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A study on hydrodynamics and mass transfer of moving liquid layers using computation fluid dynamics

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Abstract

The two-dimensional Kelvin-Helmholtz instability occurring in two immiscible co-currently moving horizontal liquid layers is studied numerically, using the volume-of-fluid method. To initialize the wave development, two different perturbation terms are implemented into the model. A three-component liquid system toluene-water-acetone is chosen, and both hydrodynamic and mass transfer studies are carried out. Numerical results are in a good agreement with experimental observations as well as the linear theory of instability.

Keywords:

Kelvin-Helmholtz instability, CFD, Liquid-liquid extraction

1. Introduction

Liquid-liquid extraction is a widespread fluid separation operation. Very often it is characterized by high complexity of flow and mass transfer phenomena which are not yet fully understood. Rigorous models necessary for the design of extraction units are not available up to now, and the design rules are mainly based on empirical correlations containing a number of parameters which are rarely based on the process physics [1]. In order to reach a better understanding of extraction processes, fundamental interfacial phenomena have to be thoroughly analyzed.

In this work, we focus on the Kelvin-Helmholtz instability (KHI). This instability represents an important phenomenon caused either by velocity or density difference across the interface between two immiscible fluids.
In the past decades, KHI has been studied extensively, both experimentally and theoretically. Experimentally, the KHI of two-immiscible liquid fluids was investigated in [2]. In these experiments, the instability occurs because of a vertical perturbation introduced when the rectangular tube is tilted by a small angle. Theoretically, the KHI is studied by the classical linear stability theory (see, for example, [3]). This theory gives reliable results for low velocity deference between the two immiscible fluids. When the difference becomes higher, the linear stability theory fails to predict the wave growth.
Recently, due to the rapid development of computational power and algorithms, direct numerical simulations have become more and more popular for studying interfacial phenomena. To track the position and motion of an interface, different methods have been developed, as, for example, the marker and cell method [4], the volume-of-fluid (VoF) method [5], the level set method [6] and the combined front-tracking/front-capturing method suggested in [7].
In [8], the level set method is used for the study of the KHI in three different cases, namely the rollup of a vortex sheet without surface tension forces, the growth of the KHI in the linear regime, and the long-time evolution of the KHI. In [9] and [10], numerical investigations of the KHI are carried out for liquid-gas systems with different ratios of density and viscosity. In both cases, the VoF method is applied together with a piecewise linear interface calculation reconstruction method.
In our work, the two-dimensional KHI is studied using the VoF method without any reconstruction algorithm, because of minor smearing observed in our simulations. The selected system is a toluene-water-acetone system, in which acetone is transferred from the toluene layer to the aqueous layer. This system is recommended as a standard one by the European Federation of Chemical Engineers for testing the performance of liquid-liquid extraction columns.

2. Model formulation and implementation

In the VoF method used to resolve the movement of the interface, a scalar quantity f is introduced, which represents the volume fraction of a mesh cell occupied by one phase. Thus, it takes values between 0 and 1 for the cells containing the interface and the values 0 or 1 away from the interface. For incompressible flows and due to the absence of phase changes, the interface location change with time is tracked by solving the following equation:

$$\frac{\partial \mathrm{f}}{\partial \mathrm{t}} + \nabla \cdot \left(\mathrm{f}\, \bar{\mathrm{u}} \right) = 0 \tag{1}$$

This equation reflects the fact that the volume of fluid function f is advected with the local fluid velocity. The governing continuity, momentum and mass transfer equations for the two-phase fluid flow are:

$$\nabla \bar{u} = 0 \tag{2}$$

$$\frac{\partial}{\partial t}\rho \bar{u} + \nabla \cdot \rho \bar{u}\bar{u} = -\nabla \bar{p} + \rho g + \mu \Delta \bar{u} \tag{3}$$

$$\frac{\partial C}{\partial t} + \bar{u} \cdot \nabla C = \nabla \left(D \nabla C \right) \tag{4}$$

where

$$\rho = f \rho_T + \left(1 - f\right)\rho_W \tag{5}$$

$$\mu = f \mu_T + \left(1 - f\right)\mu_W \tag{6}$$

As can been seen from Eqs. (2), (3), (5) and (6), the flow field is resolved using a homogeneous model. This means that the two phases share a common velocity and pressure field. The choice of the homogeneous model substantially reduces the necessary computational time. For the mass transfer studies, the transport equation is solved for the transferred component, whereas the interface is kept at thermodynamic equilibrium.

The surface tension model which is used for the VoF method is based on the continuum surface force model (see [11]). In this model, the surface tension force is represented as a volume force:

$$\bar{F}_\sigma = \left(-\sigma \kappa n\right)\delta \tag{7}$$

$$\delta = \left|\nabla f\right| \tag{8}$$

where σ is the surface tension coefficient, n is the vector normal to the interface, and κ is the surface curvature.

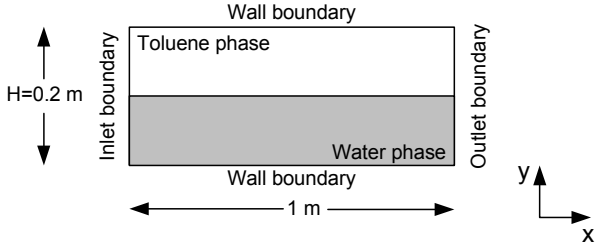

Figure 1. Geometry and boundaries of the studied two-phase domain

To complete the model formulation, the boundary and initial conditions should be defined. In Fig. 1, the two-dimensional geometry and boundaries are shown.
To examine the effect of different perturbations on the wave development, two case studies are considered. First, a perturbation is implemented into the initial condition as follows

$$U_y = - A \frac{2\pi}{\lambda} \sin(\frac{2\pi}{\lambda} x) U_x \quad (9)$$

where A is the amplitude, λ is the wave length, U_x and U_y is the vertical and horizontal velocity components, respectively. In the second case, two perturbations are used simultaneously, one as initial and one as inlet perturbation given by

$$U_y = A_{initial} \; 100 \; y \; (H-y) \cos(8\pi x) \quad (10)$$

$$U_y = A_{inlet} 100 \; y \; (H-y) \cos(2\pi t) \quad (11)$$

where t is time, $A_{initial}$ and A_{inlet} is the initial and inlet amplitude, respectively.
A uniform hexahedral structured grid is used for the two-dimensional domain, in which the system of governing equations is solved numerically. Approximately 200,000 grid elements are necessary to obtain grid independent results. A time step of $5 \cdot 10^{-4}$ is selected for all simulation to ensure that the Courant number (a stability criterion for transient moving boundary problems) is always smaller than one and in this way a stable solution is ensured. All simulations are carried out with the commercial CFD tool CFX 10.0 by Ansys Inc.

3. Results

3.1. Hydrodynamics

For the study of hydrodynamics, mass transfer was not considered and, thus Eq. (4) was not used. In Fig. 2, the wave propagation for 3 different time steps is shown for both cases. Only minor smearing of the interface can be observed. The results are in qualitative agreement with experimental data presented in [4]. Initially, the wave develops in the vertical direction with increasing amplitude. Gradually, because of the action of gravity and the upper phase flow, the vertical growth of the wave ceases. Instead, finger-like structures begin to develop.
An exponential growth of the wave with time is established as shown in Fig. 3, when the wave evolves in the vertical direction. This linear exponential growth is in accordance with the linear theory. The calculated time necessary for the wave to develop and break down is approximately 1 s in all simulations, similar

both to the experiments carried out in [2] and to the numerical simulations performed in [6].

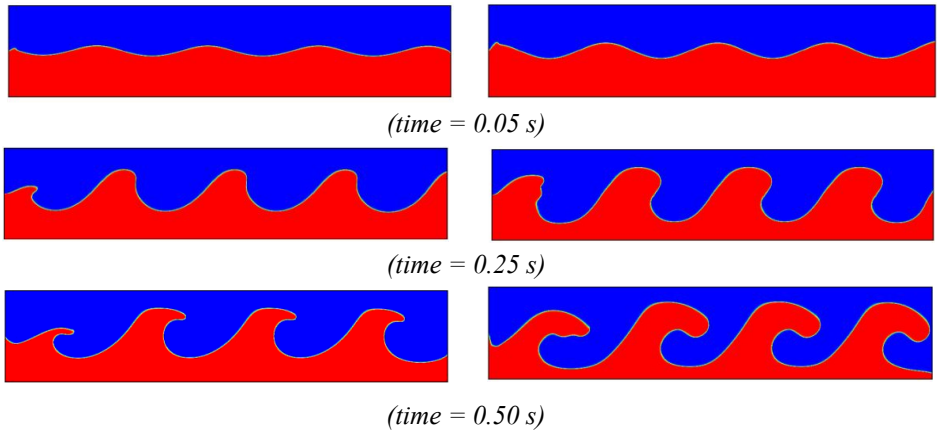

Figure 2. Wave evolutions using one perturbation term (left) and two perturbation terms (right) for $A = A_{Initial} = A_{Inlet} = 0.5$ and $\lambda = 0.2$

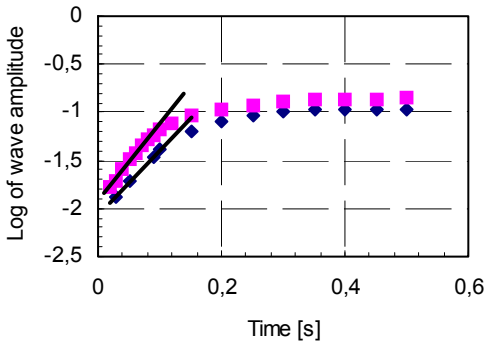

Figure 3. Wave amplitude as a function of time

3.2. Mass transfer

Acetone represents the transferring component. To describe its mass transfer, Eq. (4) is used, while thermodynamic equilibrium is implemented at the interface. In Fig. 4, the mass fraction of acetone is presented for the case in which one perturbation term (Eq. (9)) is used. It is clearly visible that mass transfer is promoted at the crest of the wave, because of the high convection at this position.

4. Conclusions

In this work, the KHI in two immiscible horizontal liquid layers is studied using the VoF method. This method is able to capture accurately the wave propagation, both when the wave develops in the vertical direction and when finger-like structure start to appear. Only minor interface smearing is observed in all simulations, and thus, accurate mass transfer calculations are possible. The mass transfer study reveals regions where it is promoted due to high convection.

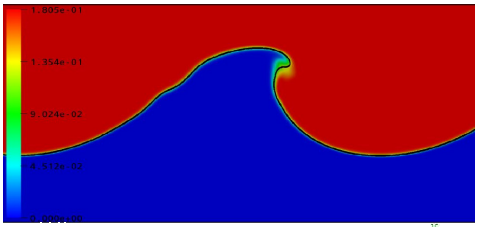

Figure 4. Mass fraction of acetone in the toluene phase at 0.25 s

In the future, the investigation will be extended to cover systems system with chemical reactions. In this way, the fundamental phenomena occurring in a reactive extraction column can be captured and analyzed.

Acknowledgements

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