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Abstract

In this paper, we present the capability of "phase_field" model of TrioCFD code to capture coupled mass transfer and hydrodynamic phenomena. For this purpose, we consider a droplet composed of one miscible and one immiscible components released in a 2D rectangular domain filled with water. Mass transfer occurs between the miscible element and the water, which leads to a variation of the density of each phase. The Boussinesq approximation for a multicomponent system is used to define the density law. The results found are in good agreement with the dynamics described from an experimental study and present a significant validation of such a model using coupled Cahn–Hilliard/Navier–Stokes equations.

Introduction

In most studies, mass transfer in a system is often separated from the hydrodynamic phenomenon involved in a two-phase flow. However, both phenomena are strongly coupled in the sense that the movement of the two-phase fluid depends on the density variation induced by the mass transfer. In order to highlight these coupled phenomena, we perform, in this work, numerical simulation where a mass transfer in a multicomponent system leads to a variation of the density and therefore affects the motion of the system. To do so, in the following, we first describe our problem and the phase field method with the associated equations implemented in "phase_field" model of TrioCFD code. Then, we present the numerical parameters of the problem with the assumptions used. Finally, we show some screenshots of the simulation and discuss the results obtained.

Description of the problem

We study the dynamics of a multicomponent droplet released in a quiescent water column, in the same spirit as (Rao et al. 2015). The droplet considered as the dispersed phase is initially composed of two components: acetonitrile (a miscible component) and chlorobenzene (an immiscible component in water). Since the density of the mixture (acetonitrile+chlorobenzene) is different from the surrounded water, the droplet tends to move up or down. In parallel, mass transfer occurs between water (the continuous phase) and the miscible element of the droplet, and therefore modifies the density of each phase. Actually, the density of the dispersed phase increases with the quantity of acetonitrile transfered while the density of the continuous phase decreases. As a result, with a droplet that is initially lighter than water, the droplet starts rising due to buoyancy effect, reaches a threshold point when the densities of both dispersed and continuous phases are equal and ends up sinking in water by gravity. In other words, the dynamics of the droplet involves hydrodynamic phenomenon with a change of densities induced by component mass transfer.

The phase-field model

The phase field method is a good candidate for simulating such coupled mass transfer/hydrodynamic phenomena. In order to describe the whole system, we couple the advective Cahn–Hilliard equations for the evolution of the molar fraction and Navier–Stokes equations for the fluid motion. For our {acetonitrile, chlorobenzene, water} ternary system, we have:

- two advective Cahn–Hilliard (CH) equations:

$$\frac{\partial x_i}{\partial t} + \mathbf{u} \cdot \nabla x_i = \nabla \cdot \left(\sum_{j \in \{a,c\}} \mathcal{M}_{i,j} \nabla \tilde{\mu}_j \right) \quad (1)$$

$$\tilde{\mu}_i = \frac{\partial \bar{G}}{\partial x_i} - \sum_{j \in \{a,c\}} \kappa_{i,j} \Delta x_j \quad (2)$$

- incompressible Navier–Stokes (NS) equations:

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla P + \sum_{i \in \{a,c\}} x_i \nabla \tilde{\mu}_i + \rho(x_a, x_c)\mathbf{g} + \eta \Delta \boldsymbol{u} \quad (3)$$

$$\nabla . \mathbf{u} = 0 \quad (4)$$

with x_i and $\tilde{\mu}_i$ are the molar fraction and chemical potential of the element i (the index a for acetonitrile and c for chlorobenzene), $\mathcal{M}_{i,j}$ the mobility, $\kappa_{i,j}$ the gradient energy, $\bar{G}$ the Gibbs energy, **u** the velocity, P the pressure, ρ the mass density, η the dynamic viscosity and **g** the gravity. The term with $\tilde{\mu}_i$ in Eq. 3 represents the capillary force within the interface, as mentioned in (Kim 2012).

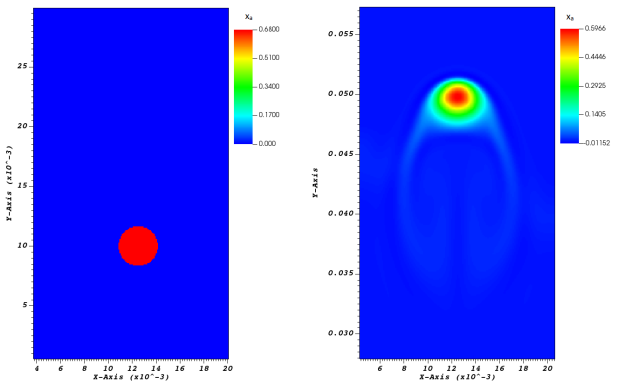
Numerical parameters of the problem

In this study, we have extended the capabilities of the "phase_field" application of TrioCFD code so that it can treat an arbitrary number of components while, so far, only binary system could be considered (Angeli, Bieder, and Fauchet 2015; Rasolofomanana, Le Tellier, and Henry 2022). The droplet has an initial diameter of 3.3 mm and is initially placed so far enough from the walls of the 2D domain to avoid edge effects. We keep the viscosity of both phases constant $\eta = 10^{-3}$ Pa.s and make sure that there is at least 4 cells within the interface so that the interface structure be captured. At equilibrium, we consider that the droplet is composed only of chlorobenzene and is heavier than the surrounded acetonitrile water mixture. To ensure this variation of the density, we define the density law by using the Boussinesq approximation for multicomponent system:

$$\rho(x_a, x_c) = \rho_0 \left(1 + \beta_a x_a + \beta_c x_c\right) \tag{5}$$

with ρ_0, β_a, β_c are respectively the density of reference, the volume expansion coefficient for acetonitrile and chlorobenzene defined from the density of each element of system.

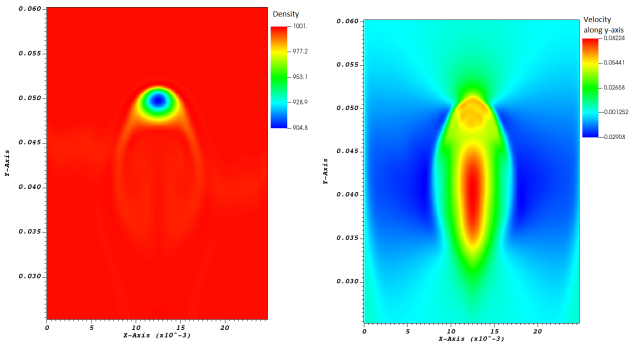
Results and Discussion



(a) t=0s **(b)** t=1.2s

Figure 1: Molar fraction of acetonitrile.

We show in Figure 1 the evolution of the molar fraction of acetonitrile and so the droplet in the water column at t=0s and t=1.2s. At initial time, we consider a circular droplet with zero interface thickness (see Figure 1a) that is lighter than the surrounded water. It is important to note that for the case presented in this paper, the initial density of the droplet is 890 kg/m^3. At t>0s, since the "phase_field" is a diffuse interface model, the interface between the two phases becomes diffuse and a mass transfer of acetonitrile occurs through it. This latter leads to a modification of the density of each phase and makes the droplet move up in the water column due to buoyancy from $y = 0.01$ to $y \sim 0.05$ in 1.2s (see Figure 1b).



(a) Density at t=1.2s **(b)** Velocity Y-axis at t=1.2s

Figure 2: Density and velocity at time t=1.2s.

Actually, one can notice in Figure 2a that at t=1.2s, the density of the droplet increases and its size becomes smaller than the initial size due to mass transfer. The rising droplet in the water column is highlighted by the velocity along y-axis in Figure 2b. These results in ascent stage are in relatively good agreement with those reported in Rao et al. 2015.

Conclusion

We have carried out a 2D simulation of the dynamics of a multicomponent droplet released in a water column using the improved "phase_field" model of TrioCFD code. Such a model can solve several equations of Cahn–Hilliard coupled with Navier–Stokes equations. In this paper, we have used the Boussinesq approximation for multicomponent system so that the mass transfer between the dispersed and continuous phases induces the droplet to rise or fall in the continuous phase. The results obtained represents quite well qualitatively the dynamics predicted for an initial lighter droplet released in a quiescient water.

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