Numerical simulation of rising droplets in liquid-liquid systems: A comparison of continuous and sharp interfacial force models

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Abstract

Simulations of single droplets rising in a quiescent liquid were performed for various initial droplet diameters. The continuous phase was water and the dispersed phase was either $n$-butanol, $n$-butyl acetate or toluene, thus resulting in three standard test systems for liquid-liquid extraction. For the simulations, a level set based code was developed and implemented in the open-source computational fluid dynamics (CFD) package OpenFOAM\textsuperscript{®}. To prevent volume (or mass) loss during the reinitialisation of the level set function, two methods published recently were used in the code. The continuum surface force (CSF) model and the ghost fluid method (GFM) were applied to model interfacial forces, and their influence on grid convergence, droplet shapes and rise velocities was investigated. Grid convergence studies show a reasonable behaviour of the GFM, whereas the CSF model is less reliable, especially for systems with high interfacial tension. The results for droplet shape and terminal rise velocity are in excellent agreement with experimental and numerical investigations from literature. The onset of oscillations is

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correctly predicted, and the influence of the smoothing of interfacial forces on velocity oscillations is studied. Simulations of oscillating droplets remain stable, but the frequencies of the velocity oscillations differ from experimental results.

**Keywords:** Droplet, Liquid-liquid extraction, Terminal velocity, CFD, Level set, Interfacial force model

1. Introduction

Transport phenomena at moving boundaries are crucial in various unit operations of process engineering, e.g. condensation, absorption and liquid-liquid extraction. Therefore, moving boundaries have been studied extensively for several decades, both experimentally and theoretically, and remain subject of ongoing research. Mass transfer in liquid-liquid extraction columns occurs at moving boundaries of rising droplets. Thus, fluid dynamics of and mass transfer in droplet swarms are essential for the design of liquid-liquid extraction. To capture these complex phenomena properly, fluid dynamics of single moving droplets should be fully understood and mastered first.

Fluid dynamics of a single droplet is governed by physical properties of the system and the size of the droplet. Relatively small droplets remain spherical and reach their terminal rise velocity after a short period of acceleration. Increasing the droplet diameter leads to higher terminal velocities. Consequently, the forces acting upon the droplet grow and deform the droplet to an ellipsoidal or oblate shape. Droplets of even larger size begin to oscillate.

Apart from the physical properties of both liquid phases, the terminal velocity also depends on the purity of the system. In pure systems, the interface remains mobile and the shear forces acting there lead to internal circulations, i.e. toroidal flow patterns in the droplet. In contrast, impurities accumulated at the interface inhibit the development of internal circulations. Thus, shear forces increase and the resulting terminal velocities are lower than in pure systems. For this reason, carefully purified systems were used in recent experimental investigations.

This work focusses on the numerical simulation of rising droplets. The most widely-used methods to simulate moving boundaries are moving mesh, front tracking and front capturing methods. Moving mesh methods (e.g. Bäumler et al., 2011; Tuković and Jasak, 2012) employ a boundary fitted grid which is moved to keep the grid nodes exactly at the interface. Thus, boundary con-
ditions at the interface can be implemented directly, resulting in a very exact and sharp representation of the two-phase flow. Problems may arise when the interface undergoes significant topological changes, such as strong droplet deformations or the coalescence of two droplets. Front tracking methods (Unverdi and Tryggvason, 1992) describe the interface with a moving mesh on a fixed grid. This approach is very accurate but requires dynamic restructuring of the interface mesh. Front capturing methods employ markers or indicator functions to locate the interface of a two-phase system. The movement of the interface is then described with a simple advection equation for the indicator function, which can be readily discretised with standard numerical methods, e.g., finite element methods (FEM) or finite volume methods (FVM). Hence, front capturing methods are robust and especially suitable for the simulation of strong interface deformations whereupon no time-consuming mesh movement or smoothing algorithms are necessary. While various front capturing methods have been proposed, the prevailing approaches of this category are the volume of fluid (VOF) method introduced by Hirt and Nichols (1981) and the level set method by Osher and Sethian (1988).

The interfacial forces are of utmost importance for the dynamic behaviour of moving boundaries. Consequently, the implementation of interfacial forces are crucial for the performance of a CFD code for two-phase flows, and various methods have been introduced. One of the earliest methods is the continuous surface stress (CSS) model of Lafaurie et al. (2000) and Gueyffier et al. (1999). Owing to its simplicity and robustness, the continuum surface force (CSF) model of Brackbill et al. (1992) is probably the most widely-used interfacial force model. By spreading the interfacial forces over a volume, the CSF model leads to a smooth transition in pressure at the interface. In contrast, the ghost fluid method (GFM) of Liu et al. (2000) and Kang et al. (2000) leads to a sharp pressure jump.

Dijkhuizen et al. (2005) used a front tracking model to simulate toluene droplets with initial diameters of 4 to 12.5 mm rising in water. Compared with the experimental data of Wegener et al. (2010) for the same system, velocity oscillations occurred for larger diameters in the simulations and showed different amplitudes and frequencies. Moreover, the rise velocities were lower in the simulations than in the experiments of Wegener et al. (2010). Wang et al. (2008) studied mass transfer from droplets in a n-butanol/water system. The moving boundary was described with the level set method and the interfacial forces were implemented with the CSF model. For one droplet diameter, numerical results for the rise velocity and a comparison of the sim-
Bertakis et al. (2010) published terminal velocities of $n$-butanol droplets rising in water obtained with the academic code DROPS (cf. Gross et al., 2006). This code employs a level set formulation of the two-phase flow discretised with finite elements; the interfacial forces are implemented with the CSF model. The results were in excellent agreement with the authors’ own experimental data. However, the simulated rise time was rather short and covered only the onset of velocity oscillations.

Eiswirth et al. (2011) studied toluene droplets rising in water using the commercial finite-element code COMSOL Multiphysics 3.3a. The two-phase flow was described with a modified level set method suggested by Olsson and Kreiss (2005) which is, in fact, very similar to a VOF approach. The CSF model was used for interfacial forces. Comparing the terminal velocities with their own experimental results and those published by Wegener et al. (2007), Eiswirth et al. (2011) found very good agreement for small droplets ($<1.5$ mm) and large droplets ($>3$ mm) as well as satisfactory agreement for medium-size droplets. Moreover, experimental and simulated droplet shapes were in excellent accordance. However, the simulated rise time was too short to show oscillations which were, consequently, not discussed.

Bäumler et al. (2011) investigated the rise of single droplets experimentally and numerically. The simulations of three standard test systems for liquid-liquid extraction were carried out with moving mesh method implemented in the academic code NAVIER. The code uses finite element discretisation, and interfacial conditions, including the interfacial forces, are implemented with a subgrid projection method. Experimental results were taken from Wegener et al. (2010) (toluene/water) and Bertakis et al. (2010) ($n$-butanol/water). Additionally, experiments for $n$-butyl acetate droplets rising in water were performed. The agreement of numerical and experimental results was excellent for all systems and over the whole range of droplet diameters. However, oscillations of large droplets led to strong mesh deformation and, eventually, to a collapse of the simulations.

The results presented in this publication were obtained with a CFD-code based on a level set formulation of the two-phase flow. The code was implemented in the open source CFD package OpenFOAM® (Open Source Field Operation and Manipulation, www.openfoam.com, cf. Weller et al. (1998)). It includes two recent methods to overcome the volume loss frequently found in level set based methods. Simulations of rising droplets in three standard test systems for liquid/liquid extraction ($n$-butanol/water, $n$-butyl
acetate/water and toluene/water) were performed with the continuous interfacial force model of Brackbill et al. (1992) and with the sharp model of Kang et al. (2000). The influence of the interfacial force model on grid convergence, droplet shape, rise velocity and the onset of oscillations was studied. Furthermore, the simulation results were compared with recent numerical and experimental investigations. In this context, a comparison with the precise boundary fitted moving mesh method of Bäumler et al. (2011) is particularly interesting.

2. Mathematical model and numerical method

The CFD code used for this publication was recently employed to study the influence of Marangoni convection on single rising droplets (Engberg et al., 2014a). In the following sections, the mathematical framework of the level set approach, the governing equations and the numerical details are outlined.

2.1. Level set method

The fundamental idea of the level set approach is to employ a function to indicate whether a point \( x \) is located in the continuous phase \( \Omega_c \) or in the dispersed phase \( \Omega_d \). For this purpose, the indicator or level set function is defined as follows:

\[
\psi(x,t) < 0 \quad \text{if} \quad x \in \Omega_d \tag{1}
\]

\[
\psi(x,t) > 0 \quad \text{if} \quad x \in \Omega_c \tag{2}
\]

Thus, the interface \( \partial \Omega = \partial \Omega_c \cap \partial \Omega_d \) is defined implicitly by the isocontour \( \psi(x_I) = 0 \), where \( x_I \) is an arbitrary point on the interface.

In principle, any sufficiently smooth function could be chosen as a level set function. However, it has been shown that a signed distance function is a particularly advantageous choice (cf. Osher and Fedkiw, 2003). It has the following properties:

\[
|\psi(x)| = \min(|x - x_I|) \quad \text{for all} \quad x_I \in \partial \Omega \tag{3}
\]

\[
|\nabla \psi| = 1 \tag{4}
\]

The movement of an interface in a velocity field \( \mathbf{v} \) can be described with the following advection equation for the level set function \( \psi \):

\[
\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi = 0 \tag{5}
\]
Due to the advection, the level set function becomes distorted and loses its properties as a signed distance function (Eqs. (3), (4)).

The procedure to restore \( \psi \) as a signed distance function is called reinitialisation and is realised by solving the following partial differential equation:

\[
\frac{\partial \psi}{\partial \tau} = \frac{\psi_0}{\sqrt{\psi_0^2 + \Delta x^2}} (\psi_0) (1 - |\nabla \psi|) + \tilde{F}
\]

where \( \tau \) is pseudo-time, \( \Delta x \) is grid spacing and \( \psi_0 \) is the initial condition

\[\psi_0 = \psi(x, \tau = 0)\]  

It has been shown that the zero level set contour \((\psi(x) = 0)\) is often displaced during the reinitialisation (cf. Sussman and Fatemi, 1999). To prevent these artificial volume changes, a forcing term \( \tilde{F} \) recently suggested by Hartmann et al. (2010) is included in the reinitialisation equation (6). The formulation of the term \( \tilde{F} \) can be found in Hartmann et al. (2010).

Equation (6) is discretised in pseudo-time with a simple explicit Euler scheme with a predictor-corrector procedure for the forcing term \( \tilde{F} \). For the spatial derivatives, the third-order WENO scheme of Jiang and Peng (2000) is used. To reinitialise \( \psi \), 10 pseudo-time steps with a step size of \( \Delta \tau = \Delta x^2 \) were performed for each (physical) time step.

Despite the forcing term \( \tilde{F} \), preliminary simulations showed that the volume was not conserved. As the droplet size has a significant influence on the terminal velocity, it is very important to conserve the droplet volume exactly. Hence, an interface shift was implemented as proposed by Gross (2008). After the reinitialisation, a new level set function \( \psi_{\text{new}} \) is calculated by subtracting a correction \( \tilde{\psi} \) from the reinitialised level set function \( \psi \):

\[\psi_{\text{new}} = \psi(x, t) - \tilde{\psi}\]

The correction \( \tilde{\psi} \) is determined iteratively in such a way that the volume described by \( \psi_{\text{new}} \) is equal to the initial droplet volume. The shifted level set field \( \psi_{\text{new}} \) is then defined as the new level set function and used for the subsequent calculations. It was found that a rather small correction of \( \tilde{\psi} \approx 10^{-3} \Delta x \) applied every second time step was required to conserve the volume. Thus, one may safely assume that the solution is not disturbed by the interface shift.

Peng et al. (1999) introduced the concept of a localised level set function:
They pointed out that it is sufficient when the level set function is a distance function in the vicinity of the interface. Consequently, only cells in a confined region close to the interface have to be reinitialised, reducing the computational effort substantially. Outside the reinitialised region, the level set function is set to a constant value. In this work, the level set function was reinitialised in four consecutive cells on each side of the interface.

2.2. Navier-Stokes equations and moving reference frame

In this work, three systems, each consisting of two immiscible isothermal liquids, are studied. The liquids can be considered as Newtonian and incompressible. Hence, the fluid dynamics is described with the mass continuity and the Navier-Stokes equations. The equations describing the two-phase system are applied in single-field formulation, i.e. one set of equations for the whole domain including both the continuous and dispersed phase:

\[
\nabla \cdot \mathbf{v} = 0
\]

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \rho \mathbf{a} + (\rho \mathbf{v} \cdot \nabla) \mathbf{v} = \nabla \cdot (\eta (\nabla \mathbf{v} + \nabla \mathbf{v}^T)) - \nabla p - \rho g + \mathbf{F}_\sigma
\]

where \(\rho\) denotes density, \(\eta\) viscosity, \(p\) pressure and \(g\) gravitational acceleration. A modified pressure without hydrostatic contribution \(p^* = p - \rho g \cdot \mathbf{x}\) is used in the simulations to simplify the specification of boundary conditions (cf. Rusche, 2002). To simulate long rise times, the centre of the computational domain is kept approximately at the centre of mass of the droplet. The acceleration term \(\mathbf{a}\) in the momentum equation (10) accounts for this moving reference frame and is determined with a procedure based on a method given by Rusche (2002) (cf. Engberg et al., 2014b).

In the present work, the discontinuities of physical properties at the interface are “smeared” over a small area to ensure numerical stability. Therefore, a smoothed Heaviside function is employed:

\[
H_\epsilon(\psi) = \begin{cases} 
0 & \text{if } \psi < -\epsilon \\
\frac{1}{2} + \frac{\psi}{2\pi} + \frac{1}{2\pi} \sin \left(\frac{\pi \psi}{\epsilon}\right) & \text{if } |\psi| \leq \epsilon \\
1 & \text{if } \psi > \epsilon
\end{cases}
\]

In equation (11), parameter \(\epsilon\) determines the thickness of the transition region from one phase to another. In terms of the grid spacing \(\Delta x\), a typical value of the smoothing parameter of \(\epsilon = 1.5\Delta x\) was chosen for the simulations.
The density $\rho$ is calculated by

$$\rho = \rho_d + (\rho_c - \rho_d)H_\epsilon(\psi)$$  \hspace{1cm} (12)$$

The viscosity $\eta$ is interpolated with a method suggested by Kothe (1998). For this purpose, the arithmetic and the harmonic mean of viscosities are calculated with the Heaviside function (11) interpolated to the cell faces (cf. Fig. 1). These mean values are then averaged according to the relative orientation of the interface normal and the cell face normal.

Two different models are used for the surface force at the interface due to the interfacial tension $F_\sigma$: the continuum surface force (CSF) model of Brackbill et al. (1992) and the ghost fluid method (GFM) of Kang et al. (2000).

For the CSF model, the interfacial force is multiplied with a smoothed delta function $\delta_\epsilon$ and, consequently, transformed into a volume force acting in a small region at the interface:

$$F_\sigma = (\sigma \kappa \nabla \psi) \delta_\epsilon(\psi)$$  \hspace{1cm} (13)$$

where $\sigma$ denotes the interfacial tension and $\kappa$ the curvature of the interface. The smoothed delta function $\delta_\epsilon$ is calculated with

$$\delta_\epsilon(\psi) = \begin{cases} 0 & \text{if } |\psi| > \epsilon \\ \frac{1}{2\epsilon} + \frac{1}{2\epsilon} \cos \left( \frac{\pi \psi}{\epsilon} \right) & \text{if } |\psi| \leq \epsilon \end{cases}$$  \hspace{1cm} (14)$$

The curvature $\kappa$ is defined as the divergence of the interface unit normal $n_I$ calculated from the level set function:

$$n_I = \frac{\nabla \psi}{|\nabla \psi|}$$  \hspace{1cm} (15)$$

$$\kappa = -\nabla \cdot n_I$$  \hspace{1cm} (16)$$

To obtain a cell averaged value, the curvature is integrated over each finite volume $V_i$:

$$\bar{\kappa}_i = -\frac{1}{V_i} \int_{V_i} \nabla \cdot n_I \, dV$$  \hspace{1cm} (17)$$

Applying the Gaussian theorem yields:

$$\bar{\kappa}_i = -\frac{1}{V_i} \oint_S n_I \cdot dS$$  \hspace{1cm} (18)$$
Equation (18) can be readily approximated within the finite volume framework as a sum over all faces of a cell. The pressure gradient at a cell face \( i + 3/2, j \) between cells \( i+1, j \) and \( i+2, j \) (cf. Fig. 1) can be discretised with

\[
\left( \frac{\partial p}{\partial x} \right)_{i+3/2,j} \approx \frac{p_{i+2,j} - p_{i+1,j}}{\Delta x}
\]  

(19)

However, problems arise when the interfacial tension leads to a discontinuity in pressure between the cell centres. Liu et al. (2000) and Kang et al. (2000) showed that the approximation of the pressure gradient (19) can be modified by inserting a ghost value \( p_i + \sigma \kappa_{i,i+1/2} \) in cell \( i \) (cf. Fig. 1) to account for...
the discontinuity. Thus, the following expression is obtained:

\[
\frac{\partial p}{\partial x}|_{i+1/2} \approx \frac{p_{i+1} - p_i}{\Delta x} - \frac{\sigma \kappa_{I,i+1/2}}{\Delta x}
\]  

(20)

where \(\kappa_{I,i+1/2}\) is the curvature interpolated to the interface (cf. Liu et al., 2000; Francois et al., 2006):

\[
\kappa_{I,i+1/2} = \frac{\bar{\kappa}_i \psi_{i+1} + \bar{\kappa}_{i+1} \psi_i}{|\psi_i| + |\psi_{i+1}|}
\]  

(21)

Brackbill et al. (1992) derived the CSF model under the assumption of a gradual change in pressure at the interface. In contrast, the GFM is a discretisation technique which takes a sharp pressure jump at the interface into account. Therefore, the CSF model leads to a smooth transition in pressure between the phases, whereas the GFM produces a pressure jump from one cell to another, which is closer to reality. Both models are used in conjunction with single-field formulations of the mass continuity and the Navier-Stokes equations.

The implementation of the GFM is more demanding and increases the computational effort. While the CSF model can be easily applied to arbitrary grids, the GFM, as currently implemented, is limited to structured orthogonal grids. With appropriate interpolation techniques, however, the GFM may be extended to arbitrary grids.

2.3. Discretisation, grid and boundary conditions

Eqs. (5), (9) and 10 were solved within a finite volume framework. As is customary in OpenFOAM®, a collocated variable arrangement was used, i.e. level set function, pressure and velocities were stored at the cell centres. Convective terms (\(\mathbf{v} \cdot \nabla\)) in Eqs. (5) and (10) were discretised with the NVD Gamma scheme introduced by Jasak et al. (1999) and time was discretised with a first-order accurate implicit Euler scheme. The time steps were constant during the simulations and in the range of 10 to 100 ms leading to maximum Courant numbers of 0.25.

The pressure-velocity coupling is achieved with a Pressure Implicit with Splitting of Operators (PISO)-algorithm (cf. Issa, 1986) adopted from the VOF-code interFoam provided with OpenFOAM® 1.7.1. For this algorithm, the continuity equation (9) is reformulated as a Poisson equation for pressure,
Figure 2: The wedge-shaped computational domain is $12d_0$ high and $5d_0$ wide. To resolve the fluid dynamics close to the droplet, the grid is refined in the centre and becomes gradually coarser towards the boundaries.

providing a correction for the velocity field. The discretised Navier-Stokes-equations and the pressure equation are solved sequentially in a predictor-corrector procedure. A detailed description of the algorithm was presented by Rusche (2002). In all simulations, three corrector steps were performed with the PISO-loop.

The droplets considered in this work are small enough to rise in a vertical path (cf. Bäumler et al., 2011). Thus, axial symmetry of the droplet was assumed, effectively reducing the computational effort. The wedge-shaped computational domain can be seen in Fig. 2. The reference frame is translated in the $z$-direction, as in the study of Bäumler et al. (2011).

In terms of the initial droplet diameter $d_0$, the computational domain is
5 \, d_0 \text{ wide and } 12 \, d_0 \text{ high. As can be seen in Fig. 2, the grid is structured and refined in the vicinity of the droplet. The size of the refined region is } d_0 \times 2 \, d_0 \text{ except for the simulation of the largest } n\text{-butanol droplet. This droplet } (d_0 = 4 \text{ mm}) \text{ deforms significantly and requires a refined region of } 1.5 \, d_0 \times 2 \, d_0. \text{ The grid spacing in the refined region is discussed in Section 3.2.}

The boundary conditions were chosen as follows: due to the moving reference frame, the velocity at the top and the outer boundary of the computational domain is equal to the frame velocity (cf. Fig. 3). At the bottom of the computational domain, a zero gradient condition is employed for velocity. Zero gradient conditions are also appropriate for the localised level set function at the top, bottom and outer boundary. The boundary conditions for the modified pressure are a constant reference pressure at the bottom and zero...
gradient conditions at the top and sides.
As can be seen in Fig. 2, the droplet is initialised as a sphere at rest in the middle of the domain.
The physical properties are taken from Misek et al. (1985) and are listed in Table 1.

Table 1: Physical properties of the investigated systems: Density $\rho$, dynamic viscosity $\eta$ and interfacial tension $\sigma$ at temperature $\vartheta$, where $d$ denotes the droplet phase and $c$ the continuous phase

<table>
<thead>
<tr>
<th>system</th>
<th>$\rho_d$ (kg/m$^3$)</th>
<th>$\eta_d$ (mPa s)</th>
<th>$\rho_c$ (kg/m$^3$)</th>
<th>$\eta_c$ (mPa s)</th>
<th>$\sigma$ (mN/m)</th>
<th>$\vartheta$ (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>toluene/water</td>
<td>862.3</td>
<td>0.552</td>
<td>997.0</td>
<td>0.890</td>
<td>35.0</td>
<td>25</td>
</tr>
<tr>
<td>n-butyl acetate/water</td>
<td>877.2</td>
<td>0.820</td>
<td>996.6</td>
<td>0.904</td>
<td>14.0</td>
<td>25</td>
</tr>
<tr>
<td>n-butanol/water</td>
<td>845.4</td>
<td>3.280</td>
<td>986.5</td>
<td>1.390</td>
<td>1.63</td>
<td>20</td>
</tr>
</tbody>
</table>

3. Results

3.1. Static droplet

Before the more difficult simulation of deformable droplets is approached, it appears reasonable to analyse a problem having an analytical solution to assess the two interfacial force models. The static droplet is a popular benchmark for interfacial force models. A 2D “droplet” with a diameter of $d_0 = 4$ mm was initialised in a quiescent continuous phase. The size of the two-dimensional domain was 8 mm $\times$ 8 mm. Both phases had similar densities (1000 kg/m$^3$) and viscosities (10$^{-3}$ Pa s) and the interfacial tension was 0.073 N/m. The gravitational acceleration was not taken into account. Therefore, no flow should develop and the pressure jump at the interface is given by the Young-Laplace-equation:

$$\Delta p_{\text{exact}} = \sigma \kappa = \frac{2 \sigma}{d_0} = 36.5 \text{ Pa s} \quad (22)$$

A time step of $\Delta t = 10^{-6}$ s was calculated. All systems of equations were solved with a tolerance of $10^{-12}$.

For a quantitative comparison of the results, four quantities were defined (cf. Francois et al., 2006):

- $|v_{\text{max}}|$, i.e. the magnitude of the maximum velocity
\[ \Delta p_{\text{tot}} = \bar{p}_d - \bar{p}_c , \]
where \( \bar{p}_d \) and \( \bar{p}_c \) are the arithmetic averages of the pressures in the dispersed \((\psi \leq 0, N_d \text{ cells})\) and the continuous \((\psi > 0, N_c \text{ cells})\) phase, respectively:
\[
\bar{p}_d = \frac{1}{N_d} \sum_{i=1}^{N_d} p_i \quad \text{and} \quad \bar{p}_c = \frac{1}{N_c} \sum_{i=1}^{N_c} p_i
\]

\[ \Delta p_{\text{part}} = \bar{p}_{\text{part},d} - \bar{p}_{\text{part},c} \]
For the arithmetic averages, only cells with \( H_{\epsilon,i} = 0 \) (for \( \bar{p}_{\text{part},d} \)) or \( H_{\epsilon,i} = 1 \) (for \( \bar{p}_{\text{part},c} \)) are taken into account. Thereby, the transition region of the CSF model is not included.

\[ \Delta p_{\text{max}} = p_{\text{max}} - p_{\text{min}} , \]
where \( p_{\text{max}} \) is the maximum and \( p_{\text{min}} \) the minimum pressure in the computational domain.

The relative error \( E \) of the pressure differences was calculated according to
\[
E = \frac{\left| \Delta p - \Delta p_{\text{exact}} \right|}{\Delta p_{\text{exact}}} \tag{23}
\]

The results for various grid spacings are compiled in Table 2. Regarding the maximum velocities, the results indicate that spurious currents are reduced with grid refinement when the GFM is used. In contrast, with the CSF model, grid refinement increases the magnitude of the maximum velocity. Moreover, \( |v_{\text{max}}| \) is in all cases larger with the CSF model than with the GFM.

Due to the transition region, \( E_{\text{tot}} \) is large for the CSF model on coarse grids and decreases with grid refinement. Consequently, the error is significantly smaller when the transition region is not included \( (E_{\text{part}}) \), and a reasonable agreement with the exact pressure jump is achieved. Nevertheless, the error increases with the last level of refinement. The same conclusions apply to \( E_{\text{max}} \).

For the GFM, \( E_{\text{tot}} \) is relatively small in all cases and decrease consistently with grid refinement. A comparison of \( E_{\text{tot}} \) and \( E_{\text{part}} \) shows that no significant deviations from the exact pressure difference occur at the interface.

| \( \Delta x \) | \( \mu \text{m} \) | \( |v_{\text{max}}| \) | \( \mu \text{m/s} \) | \( E_{\text{tot}} \) | \( \% \) | \( E_{\text{part}} \) | \( \% \) | \( E_{\text{max}} \) | \( \% \) |
|---|---|---|---|---|---|---|---|---|---|
| 400 | 2.17 | 12.5 | 1.085 | \( \Delta p_{\text{exact}} \) | 1.929 | \( \Delta p_{\text{exact}} \) | 1.140 | 0.971 | 0.961 | 3.546 |
| 200 | 4.15 | 6.55 | 0.183 | 0.822 | \( \Delta p_{\text{exact}} \) | 0.294 | 0.230 | 0.232 | 0.988 |
| 100 | 9.83 | 3.48 | 0.017 | 0.664 | \( \Delta p_{\text{exact}} \) | 0.119 | 0.055 | 0.055 | 0.270 |
| 50  | 19.7  | 1.56 | 0.050 | 0.782 | \( \Delta p_{\text{exact}} \) | 0.044 | 0.025 | 0.026 | 0.071 |
While $E_{max}$ is larger for the GFM than for the CSF model on coarse grids, it shows a better grid convergence with the GFM. On the finest mesh, $E_{max}$ obtained with the GFM is one order of magnitude smaller than the corresponding error of the CSF model.

For this simple test case, results obtained with the GFM are quantitatively better in most cases. In contrast to the CSF model, the GFM shows a better and more consistent convergence with grid refinement. These conclusions disagree with those of Francois et al. (2006) who observed a similar behaviour of both models when a good curvature approximation was used. At the same time, our results are in accordance with the conclusions of Kang et al. (2000), as well as some other works. In comparison with the numerical results of Francois et al. (2006), two factors might contribute to the different findings: Francois et al. (2006) used a discretisation procedure which led to an exact balance of interfacial and pressure forces in the static case. As noted by Rusche (2002), however, this is not guaranteed for the current implementation of the PISO-algorithm. Moreover, the smoothed delta function with $\epsilon = 1.5\Delta x$ distributes interfacial forces over a broader region than the VOF-code of Francois et al. (2006). The results show that under these circumstances, a sharp approach leads to a better balancing of interfacial and pressure forces and, consequently, to a reliable grid convergence.

3.2. Grid convergence of the terminal rise velocity

To assess the grid convergence of the terminal rise velocity, droplets with an initial diameter of $d_0 = 2$ mm were simulated for all systems with various grid spacings. The resulting terminal rise velocities are compiled in Table 3. For the $n$-butanol/water system, grid-independent results are obtained with

<table>
<thead>
<tr>
<th>$d_0/\Delta x$</th>
<th>n-butanol/water</th>
<th>n-butyl acetate/water</th>
<th>toluene/water</th>
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<tr>
<td></td>
<td>CSF</td>
<td>GFM</td>
<td>CSF</td>
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<tr>
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<td>55.92</td>
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<td>87.53</td>
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<td>88.90</td>
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<tr>
<td>120</td>
<td>–</td>
<td>–</td>
<td>88.96</td>
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</tbody>
</table>
a grid spacing of $d_0/\Delta x = 60$ and $d_0/\Delta x = 80$ for the GFM and the CSF model, respectively.

Slightly finer grids are required for the $n$-butyl acetate/water system. The interfacial tension of the $n$-butyl acetate/water system is almost one order of magnitude higher than that of the $n$-butanol/water system. Consequently, the interfacial force model is far more important in this case. While the GFM shows reasonable grid convergence, the convergence behaviour of the CSF model is less clear.

The toluene/water system possesses the highest interfacial tension among the three systems investigated. Therefore, it is the most challenging test system for the interfacial force models in this study. The results show a very good convergence for the GFM, but a less reliable behaviour of the CSF model. The grid convergence study affirms the conclusion of the static droplet test case: while grid convergence was achieved with the GFM in all cases, the CSF model was less reliable. This finding reflects the consistent reduction of spurious currents with grid refinement achieved with the GFM – a quality which is particularly important for systems with high interfacial tension (e.g. toluene/water).

Furthermore, the results show that a grid spacing of $d_0/\Delta x = 80$ leads to good results which deviate only marginally from those obtained with the finer grids. This conclusion was also confirmed for other droplet diameters. Hence, the simulation results presented in following sections were obtained with this grid spacing.

3.3. Droplet shape

The droplet shape is defined by the isocontour $\psi(x,t) = 0$ which can be obtained in the post processing procedure. In Fig. 4, some droplet shapes for the $n$-butanol/water system are shown. The shapes agree well with those presented by Bertakis et al. (2010). In accordance with Bäumler et al. (2011), we observed a vortex in the wake of droplets with $d_0 > 2$ mm. Furthermore, we found a secondary internal circulation for $d_0 = 3.48$ mm and $d_0 = 4$ mm which is presented in Fig. 5. This phenomenon can be explained by the very flat shape in conjunction with the vortex in the wake of these droplets.

The aspect ratio $\mathcal{E}$, i.e. the ratio of the two principal axes, was determined graphically from the droplet shapes. Both for the CSF model and the GFM, the agreement with the simulation results of Bäumler et al. (2011) is excellent, as can be seen in Table 4. Oscillations were observed for droplets with $d_0 \geq 3$ mm. This is in line with Bertakis et al. (2010) and Bäumler et al.
Figure 4: Simulated droplet shapes of the $n$-butanol/water system at times 0.1 s, 0.2 s, 0.3 s, 0.4 s, 0.5 s and 0.6 s (left to right); the initial droplet diameters are 2 mm, 3 mm, 3.48 mm and 4 mm (top to bottom). The GFM was used for the simulations.

Figure 5: The streamlines of a $n$-butanol droplet with $d_0 = 4$ mm rising in water reveal a vortex in the wake of the droplet and two internal circulations.
Table 4: Aspect ratios of the system $n$-butanol/water from this study obtained with the CSF model ($\varepsilon_{CSF}$) and the GFM ($\varepsilon_{GFM}$) and simulation results from Bäumler et al. (2011) ($\varepsilon_{Navier}$)

<table>
<thead>
<tr>
<th>$d_0$ (mm)</th>
<th>$\varepsilon_{CSF}$</th>
<th>$\varepsilon_{GFM}$</th>
<th>$\varepsilon_{Navier}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00</td>
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<td>0.95</td>
<td>0.95</td>
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<td>0.84</td>
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<tr>
<td>3.00</td>
<td>0.35</td>
<td>0.36</td>
<td>0.36</td>
</tr>
</tbody>
</table>

The aspect ratios obtained for the $n$-butyl acetate/water system are given in Table 5. A comparison with the aspect ratios determined by Bäumler et al. (2011) shows very good agreement for both interfacial force models. In accordance with Bäumler et al. (2011), shape oscillations occur for droplets with $d_0 = 4$ mm in simulations with both interfacial force models.

Table 5: Aspect ratios of the system $n$-butyl acetate/water from this study obtained with the CSF model ($\varepsilon_{CSF}$) and the GFM ($\varepsilon_{GFM}$) and simulation results from Bäumler et al. (2011) ($\varepsilon_{Navier}$)

<table>
<thead>
<tr>
<th>$d_0$ (mm)</th>
<th>$\varepsilon_{CSF}$</th>
<th>$\varepsilon_{GFM}$</th>
<th>$\varepsilon_{Navier}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>1.50</td>
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<td>0.97</td>
<td>0.97</td>
</tr>
<tr>
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<td>0.79</td>
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<tr>
<td>3.50</td>
<td>0.55</td>
<td>0.56</td>
<td>0.55</td>
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</table>

Some droplet shapes for the toluene/water system are shown in Fig. 6. The qualitative agreement of the simulated shapes of this work with the experimental and numerical results of Eiswirth et al. (2011) is apparent. In comparison with the CSF model, the GFM leads to aspect ratios closer to the results of Bäumler et al. (2011) (cf. Table 6). Similar to Bäumler et al. (2011), we found shape oscillations for droplets with $d_0 = 4.4$ mm in the simulation with the CSF model. In simulations with the GFM, oscillations occurred already for droplets with $d_0 = 4$ mm. This finding will be discussed further in Section 3.5.
Figure 6: Simulated droplet shapes of the toluene/water system at times 0.1 s, 0.2 s, 0.3 s, 0.4 s, 0.5 s and 0.6 s (left to right); the initial droplet diameters are 2 mm, 3 mm and 4 mm (top to bottom). The GFM was used for the simulations.

Table 6: Aspect ratios of the system toluene/water from this study obtained with the CSF model (\(\mathcal{E}_{\text{CSF}}\)) and the GFM (\(\mathcal{E}_{\text{GFM}}\)) and simulation results from Bäumler et al. (2011) (\(\mathcal{E}_{\text{NAVIER}}\))

<table>
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<tr>
<th>(d_0) (mm)</th>
<th>(\mathcal{E}_{\text{CSF}})</th>
<th>(\mathcal{E}_{\text{GFM}})</th>
<th>(\mathcal{E}_{\text{NAVIER}})</th>
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<tr>
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<td>–</td>
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3.4. Terminal rise velocity

In this section, the results for the drop rise velocity are presented and compared with experimental and numerical results from the literature. A qualitative representation of the transient droplet rise velocity is shown in Fig. 7. The droplet rise velocity usually increases to a maximum $v_{\text{max}}$ before slowing down and reaching the terminal, or characteristic mean velocity $v_{\text{cha}}$ (cf. Wegener et al., 2010). The upper curve (b) in Fig. 7 depicts the rise velocity of a larger droplet with oscillations around the mean velocity $v_{\text{cha}}$. In Fig. 8, terminal rise velocities for $n$-butanol droplets in water are shown together with the results of Bertakis et al. (2010) and Bäumler et al. (2011) as well as the corresponding relative deviations. With both interfacial force models, an excellent agreement with the numerical results of Bäumler et al. (2011) is achieved. Both numerical and experimental values of the terminal rise velocity published by Bertakis et al. (2010) show a distinct maximum obtained for a droplet diameter of approximately 2.5 mm and a rapid decrease for larger droplets. In contrast, our simulations and those of Bäumler et al. (2011) predict a less pronounced maximum velocity for larger droplets with initial diameters in the range of 3.1 mm to 3.5 mm. Recently, Komrakova et al. (2013) published terminal rise velocities of $n$-butanol droplets in water obtained with a Lattice Boltzmann method. In their study, the maximum rise

![Figure 7](image_url)  
Figure 7: Qualitative representation of the transient droplet rise velocity as a function of time. The lower curve (a) applies for circulating droplets and the upper curve (b) for oscillating droplets. The maximum velocity $v_{\text{max}}$ and the characteristic mean velocity $v_{\text{cha}}$ are marked.
velocity was found for the droplet with $d_0 = 3.8$ mm. As noted by Bäumler et al. (2011), the simulated times of Bertakis et al. (2010) were slightly too short to reach the terminal rise velocity for large droplets. Consequently, deviations are found for droplets with $d_0 \geq 3$ mm. The terminal rise velocities for $n$-butyl acetate droplets in water from this work, the results of Bäumler et al. (2011) and their relative deviations are shown in Fig. 9. The results for the $n$-butyl acetate/water system show the difference between the interfacial force models more clearly: A very good agreement with the simulation results of Bäumler et al. (2011) is obtained with the GFM, while the CSF model leads to larger deviations, cf. Fig. 9 (b). The maximum deviation is found for the smallest droplet ($d_0 = 1$ mm) which possesses the highest jump in pressure at the interface. Furthermore, a reasonable agreement with the experimental results of Bäumler et al. (2011) is achieved with both models, cf. Fig. 9 (c), (d).

Our results for the terminal rise velocities for toluene droplets in water and those of Wegener et al. (2010) and Bäumler et al. (2011) as well as their relative deviations are shown in Fig. 10. The results obtained with the CSF model deviate distinctly from those with the GFM and the data of Bäumler et al. (2011). Similar to the previous system, the result for the smallest droplet ($d_0 = 1$ mm) obtained with the CSF model shows the largest deviations, cf. Fig. 10 (b). With the GFM, a very good agreement with the simulation results of Bäumler et al. (2011) is achieved. For both interfacial force models, the simulated terminal rise velocities agree well with the experimental maximum velocities of Wegener et al. (2010).

Transient rise velocities of toluene droplets with $d_0 = 2$ mm and $d_0 = 3.5$ mm simulated with the GFM are presented in Fig. 11 with the corresponding experimental data of Wegener et al. (2010). In both cases, a good agreement is achieved. Deviations during the acceleration phase can be explained with different initial conditions: While the simulated droplets are initialised as spheres, the experimental droplets are produced with a capillary and deform during the detachment. In all cases, the acceleration phase is terminated after $1$ s or less.

The results presented in this section are in line with the findings of Section 3.1: In comparison with the CSF model, the GFM reduces spurious currents. This is especially important in cases with high interfacial tension and large curvatures (i.e. for small droplets).

The numerical values for the terminal rise velocity of all cases considered in this work are compiled in Table 7.
Figure 8: Terminal rise velocity of n-butanol droplets in water:
(a) The numerical results from this work in comparison with simulations from Bäumler et al. (2011) as well as experimental and numerical results from Bertakis et al. (2010)
(b) Relative deviation from the simulation results of Bäumler et al. (2011) for the CSF model (+) and for the GFM (×)
(c) Relative deviation from the experimental results of Bertakis et al. (2010) for the CSF model (+) and for the GFM (×)
(d) Relative deviation from the simulation results of Bertakis et al. (2010) for the CSF model (+) and for the GFM (×)
Figure 9: Terminal rise velocity of $n$-butyl acetate droplets in water:
(a) The simulation results from this work in comparison with experimental and numerical results from Bäumler et al. (2011).
(b) Relative deviation from the simulation results of Bäumler et al. (2011) for the CSF model (+) and for the GFM ($\times$)
(c) Relative deviation from $v_{max}$ of Bäumler et al. (2011) for the CSF model (+) and for the GFM ($\times$)
(d) Relative deviation from $v_{char}$ of Bäumler et al. (2011) for the CSF model (+) and for the GFM ($\times$)
Figure 10: Terminal rise velocity of toluene droplets in water:
(a) The numerical results from this work in comparison with simulations from Bäumler et al. (2011) and experimental results from Wegener et al. (2010).
(b) Relative deviation from the simulation results of Bäumler et al. (2011) for the CSF model (+) and for the GFM (×)
(c) Relative deviation from $v_{\text{max}}$ of Wegener et al. (2010) for the CSF model (+) and for the GFM (×)
(d) Relative deviation from $v_{\text{cha}}$ of Wegener et al. (2010) for the CSF model (+) and for the GFM (×)
Figure 11: Transient rise velocity of toluene droplets in water: Simulation results with the GFM (lines) and experimental data of Wegener et al. (2010) (symbols).
Table 7: Numerical results for the terminal rise velocity in mm/s for all cases considered in this work.

<table>
<thead>
<tr>
<th>$d_0/\Delta x$</th>
<th>$n$-butanol/water</th>
<th>$n$-butyl acetate/water</th>
<th>toluene/water</th>
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<td>CSF</td>
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</table>
3.5. Oscillations and stability

In simulations of the \( n \)-butanol/water system, oscillations occur for droplets with \( d_0 \geq 3 \) mm. However, the amplitude of the oscillations decreases and eventually, a constant rise velocity and droplet shape is reached. This behaviour is shown in Fig. 12 for a droplet with \( d_0 = 4 \) mm, simulated with both the CSF model and the GFM.

In contrast, the \( n \)-butyl acetate droplet with \( d_0 = 4 \) mm and the toluene droplet with \( d_0 = 4.4 \) mm show oscillations with constant amplitude and frequency. As mentioned in Section 3.3, toluene droplets with an initial diameter of 4.4 mm show oscillations when the CSF model is used, whereas with the GFM, oscillations occur for smaller droplets (\( d_0 = 4 \) mm). This finding can be explained with Fig. 13. In the simulations discussed previously, the smoothing parameter of the transition region was \( \epsilon = 1.5 \Delta x \). When the smoothing parameter is increased to \( \epsilon = 3 \Delta x \), toluene droplets with \( d_0 = 4.4 \) mm simulated with the CSF model do not oscillate. In contrast, oscillations are found in the rise velocity simulated with the GFM. Apparently, simulation results are very sensitive to the smoothing of interfacial forces and excessive smoothing may even lead to an erroneous prediction of droplet dynamics.

Comparing the simulated rise velocities with the experimental results of Wegener et al. (2010), we find a similar amplitude of approximately 10 to 15 mm/s in the velocity oscillations. Nevertheless, the frequencies (or periods) of the velocity oscillations obtained from the simulations are very different from experimental results: The order of magnitude of the periods in our simulations is 0.1 s, whereas Wegener et al. (2010) determined periods of approximately 1 s experimentally. For oscillating droplets, axial symmetry cannot be assumed and droplets should be simulated fully three-dimensional. Consequently, it is likely that 3D effects which cannot be reproduced in our simulations are responsible for the different frequencies.
Figure 12: Transient rise velocities of a $n$-butanol droplet with $d_0 = 4$ mm rising in water, simulated with the CSF model and the GFM.

Figure 13: Transient rise velocities of a toluene droplet with $d_0 = 4.4$ mm rising in water, simulated with the CSF model and the GFM. In both cases, the smoothing parameter of the transition region was set to $\epsilon = 3\Delta x$. 
4. Conclusions

In this paper, the results of numerical simulations of single droplets rising in a quiescent liquid are presented. Three standard test systems for liquid-liquid extraction were investigated: n-butanol/water, n-butyl acetate/water and toluene/water in which water represents the continuous phase. Assuming axial symmetry of the droplet, we simulated droplets with various diameters up to the onset of oscillations. For the simulations, a CFD code based on a level set formulation of the two-phase flow was developed and implemented in the open-source CFD package OpenFOAM®. A well-known drawback of the level set method is the volume change during reinitialisation. Applying two recently published methods, we were able to overcome this problem. Furthermore, two interfacial force models were applied in this work: the widely-used CSF model, which leads to a smooth transition in pressure at the interface, and the GFM, which results in a sharp jump. The influence of the interfacial force model on the shape and the dynamic behaviour of the droplets was studied.

For the theoretical test case of a static droplet as well as for rising droplets in all three test systems, grid convergence was achieved with the GFM. In contrast, the CSF model showed a less reliable behaviour with respect to grid refinement.

Regarding droplet shapes and terminal rise velocities, good agreement with recent numerical investigations by Bäumler et al. (2011) and Bertakis et al. (2010) was found with both interfacial force models. The results obtained with the GFM agree particularly well with the numerical results of Bäumler et al. (2011). The comparison of terminal rise velocities, droplet shapes and onset of oscillations obtained from our simulations with experimental results published by Bertakis et al. (2010), Wegener et al. (2010) and Bäumler et al. (2011) is equally satisfactory for both interfacial force models. The only distinct discrepancy was found in the n-butanol/water system for droplets with \( d_0 \geq 3 \) mm. Bertakis et al. (2010) found a pronounced maximum in the terminal rise velocity for droplets with \( d_0 \approx 2.5 \) mm, both experimentally and numerically. Similar to Bäumler et al. (2011), our simulations show a less pronounced maximum velocity for larger droplets with initial diameters in the range of 3.1 mm to 3.5 mm. Komrakova et al. (2013) found the maximum rise velocity for droplets with \( d_0 = 3.8 \) mm. Future experimental and numerical investigations should clarify the tendency for larger droplets in this system.
The onset of oscillations predicted with our simulations compares favourably with numerical and experimental results from literature (Bäumler et al., 2011; Bertakis et al., 2010; Wegener et al., 2010). However, it was shown that excessive smoothing of interfacial forces with the CSF model can lead to an unphysical stabilisation of the droplet. In contrast, this problem does not occur with the GFM.

The results presented in this paper show that a satisfactory simulation of droplets can be achieved with both the CSF model and the GFM. Nevertheless, the GFM results in lower spurious currents which, furthermore, are consistently reduced with grid refinement. These properties are reflected in the simulated rise velocities and in a reliable performance with respect to grid refinement.

5. Acknowledgement

We would like to thank Dr. Mirco Wegener for the experimental data.
References


