A SIMPLE MODEL TO DESCRIBE DIMPLE DYNAMICS

ALEJANDRO J. ACEVEDO-MALAVÉ, ELOY SIRA and MÁXIMO GARCÍA-SUCRE

SUMMARY

A model based on the hydrodynamics equations that allows to describe the dynamics of a dimple, once it has formed, is proposed. The Navier-Stokes equations are considered, and two fundamental approaches are used to simplify the mathematical treatment of the hydrodynamics equations. Certain conditions are considered that must be fulfilled at the interface, which serve to close the system of differential equations and lead to an evolution equation that describes the interfacial film dynamics. With the intention of solving this equation, the method of finite differences has been used.

Very different mechanisms are known to take place in the problem of emulsion stability (Kashchiev and Exerowa, 1980; Exerowa *et al*., 1983; Ivanov, 1988; Bibette, 1992; Bibette *et al*., 1992; Sonin *et al*., 1994; Kabalnov and Wennerström, 1996). Depending on the thickness of the interfacial film, diverse factors must be taken into account that have a marked influence on the physics of the problem. When thickness of the interfacial film is <300nm, the electrostatic interactions must be taken into account. Mathematically is necessary to include a disjoining pressure $\Pi \neq 0$.

It has been reported that one of the most important factors within the stability problem of emulsions is the coalescence process, which is related to the stability of the interfacial film (Vrij, 1966; Vrij and Overbeeck, 1968; Ivanov *et al*., 1969; Sharma and Ruckenstein, 1987).

When drops approach each other in an emulsified system, the coalescence process begins. In this process, the liquid between the drops drains off until the two drops hit and a new one of a greater volume forms (Denkov *et al*., 1991; Kralchevsky *et al*., 1991; Tsekov and Radoev, 1992; Danov *et al*., 1993; Jaeger *et al*., 1994; Ivanov and Kralchevsky, 1997). This process can be divided into two stages: i) the drops approach each other without deformation until, at a certain distance between them a flat circular film appears, and ii) the thickness of this film begins to diminish from a certain separation, until it arrives to the critical separation and the two drops form a larger one.

Before coalescence occurs, a protuberance in the shape of a hole forms at the interfacial film, which depending on its dynamics can oscillate until disappearance or can coalesce, if the two drop surfaces are superposed (Ivanov, 1988; Velev *et al*., 1993; Hartland and Jeelani, 1994; Chesters and Bazhlekov, 2000; Yeo *et al*., 2001; Yeo *et al*., 2003). This protuberance is known as a dimple (Figure 1).

In this paper, a hydrodynamic model based on the quasi-static and lubrication approaches is proposed, allowing the simulation the dimple evolution.

Mathematical formulation of the model

The fundamental object of this study is to construct a model that allows to simulate the dimple dynamics. With this purpose, the Navier-Stokes equations for the interfacial film and the disperse phase were considered in the spirit of the quasi-static and the lubrication approximations.

The lubrication approximation is very useful to simplify the

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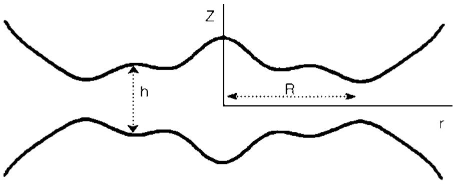

Figure 1. Collision between two droplets.

hydrodynamics equations, being applicable under the following conditions:

- The space between the two surfaces is small in comparison with the radius of the interface film (h(r,t) <<R, where h(r,t): thickness of the interface film and R: its radius).

- The inertial forces that act on the interface film are smaller than viscous forces (small Reynold number).

- The "z" component of the velocity is smaller than its radial component.

- The dependencies on angular velocity are very small.

- The variation of v_r with r is much smaller than its variation with z ($\partial v_r/\partial r << \partial v_r/\partial z$).

In agreement with the previous suppositions, the Navier-Stokes equations in cylindrical coordinates take the form

$$\frac{\partial h}{\partial t} = -\frac{1}{r}\frac{\partial (hur)}{\partial r} \tag{1}$$

$$\tau = -\frac{h}{2}\frac{\partial P}{\partial r} \tag{2}$$

where u: interface velocity, and τ: radial component of the stress tensor.

The equations for the flow inside the drops are given by the equation of continuity for an incompressible fluid and the Navier-Stokes equation within the quasi-static approximation, so that

$$\nabla \cdot v = 0 \tag{3}$$

$$-\nabla P_d + \mu_d \nabla^2 v = 0 \tag{4}$$

where P_d: pressure at the dispersed phase, and μ_d its viscosity.

On the interfacial film the following conditions must be satisfied:

$$u = v_r \tag{5}$$

and the sum of the shear stress of the dispersed phase and the interfacial film must be zero, so that:

$$\tau + \tau = 0 \tag{6}$$

In order to obtain an adimensional system of equations, the variables of the system are scaled according to the following relationships:

$$r' = \frac{r}{R_{eq}};\ h' = \frac{h}{R_{eq}};\ t' = \frac{tV}{R_{eq}}$$
$$\tau' = \frac{\tau R_{eq}}{\mu_d V};\ P' = \frac{P R_{eq}}{\mu_d V}$$
$$u' = \frac{u}{V};\ v' = \frac{v}{V} \tag{7}$$

where R_{eq}: drop radius, and V: approach velocity between the droplets.

Now, the equation system has only one parameter, which is the capillary number (Ca= $\mu_d V/\sigma$, where σ: interfacial tension). This parameter can be eliminated carrying out the following scaling on the system variables:

$$r^* = \frac{r'}{Ca^{1/3}};\ h^* = \frac{h'}{Ca^{2/3}}$$
$$t^* = \frac{t'}{Ca^{2/3}};\quad \tau^* = \tau' Ca^{2/3}$$
$$P^* = P'Ca;\ u^* = u'Ca^{1/3}$$
$$v^* = v'Ca^{1/3} \tag{8}$$

The adimensional system of equations is:

$$\frac{\partial h^*}{\partial t^*} = -\frac{1}{r^*}\frac{\partial (h^* u^* r^*)}{\partial r^*} \tag{9}$$

$$\tau^* = -\frac{h^*}{2}\frac{\partial P^*}{\partial r^*} \tag{10}$$

$$\nabla^* \times v^* = 0 \tag{11}$$

$$-\nabla^* P_d^* + \nabla^{*2} v^* = 0 \tag{12}$$

$$u^* = v_r^* \tag{13}$$

$$\tau^* = \tau_d^* = 0 \tag{14}$$

$$P^* = 2 - \frac{1}{2}\Delta^* h^* \tag{15}$$

where Δ*: adimensional Laplacian operator acting over h*(r*,t*) in cylindrical coordinates.

The central idea of this section is to obtain from the equation system (Eqs. 9-15) one equation for the surface h*(r*,t*) without the unknown variable u*. For this purpose, Eq. 10 is inserted in Eq. 14, so that

$$-\frac{h^*}{2}\frac{\partial P^*}{\partial r^*} + \tau_d^* = 0 \tag{16}$$

$$\text{where}\quad \tau_d^* = 2\frac{\partial v_r^*}{\partial r^*} \tag{17}$$

If, additionally, the fact that at the interface u*= v_r^* is taken into account, then

$$\frac{\partial u^*}{\partial r^*} = \frac{h^*}{4}\frac{\partial P^*}{\partial r^*} \tag{18}$$

and the pressure gradient can be calculated from Eq. 15. The resulting equation is inserted in Eq. 18, thus giving

$$\frac{\partial u^*}{\partial r^*} = -\frac{h^*}{8}\frac{\partial (\Delta^* h^*)}{\partial r^*} \tag{19}$$

Now, manipulating Eq. 9,

$$-\frac{\partial h^*}{\partial t^*} = u^*\frac{\partial h^*}{\partial r^*} + \left(\frac{u^*}{r^*} + \frac{\partial u^*}{\partial r^*}\right)h^* \tag{20}$$

On Eq. 20, the term in parenthesis is zero (continuity equation), so that

$$-\frac{\partial h^*}{\partial t^*} = u^*\frac{\partial h^*}{\partial r^*} \tag{21}$$

The derivative of Eq. 21 with respect to r* is

$$-\frac{\rightarrow^2 h^*}{\partial r^* \partial t^*} = \frac{\partial u^*}{\partial r^*}\frac{\partial h^*}{\partial r^*} + u^*\frac{\partial^2 h^*}{\partial r^{*2}} \tag{22}$$

Next, u* from Eq. 21 is introduced in Eq. 22, to obtain

$$\frac{\partial^2 h^*}{\partial r^* \partial t^*}\frac{\partial h^*}{\partial r^*} - \frac{\partial^2 h^*}{\partial r^{*2}}\frac{\partial h^*}{\partial t^*} = \frac{h^*}{8}\frac{\partial (\Delta^* h^*)}{\partial r^*}\left(\frac{\partial h^*}{\partial r^*}\right)^2 \tag{23}$$

On the other hand, if the surfactant is absent there are no Marangoni stresses on the drops surfaces, so that Eq. 12 takes the form

$$\nabla^{*2} v^* = 0 \tag{24}$$

but the radial component of the vector field in Eq. 24 is

$$\nabla^{*2} v^*\Big|_{r^*} = \nabla^{*2} v_r^* - \frac{1}{r^{*2}} v_r^* = 0 \tag{25}$$

Taking into account that at the interface u*= v^*_r and inserting Eqs. 19, 21 and 23 in Eq. 25, it is obtained

$$\frac{\partial^2 h^*}{\partial r^* \partial t^*}\frac{\partial h^*}{\partial r^*} - \frac{\partial h^*}{\partial t^*}\left(\frac{\partial^2 h^*}{\partial r^{*2}} + \frac{h^*}{r^{*2}}\right) = -\frac{h^{*2}}{8}\frac{\partial h^*}{\partial r^*}\left(\frac{1}{r^*}\frac{\partial (\Delta^* h^*)}{\partial r^*} + \frac{\partial^2 (\Delta^* h^*)}{\partial r^{*2}}\right) \tag{26}$$

and in turn, Eq. 26 can be manipulated so as to lead to

$$\frac{\partial^2 h^*}{\partial t^* \partial r^*}\frac{\partial h^*}{\partial r^*} r^* - \frac{\partial h^*}{\partial t^*}\left(r^*\frac{\partial^2 h^*}{\partial r^{*2}} - \frac{\partial h^*}{\partial r^*}\right) = 0 \tag{27}$$

The initial and boundary conditions of the problem are

$$h(r,0) = h_0 + me^{-r^2} \text{ if } r \le R$$
$$h(R,t) = h_0 \tag{28}$$
$$\text{and } \left.\frac{\partial h}{\partial r}\right|_{r=0} = 0$$

where R: interfacial film radius, and m: a real number with value of 0.5.

Eq. 27 is the evolution equation for the interfacial film of thickness h*, which was solved numerically using the finite differences method.

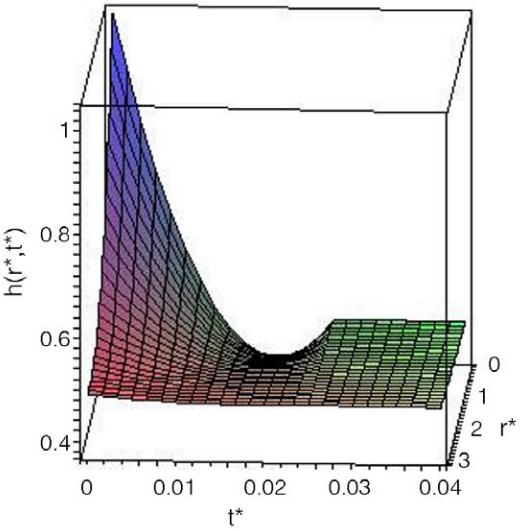

Figure 2. Evolution of interfacial film thickness h*(r*,t*).

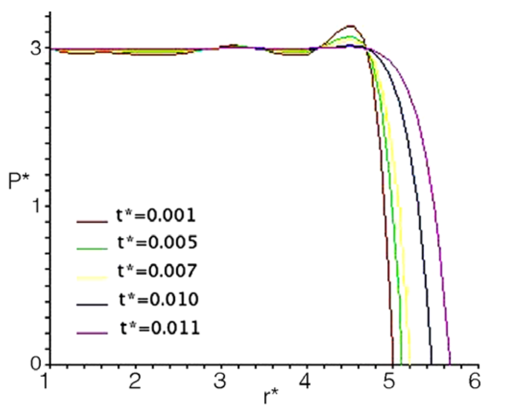

Figure 3. Dependence of the pressure vs position for some values of time.

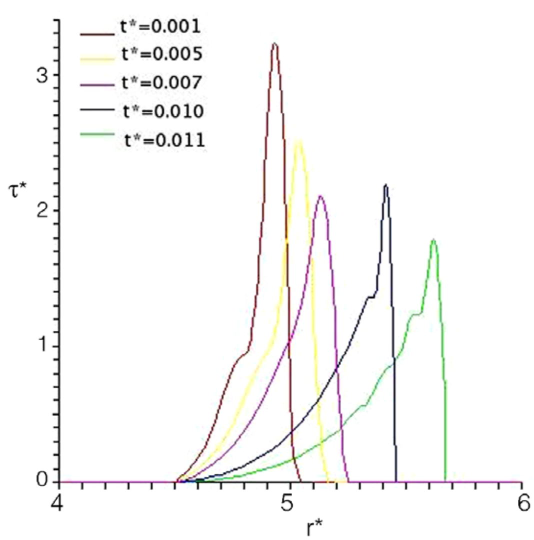

Figure 4. Dependence of the radial component of the stress tensor vs position for various time values.

Results

The resolution of the evolution equation allows to know the front-wave dynamics at the interfacial film. As initial condition, a Gaussian form disturbance was used in order to simulate the dimple dynamics.

The evolution of the thickness h* of the interfacial film with respect to position and time is shown in Figure 2. It can be seen that the initial disturbance in Gaussian form decreases with time, until it reaches a maximum amplitude and finally returns without the interfacial film broken (the rupture of the interfacial film is the last stage of the coalescence process). Also, it can be observed that the zones near the edges of the interfacial film remain approximately stable. This is a consequence of the approach employed in the development of the model, where an approximately laminar flow draining towards the outside of the film has been assumed.

In the drainage process there are changes in the pressure field on the interfacial film. In Figure 3 it can be observed that the pressure field remains constant for each t up to r* =5, and thereafter the pressure field decays down to zero. Also, it can be seen that the pressure distribution tends to grow with time, which means that the pressure grows when the liquid interface drains towards the outside.

At the center of the interfacial film pressure remains constant with a value of 2, which means that in this region the term $\frac{1}{r^*}\frac{\partial h^*}{\partial r^*}$ of $\Delta^* h^*$ is annulled with its second derivative $\frac{\partial^2 h^*}{\partial r^{*2}}$.

The behavior of the radial component of the viscous stress tensor can be appreciated in Figure 4. It is observed that for values of r* <4.5 the stress is zero. For values of r* >4.5 stress grows up to a maximum value and finally it decreases until being annulled.

When the liquid interface drains towards the outside it is observed that stress decreases, until the dimple drains completely out of the drop surface.

Conclusions

A model based on Navier-Stokes equations that describes dimple dynamics was elaborated. To this end, the hydrodynamic equations were considered in the spirit of two fundamental approaches, the quasi-static and the lubrication approximations.

The resolution of the evolution equation allows to know how does the dimple dynamics develop.

By solving the evolution equation, the dependence of the interfacial film thickness on position and time was obtained. An initial disturbance in Gaussian form decreased with time until reaching maximum amplitude and no coalescence was observed.

The pressure field diminished with time, from the center of the interfacial film to the barrier ring. This behavior was inverted when the dimple changed its concavity.

When the liquid interface drained towards the outside, the stress on the interfacial film diminished from the barrier ring to the center, and this tendency was inverted when the dimple returned to the equilibrium position.

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UN MODELO SENCILLO PARA LA DESCRIPCIÓN DE LA DINÁMICA DE UN DIMPLE

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RESUMEN

Se propone un modelo que permite la descripción de la dinámica de una depresión superficial (dimple) una vez que se ha formado. Las ecuaciones de Navier-Stokes son consideradas, y dos enfoques fundamentales son utilizados para simplificar el tratamiento matemático de las ecuaciones hidrodinámicas. Se consideraron ciertas condiciones que deben cumplirse en la interfase, las cuales sirven para completar el sistema de ecuaciones diferenciales y llevan a una ecuación de evolución que describe la dinámica de la película interfacial. A fin de resolver la ecuación se utilizó el método de diferencias finitas.

UM MODELO SIMPLES PARA A DESCRIÇÃO DA DINÂMICA DE UM DIMPLE

Alejandro J. Acevedo-Malavé, Eloy Sira e Máximo García-Sucre

RESUMO

Propõe-se um modelo que permite a descrição da dinâmica de uma depressão superficial (dimple) após ter se formado. As equações de Navier-Stokes são consideradas, e dois enfoques fundamentais são utilizados para simplificar o tratamento matemático das equações hidrodinâmicas. Consideraram-se certas condições que devem cumprir-se na interfase, as quais servem para completar o sistema de equações diferenciais e conduzem a uma equação de evolução que descreve a dinâmica da película interfacial. A fim de resolver a equação se utilizou o método de diferenças finitas.