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TRANSPORT PHENOMENA AND FLUID MECHANICS

An improved subgrid scale model for front-tracking based simulations of mass transfer from bubbles

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Abstract
Gas–liquid bubble column reactors are often used in industry because of their favorable mass transfer characteristics. The bubble mass boundary layer in these systems is generally one order of magnitude thinner than the momentum boundary. To resolve it in simulations, a subgrid scale model will account for the sharp concentration variation in the vicinity of the interface. In this work, the subgrid scale model of Aboulhasanzadeh et al., Chem Eng Sci, 2012, 75:456–467 embedded in our in-house front tracking framework, has been improved to prevent numerical mass transfer due to remeshing operations. Furthermore, two different approximations of the mass distribution in the boundary layer have been tested. The local and global predicted Sherwood number has been verified for mass transfer from bubbles in the creeping and potential flow regimes. In addition, the correct Sherwood number has been predicted for free rising bubbles at several Eötvös and Morton numbers with industrial relevant Schmidt numbers (10^3–10^5).

KEYWORDS
boundary layer, bubble columns, front tracking, mass transfer, subgrid scale modeling

1 INTRODUCTION

Because of the many industrial applications in chemical, biochemical, and petrochemical industries, the mass transfer in gas–liquid systems has been widely studied for decades. Such studies aim to obtain a better understanding of the complex hydrodynamics that govern the mass transfer characteristics impacting reactor design and scale-up. However, detailed investigation of mass transfer in gas–liquid systems is still challenging. Experimental studies face challenges with respect to available measuring techniques, which are either intrusive or limited by the data that can be obtained. Numerical studies on the other hand are limited by computational power. This limiting factor of numerical simulations can partly be overcome using a multiscale modeling approach. In this approach, correlations obtained from small-scale simulations are used in large-scale simulations to accurately capture the small-scale phenomena without resolving these.

Direct numerical simulations (DNS) are mostly used to obtain these correlations. In DNS the bubble shape is resolved hence they are able to resolve the relevant length and time scales of the hydrodynamics without any rigorous assumptions. In DNS, there exist two categories of techniques to model a gas–liquid interface: front capturing (FT) and front tracking (FT). The main front capturing techniques are the volume of Fluid (VOF) method and the Level Set (LS) method. In these methods, the bubble interface is obtained implicitly by reconstruction. In the VOF method the interface is obtained from a color function, which generally is the phase fraction making the method inherently mass conservative. However, the calculation of surface properties, for example, the surface tension, is difficult. Furthermore,
the automatic merging of bubbles when their interfaces occupy the same grid cell might lead to artificial coalescence of bubbles. The LS method improves the calculation of the surface tension by tracking the surface via a distance function to the surface. Compared to VOF however, it is more difficult to strictly obey mass conservation. In the FT method, the interface is explicitly tracked by Lagrangian marker points. Although the explicit tracking of the interface prevents automatic coalescence, the advection of the marker points is performed with the local velocity making the method nonconservative.

When these methods are used to determine mass transfer in gas-liquid systems by means of solving a species convection-diffusion equation with proper conditions at the gas-liquid interface, a problem arises due to the very thin mass boundary layer that exists because of the typically high Schmidt numbers (Sc) of liquids. To resolve this mass boundary layer, a high grid density is necessary, which will lead to high computational power requirements.

To still be able to study mass transfer, different approaches have been taken. Bothe et al., Bothe and Warnecke, Onea et al., Alke et al. and Hayashi and Tomiyama have used one uniform grid to resolve both the hydrodynamics and the species transfer while simulating mass transfer from single (deformable) bubbles, Taylor bubbles, or bubble trains. To keep the computational requirements reasonable, the simulations were performed in 2D, with a axisymmetric domain and/or at low Sc. Because a high Sc only influences the smallest length scale for species transfer, several researchers used separate grids for the hydrodynamics and the species transfer. In this approach both grids are uniform and regular, which makes interpolation of the velocity field to the more refined species transfer grid possible. Davidson and Rudman investigated the mass transfer of deformable bubbles with this technique. Reactive mass transfer was studied by Koynov et al. and Radl et al. Darmana et al. used it to simulate single bubbles in 3D at a low Sc and Roghair et al. used the two-grid approach to investigate the mass transfer in bubble swarms. These simulations were still limited to moderate Sc (Sc = 1–430).

The high resolution is only required in the regions with high gradients. Therefore, many researchers have used unstructured meshes, which are refined at the interface and coarse in bulk regions. Jung and Sato, Dani et al., Wylock et al., Colombet et al. and Deising et al. have used these local refinement techniques to study single bubbles and Hayashi and Tomiyama have used it to simulate Taylor flow bubbles. The disadvantage of an unstructured mesh is that it should move with the bubble. Therefore Jung and Sato, Dani et al., Wylock et al. and Colombet et al. used fixed particle/bubble shapes. With this method, Colombet et al. was able to simulate cases with Sc up to 20,000 in a 2D and axisymmetric domain.

In the last decade, the Center for Smart Interfaces and the Institute for Mathematical Modeling and Analysis groups in Darmstadt have worked on a subgrid scale model for the VOF method that can resolve the thin boundary layer inexpensively. The subgrid scale model uses an analytical solution with a fitted parameter, the local boundary layer thickness, to capture the steep concentration gradient. From this concentration gradient the mass transfer flux is determined. In Bothe and Fleckenstein the model was improved to be able to handle Henry numbers different from unity. In Gründing et al. the model was extended to handle reactive boundary layers. Weiner and Bothe recently further improved the quality of the model by different fitting and correction steps. They were able to simulate up to a Sc of 10^7 while deviating less than 1% from the reference value. The simulation was in 3D but symmetry planes were used.

Aboulhasanzadeh et al. also introduced a subgrid scale model to reduce the computational requirement, but for the FT method. In this subgrid scale model, the mass boundary layer is approximated by a simplified version of the advection–diffusion equation near the interface, while the rest of the domain is solved by the Finite Volume Method. The 2D version of this implementation was validated with DNS simulations on a fine grid for single, spherical and ellipsoidal bubbles at moderate Reynolds numbers, Re, and Sc. When the method was extended to 3D, the model was also validated against experimental results. The method was furthermore used to simulate the effect of multiple bubbles interacting. The original method of Aboulhasanzadeh et al. and its extensions did not perform any extra operations for mass conservation during the remeshing procedure of the FT markers (personal communication). This will result in numerical movement of mass during the remeshing procedure. In addition, due to the growth or shrinkage of the marker during remeshing, artificial sources or sinks of mass will be created and species will not be conserved. In this article, we will improve the method to accurately conserve species during the remeshing procedure.

In addition, Aboulhasanzadeh and Tryggvason use a second order polynomial to approximate the profile in the boundary layer. To improve the approximation, we will change this to an error function. In the present study, the improved method will be verified and validated over a wide range of physical properties of the gas-liquid system covering a large part of the Grace bubble diagram. This article starts with an introduction to the applied FT method. Following, the implementation of the mass boundary layer model is given. The obtained model is verified in the next section. The article ends with the validation results of single rising bubbles and some conclusions.

## 2 | FRONT TRACKING

The FT method used in the present study is based upon the method of van Sint Annaland et al., Dijkstra et al., and Roghair et al. This method solves the continuity equation and the Navier–Stokes equation for incompressible flows using a one field approximation:

$$\nabla \cdot \mathbf{u} = 0$$  

$$\rho \frac{\partial \mathbf{u}}{\partial t} = -\nabla p - \rho \nabla \cdot (\mathbf{u} \mathbf{u}) - \nabla \cdot \tau + \rho g + F_s$$  

$F_s$ in Equation (2) is a force density accounting for the surface tension arising from the interfaces. This force is directly calculated.
from the triangular markers using the pull force method.9 In this method, the tensile force on a marker, $m$, of adjacent markers is computed using the joint tangent, $tm$, and the normal vector, $nm$, $c$.

$$F_{s,m} = \frac{1}{2} \sum_{i} \sigma (t_{mi} \times n_{mi})$$ (3)

The obtained force is mapped from marker $m$ to the closest Eulerian grid cell by using mass-weighting.2 The mismatch between the discrete representation of the surface tension and the pressure gradient leads to undesirable spurious currents. To alleviate problem, the method is expanded with a so-called pressure-jump correction.36 Equations (1) and (2) are solved on a fixed Cartesian grid with a staggered arrangement of pressure and velocity variables. The Finite Volume Method with the two-step projection-correction method is used. The convection term is treated explicitly. The viscous terms are treated semi-implicitly where the implicit part of the viscous terms and the pressure correction are solved using a second order central difference scheme. Both the implicit part of the viscous terms and the pressure correction are solved using a Block ICCG matrix solver. Details on the numerical procedure can be found in van Sint Annaland et al.,35 Dijkhuizen et al.,36 and Roghair et al.37

In FT the bubble interface is modeled by a number of unstructured triangular meshes. Each triangular cell in the mesh is called a marker. The points creating these markers are advected with the local velocity using a fourth order Runge-Kutta scheme. The local velocity is spatially interpolated with a third order spline interpolation. Due to the advection of these marker points by the local velocity the bubble interface deforms over time and the mesh quality decreases. Therefore, three different remeshing operations are implemented which are edge splitting, edge merging, and edge swapping.8,9 To improve the grid quality even further, the marker points are more evenly distributed via the smoothing algorithm of Kuprat et al.40 Finally, the advection of the markers and the remeshing procedure will lead to small volume changes, which become significant when a large number of time steps are simulated. To overcome these numerical volume changes, the volume errors are corrected by distributing the volume loss or gain over the entire surfaces.20

The local phase fraction is computed geometrically using the markers.36 The local averaged density, $\rho$, and viscosity, $\mu$, are evaluated at the embedded interface from the properties of both phases, using normal and harmonic averaging, respectively.41 Full details of the numerical approach can be found in Roghair et al.20

3 | MASS TRANSFER

The species distribution in the gas-liquid system can be obtained by solving the advection–diffusion equation.

$$\frac{\partial c}{\partial t} + (u \nabla) c = D \nabla^2 c$$ (4)

In this equation $c$ is the mass concentration and $D$ the mass diffusion coefficient. In the bulk region, that is, away from the bubble, gradients are low. The advection–diffusion equation can, hence, be discretized on a relatively coarse grid, which coincides with the hydrodynamics grid. The diffusion term is treated implicitly using a second order central differencing scheme while the convection term is discretized explicitly using the Van Leer scheme. Although the mass transfer between the two phases is handled by the subgrid scale model, which will be described below, the convection equation will also be evaluated in cells inside the bubble. Therefore, the cells inside the bubble are initialized at zero concentration.

In the region close to the bubble, the concentration gradients are too large and cannot be captured with the coarse hydrodynamic grid. Therefore, a simplified version of the advection–diffusion equation is solved following the approach of Aboulhasanzadeh et al.31 The simplified advection–diffusion equation is embedded with the FT markers of the mobile interface. When the approximated mass boundary layer exceeds a certain limit thickness, $\delta_0$, the mass is transferred to the Eulerian grid as a source term in Equation (4).

The approximated solution of the mass boundary layer is given by Aboulhasanzadeh et al.31:

$$\frac{d c}{d t} = n \gamma \frac{\partial c}{\partial n} + D \frac{\partial^2 c}{\partial n^2}$$ (5)

where $\gamma$ is the strain rate defined as $\gamma = \frac{\partial v}{\partial n}$, $n$ is the direction normal to the marker, and $u_n$ is the normal velocity component. Equation (5) indicates that during the advection of the bubble, the mass boundary layer changes by compression (or expansion) of the boundary layer by the flow field as well as by diffusion in the normal direction. In this approximation, the concentration of each marker is assumed to change only in the direction perpendicular to the bubble surface, $n$. The effects of curvature as well as tangential diffusion are neglected. Tangential convection is incorporated via the movement of the marker.

To solve the simplified equation, the mass per marker is defined. More precisely, it is the mass in the boundary layer per unit interface area, that is, $M_0 = \int c(n) dn$ where $\delta_0$ is a simulation setting defining the region of the boundary layer approach. The time evolution of the total mass is obtained by integrating Equation (5) over $\delta_0$.

$$\frac{d M_0}{d t} = -\gamma M_0 \frac{\partial c}{\partial n}|_{\delta_0} + n c_0 \delta_0 + D \frac{\partial c}{\partial n}|_{\delta_0}$$ (6)

The two later terms are transferred to the Eulerian grid if the boundary layer thickness $\delta$ exceeds the threshold thickness $\delta_0$, using polynomial weighing.19 To evaluate Equation (6), the concentration
profile is approximated by a second order polynomial in the approach of Aboulhasanzadeh et al.\textsuperscript{31} given by:

\[
c(n) / c_0 = \begin{cases} 
(1 - \frac{n}{\delta})^2 & \text{for } n < \delta \\
0 & \text{for } n \geq \delta 
\end{cases}
\] (7)

\(M_0\) is calculated explicitly after which the corresponding \(\delta\) is calculated to match \(M_0\).

Although, the approximation of the profile using a second order polynomial is beneficial for the calculation of the boundary layer thickness, \(\delta\). The exact concentration profile given in Equation (8) can also be used, which will improve the subgrid scale approximation. In this case, the Newton–Raphson method is used to calculate the \(\delta\) needed for the evaluation of \(M_0\).

\[
c(n) / c_0 = \text{erfc}\left(\frac{n}{\delta}\right)\] (8)

3.1 Remeshing

\(M_0\), the mass density, is stored for every marker at every time step. When changing the number of markers or changing their size during remeshing (see Figure 1), the values of \(M_0\) need to be updated in an appropriate way. In this work, the method of Aboulhasanzadeh et al.\textsuperscript{31} is extended to correct the mass in the boundary layer in each remeshing operation.

For edge splitting and edge swapping (Figure 1a,c), the operations are relatively easy. During edge splitting, the edge between two markers is split, leading to four markers. The concentration of the new markers is set to the concentration of the parent marker. For edge swapping, the way two markers are connected changes. The mass of these new markers is set to the average \(M_0\).

During edge collapsing (Figure 1b), a marker point is removed leading to the removal of two markers. The removal of the markers will cause all surrounding markers to change size. In addition, the mass from the removed markers should also be distributed over the surrounding markers. To accurately distribute the mass, the total mass of all involved markers is determined before the edge collapsing. After the remeshing operation, the loss of mass is calculated which is distributed to the markers that increased in size proportional to their size increase.

The last operation is edge smoothing, Figure 1d. Edge smoothing has a lot in common with edge collapsing, because all involved markers change slightly in size during the displacement of the edge. Therefore, the same procedure as for edge collapsing is applied. This procedure introduces artificial movement of mass, but it is expected to be minor.

4 Verification

To verify the correct implementation of the extended model, a spherical bubble is subjected to Stokes flow and potential flow conditions, respectively. The Sherwood number (Sh) from the simulations will be
determined using \( \delta_0 = -\frac{2\Delta x}{\mu} \) which is calculated in the subgrid scale model. Besides the average \( Sh \) over all markers, the local \( Sh \) is determined as the average of the markers that lay in a certain angle range \( (2\gamma) \) with \( \theta = 0^\circ \) at the top of the bubble and \( \theta = 180^\circ \) at the bottom. The computed \( Sh \) are time-averaged over the last 2 s of the simulation. The simulation settings are given in Table 1.

### 4.1 Stokes flow

For the first test, the bubble is placed in a velocity and pressure field following from the Hadamard-Rybczynski solution\(^4^2\),\(^4^3\) by fixing the velocity components and the pressure on the grid while using a moving frame of reference on the bubble.\(^2\) In this case, the local and global \( Sh \) is given by

\[
\frac{Sh(\theta)}{\sqrt{Pe}} = \sqrt{\frac{3}{\pi}} \frac{1 + \cos\theta}{\sqrt{2 + \cos\theta}} \sqrt{\frac{1}{1 + \kappa}}
\]

\[
\frac{Sh}{\sqrt{Pe}} = \frac{1}{2} \int_0^\gamma \sin(\theta) Sh(\theta) d\theta = \sqrt{\frac{4}{3\pi} 1 + \Delta x}
\]

where \( Pe \) is the Peclet number defined as \( \frac{\mu u}{D} \), where \( u \) is the bubble rise velocity.

Time and grid dependency studies have been performed, where doubling the resolution would give differences of less than 0.1 and 0.2%.

### 4.2 Potential flow

For potential flow the approach is similar to that of the Stokes flow test. The applied velocity and pressure field is obtained from Clift et al.\(^4^4\) The analytical local and global \( Sh \) in potential flow are given in Equations (11) and (12), respectively.

\[
\frac{Sh(\theta)}{\sqrt{Pe}} = \sqrt{\frac{3}{\pi}} \frac{1 + \cos\theta}{\sqrt{2 + \cos\theta}} \sqrt{3}
\]

\[
\frac{Sh}{\sqrt{Pe}} = \frac{1}{2} \int_0^\gamma \sin(\theta) Sh(\theta) d\theta = \sqrt{\frac{4}{\pi}}
\]

The global \( Sh \) with the second order polynomial profile was overestimated with 1.7%, while the error function profile underestimated the global \( Sh \) with 0.6%. In Figure 3, the local \( Sh \) from the simulations again follows the analytical solution reasonably well, where the error function yields better results at the upper hemisphere.

### 5 Validation

Besides verification, the model was validated for the case of mass transfer from a single rising bubble to the surrounding liquid. Two qualitatively different cases were considered, namely bubbles that remain nearly spherical and wobbling bubbles. The computed \( Sh \) from the simulations will be compared to the literature correlations summarized in Table 2.

---

### Table 1

| Setting                          | Value |
|----------------------------------|-------|
| Bubble diameter                 | 0.0032 m |
| Bubble resolution               | 40 Cells |
| Domain size                     | 2.5 \( \times \) 2.5 \( \times \) 2.5 \( \Delta x \) |
| Time step                       | 0.000001 s |
| Simulation time                 | 6.0 s |
| Viscosity ratio \( \kappa \)     | 0.185 |
| Velocity                        | 0.05 m/s |
| Peclet number                   | 160,000 |

---

FIGURE 2 Local Sherwood number in Stokes flow for original model and error function model [Color figure can be viewed at wileyonlinelibrary.com]
In these correlations the Reynolds number, that is, the dimensionless rise velocity, is an important parameter. In our simulations we, however, specify the material properties and bubble size/shape and the rise velocity is an outcome. In dimensionless terms the Morton and Eötvös numbers are specified and the Reynolds number results.

### Table 2: Correlations used for the validation of the mass transfer model

| Shape          | Validity                      | Correlation                                                                                                                                                                                                 | Accuracy | References                  |
|----------------|-------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-----------------------------|
| Spherical      | Low Re creeping flow          | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \)                                                                                                                                                                   | 7%       | Lochiel and Calderbank     |
| Spherical      | All Re all Pe                 | \( Sh = 1 + \left( 1 + \left( \frac{2.5}{Pe_{\text{max}}} \right)^{2/3} \right)^{3/4} \)                                                                                                       | 12%      | Colombet et al.             |
| Spherical      | \( Re < 10 \)                 | \( Sh \) = \left( 0.65 + 0.06 \sqrt{Re} \right) \sqrt{Pe}                                                                                                                                              | 5%       | LeClair and Hamielec       |
| Spherical      | \( Re > 1 \)                  | \( Sh = 0.651 \sqrt{Pe} \left( 1.032 + \frac{0.68}{Re^{0.7}} + \frac{1.60 - 0.68}{Re^{2.7}} \right) \)                                                                                          |           | Feng and Michaelides      |
| Spherical      |\( Re < 100 \ Pe > 1 \)      | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1 - \frac{1}{1 + 0.9 \sqrt{Re^{0.7}}} \right) \)                                                                                                      | 10%      | Takemura and Yabe          |
| Spherical      | \( Re > 25 \)                 | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1 - \frac{2 + 3.4 \sqrt{Re^{0.7}}}{1 + \sqrt{Re^{0.7}}} \right) \)                                                                                      | 10%      | Lochiel and Calderbank     |
| Spherical      | \( Re > 70 \)                 | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1 - \frac{1}{Re^{0.7}} (2.89 + 2.15 \sqrt{Re^{0.7}}) \right) \)                                                                                      | 5%       | Weber                      |
| Spherical      | \( Re > 50 \)                 | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1 - \frac{2 + 3.4 \sqrt{Re^{0.7}}}{1 + \sqrt{Re^{0.7}}} \right) \)                                                                                      |           | Winnikow                   |
| Spherical      | Intermediate Re Sc \( \rightarrow \infty \)  | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1 - \frac{1}{\left( 1 + \left( \sqrt{Re^{0.7}} \right) \right)^{1/2}} \right) \) with \( n = \frac{4}{3} + 3e \) |           | Clift et al.               |
| Spherical      | High Re potential flow        | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \)                                                                                                                                                                   |           | Boussinesq                 |
| Ellipsoidal,   | \( Re > 100 \)                | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1 - \frac{1}{\left( 1 + \left( \sqrt{Re^{0.7}} \right) \right)^{1/2}} \right) \) with \( n = \frac{4}{3} + 3e \) |           | Lochiel and Calderbank     |
| Wobbling       | \( Mo < 4 \times 10^{-8} \)  | \( Sh = \frac{2}{\sqrt{3}} \sqrt{1.8PeSc} \) with \( Sc = 0.0013Re^{0.23} \)                                                                                                                          | 10%      | Bork et al.                |
| Wobbling       | \( 10^3 < Re_{ab} < 10^6 \) | \( Sh = \frac{2}{\sqrt{3}} \sqrt{1.8PeSc} \) with \( Sc = 0.0013Re^{0.23} \)                                                                                                                          | 10%      | Bork et al.                |
| Wobbling       | \( 3 \text{ mm} < d_b < 10 \text{ mm} \) | \( Sh = 2 + 0.015Re^{0.7} Sc^{0.7} \)                                                                                                                                                                    |           | Brauer and Mewes           |
| Wobbling       | \( M < 10^{-6} \)             | \( Sh = 1.2 \left( \frac{d_b}{Re} \right) \left( f_{N} = \frac{4}{3} \left( d_b^{2/3} + 3 \right) \right)^{1/2} \)                                                                                       |           | Anderson                   |
| Wobbling       | \( M < 10^{-6} \)             | \( Sh = \frac{2}{\sqrt{3}} \sqrt{Pe} \left( 1.1 + 0.027 \sqrt{We} \right) \)                                                                                                                        |           | Montes et al.              |

**Figure 3** Local Sherwood number in potential flow for original model and error function model [Color figure can be viewed at wileyonlinelibrary.com]

**Figure 4** The simulations performed for validation of the terminal rise velocity, shape and Sherwood number [Color figure can be viewed at wileyonlinelibrary.com]
Therefore, we will first, briefly, present the hydrodynamic validation of the simulations.

To validate the hydrodynamics, we have used the Grace diagram as is done by others before.\textsuperscript{35,58-60} Furthermore, we checked the simulated Reynolds number against the correlation proposed by Tomiyama et al.\textsuperscript{61}:

\[
C_D = \frac{4d_b}{3 \rho v g} \left( \frac{(1 - \rho_b)}{\rho} \right) = \max \left\{ \min \left\{ \frac{16}{Re} \left( 1 + 0.15 Re^{0.687} \right), 48 \frac{8}{Re} \right\} \right\}
\]

(13)

To obtain this correlation Tomiyama used experiments with demineralized water, rather than with ultra-purified water. Dijkhuizen et al.\textsuperscript{62} investigated the effect of using demineralized water instead of ultra-purified water. They found that the correlation of Tomiyama consistently overestimates the drag force for Reynolds numbers above 500. Therefore Dijkhuizen et al. proposed a new correlation which uses the Reynolds dependent part from Mei et al.\textsuperscript{63}

\[
C_D = \frac{\sqrt{C_D(Re)^2 + C_D(Eo)^2}}{2} \left( \frac{12}{Re} + 0.75 \left( 1 + \frac{3.315}{\sqrt{Re}} \right) \right)^{-1}
\]

(14)

\[
C_D(Re) = \frac{4Eo}{Eo + 9.5}
\]

(15)

\[
C_D(Eo) = \frac{24}{Re} \left( 3 \left( \frac{12}{Re} + 0.75 \left( 1 + \frac{3.315}{\sqrt{Re}} \right) \right)^{-1} \right)
\]

(16)

For the validation of the mass transfer, the correlations displayed in Table 2 are used. The Peclet number and the aspect ratio (E) are

\[
\text{TABLE 3} \quad \text{Settings used for the validation of the 20 points in Figure 4}
\]

| Bubble diameter | 0.0015–0.0069 m |
|----------------|------------------|
| Bubble resolution | 20 Cells |
| Initial bubble shape | Spherical |
| Domain size | 100 × 100 × 20Z Cells |
| Initial bubble position | 50 × 50 × 60 % |
| Initial concentration (c₀) | 1.0 Kg/m³ |
| Time step | 10⁻⁶–10⁻⁵ s |
| Dimensionless simulation time | 100 |
| Viscosity ratio | 48–66 |
| Density ratio | 640–908 |
| Eötvös number | 0.2–60 |
| log Morton number | −11–1 |

Note: Z is the domain height, which is given in Table 4 for each simulation.

\[
\text{TABLE 4} \quad \text{Simulated Reynolds numbers (S) compared to the experimental and numerical results. Simulated Reynolds numbers (S) compared to the experimental and numerical results as obtained from the Grace diagram (G), the correlation of Tomiyama (T) and the correlation of Dijkhuizen et al. (D). Also the simulated Sherwood values with the second order polynomial (p2) and the error function (erf) are reported together with the Sherwood number predicted with the correlation of Takemura and Yabe (T), Lochiel and Calderbank (L) and Anderson (A)}
\]

| # | Eo | log (Mo) | Pe | Sc | Z | Reynolds | Sherwood |
|---|---|--------|---|---|---|----------|----------|
|   |   |        |   |   |   | S | G | T | D | p2 | erf | T | L | A |
| 1 | 0.2 | −11 | 5.1e5 | 1.1e3 | 7 | 470. | 354. | 544. | 581. | 758. | 741. | 742. | 752. |
| 2 | 0.2 | −9 | 3.1e5 | 3.5e3 | 7 | 89.9 | 100 | 78.4 | 98.4 | 518. | 507. | 526. | 521. |
| 3 | 0.2 | −7 | 1.5e5 | 1.1e4 | 7 | 13.5 | 13.8 | 12.7 | 14.1 | 297. | 290. | 312. | 191. |
| 4 | 0.2 | −5 | 5.8e4 | 3.5e5 | 6 | 1.68 | 1.56 | 1.91 | 2.00 | 171. | 167. | 172. |
| 5 | 1 | −11 | 9.0e5 | 9.2e2 | 8 | 977. | 936. | 888. | 1048 | 1004 | 981. | 1080 |
| 6 | 1 | −9 | 9.7e5 | 2.9e3 | 7 | 331. | 321. | 281. | 323. | 976. | 953. | 1080 |
| 7 | 1 | −7 | 7.6e5 | 9.2e3 | 7 | 82.1 | 78.5 | 87.7 | 85.7 | 791. | 773. | 815. | 806. |
| 8 | 1 | −5 | 4.2e5 | 2.9e4 | 7 | 14.4 | 11.6 | 13.8 | 15.2 | 502. | 491. | 529. | 344. |
| 9 | 1 | −3 | 1.7e5 | 9.2e4 | 6 | 1.89 | 1.75 | 2.10 | 2.21 | 299. | 292. | 298. |
| 10 | 2 | −11 | 1.2e6 | 8.1e2 | 10 | 1448 | 1214 | 1158 | 1308 | 1027 | 1004 | 1106 |
| 11 | 2 | −9 | 1.4e6 | 2.6e3 | 10 | 550. | 485. | 366. | 412. | 1010 | 987. | 1106 |
| 12 | 2 | −7 | 1.2e6 | 8.1e3 | 6 | 146. | 142. | 116. | 125. | 947. | 924. | 924. |
| 13 | 2 | −5 | 8.0e5 | 2.6e4 | 8 | 30.9 | 29.0 | 29.4 | 31.3 | 726. | 710. | 772. | 687. |
| 14 | 2 | −3 | 3.9e5 | 8.1e4 | 7 | 4.75 | 4.91 | 5.10 | 5.36 | 452. | 442. | 466. |
| 15 | 10 | −11 | 1.4e6 | 6.3e2 | 10 | 2266 | 2000 | 1977 | 2010 | 1028 | 1004 | 1114. |
| 16 | 10 | −9 | 1.4e6 | 2.0e3 | 10 | 698. | 710. | 625. | 635. | 1008 | 981. | 1114. |
| 17 | 10 | −7 | 1.5e6 | 6.3e3 | 10 | 246. | 246. | 198. | 200. | 987. | 964. | 1114. |
| 18 | 10 | −5 | 1.4e6 | 2.0e4 | 9 | 72.1 | 71.5 | 62.5 | 61.6 | 992. | 969. | 969. |
| 19 | 10 | −3 | 1.0e6 | 6.3e4 | 8 | 16.1 | 16.3 | 18.5 | 16.6 | 769. | 752. | 824. | 579. |
| 20 | 10 | −1 | 5.1e5 | 2.0e5 | 7 | 2.56 | 2.40 | 2.97 | 3.05 | 504. | 493. | 515. |
was also found by Brauer and Mewes.64 The required height of the bubble diameters in horizontal direction was found to be sufficient, and the bubble resolution were investigated. A domain size of five

908 and the viscosity ratio from 48 to 66 (roughly corresponding to an air-water system). For three cases the influence of the domain size is the rise velocity predicted by the Grace diagram.

In total, 20 different simulations are performed, which are marked in Figure 4. The density ratio in these simulations range from 640 to slightly outside, but mostly within 10% accuracy of the literature values.57,65 between the range defined by the different literature results or number from literature. The simulation results generally lie in the simulations generally predict a lower Sh, but the predictions are within 10% of the Sh calculated from the correlations. For Cases 13 and 19 a lower Sh in the simulation compared to the literature values is expected because those bubbles are significantly deformed whereas all the empirical correlations assume spherical bubbles. The aspect ratios of Cases 13 and 19 are 1.26 and 1.46, respectively. For high Reynolds numbers deformation is beneficial for the mass transfer,45 but for low Reynolds numbers deformation actually leads to lower Sh.68 The Sh of Case 1 appears to be too small, it matches, however, with experiments reported in Winnikow.50

For nonspherical bubbles the Sh from the correlations are plotted against the Sh from the simulation with the error function in Figure 5b. The Sh obtained from the correlation of Lochiel and Calderbank46 and Montes et al.56 assume potential flow leading to too high Sh. For Case 16 the simulation result agrees quite well with the correlations of Bork et al.53 and Brauer and Mewes.54 Overall the best agreement is found with the correlation of Anderson.55 However this correlation is only valid for oscillating bubbles. To the author’s knowledge, there are no correlations reported in the ellipsoidal regime where shape oscillations are minor and the Reynolds number is moderate. Hence, Case 18 remains uncompared with correlations. Figueroa-Espinoza and Legendre,68 proposed a correction factor \( f(E) = 1 - 0.13(E - 1) \) for the Sh when \( Re \approx 10 \). For \( Re = 100 \) and high \( Sc \), Sh is almost constant for different aspect ratios. For Case 18, \( Re = 72 \) and the aspect ratio is 2.18. Combining this with the correlation of Weber49 for a sphere, the Sh is 6.2% too low for the erf function profile and 4.1% for the second order polynomial. The difference between the error function profile and the second order polynomial is 2.35% in all cases.

In Figure 6, the obtained concentration profiles of some cases are given. Case 5 corresponds to a steady wobbling bubble. The double wake arises when the bubble drastically changes its horizontal direction, that is, at the inflection point. After the inflection point the wake stabilizes again and forms one single wake until the next inflection point is encountered and the wake again splits in two. In Case 17 the
wobbling is more unsteady and hence a more complex wake is observed. The global Sh for this type of wobbling bubbles oscillates together with the bubble trajectory. In Figure 7, the global Sh is plotted together with the Reynolds numbers in the two directions perpendicular to the rise direction for Case 17. The bubble follows a zigzag path and the Sh is found to oscillate with the same frequency as the zigzag frequency. Lastly, Case 19 is an ellipsoidal bubble with a steady path. For this bubble and all other bubbles, which follow a steady path, spherical, or ellipsoidal, one straight wake is following the bubble.

When closely looking at the top of the bubbles, an increased concentration is observed. This concentration is not a result of the subgrid scale model transferring concentration to the grid, but is actually mass that diffuses from the bottom of bubble into the bubble since we do not initialize the bubble concentration on the grid. This effect was also discussed by Aboulhasanzadeh et al. 31

**Figure 6** 2D concentration profile at the center of the domain (a–c) and 3D concentration profile (d–f) for different cases [Color figure can be viewed at wileyonlinelibrary.com]
however, the amount of mass that diffuses into the bubble was found to be small.

6 | CONCLUSIONS

In the present article, the subgrid scale model of Aboulhasanzadeh et al.\textsuperscript{31} has been improved, verified, and validated. Two different profiles have been used in this work: an approximate profile (a second order polynomial) and the exact profile (the error function). Furthermore, a new procedure is applied to redistribute the mass during remeshing and the effect of the different remeshing operations has been studied.

The verification tests showed that the improved subgrid scale model is not only capable of finding the correct global Sh, but also the correct local Sh. While with the second order profile the Sh was overestimated slightly, especially at the upper hemisphere, the error profile underestimated the Sh slightly. The origin of the underestimation was found at the bottom of the bubble where $\delta$ becomes large and Newton’s method is incapable of correctly estimating $\delta$ due to asymptotic behavior. Furthermore, it was found that the proposed remeshing procedure is necessary, especially for smoothing, to obtain the correct local Sh.

The 20 simulations of free rising bubbles showed that the subgrid scale model is capable of capturing the Sh for all bubble shapes with $Eo < 40$ within $\pm 15\%$ of the literature correlations. Furthermore, the Sh obtained with the second order profile and exact profile were found to constantly differ $2.3\%$ from each other.

An investigation of the concentration profile showed that there is some concentration diffusing back into the bubble on the grid. While the amount is small, this phenomenon can cause problems for more complex systems like bubbles interacting in a swarm. Model improvements related to this coupling of the boundary layer and the bulk region will be part of future work.

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