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DIRECT NUMERICAL SIMULATION OF THE EFFECTIVE DRAG IN GAS-LIQUID-SOLID SYSTEMS

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ABSTRACT
Due to the increase in the oil prices and the depletion of the oil reserves, Fischer-Tropsch processes for the production of synthetic fuels, methanol synthesis and other gas-to-liquid processes are rapidly gaining interest. These reactions are commonly performed in slurry bubble columns, i.e. three-phase gas-liquid-solid reactors. Although slurry bubble columns are already widely used, challenging scale-up and operational issues are encountered when these reactors are used for the Fisher-Tropsch process. To improve the fundamental understanding of these complex reactors, this work focuses on the effective drag acting on particles and bubbles in dense flows, using Direct Numerical Simulations. We combined the Front Tracking method of Roghain et al. (2013b) and the second order implicit Immersed Boundary method of Deen et al. (2012), resulting in a resulting hybrid Front Tracking Immersed Boundary method that is able to simulate dense three phase flows and quantify the effects. For a system consisting of 2 mm bubbles and 1 mm particles, effective drag closures are developed for both the bubbles and the particles at several phase volume fractions. In future research, the developed methodology will be applied to study the effect of the bubble and particle size and their ratio as well as heat and mass transfer.

Keywords: Multiphase flow, Slurry bubble column, multiscale modeling, gas-liquid-solid flows, fluid structure interaction, Front Tracking, Immersed Boundary method.

NOMENCLATURE

Greek Symbols

α Void fraction.
μ Viscosity, [Pa·s].
ρ Density, [kg/m³].
σ Surface tension coefficient, [N/m].
τ Stress tensor, [Pa].
ϕ Solid volume fraction.
ψ Velocity component, [m/s].
ω Rotational velocity, [1/s].

Latin Symbols

a, b, C Coefficient.
d Diameter, [m].
DNS Direct Numerical Simulation.
Eö Eötvös number, \( g d_b^2 \Delta \rho / \sigma \).
F Force density or Force, [N/m³] or [N].

Sub/superscripts

b Bubble.
B Buoyancy.
c Central.
col Due to particle-particle collisions.
D Drag.
g Gas phase.
l Liquid phase.

FT Front Tracking.
g Gravity acceleration, [m/s²].
IB Immersed Boundary.
I Moment of inertia , [kg·m²].
MCFD Multiphase Computational Fluid Dynamics.
Mo Morton number, \( g d_b^2 \Delta \rho / (\rho l^3 \sigma) \).

INTRODUCTION

The interest in Fischer-Tropsch processes for the production of synthetic fuels, methanol synthesis and other prominent gas-to-liquid processes has rapidly expanded in recent years, due to depletion of oil reserves and increasing oil prices. In these gas-to-liquid processes, a reactant gas is converted into liquid products over a solid catalyst. These type of three-phase gas-liquid-solid processes are often performed in slurry bubble columns. To accurately scale-up and design these columns, the fundamental understanding of the complex three phase interactions needs to be improved (Kantarci et al., 2005; Wang et al., 2007; Yang et al., 2007; Pan et al., 2016).
The introduction of particles in a bubble column causes a decrease in the bubble size and an increase in the void fraction. Besides, the bubble rise velocity decreases with increasing solids volume fraction even when neutrally buoyant particles are used (Kantarcı et al., 2005; Wang et al., 2007; Hooshyar et al., 2013; Baltussen et al., 2013; Pan et al., 2016). By using neutrally buoyant particles, Hooshyar et al. (2015) reported that the interaction mechanism depends on the Stokes relaxation time of the particles. When the Stokes relaxation time is relatively small, the bubble rise velocity is only affected via an increase in the apparent viscosity. For larger particles, which also have a larger Stokes relaxation time, the bubble rise velocity is only slightly influenced by the change in the apparent viscosity, while the main effect is caused by the encounters between the particles and the bubbles.

Because slurry bubble columns are often several meters in diameter and tens of meters in height, it is not possible to resolve all the details of the bubble-particle interactions for a full slurry bubble column. Therefore, a multiscale modeling approach is used to simulate industrial size columns. In this approach, coarse grained models, which do not capture the the particle/bubble scale transport phenomena (like the Euler-Lagrange or Euler-Euler models), need closures for the bubble-bubble, bubble-particle and particle-particle interactions. This effective drag acting on the particles and the bubbles in dense can will be determined using smaller scale Euler-Lagrange or Euler-Euler models, need closures for the particle/bubble scale transport phenomena (like the full slurry bubble column. Therefore, a multiscale modeling method of Deen et al. (2013a) combined a front capturing method with a IB method. In FT, the bubbles are treated explicitly. The diffusion terms are discretised using a second order (1D) polynomial fit, each neighboring fluid node inside a particle can be eliminated from equation 3.

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

(1)

\[ \rho \frac{d \mathbf{u}}{dt} = -\rho \nabla p - \rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \mathbf{\tau} + \rho \mathbf{g} + \mathbf{F}_d \]  

(2)

Because the velocity field is continuous across the gas-liquid interface, the Navier-Stokes equations can be solved using an one-field approximation. The surface tension at the gas-liquid interface is taken into account by an extra force density, \( \mathbf{F}_d \), which is introduced near the interface. This force is directly calculated from the triangular mesh by summing the tensile forces exerted by the three neighboring markers, triangular element, on a reference marker and subsequent force mapping to the Eulerian grid using mass-weighing (Dijkstra et al., 2010b; Roghair, 2012). To alleviate the parasitic currents that arise due to the mismatch between the discretisation of the surface tension and the pressure field, the surface tension calculations is augmented with the so-called “pressure-jump correction” (Renardy and Renardy, 2002; Francois et al., 2006; Dijkstra et al., 2010b). The local density and viscosity are obtained by normal and harmonic averaging, respectively.

The no-slip boundary condition at the particle surface is taken into account implicitly. At the level of the discretised Navier-Stokes equations, each velocity component at a certain node in the fluid, \( \psi_c \), can be described as a function of the velocity components of the neighboring nodes, \( \psi_{nb} \), with equation 3.

\[ a_c \psi_c + \sum_{nb} a_{nb} \psi_{nb} = b_c \]  

(3)

where the coefficients \( a_{nb} \) indicate the coupling of the velocity at node \( c \) with the velocities of the neighboring nodes, \( nb \).

Using a second order (1D) polynomial fit, each neighboring fluid node inside a particle can be eliminated from equation 3. Together with the local velocity field and the velocity at the particle surface, the coefficients of the two velocity nodes involved in the polynomial fit are adjusted. A similar function is obtained for fluid nodes that are in close proximity of two particles, when there is only 1 grid point in between the particles, by using the velocity of the central node and the velocity of both particles. Because both equations are singular when the particle surface is close to the central cell, a linear fit is used when the distance between the surface and the central point is less than \( 10^{-4} \) times the grid size. The velocity field given by equation 2 is obtained on a staggered grid using a projection-correction method. In the projection step, all terms in this equation are treated explicitly except for the diffusion term, which is treated semi-implicitly. The implicit part of the diffusion term is chosen such that it only depends on the velocity component that is solved for, whereas the remaining (small) terms are treated explicitly. The diffusion terms are discretised using
a second order central difference scheme, while a second order flux-delimited Barton scheme is used for the convective terms. The projected velocity field is corrected to satisfy the continuity equation (equation 1). The equations in both the projection step and the correction step are solved using a OpenMP parallelised block ICCG matrix solver.

**Particles**

When the velocity field is calculated, the positions of the particles, \( m \), are updated by solving the Newtonian equations of motion:

\[
V_m \rho_m \frac{d\omega_m}{dt} = mg + \oint_{r_m} (\mathbf{r} \times \mathbf{n}) dS + \iiint_{\Omega_m} -\nabla p dV + F_{d,\text{col}}
\]

(4)

\[
I_m \frac{d\mathbf{\omega}_m}{dt} = \oint_{r_m} (r_{i,j,k} - r_m) \times (\mathbf{r} \times \mathbf{n}) dS
\]

(5)

where the moment of inertia is given by:

\[
I_m = \frac{1}{10} V_m \rho_m d_m^2
\]

(6)

In the three-phase system, the transpose part of the Stokes stress tensor in equation 4 and 5 should be included, because the viscosity is not constant. Both the pressure gradient and the velocity gradients, which are needed in the stress tensor, can be obtained directly from the second order fit, which was used to apply the no-slip boundary condition.

In the continuous limit, the calculation of the pressure force can be performed with either a surface integral or a volume integral using Gauss’s theorem. Although the pressure inside the particle is unknown, the volume integral of the pressure gradient over the total particles will effectively result in a calculation depending on the pressures outside the particle due to the employed discretisation. When the calculation via the surface integral and the volume integral are compared with the results of Zick and Homsy (1982), the calculation of the force via the surface integral is not able to accurately capture the drag of a particle in a dense array. Therefore, the drag force will be calculated via the volume integral in this paper.

The interactions between the particles are included using a hard sphere model (Hoomans et al., 1996). Therefore the drag force as discussed before does not include the collisions with other particles. However, the collisions with the bubbles are not separately treated and therefore their effects will be lumped in the drag force.

**Bubbles**

Following the update of the particle positions and velocities, the position of the bubbles is updated. Every marker point at the surface is displaced separately with the local velocity, which is interpolated from the Eulerian grid using cubic spline interpolation, by fourth order Runga-Kutta time stepping. Because each marker point is advected separately, the bubbles will change both its position and its shape. Nevertheless, this also changes the distance between the marker points leading to a decreased surface mesh quality. To restore the mesh quality, the surface is remeshed, using four elementary operations: edge splitting, edge collapsing, edge swapping and smoothing (Roghair, 2012).

Due to the separate advection of the marker points and the remeshing, small volume changes in the bubble volume arise, which accumulate over the total simulation time. To locally restore the volume losses during the remeshing a smoothing procedure described by Kuprat et al. (2001) is implemented. Moreover, the volume changes due to the separate advection of each marker are compensated by distributing the lost volume over all the interface cells. This procedure might cause unphysical overlap with other bubbles and particles. Marker points that are close to another bubble or particle, within the maximal edge length of a marker, are therefore excluded from this operation.

**Simulation set-up**

The simulations are started with a random initial configuration of bubbles and particles, generated using a Monte-Carlo method. In this method, the dispersed elements (bubbles/particles) are first placed in a lattice structure in the domain. Subsequently, each element is displaced slightly 200 times. The procedure is repeated until no overlap between the elements is found.

In the simulations, periodic boundaries are used to mimic an infinite bubble/particle swarm. To ensure that the finite box size does not influence the results, a minimum number of bubbles and particles is required. Roghair et al. (2011) and Bunner and Tryggvason (2002) established that the minimum number of bubbles needed is 12. By changing the number of particles for simulations with the settings of table 1, there is no effect when the number of particles exceeds 40. Therefore, the minimum number of bubbles and particles used in the simulations is conservatively set to respectively 16 and 60.

Besides the number of bubbles and particles, the resolution of both the particles and the bubbles should be sufficient to obtain grid independent results. Dijkstrauijen et al. (2010a) showed that at least 20 grid cells across a bubble diameter are needed in the used FT method. Furthermore, simulations using again the settings of table 1 with a different resolution for the particles showed negligible effect of the grid resolution. Therefore, the number of grid cells inside a particle and a bubble diameter is set to 10 and 20, respectively.

To study the effect of the void fraction and the solids volume fraction, 27 different simulations have been performed, which are grouped in four different cases listed in table 2. All

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Void fraction, ( \alpha )</td>
<td>0.30</td>
<td></td>
</tr>
<tr>
<td>Solid volume fraction, ( \phi )</td>
<td>0.05</td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
<td>171</td>
<td></td>
</tr>
<tr>
<td>Grid size</td>
<td>1.0 \times 10^{-4}</td>
<td>m</td>
</tr>
<tr>
<td>Time step</td>
<td>1.0 \times 10^{-5}</td>
<td>s</td>
</tr>
<tr>
<td>Bubble diameter</td>
<td>2.0 \times 10^{-3}</td>
<td>m</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>1.0 \times 10^{-3}</td>
<td>m</td>
</tr>
<tr>
<td>Liquid density</td>
<td>1.0 \times 10^3</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Liquid viscosity</td>
<td>1.0 \times 10^{-3}</td>
<td>Pas</td>
</tr>
<tr>
<td>Gas density</td>
<td>100.0</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Gas viscosity</td>
<td>1.8 \times 10^{-5}</td>
<td>Pas</td>
</tr>
<tr>
<td>Solids density</td>
<td>2.0 \times 10^3</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Surface tension</td>
<td>0.073</td>
<td>N/m</td>
</tr>
<tr>
<td>Normal restitution coefficient</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>Tangential restitution coefficient</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>Friction coefficient coefficient</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>– log(Mo)</td>
<td>10.6</td>
<td></td>
</tr>
<tr>
<td>Eo</td>
<td>0.48</td>
<td></td>
</tr>
</tbody>
</table>
Table 2: Gas fraction, solids volume fraction and averaging time for the four different cases studied to determine the effect of solids volume fraction and the void fraction. All cases have the same settings as listed in table 1, except for the parameters listed here.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\alpha$</th>
<th>$\phi$</th>
<th>$t_{avg}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.20</td>
<td>0.02...0.14</td>
<td>0.8</td>
</tr>
<tr>
<td>2</td>
<td>0.40</td>
<td>0.02...0.14</td>
<td>0.25...0.8</td>
</tr>
<tr>
<td>3</td>
<td>0.15...0.45</td>
<td>0.05</td>
<td>0.55...0.8</td>
</tr>
<tr>
<td>4</td>
<td>0.15...0.45</td>
<td>0.10</td>
<td>0.8</td>
</tr>
</tbody>
</table>

According to figure 1, the drag coefficient of the bubbles increases with increasing void fraction and solids volume fraction. The increase of the relative drag force with increasing void fraction was also determined in two-phase flows (Roghair et al., 2011; Martínez-Mercado et al., 2007). However, the effects in the three-phase flow are larger due to the addition of particles, which is in good agreement with the experimentally observed decrease in the bubble rise velocity upon the introduction of particles (Kantarci et al., 2005; Wang et al., 2007; Hooshyar et al., 2013; Pan et al., 2016). The data of figure 1 was used to derive a correlation for the relative bubble drag coefficient. With respect to the form of the correlation, we constrained the form such that the correlation will lead to the correlation of Roghair et al. (2011) in the limit that there are no particles ($\phi = 0$) and that the drag coefficient of a single bubble ($\alpha = 0$) is higher in a liquid containing particles. This resulted in the fit in equation 9.

$$C_{D,rel} = 1 + \frac{18}{E_0} \alpha + 1.8 \cdot 10^5 \alpha^2 \varphi^{1.1} + 2.7 \cdot 10^3 \varphi^2$$ (9)

In addition to the close match of the symbols and the lines in figure 1, the parity plot of figure 2 shows that most of the results are within 10% of the fit. On average, the differences between the correlation and the simulation results amounts 7.6%, which is less than the spread in results obtained by using different initial conditions. The maximum difference, which is obtained for low solids volume fractions and low void fractions, is 20%.

Secondly, the effect of the bubbles on the drag coefficient of the particles can be determined in a similar manner as the drag coefficient of the bubbles. In the case of the particles, the drag coefficient is now normalized with the drag coefficient of a single particle in an infinite fluid, given by Schiller and Nauman (Clift et al., 1978):

$$C_{D,\text{inf},p} = \frac{4d_p(p_l - p_p)g}{3\rho_p w^2} = \frac{24}{R_{ep}^{0.687}} \left(1 + 0.15 R_{ep}^{0.687}\right)$$ (10)

The resulting relative drag coefficient is given by:

$$\frac{C_{D,rel}}{C_{D,\text{inf},p}} = \left[1 - \frac{\alpha p_l - p_p}{\rho_l - \rho_p}\right] \frac{1}{\left(\frac{\varphi}{\rho_l - \rho_p}\right)}$$ (11)

Figure 3 clearly shows that the drag force on the particles occasionally changes direction. In these circumstances, a bubble and particle will mutually rise, because the combination of one bubble and one particle is buoyant with respect to the liquid. The large standard deviations indicate that particles have two different modes: almost free movement and movement that is obstructed by bubbles. Because particles appear to alternate between these modes, the standard deviations are much larger than the averaged drag coefficient. The calculation of the drag coefficient will be improved when the drag coefficient is calculated for each of these two modes separately. However, this is beyond the scope of this work. In addition, the simulations of case 2 with a solids fraction of 8% only show a difference of 8% for the drag coefficient of the particles.

The obtained drag coefficients are also fitted to quantify the effect of the void fraction and the solids volume fraction on the drag coefficient. The correlation should meet two criteria: the relative drag coefficient of the particles should be equal to 1 when the solids volume fraction and the void fraction are zero. Secondly, it is expected that the drag coefficient of a
Figure 1: Effect of the solids volume fraction, figure a, and the effect of the void fraction, figure b, on the normalized drag coefficient of the bubbles. The drag is normalized using equation 8. The lines in the figures represent the fit of equation 9. The bars indicate the standard deviation.

In addition to a proper capture of the trends in the drag coefficient, the parity plot in figure 4 shows an average absolute difference between the simulation and the correlation results of only 7.1% with a maximum of 22.5%.

The increase of the drag coefficients of both the bubbles and the particles can partly be explained by the micro structuring of the bubbles. The bubbles cluster in a dynamic system of horizontal layers, as shown in figure 5. The horizontal clustering was already observed by Roghair et al. (2013b) for bubble swarms and by Baltussen et al. (2013) for slurries, and is probably caused by the lack of large scale circulations. The clustering of the particles prevails due to hindrance by the bubbles. The particles partly cluster on top of the bubbles, effectively hindering the rise of the bubbles, which decreases the particle velocity or even reverses its direction. The particles will eventually roll down the side of the bubble, due to a combination of buoyancy forces and surface tension.

CONCLUSION

In this paper, a combined FT second order implicit IB method was used to simulate dense bubble/particle swarms. By using this method, the effect of the void fraction and the solids volume fraction on the drag coefficient of 1 mm particles and 2 mm bubbles was determined. For both the particles and bubbles, a combined effect of the void fraction and the solids volume fraction was found on the drag coefficient. Using the simulation results, drag correlations for both the bubbles and the particles were developed, which provides an accurate description for $15\% \leq \alpha \leq 50\%$ and $2\% \leq \phi \leq 14\%$.

Because of the limited range in physical properties, particle and bubble diameter used in this paper, the applicability of the obtained correlations is limited to the range of conditions investigated. To obtain a broader applicability, the simulation
range should be extended. Preliminary results to assess the effect of the bubble diameter show similar trends in void fraction and solids volume fraction. An increasing bubble diameter will lead to a decrease in the drag coefficient for both the bubbles and the particles. It is expected that the size of the particles will influence the drag coefficient. However, because the increase of inertia of the particles might lead to larger deformation and even to break-up of the bubbles, it is hard to predict the effect of the particle size on the drag of both particles and bubbles.

Simulating particles with a high inertia in combination with bubbles with a relatively low surface tension is still difficult for the FT-IB model. In such cases, particles can fall through bubbles, leading to the formation of a doughnut shaped bubble or even the break-up of the bubble. To enable capturing these events, a break-up model needs to be included in the method. Another option is to combine the currently used FT model with the Volume of Fluid model, which prevents unphysical merging of the bubbles while break-up is incorporated in the model (Torres and Brackbill, 2000; Walker et al., 2013). Another option is to implement FT without connectivity, like the Local Front Reconstruction Method (Shin and Juric, 2002).

Although the second order IB method is tested thoroughly, the rotation of freely moving particles at high Reynolds numbers is not accurately calculated. However, the disturbance of the bubbles and the frequent collisions with both particles and bubbles are expected to diminish any effect of unphysical rotation. To prevent any unphysical rotation of the particles, the calculation of the rotational velocity should be improved.

Finally, the currently used size ratio between the bubbles and the particles ($d_b/d_p = 2$) is much larger than the ratio which is common in slurry bubble columns ($d_b/d_p \approx 10 - 100$). To obtain a realistic effect of the particles on the drag of the bubbles and vice versa, this diameter ratio should be decreased drastically. Clearly this will put challenges on the allowable number of grid cells, which can probably only be solved by applying adaptive grid refinement.

Figure 3: Effect of the solids volume fraction (a), and the effect of the void fraction (b) on the normalized drag coefficient of the particles. The drag is normalized using equation 11. The lines in the figures represent the fit of equation 12. The bars indicate the standard deviation.

Figure 4: Parity plot containing the relative drag coefficient of the particles obtained from the simulations and the correlation given by equation 12. The dashed lines indicate an error of 10%.
Figure 5: Two snapshots of a simulation with a void fraction of 25% and a solids volume fraction of 5%. Figure (a) and (d) show both the particles and the bubbles, while the middle and the right figures only show the bubble configuration and the particle configuration.

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