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Numerical Modeling of the Processes of Coagulation and Dispersion of Drops in Electric Field

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Abstract

Results of the physical and mathematical modeling of the processes of producing and disintegrating water-oil emulsions using the COMSOL Multiphysics software, as well as of electric fields, velocity fields, and pressure fields, under boundary conditions that correspond to the apparatuses under development are presented. Based on the analysis of the data obtained, different versions of the design of electric dispersers and electric dehydrators are proposed.

Key words: Electric dispersers; Design; Modernization; Physicochemical characteristics; Emulsion; Model fluids; Drop diameter; Field strength

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INTRODUCTION

Analytical calculation of processes of destruction and the interaction of water droplets in oil in an electric field is only possible for a limited number of cases. That is why numerical modeling of the processes of creation and destruction of emulsions in electric fields is a promising area of research.

Taylor[1] did theoretical analysis of droplet deformation under the influence of an external electric field. Relationship between the droplet D and the deformation strength of the electric field he represented as:

$$D = \frac{9 f_d(R,Q,\lambda)}{8(2+R)^2} Ca_E$$

where $f_d(R,Q,\lambda)$ is a function of

$$f_d(R,Q,\lambda) = R^2 + 1 - 2Q + \frac{3}{5}(R-Q)\frac{(2+3\lambda)}{(1+\lambda)}$$

Accuracy of the theory for small deformations Taylor drops proved by several authors[2]. Sherwood[3] based on the method proposed settlement boundary integrals of Laplace's equation and the Stokes equation, i.e. divided the problem into two parts: the calculation of the electric field, the calculation of the velocity field in liquids. Initially, he has calculated electric field distribution on the surface of the drop, and after the jump of the electric field at the interface was calculated, he has determined fluid velocity field.

In[4,5] analyzed the mechanisms of deformation and fracture drops. The influence of the relative viscosity on the stability of drops and defined the limits of applicability of the proposed method of boundary integrals was studied. Authors[6,7] have considered the final deformation of water droplets, but have neglected by the effects of viscosity, which play an important role for emulsions.

Model of weakly conducting fluid with the two drops was used in[8]. Viscous interactions between two drops were investigated in[9].But the effect of the relative motion of the droplets not taken into account.

The motion of two drops in a uniform electric field using a weakly conducting fluid was studied in[10]. Mutual influence of turbulence and electric field on the behavior of emulsions was studied in[11-14]. Shown, that turbulence promotes rapprochement drops, while the electric field destroys the adsorption film and increases the likelihood of a successful merger of droplets in contact.

Previously we have reported the results of studies of processes of destruction and merging of droplets in weakly conducting liquids received by numerical methods[15-17].

In this paper, we present the model of fracture and merge droplets in weakly conducting liquids, which in the Navier-Stokes equations take into account additional Coulomb and polarization forces.

The results are compared with the results of other authors using dimensionless parameters.

1. EXPERIMENT

The processes of the dispersion and coagulation of water in low-conducting fluids were modeled using COMSOL Multiphysics software. The electrocoagulation unit proposed in COMSOL was taken as the basis. This unit employs two modules, i.e., the AC/DC Module and the Microfluidics Module. The AC/DC Module makes it possible to model dc and ac electric fields in a working zone with various shapes and dimensions, as well as to determine the spatial and time distributions of the parameters such as the electric conductivity and dielectric constant. The Microfluidics Module includes applications that describe the flow dynamics in both a homogeneous and multiphase fluid in the working zone under the effect of various volume forces.

These processes were modeled based on the equations that describe the flow of an incompressible fluid between two electrodes for the schemes shown in Figure 1. A low-conductive fluid with one or two water drops moves between the electrodes. The top and bottom boundaries are the entry and exit of the low-conductive fluid; the charged and grounded electrodes are arranged on the right and left.

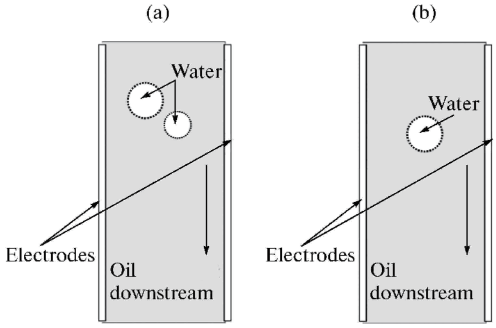

Figure 1
Schematics of the Model of (a) the Coalescence and (b) the Disintegration of Water Drops

The system of equations that is solved during the modeling includes the generalized version of the Navier-Stokes equations with an additional electric field force and the flow continuity equation:

$$\begin{cases} \rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u = \nabla \cdot [-pI + \eta(\nabla u + (\nabla u)^T)] + \\ +F_{st} + \rho g + F, \\ \nabla \cdot u = 0, \end{cases}$$

where ρ is the density (kg/m^3), u is the flow velocity (m/s), η is the dynamic viscosity (Pa·s), p is the pressure (Pa), I is the identity tensor, $\eta(\nabla u+(\nabla u)^T)$ is the viscous stress tensor, g is the acceleration of gravity (m/s^2), F_{st} are the forces at the interface (N/m^3), and F is the additional electric field volume force (N/m^3).

To trace the movement of the phases at the interface of the fluids, the following system of equations is used:

$$\begin{cases} \frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nabla \cdot \frac{3\chi\sigma\varepsilon}{2\sqrt{2}} \nabla \psi \\ \psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi, \end{cases}$$

where σ is the surface tension coefficient (N/m); ε is the numerical parameter (m) that determines the thickness of the interface of the fluids, i.e., the zone where the phase variable ϕ changes from -1 for water to +1 for oil; and x is the numerical parameter that characterizes the mobility of the interface.

The electric potential was calculated as follows:

$$-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla V) = 0$$

where ε_0 is the dielectric constant in vacuum and s_r is the relative dielectric constant of the fluid.

The relative dielectric constant was determined as a function of the internal volume fractions of both fluids as follows:

$$\varepsilon_r = \varepsilon_{r1} Vf1 + \varepsilon_{r2} Vf2$$

where ε_{r1} and ε_{r2} are the relative dielectric constants of oil and water, respectively; $Vf1$ is the volume fraction of the first fluid, i.e., water; and $Vf2$ is the volume fraction of the second fluid, i.e., oil.

The electric field's strength was calculated using the following formula:

$$E = -\nabla \cdot V$$

The electric force in the Navier—Stokes equation was found as follows:

$$F = -\frac{\varepsilon_0 \varepsilon_r E^2}{\sigma_e} \nabla \sigma_e$$

The electric conductivity was determined as a function of the internal volume fractions of both fluids as follows:

$$\sigma_e = \sigma_{e1} Vf1 + \sigma_{e2} Vf2$$

where σ_{e1} and σ_{e2} are the electric conductivities of castor oil and water, respectively.

Figure 2 shows the results of the numerical modeling of the process of the disintegration of water drops with different electric conductivity (saltiness) in an oil product under the effect of an electric field. The modeling was carried out for 4 mm in diameter water drops with an electric conductivity of 3 × 10^{-4} (ohm cm)$^{-1}$ placed into the 70 × 40 mm interelectrode space. Figure 2a illustrates the results of calculating the distribution of the electric field potential in the vicinity of the drop interface. The results of calculating the velocity field (Figure 2b) allow us to draw the conclusion that the two vortices that appear in the continuum are responsible for the pattern of the disintegration of the drop. The application and amplification of the electric field lead to the retardation of the drop. The interaction of the incoming flow with the drop results in the formation of a Carman track. Behind a stationary or slowly moving object, vortices appear that interact with the mobile interface. The drop deforms and then disintegrates along the electric force lines. The study's results have shown that the mechanism of the disintegration of the drop is governed by not only its dimensions but also, to a substantial extent, by the hydrodynamic and electrophysical properties of the fluids that form the emulsion, as well as by the electric parameters of the system.

The conductivity of the oil and water strongly depends on the concentration of various substances in them; as a result, the electric conductivity of the oil emulsions is governed not only by the amount of water contained and its dispersity but also by the amount of salts and acids dissolved. The experiments and modeling were carried out using model fluids with properties whose range overlaps to the best extent possible the properties of the available water-oil emulsions.

A full-scale experiment was previously performed to study the behavior of a water drop in castor oil. The properties of castor oil are within the range of the possible hydrodynamic and electrophysical properties of oil. In addition, castor oil is transparent, which makes it possible to easily observe and record the occurring processes.

Time = 0.545 Surface: Volume fraction of fluid 1 (1) Contour: Electric potential (V) Contour: Volume fraction of fluid 1 (1)

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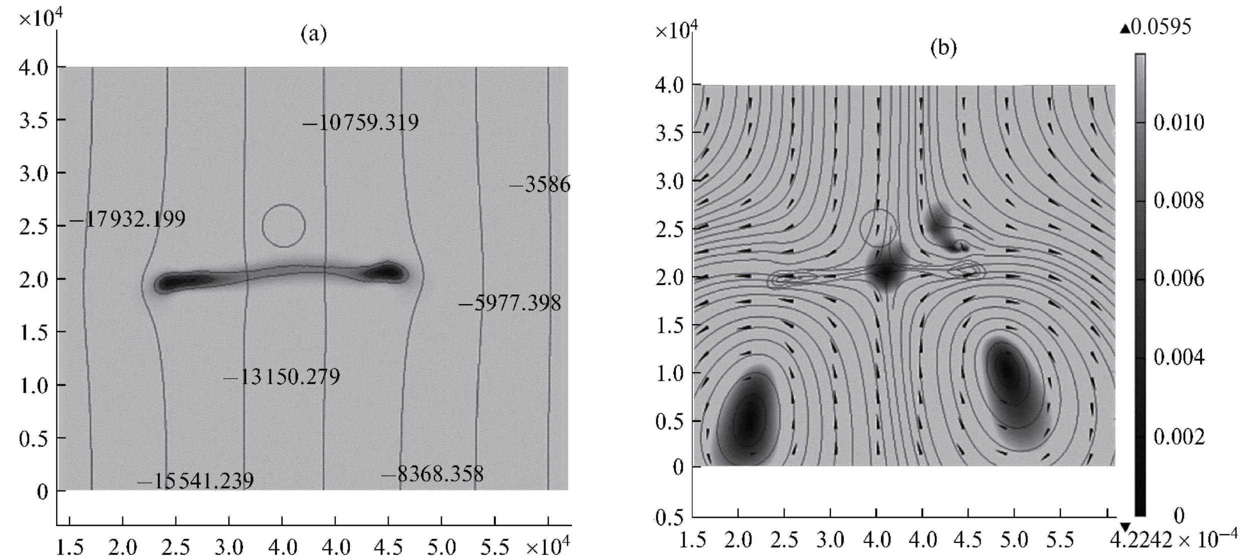

Figure 2
Results of the Numerical Modeling of the Disintegration of Water Drops With Electric Conductivity of 3 × 10^{-4} (Ohm cm)$^{-1}$ in Oil Products Obtained at Potential Difference Between the Electrodes of 4 kV/cm and the Initial Drop Diameter of 4 mm: (a) Electric Field; (b) Velocity Field

RESULTS

Numerical simulation results are presented as the degree of deformation $D = \frac{d_{\max} - d_{\min}}{d_{\max} + d_{\min}}$ ($d_{\max}$ and $d_{\min}$- the maximum and minimum diameters of deformed drop) from the electric capillary number and Weber number $We = \frac{\varepsilon_0 \varepsilon R_0 E_\infty^2}{\sigma}$. If D>0, the drop is pulled across the field (prolate spheroid), and if D<0, the drop is compressed by the field (oblate spheroid).

The results of physical experiments deformation of water droplets (3.06, 4.8, 5.4, 6.6, 7.8, 8.58 mm) in castor oil presented in Figure 3. It is clear that up to the strain D = 0.07, the experimental results agree with those obtained analytically based on the theory of small deformations of weakly conducting liquids proposed by Taylor. For large deformations observed significant deviation from analytical calculation.

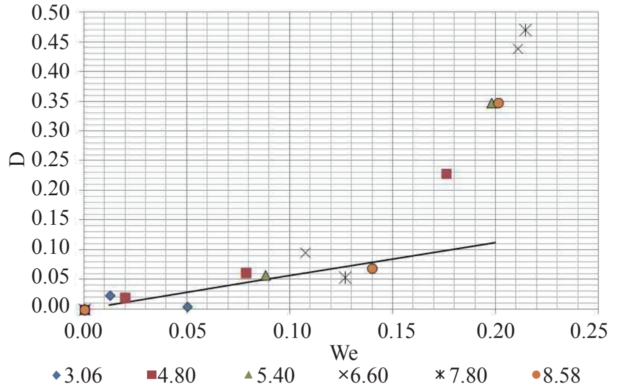

Figure 3
Effect of Weber Number We on the Degree of Deformation D Drops of Water in Castor Oil: Solid Line - Results of Analytical Calculation of the Theory of Small Deformations of Weakly Conducting Liquids Proposed Taylor; Markers - Results of Physical Experiments for Droplet With Different Diameter, mm

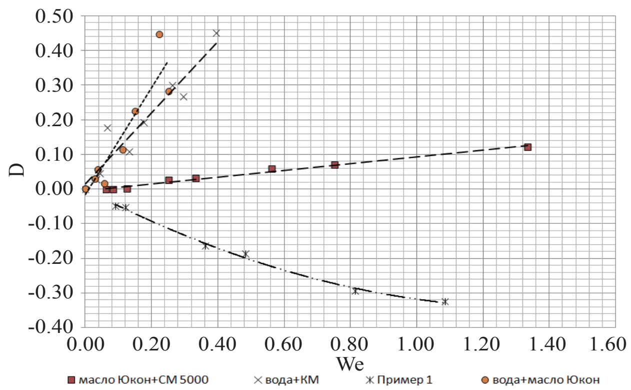

Figure 4
Effect of Weber number We on the degree of deformation D: line - the results of analytical calculation of the theory of small deformations of weakly conducting liquids proposed by Taylor. Markers - results of numerical experiments for different pairs of liquids: drops of castor oil in the silicone oil 5000 (◊ - castor oil + silicone oil 5000); Yukon oil droplets in silicone oil 5000 (□ - Yukon oil +silicone oil 5000); drops of water in castor oil (× - castor oil + water) drops of water in Yukon oil (○ - water + Yukon oil)[18,19]

Numerical experiments for liquid systems given in[18,19] with use the proposed model was performed also. The results were compared with analytical calculations based on the theory of small deformations of weakly conducting liquids proposed by Taylor (Figure 4). Their good agreement was derived. This indicates the adequacy of the proposed numerical model and the possibility of using this model to predict the behavior of weakly conducting liquids for small deformations.

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