

Application of the Least Square Finite Element Method in the Evaluation of the Rheological Behaviour of Dilute Polymeric Emulsions in Simple Shear Flow

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ABSTRACT

The advection of the interface in the creeping flow of a two-phase liquid system is predicted using an in-house developed three-dimensional least squares finite element (LSFEM) computer code, which is based on the volume of fluid method (VOF) and applied locally in the interface area.

Moreover, a criterion for an appropriate definition of the interface thickness is suggested, which is employed to evaluate the surface tension forces, using the derivative of the volume fraction on the Gaussian points of each element.

Finally, the deformation of the second phase, which is assumed to be a drop, in the simple shear flow is satisfactorily compared with available data in the literature; and it is shown that even for the case that both phases have equal viscosities, the apparent viscosity of the dilute two-phase emulsion is affected by the surface tension and the second phase size.

INTRODUCTION

Moving boundary and evaluating the position of the interface is the concern of many flow problems [1], such as mixing and morphological development in two-phase flows. Therefore, many researches have devoted their attention to capture or track the interface using Eulerian, Lagrangian or mixed approaches [2]. Here we have employed the volume of fluid method

(VOF), which captures the interface using Eulerian formulation [3].

There exist at least three challenges for the evaluation of the interface in all of the Eulerian methods, including VOF: (i) a proper solver for the advection equation, (ii) a direct interface reconstruction method and, (iii) a precise method for the surface tension force calculation. Certainly, different methods are purposed to provide a better solution for the mentioned problems [4-8].

In the current research we have adjusted a least square finite element method to have a stable solution for the interface displacement equation, which is totally governed by advection terms. Also, the first and the second derivatives of the volume fractions on the Gaussian points of each element are used to calculate the interface curvature and the surface tension force, as a result.

Then, using the derivatives of the velocity on the walls, the apparent viscosity of the dilute two-phase emulsion is calculated and it is shown that the value of the apparent viscosity changes as the second phase changes; also its final value is a function of second phase size and surface tension.

MATHEMATICS AND SOLUTION

Here we direct our attention to the creeping flow of an incompressible Newtonian fluids, therefore the equations of motion can be stated as follows:

$$-\mu \nabla^2 \mathbf{u} + \nabla P = \sigma \kappa \mathbf{n} \delta \quad (1)\text{-a}$$

$$\nabla \cdot \mathbf{u} = 0 \quad (1)\text{-b}$$

where ∇ and $\nabla^2 = \nabla \cdot \nabla$ are Nabla and Laplace operators, respectively; and “.” stands for the dot product. P and μ are pressure and Newtonian viscosity in the flow domain, correspondingly. The vectors $\mathbf{x} = (x, y, z)$ and $\mathbf{u} = (u, v, w)$ denote location and velocity of any arbitrary point, for a three-dimensional flow field in the Cartesian coordinate. The term on the RHS of equation (1-a) is the contribution of the surface tension, in which the scalar value of σ is the surface tension coefficient. The curvature of the interface and its normal are denoted by κ and \mathbf{n} , respectively. δ is Dirac’s distribution function.

The advection of the interface can also be described by equation (2):

$$\frac{\partial F}{\partial t} + \mathbf{u} \cdot \nabla F = 0 \quad (2)$$

where t denotes time and the volume fraction of each arbitrary point is shown by F , which will be defined later in equation (3).

The equations of motion (equations 1-a and 1-b) can be solved using Galerkin finite element method [9], as described in [10 and 11]. However, a least squares finite element method [12] is used to obtain a stabilized solution for equation (2), which is totally governed by the advection terms. It is worth to mention that the solution domain of the recent equation is considered to be the elements, which at least one of their nodes are closer to interface than interface thickness (Will be described later). We have employed cuboid elements to discretize the domain and tri-linear interpolation functions are used for pressure and volume fraction and tri-quadratic interpolation function for velocity components.

Interface

The volume fraction parameter determines the position of the interface as well as its curvature and normal direction. Therefore, a precise evaluation of the mentioned parameter is vital for a better prediction of the second phase deformation. In order to achieve this target, a new criterion for the interface thickness assumption and a new method for evaluating the second derivative of the volume fraction are suggested.

In this research, we have proposed that the curvature and the normal direction, in each active element (element with the interface) to be calculated using the derivatives of the nodal values of the volume fraction on the Gaussian points of the $3 \times 3 \times 3$ stencil around each active element. Therefore, it is expected that all of the involved nodes in the mentioned element to be inside the interface region. This condition can be fulfilled if the interface radius (R_i), or half of the interface thickness, to be three times the greatest diagonal in the meshing system. Therefore, the nodal values of the volume fraction can be defined, as equation (3):

$$F = \begin{cases} \frac{1}{2} + \frac{1}{2} \frac{d}{R_i} & d > R_i \\ \frac{1}{2} - \frac{1}{2} \frac{d}{R_i} & d < R_i \\ \frac{1}{2} & d = 0 \end{cases} \quad (3)$$

where d is the minimum distance between each node and the interface.

VERIFICATION

In order to investigate the correctness of our method, a comparison has been made between our results and the available data in the literature [13 and 14], in a simple shear flow as shown in figure (1).

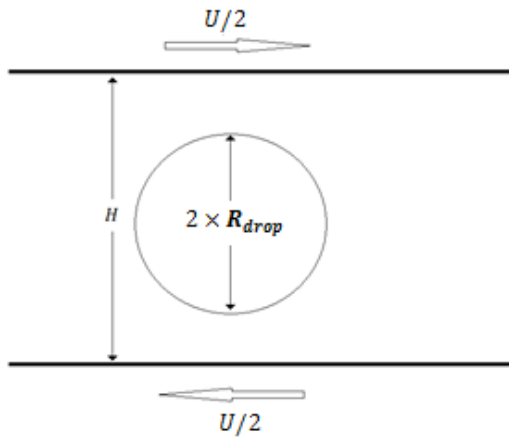


Figure 1. An immiscible droplet with the radius of R_{drop} in simple shear flow

In Figure 1 the gap between the moving plates in the simple shear flow is denoted by H and R_{drop} is the radius of the undeformed sphere-like droplet. The upper and lower plates move with the velocities of $U/2$ and $-U/2$; respectively; therefore, the average shear rate is defined by $\bar{\gamma} = U/H$. The ratio of the viscous to surface tension forces is also defined by Capillary number, as stated in equation (4):

$$Ca = \frac{\mu \bar{\gamma} R_{drop}}{\sigma} \quad (4)$$

μ is the viscosity of the main phase, which is equal to the second phase viscosity, as an assumption.

In our first example, we have studied case (4) of figure (2) in [13]. Figure (2) illustrates the steady shape of a droplet with $Ca = 0.1$ and $R_{drop} = \frac{1}{2}H$, which comply perfectly with the experimental results.

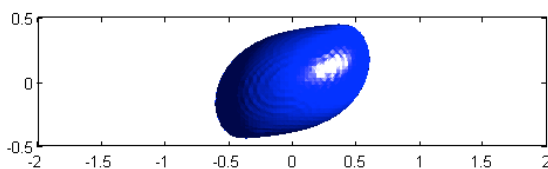


Figure 2. The steady shape of a droplet with $Ca = 0.1$ and $R_{drop} = \frac{1}{2}H$, reproducing case (4) of figure (2) in [13].

This method can also predict the droplet breakup, as shown in figure (3).

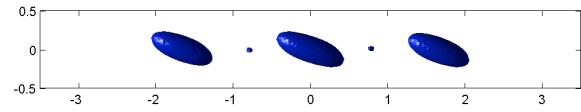


Figure 3. The steady shape of a droplet with $Ca = 0.46$ and $R_{drop} = 0.35H$, reproducing case (1) of figure (3) in [13].

VISCOSITY OF THE DILUTE EMULSION

Here the effect of a single droplet deformation on the apparent viscosity of a two-phase flow is studied. In order to calculate the apparent viscosity of the dilute emulsion, the following correlation is used:

$$\frac{\mu_a}{\mu} = \frac{\dot{\gamma}_w}{\bar{\gamma}} \quad (5)$$

where $\dot{\gamma}_w$ and μ_a are the shear rate at walls and apparent viscosity, respectively.

Figure (4), shows the trend of the viscosity changes before equilibrium for different values of Capillary numbers, when the diameter of the droplet is 0.7 of the gap.

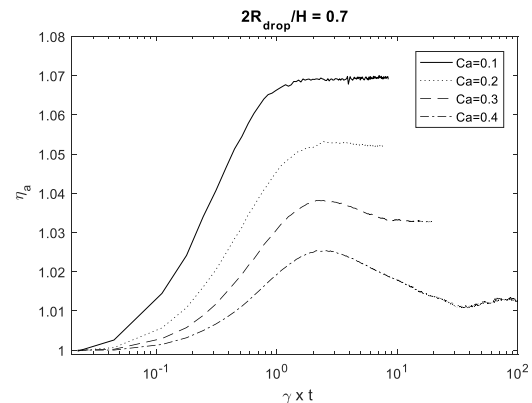


Figure 4. Trend of the viscosity changes by time (t) for $R_{drop}/H=0.7$

According to figure (4), it is observed that by decreasing of the Capillary number, the value of the equilibrium viscosity increases, which can be attributed to higher values of the surface tension forces. Also, it is shown that the viscosity experiences a

fluctuation before equilibrium for larger values of Capillary number. Similar behaviour has also been observed for the shape of droplet before the equilibrium [13 and 14].

By increasing the droplet size, the viscosity and its fluctuation will increase as well, as shown in figure (5):

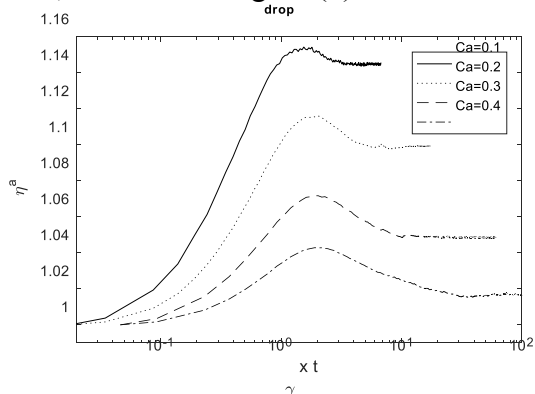


Figure 5. Trend of the viscosity changes by time (t) for $R_{drop}/H=0.9$

CONCLUSION

A computer code has been developed to predict the flow field parameters and the interface advection using Galerkin finite element and least squares finite element methods, respectively. Moreover, a criterion for choosing the suitable interface thickness has been suggested, which is used to defined the nodal values of the volume fraction. Also, the surface tension forces in each active element have been calculated using the derivatives of the volume fraction at the Gaussian points around the element with interface.

It has been shown that this model can predict perfectly the second phase deformation at low and high values of the capillary number. Finally, the effect of the second phase deformation on the apparent viscosity of the dilute emulsion has been studied and it has been shown that increasing the surface tension as well as second phase size can give a rise to the apparent viscosity of the emulsion, even when two phases have similar viscosities.

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