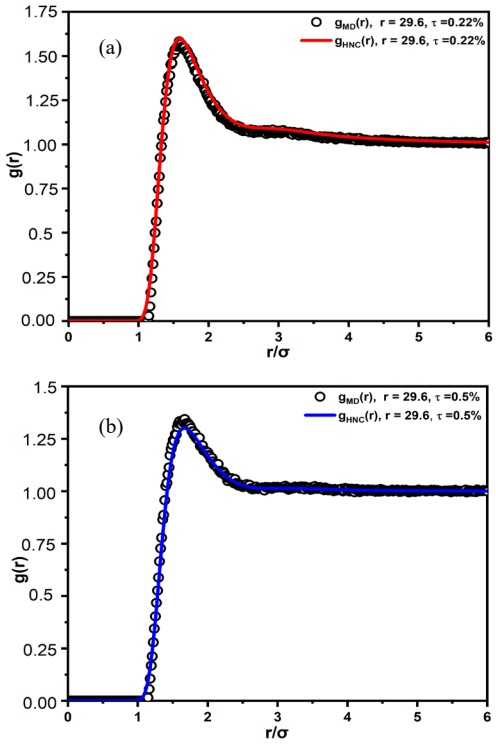
k_BT / R^3 for pressure P, and $R\sqrt{k_BT / m}$ for the diffusion coefficient D_c. Our objective through the use of (MD) simulations is to validate the structural properties obtained from the numerical study and then explore the dynamics of studied system.

4. RESULTS AND DISCUSSION

4.1. Characteristics of the Structure

Figure 2 shows a comparison of the RDF, $g(r)$ obtained from the HNC approximation and MD simulations, as a function of r/σ. Firstly, it should be noted that for all quantities of added CpCl τ (+0.22%, +0.5%, +0.75%, +1%), $g(r)$ curves are generally in good agreement. Second, due to the low volume fraction studied, $\Phi = 2.8\%$, the appearance of $g(r)$ displays a single correlation peak. For low charge rates, τ=+0.22%, τ=+0.50% (Figures 2a, 2b), as mentioned for the potential and despite the repulsive effect created by the inclusion of charges, the attractive effect is still present. Therefore, the presence of bridging effects is indicated by the appearance of a single, narrow, and highly pronounced correlation peak, explaining the good localization of droplets at d~233 Å (τ=+0.22%). Increasing the charge rate, τ=+0.5%, weakens the bridging between droplets, consequently, the correlation peak is less intense and the inter-droplet distances are slightly larger, around d~238Å (τ=+0.50%).

For high charge rates, τ=+0.75%, τ=+1% (Figure 2c, Figure 2d), the bridges have disappeared, and the electrostatic repulsion has completely overridden the attractive effect of PEO-2m. The correlation peak is weakly pronounced and very broad, indicating a weak correlation between the particles in the studied system (τ=+0.75%: d~293Å, and τ=+1%: d~319Å).



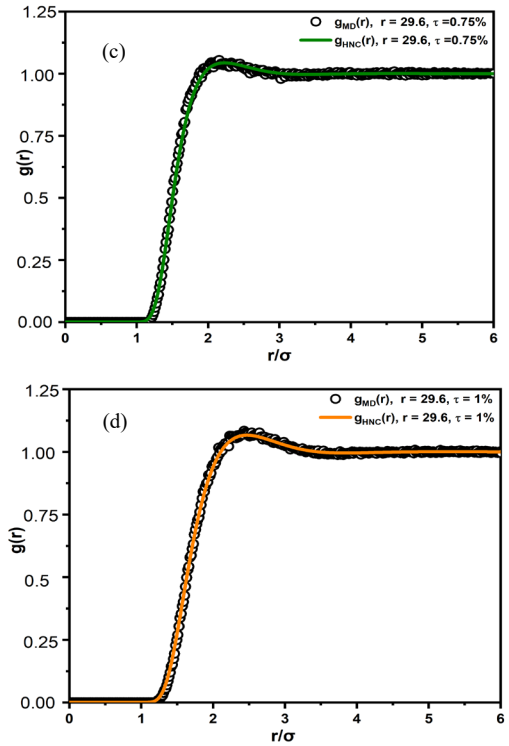


Figure 2. Radial distribution function $g(r)$ from HNC and MD simulations, for different CpCl concentrations τ (0.22%, 0.50%, 0.75%, 1%)

These results are consistent with similar investigations [10, 11, 20], which have examined the impact of charges on the structure and stability of a mixed MEs/Polymers system. It should be noted that having stable MEs is highly recommended in enhanced oil recovery applications [25, 26]. In the pharmaceutical industry, it is essential to have a mixed MEs/Polymers system that can be easily stabilized by the addition of controlled amounts of charges to ensure targeted drug delivery [27, 28].

4.2. Thermodynamic Properties

This paragraph aims to track the process of transforming bridges between MEs droplets into loops by gradually increasing the charge rate τ. To do this, we study the variations of the coefficient of diffusion, D^*, and the viscosity, η^*, as functions of τ (+0.22%, +0.5%, +0.75%, +1%). In Figure 3, the first quantity to consider is the behavior of the reduced diffusion coefficient D_c^*; the progressive addition of charges reduces the attraction between the MEs and increases the electrostatic repulsive effect, thus slowing down the mean square displacement of the particles.

This directly influences the behavior of the coefficient of diffusion, which decreases exponentially with increasing τ. Regarding viscosity, as shown in Equation (18), η is inversely proportional to D, so an increase in τ causes a progressive increase in the system's viscosity. Thus, for τ=+1%, the system becomes viscoelastic. All results are summarized in Table 1. This dependence of the diffusion coefficient and viscosity on the charge rate is very useful for controlling the diffusion of MEs for enhanced oil recovery applications [29, 30].

Table 1. Dimensionless thermodynamics properties for different charges rates τ

Samples	D_c^*	η^*
r=0, τ=0%	1.72	0.0232
r=29.6, τ=0.22%	1.79	0.0214
r=29.6, τ=0.5%	1.72	0.0228
r=29.6, τ=0.75%	1.68	0.0235
r=29.6, τ=1%	1.66	0.0241

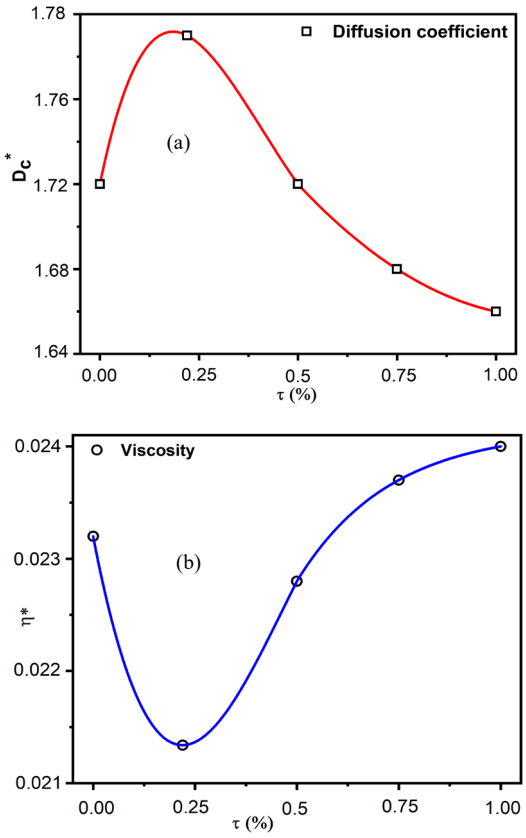


Figure 3. The diffusion coefficient D_c* and the viscosity η* as a function of τ

5. CONCLUSION

In In this work, we examined the thermodynamic and structural characteristics of a mixed system, consisting of highly diluted neutral MEs (Φ=2.8%), to which a telechelic polymer PEO-2m has been added in large quantities (r=29.6). The progressive addition of the cationic surfactant CpCl reduces the attraction between the droplets and increases the electrostatic repulsive effect. Thus, the potential barrier increases proportionally to the rate of charges per ME. Regarding the structure, the good agreement observed between the RDF, $g(r)$ obtained from the HNC approximation and MD simulations confirms the appropriate choice of the interaction potential. Moreover, as τ increases, the correlation peak becomes less pronounced and very broad, indicating a weak correlation between MEs droplets. Indeed, having a MEs and Polymers complexes, that can be easily stabilized by the addition of controlled amounts of charges is highly recommended in industrial applications, particularly in enhanced oil recovery and drug delivery. Concerning the dynamics of the studied system, the increase in charge rate slows down the mean square displacement of MEs, leading to an exponential decrease in the diffusion coefficient and a progressive increase in the system's viscosity. For high charge rates, τ=+1%, the system becomes viscoelastic. Finally, we suggest that this study could be extended to investigate the structural and dynamic properties of the system for other volume fractions (dilute and concentrated cases) with different types and quantities of polymers, in order to numerically reproduce the phase diagram of this system for better application in enhanced oil recovery.

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