CFD–DEM model for coupled heat and mass transfer in a spout fluidized bed with liquid injection

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HIGHLIGHTS

• We present a systematic CFD–DEM model development and validation.
• We study coupled heat and mass transfer phenomena in a spout fluidized bed.
• We studied the effect of liquid injection in the presence of draft plates.
• The simulation results agree well with experimental data.

ARTICLE INFO

Article history:
Received 20 July 2015
Received in revised form 20 October 2015
Accepted 14 November 2015
Available online 29 November 2015

Keywords:
Spout fluidized bed granulator
Liquid injection
Wet restitution coefficient
CFD–DEM
Heat and mass transfer
Liquid evaporation

ABSTRACT

In this paper, we present a novel CFD–DEM model for coupled heat and mass transfer in a spout fluidized bed with liquid injection. In our CFD–DEM approach both particles and droplets are treated as discrete elements. Before actual simulations were conducted, a number of tests were performed to determine the optimum particle collision time step by analysing the error in the prescribed restitution coefficient (difference between defined and applied values). Subsequently we test the model for a selected case as a proof-of-principle. In this test case, the effect of liquid injection on dynamics of a pseudo-2D spout fluidized bed with draft plates was demonstrated for the fluidized bed-spouting-with-aeration (dispersed spout) regime with injection of water droplets. The computational results were compared with experimental results that were obtained through a unique combination of particle image velocimetry (PIV) and infrared thermography (IRT).

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1. Introduction

Gas–solid spout fluidized beds with liquid injection are commonly used in a number of applications comprising physical and/or chemical transformations. This is because these beds combine features from both the spouted and fluidized beds with intense gas–solids mixing and efficient heat and mass transfer. Detailed discussion of other distinguishing features of spout fluidized beds can be found in [1,2]. Since the development of the spout fluidized bed [3] a series of modifications were suggested to improve the bed performance, such as various geometrical configurations (rectangular, conical bottom, slotted rectangular, multiple and elevated spout) and insertion of a draft tube inside the bed. The insertion of a draft tube in a spout fluidized bed comprises an additional flexibility to control the particle velocity, bed porosity and gas residence time by adjusting the operating parameters and the geometrical configurations, e.g. the entrainment height and the draft tube dimensions. Chemical processes that use gas–solid spout fluidized beds with draft plates and liquid injection through a nozzle include particle granulation and coating, and olefin polymerisation. In the former a liquid binder (suspensions, solutions and melts) is atomised in the bed of fluidizing particles. The binder sticks to the particle and the solvent evaporates from the particle surface, resulting in a layer-wise progressive particle growth. Excessive penetration of the liquid into the interior of particles can be avoided by a fast drying. This layering of the liquid usually results in a uniform dried liquid layer around the particle to form bigger granules [4]. In polymerisation, the catalyst particles (anion, cation, free-radical, Ziegler–Natta etc.) are fluidized under reactive
operating conditions using a monomer gas. The exothermic reaction heat generated can be effectively removed by liquid (monomer/solvent) injection, because the latent heat of the evaporation leads to a very large heat removal rate. These processes often involve transfer of components from the liquid phase to the gas phase and associated latent heat effects.

However, during these processes a small change in the operating conditions can potentially lead to an imbalance between the rate of liquid injection and the evaporation rate. This eventually contributes to a poor bed performance due the local de-fluidization and enhanced agglomerate/particle–lump formation. In addition, intense evaporation often leads to the accumulation of a thick
vapour layer around the particle, which may inhibit the direct particle–droplet contact i.e. non-wetting contact or Leidenfrost regime [5]. Under these conditions, the heat flux near the contact area significantly decreases, despite the high temperature gradient across the vapour boundary layer. Furthermore, wet particles often collide with wet, dry or partially wet particles, which can lead to agglomeration and a significant variation in the physical properties and appearance. This may lead to bigger agglomerates, which defluidize. Additionally, the local process conditions and moisture distribution also strongly influence the adhesive properties of the wet particles, overall drying rate and agglomeration kinetics. A detailed understanding of the complex multi-phase and multi-scale interactions together with the particulate flow transitions, and coupled heat and mass transfer are of primary importance for the process design and scale-up. This can either be achieved by performing dedicated experiments or detailed numerical simulations. The experimental studies reported in literature for gas–solid fluidized beds include: dynamic pressure drop analysis [6], temperature measurements near the injection point, X-ray imaging [7] and triboelectric probe measurements [8]. However, these techniques either provide point information or possess a low resolution with complex image post processing. Hence, these are less adequate for probing localised conditions in transient systems. Moreover, it is troublesome to perform experiments on an industrial scale, because it is difficult to access the relevant areas experimentally. Numerical simulations can offer a platform that can be used to obtain better insight in temperature, moisture distributions, local and overall heat and mass transfer characteristics. CFD–DEM models are typically used as learning models, i.e. to generate understandings of micro-scale phenomena and to develop practical (e.g. constitutive) expressions that can be used to close more coarse grained models, such as the Euler–Euler model. Literature study reveals that comparatively extensive work has been performed in the field of momentum transfer, whereas limited information is available on heat and mass transfer aspects with liquid injection. [9] performed Eulerian–Eulerian simulations to study the dynamics of gas–solid spouted bed with a draft tube and liquid injection, and compared their results with experiments. [10] studied the particulate flow behaviour in spout fluidized beds for two flow regimes by using an extended CFD–DEM embedding a variable restitution coefficient based on the moisture content with liquid evaporation. Their results indicate that the evaporation rate significantly alters the restitution coefficient, and hence the bed dynamics. [11] studied variation in mixing characteristics in a 3D rectangular spouted bed under dry and wet conditions using CFD–DEM simulations by considering the liquid bridge forces using the Mikami model (based on liquid volume, separation distance and contact angle). With increase in the liquid injection the mixing rate decreases due to the dominant liquid bridge forces which significantly suppress the particle mobility. Additionally, the granular temperature also decreased due to the higher energy dissipated during the wet particulate collisions. [12] performed coupled CFD–DEM simulations considering particle wetting to study the particulate flow in gas–solid fluidized bed and Wurster-coater spray granulator. Their results indicate that the use of a Wurster-coater leads to more narrow particle residence time distribution as compared to the top-sprayed fluidized bed, which exhibits more homogeneous particle wetting.

In this work, a novel discrete element model (DEM) incorporating detailed descriptions of coupled heat and mass transfer is presented and used to simulate the bed dynamics. This model was selected, because it resolves the particulate flow at the level of individual particles and can provide information about various forces acting on the particles and droplets. In the model, the gas phase transport phenomena were considered by solving momentum, energy and species balance equations, whereas the motion of individual spherical particles was described by Newton’s law of motion with a soft sphere collision model, along with heat and mass balances for the particles. The fluid–particle heat and mass transfer coefficients were evaluated using empirical Nusselt and Sherwood correlations. Additionally, various tests were conducted to verify the heat and mass transfer implementation by comparing the obtained results with analytical solutions. Further, as a proof of principle the dynamics of a pseudo-2D spout fluidized bed with glass particles \(d_p = 1\) mm and \(\rho_p = 2526\) kg/m\(^3\) were investigated by injecting water droplets with a mean size \(d_l\) of 60 \(\mu\)m (±30 \(\mu\)m) for the fluidized bed-spooling-with-aeration (dispersed spout) regime. The computational results in terms of pressure drop, wet particulate flow patterns were compared with previously obtained experimental data through combined particle image velocimetry (PIV) and infrared thermography (IRT) [13]. Moreover, simulations for spout fluidized bed without draft plates were performed to quantify the distribution of hot and cold spots.

Although the CFD–DEM model obtains the collisions between wet particles in a deterministic manner, in reality however, the droplets impacting on the particles undergo various stages like spreading, stretching, recoiling and rebounding, which are difficult to reproduce. So, the net effect arising due to the various forces at impact (surface tension, contact between the particle and the wall, viscous and capillary) with liquid injection were lumped by estimating the wet restitution coefficient using a model/correlation using experiments as reported by [14]. The energy dissipation during the wet collisions is more important than the actual collision behaviour. Also, the atomisation phenomena are difficult to model, so therefore in this study droplets were injected with a mean size based on experimental data based on high speed digital images. Moreover, detailed information about the post-collision spreading of the droplet has been neglected due to the low droplet to particle diameter ratios. In our work the droplet injection rates are about \(O(10^6)\) droplets per second. In systems with much higher injection rates, a volumetric approach of droplet injection (using droplet parcels rather than the individual droplets) might be more practical [15]. In the model the following assumptions were made for simplification:

1. The droplets are injected at low droplet Weber number \((W_e < 1)\) hence droplet breakage can be neglected. This assumption can be defended by the fact that most droplet breakage takes place in a very small region close to the nozzle, after which the droplets are small enough to keep their size.
2. After particle–droplet collisions, the droplets are assumed to form an uniform liquid layer around the particles i.e. partial-particle wetting can be neglected. In future work this assumption can be replaced by a more rigorous one, i.e. the assumption that dry and wet patches are distributed randomly over the particle surface.

![Fig. 1. Schematic illustration of the formation of an uniform liquid layer around the particle after particle–droplet collision.](image-url)
3. At low Biot number \((Bi < 1)\) an uniform particle temperature gradient was assumed across the particles. This assumption is fair for the particle sizes studied in this work \((d_p = 1\, \text{mm}, Bi = 0.1)\).

4. Conductive heat exchange during particle–particle and particle–wall collisions and bed wall heat losses were neglected. This assumption can be made provided that the particles are in free flight most of the time, which is typically the case in fluidized systems.

5. It is assumed that there is no heat transfer through radiation, which implies that the absolute temperatures are relatively low (i.e., below 100 °C).

6. It is assumed that there are no heat and mass transfer resistances across the liquid film.

2. Model description

In this study the simulations were carried out by extending the in-house developed CFD–DEM model reported previously by van Buijtenen et al. [10]. A detailed description of the governing equations, motion of the droplets, particle–particle and particle–droplet interactions can be found in the work of van Buijtenen et al. [10]. The treatment of the particle colliding with the draft plates was explained by Sutkar et al. [16].

2.1. Gas phase motion

The gas-phase transport phenomena were computed by solving the volume-averaged Navier–Stokes equations accounting for the local porosity and the drag force exerted by the particles and the droplets.

2.2. Particle and droplet motion

The motion of each individual particle \((a = p)\) and droplet \((a = d)\) is calculated using Newton’s law of motion:

### Table 1

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
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<tbody>
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<td>(\rho_s)</td>
<td>1.29</td>
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</tr>
<tr>
<td>(\mu_g)</td>
<td>(1.8 \times 10^{-5})</td>
<td>kg/(m s)</td>
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</tr>
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<td>–</td>
</tr>
<tr>
<td>(d_p)</td>
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<td>m</td>
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<tr>
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### Table 2

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<td>(\mu_g)</td>
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<td>kg/(m s)</td>
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<tr>
<td>(C_{p,s})</td>
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<td>J/(kg K)</td>
</tr>
<tr>
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<td>m³</td>
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</tr>
<tr>
<td>(d_p)</td>
<td>(1 \times 10^{-3})</td>
<td>m</td>
</tr>
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</tr>
<tr>
<td>(C_{p,g})</td>
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<td>J/(kg K)</td>
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<tr>
<td>(T_{\text{bed}})</td>
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<td>K</td>
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<tr>
<td>(T_{g,0})</td>
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<td>K</td>
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### Table 3

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<tr>
<td>(u_g)</td>
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<td>m/s</td>
</tr>
<tr>
<td>(w_{g,0})</td>
<td>0.005</td>
<td>kg/kg</td>
</tr>
<tr>
<td>(w_g)</td>
<td>0.5</td>
<td>kg/kg</td>
</tr>
<tr>
<td>(T_{\text{bed}})</td>
<td>349</td>
<td>K</td>
</tr>
<tr>
<td>(D_{p,d})</td>
<td>(2.11 \times 10^{-5})</td>
<td>m²/s</td>
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</table>
\[ m_a \frac{d\tilde{v}_a}{dt} = \tilde{F}_g + \tilde{F}_D + \tilde{F}_P + \sum_{b, \alpha} (\tilde{F}_{ab}) \]

where the forces on the RHS respectively are due to gravity, drag, the far field pressure, and the contact force with other particles and/or confining walls \( b \). The drag and far field pressure forces were determined by considering two-way coupling. For the drag force the closure by Beetstra et al. [17] was used.

The angular momentum is only solved for the particles and is described by:

\[ I_a \frac{d\tilde{\omega}_a}{dt} = \sum_{b, \alpha} (R_{ab} \tilde{\omega}_{ab} \times \tilde{F}_{ab}) \]

where the torque is due to tangential forces resulting from contacts with other particles and/or the walls. Note that the collisional forces between the droplets were neglected due to the small size of the droplets. As a result, there is no need to solve an equation for the angular momentum of the droplets.

For the calculation of the forces acting on small droplets the gas phase properties were mapped from Eulerian grid to the Lagrangian points using mapping windows with a size equal to the grid size, keeping the computational overhead low. The forces acting on the particles were determined by mapping the gas velocity and pressure gradient using a tri-linear interpolation.

The particle–particle interaction forces were estimated using a linear soft-sphere model [18]. In this model, the particles are

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Fig. 4. Comparison of the computed steady state dimensionless gas phase concentration profile with an analytical solution obtained from a 1D-heterogeneous plug flow model for coupled heat and mass transfer (symbols indicate the simulation results; lines indicate the analytical solution at different superficial gas velocities).

Fig. 5. Schematic of simulated geometry of spout fluidized bed with draft plates.
assumed to overlap/deform during the contact and the contact forces were calculated using a mechanical analogy consisting of a spring (for particle overlap), dash-pot (for viscous dissipation) and slider (for friction between the particles). This arrangement provides a flexibility to estimate the energy dissipation due to the non-ideal particle collisions using input parameters as spring stiffness, damping coefficient, restitution coefficient (in normal and tangential directions) and the friction coefficient.

The particle–droplet collisions were treated in a similar manner as described by van Buijtenen et al. [10]. That is, the colliding droplets always transfer their mass, volume and momentum to the particle. This leads to an increase in the particle mass and associated momentum, given by [19]:

$$m'_p = m_p + m_d$$

$$V'_p = V_p + V_d$$

$$m'_p \ddot{v}'_p = m_p \ddot{v}_p + m_d \ddot{v}_d$$

where $m_p$, $V_p$ and $\ddot{v}_p$ are respectively the new particle mass, volume and acceleration after the droplet impact. The angular velocity ($\dot{\omega}_p$) and the position vector ($\vec{r}_p$) of the particles were assumed to be unaffected by particle–droplet interactions. Further, break-up of the droplets after the impact on the particle is neglected and after the impact the droplets are removed from the simulation domain. These assumptions are valid in case of small droplet to particle diameter ratio. Upon a droplet–particle impact, the droplet is assumed to form a uniform liquid layer around the particle without changing the particle shape (i.e. the particle remains spherical) as shown in Fig. 1. This assumption only makes sense if particles are hit by large numbers of droplets, which is typically the case in the spray zone of a spout-fluidized bed. Once particles are wet, their collision properties significantly alter due to the presence of a liquid layer, which leads to an increase in the collisional energy dissipation during wet particle–particle interaction. This effect can be modelled by using a variable restitution coefficient that depends on the moisture content, physical properties of the liquid and the impact velocity. Recently, van Buijtenen et al. [10] performed simulations for a wet system with a variable restitution coefficient as a function of moisture content only. In reality, at low velocities and/or high viscosity particles will stick together to form agglomerates with zero restitution coefficient. However, in their simulations the restitution coefficient never becomes zero. In this work a simplified model proposed by Davis et al. [14] has been used to quantify the wet restitution coefficient in both the normal and tangential directions as:

$$e_{wat} = \begin{cases} e_{dry}(1 - \frac{\mu}{C_1}) & \text{if } St > St_c \\ 0 & \text{if } St < St_c \end{cases}$$

where $e_{dry}$ is the dry restitution coefficient and $St$ is the Stokes number. No particle rebound was observed at $St > St_c$ due to significant loss of particle kinetic energy in the liquid (viscous dissipation). The limiting value of the critical Stokes number ($St_c$) depends on the physical properties of liquid and solid, the relative particle velocity at impact ($V_{p,rel}$), and the sum of the liquid layer thicknesses of both particles ($\delta_l$).

### 2.3. Gas phase heat and mass transfer

The gas phase temperature was obtained by solving the thermal energy equation:

$$\frac{\partial}{\partial t} (\varepsilon \rho g H_g) + \nabla \cdot (\varepsilon \rho g \vec{u}_g H_g) = -\nabla \cdot (\varepsilon \vec{q}_h) + S_h$$

where the change in enthalpy of the gas $dH_g$ can be expressed as the product of the specific heat of the gas at constant pressure and the change in gas temperature $dH_g = C_p g dT_g$. $S_h$ represents the source term for interfacial heat transfer:

$$S_h = \frac{1}{V_{cell}} \sum_{r=1}^{N_c} \delta(\vec{r} - \vec{r}_a) h_g A_g (T_g - T_{eq})$$

where $\delta(\vec{r} - \vec{r}_a)$ represents the discrete delta function that maps the heat exchange from the particle/droplet positions $\vec{r}_a$ to the grid position $\vec{r}$. It is approximated by using a tri-linear interpolation, which is common practice in cases where the discrete elements are much smaller than the grid spacing.

The conductive heat flux ($\vec{q}_h$) is calculated with:

$$\vec{q}_h = -k_{eff} \nabla T_g$$

where the effective conductivity ($k_{eff}$) is given by:

$$k_{eff} = 1 - \frac{1}{e} k_g$$

Finally, the heat transfer coefficient for the heat exchange between the gas and the particles/droplets ($h_g$) was evaluated using the empirical Nusselt correlation given by Gunn [20]:

$$Nu_a = (7 - 10e + 5e^2) \left[ 1 + 0.7 Re_a^{0.2} Pr^{0.33} \right] + (1.33 - 2.4e + 1.2e^2) Re_a^{0.2} Pr^{0.33}$$

where the dimensionless numbers are defined as follows:

$$Nu_a = \frac{h_d d_a}{k_g}; \quad Re_a = \frac{\varepsilon_{eff} u_{eff} d_a - \vec{v}_g |d_a|}{u_g}; \quad Pr = \frac{\mu_g C_p g}{k_g}$$

The mass fraction of the moisture was obtained by solving a species balance equation:

$$\frac{\partial}{\partial t} (\varepsilon \rho_g w_g) + \nabla \cdot (\varepsilon \rho_g \vec{u}_g w_g) = -\nabla \cdot (\varepsilon \vec{q}_m) + S_m$$

where the source ($S_m$) is due to interfacial mass transfer:

$$S_m = \frac{1}{V_{cell}} \sum_{r=1}^{N_c} \delta(\vec{r} - \vec{r}_a) k_m A_g (w_g^* - w_g)$$

$\vec{q}_m$ represents the mass transfer flux as a function of the effective gas diffusivity ($D_{eff,g}$) and the gradient of the gas phase mass fraction of the moisture ($w_g$):
The mass transfer coefficient for the gas phase \( (k_m) \) was evaluated using the correlation of [20] for mass transfer based on the Sherwood number:

\[
Sh_a = \frac{(-7 - 10e + 5e^2) \left[ 1 + 0.7 \, Re_a^{0.2} \, Sc^{0.33} \right] + (1.33 - 2.4e + 1.2e^2) \, Re_a^{0.7} \, Sc^{0.33}}{2.4e - 1.2e^2} \tag{16}
\]

where the dimensionless numbers are given by:

\[
Sh_a = \frac{k_s d_a}{D_{eg}}; \quad Re_a = \frac{\varepsilon \rho_a |\bar{u}_a - \bar{v}_a| d_a}{\mu_g}; \quad Sc = \frac{\mu_g}{\rho_g D_{eg}}
\]

### 2.4. Particle and droplet phase heat and mass transfer

The heat and mass transfer from the particle and droplets to the gas phase and vice-versa was estimated by solving the particle-/droplet heat and mass balances:

\[
m_a C_{pa} \frac{dT_a}{dt} = h_i A_i (T_a - T_g)
\]

\[
\frac{dm_i}{dt} = k_m A_i \left( w_{g}^{f} - w_{g}^{i} \right)
\]

For two-component systems without chemical reaction a thermodynamic equilibrium exists at the gas–liquid interface (note that we assume no heat and mass transfer resistance in the liquid
Hence the saturated mass concentration of liquid in the gas phase \( w_{\text{eq}} \) at the interface was determined by using the Clapeyron equation:

\[
\frac{dP}{dT}_{\text{eq}} = \frac{\Delta H_{\text{evap}}}{R \Delta T}
\]

which is expressed as a function of the interface particle temperature, partial pressure and the heat of evaporation \( \Delta H_{\text{evap}} \). The interfacial particle temperature will adjust itself in such a way that at steady state the rate of heat transfer will balance the equivalent rate of heat transfer associated with the mass transfer. A schematic representation of interfacial parameters is given in Fig. 2.

### Table 6
Numerical simulation settings.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
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</thead>
<tbody>
<tr>
<td>( X_{\text{max}} \times Y_{\text{max}} \times Z_{\text{max}} )</td>
<td>0.08 \times 0.015 \times 0.18</td>
<td>m³</td>
</tr>
<tr>
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<td>–</td>
</tr>
<tr>
<td>( N_p )</td>
<td>82,505</td>
<td>–</td>
</tr>
<tr>
<td>( k_b )</td>
<td>10³</td>
<td>N/m</td>
</tr>
<tr>
<td>( \Delta t_g )</td>
<td>2 \times 10^{-3}</td>
<td>s</td>
</tr>
<tr>
<td>( \Delta t_p )</td>
<td>1 \times 10^{-4}</td>
<td>s</td>
</tr>
<tr>
<td>( \Delta t_{\text{int}} )</td>
<td>1 \times 10^{-3}</td>
<td>s</td>
</tr>
</tbody>
</table>

Fig. 7. Snapshots of wet particulate flow patterns for the fluidized bed spouting-with-aeration (dispersed spout) regime: simulated positions and radius \( r_p \) of the wet particles only, along with the gas volume fraction \( \varepsilon \) (a–d), particle configuration from high speed visual experiments (e–h), and particle temperatures from IR thermography (i–l). Note that the wet particles shown in the simulation snapshots were enlarged to make them easier to see.
3. Model verification

In this section we present various tests that were conducted to verify the heat and mass transfer implementation. The computational results are compared with analytical solutions. Subsequently, we studied the optimum particle collision time step in view of the expected strongly dissipative particle-particle collisions.

3.1. Gas-particle heat transfer coupling

To test the implementation of the heat balances, initially a fixed bed without heat transfer was considered by passing a gas through a fixed bed of stationary particles (see Table 1 and 2 for simulations settings). The obtained pressure drop was determined and compared with the Ergun equation. More details about the boundary conditions and analytical solution can be found in [21]. The simulation results show 2.8% over-prediction of the pressure drop as compared with the value obtained from the Ergun equation (200 Pa/m).

Additionally a similar fixed bed test was performed, this time including heat transfer. In this test case, a fixed bed of cold particles and cold fluid (at 300 K) were heated by injecting a hot fluid (400 K) through the bed at 0.25 m/s. During this process, the cold particles and the fluid in the domain heat up with time, leading to a heat front moving through the bed. The simulations settings are shown in Table 2.

The computational results were verified by comparing them with the solution of a 1D-convection equation, which takes into account the heat-exchange between the fluid and the particle phases. The axial heat dispersion is neglected due to the high Péclet number (Pe = 24,996). The energy balance equations for the gas and particle phases are respectively given by:

\[ \dot{e}_g \rho_g C_p g \frac{\partial T_g}{\partial t} = -\dot{e}_g \rho_g C_p g u_g \frac{\partial T_g}{\partial z} - h_g a_p (T_g - T_p) \quad (20) \]

\[ (1 - \varepsilon) \rho_p C_p p \frac{\partial T_p}{\partial t} = -h_g a_p (T_g - T_p) \quad (21) \]

where \( a_p = 6(1 - \varepsilon)/d_p \) is the specific fluid-particle surface area. We note here that particle-particle heat transfer is not included in these equations, in line with the assumptions made earlier for cases of fluidized systems. For realistic studies of heat transfer in a packed bed, one would obviously need to include this heat transfer mechanism too. The analytical solution for the given system can be found in [22]. A comparison of the temperature along the height with time is shown in Fig. 3, which indicates a very good agreement. This confirms that the gas-particle heat transfer coupling has been implemented correctly.

3.2. Coupled heat and mass transfer

Verification of the coupled heat and mass transfer was done by passing a fluid through a fixed bed of stationary particles kept at a fixed temperature (349 K) with an initial mass fraction i.e. 100 times lower than the inlet mass fraction (0.005 kg of water/kg of air). A test simulation was performed with almost similar simulation settings as given in Table 2. The other additional settings are shown in Table 3.

The computed axial profiles were compared with an analytical solution obtained from a 1D-heterogeneous plug flow model (see Eq. (22)):

\[ \left( \frac{w_s}{w_{s0}} \right) = \exp \left[ -\frac{k_m d_p}{u_z} \right] \quad (22) \]

In this model axial dispersion of the species is neglected, whereas the mass transfer coefficient \( k_m \) was estimated from an empirical Sherwood correlation based on [20], see Eq. (16). A comparison between the steady-state axial profiles of the fluid concentration and the analytical solution obtained from the 1D-heterogeneous plug flow model is shown in Fig. 4. The numerical and analytical results agree very well, which confirms that the coupled heat and mass transfer has been implemented correctly.

3.3. Time step analysis

In DEM, the instantaneous motion of individual particles is determined by solving the Newton’s motion equations for every time step and contact forces between the particles and its immediate neighbours were calculated by means a soft sphere approach. Contacts between neighboring particles is generally checked in a region with a diameter of five times the particle diameter, leading to a so-called neighbour list. The accuracy and stability of the simulations not only depends on the particle collision time step \( \Delta t_{tnbr} \) but also on the time step used for updating the neighbour list \( \Delta t_{nhbr} \). The overall efficiency of the CFD-DEM code depends on the choice of both \( \Delta t_{tnbr} \) and \( \Delta t_{nhbr} \). A big time step leads to a shorter simulation run time, but also to unrealistic simulation results. On...
the other hand, a small time step will often minimize simulations errors, but with the penalty of a dramatic rise in the total simulation run time [24,23]. [25] reported that the value of the time step does not significantly influence the bed dynamics at a high restitution coefficient (in the range of 0.9). But, during wet DEM simulations the restitution coefficient may vary anywhere between 0 and 0.97 (for a glass particle). Therefore, the effect of the time step on the accuracy of the particle collision computation was assessed. To this end, a number of tests were computed, wherein two particles were allowed to collide with a given impact velocity and input restitution coefficient ($\varepsilon_{in}$), and post collisions velocities were used to determine the restitution coefficient, $\varepsilon_{cal}$ (i.e. ratio of the particle impact velocity after and before the collision) that actually prevailed. Ideally the input restitution coefficient and the realised restitution coefficient are the same. The absolute difference between the input and realised values of restitution coefficient were determined and time steps with a small error were selected for further simulations. The computed results are summarised in Table 4. We selected $\Delta t_p = 1 \times 10^{-6}$ s for further simulations and here the error is sufficiently small.

4. Results and discussion

To demonstrate the model capabilities, we will now present simulation results for a spout fluidized bed containing glass particles subject to liquid injection. The bed is operated in the so-called fluidized bed spouting-with-aeration (dispersed spout) regime. In this regime the spout velocity is set to $U_{sp}/U_{mf} = 25.4$, whereas the auxiliary or background velocity is set to $U_{bg}/U_{mf} = 1.25$. Liquid is injected into the bed through a nozzle in a bottom spray configuration. The obtained results are expressed in terms of particulate...
flow patterns, pressure drop, particle velocity and temperature. We compare the computational results with experimental data obtained by non-intrusive methods [13].

4.1. Geometrical configuration and simulations settings

Simulations were carried out for a pseudo-2D spout fluidized bed geometry (as shown in Fig. 5) of the dimensions $W \times D \times H = 0.08 \times 0.015 \times 0.18 \text{ m}^3$ with spout dimensions of $W_{sp} \times D_{sp} = 0.006 \times 0.015 \text{ m}^2$. Two symmetrical draft plates, each of dimension $W_{dt} \times D_{dt} \times H_{dt} = 0.005 \times 0.015 \times 0.8 \text{ m}^2$, were positioned inside the bed at a distance of 3 cm from the side walls and at an entrainment height $h$ of 1.5 cm from the bottom of the bed. The bed was initially filled to a height of $H_0 = 6.5 \text{ cm}$. The physical properties of the particles and the gas, and the numerical settings used in the CFD–DEM simulations are listed in Tables 5 and 6. The hydrodynamic and thermal behaviour of the spout fluidized bed were monitored by synchronising a visual camera and an infrared (IR) camera. Here it should be noted that the experiments were performed by maintaining a constant back plate temperature of $30 \text{ °C}$. This technique allows non-intrusive identification of the wet and dry zones inside the bed. Moreover, the visual images were used to obtain quantitative flow information through PIV, whereas the thermal behaviour of the bed was determined from IR images by means of IRT. More details about the experimental set-up, arrangement of cameras, post processing of images with mapping, averaging and masking can be found in [13]. Additionally, instantaneous pressure measurements were performed using pressure sensors located in the middle of the annulus, just above the distributor plate. These measurements were done for 4 minutes at a data acquisition rate of 50 Hz.

4.2. Particle flow pattern

Snapshots of the prevailing particle flow patterns obtained from the CFD–DEM simulations are shown in Fig. 6 for the cases with and without draft plates. It can clearly be seen that in the case with draft plates the flow is very well structured in a spout section with high velocity particle up flow and a annular section with particle down flow. In the case without draft plates, similar patterns are observed, with an important difference however. In this case, there is a substantial exchange of particles between the two sections.

Fig. 7 shows snapshots of the prevailing particle distribution and gas volume fraction obtained from both the CFD–DEM simulations and the experiments. During both simulations and experiments, at the start of the liquid injection the particles in the vicinity of the spout entrance become wet and accelerate upwards through the draft plates to a certain height. After reaching a certain height, particles move laterally and subsequently lose their momentum and move down into the annulus. This continuous upward and downward transport of the particles leads to a steady particle circulation pattern, with relatively high particle velocities inside the draft plates. From Fig. 7(a)–(d) it can be seen that the distribution of the particle size is more or less homogenous. As
the time progresses, the liquid injection results in a pronounced particle movement in the annulus with periodic slugging, which is mainly attributed to the pronounced gas bypassing from the wet spout region to the dry annulus (see Fig. 7(b)). Here it is noted that, the simulations show less pronounced slugging behaviour as compared with the experiments (see Fig. 7(f)). After \( t = 1 \) s, a uniform liquid distribution was observed (see Fig. 7(c) and (k)) in the spout and annulus without any slugs/bubbles and a bed height equal to \( \approx 14.5 \) cm).

4.3. Pressure drop

The variation in pressure drop is shown in Fig. 8 for both simulations and experiments under wet conditions. During the simulations, a stable pressure signal was observed with only minor fluctuations, unlike the experiments, which illustrate intense periodic fluctuations. The former is due to the stable circulatory bed behaviour with formation/break-up of small bubbles in the annulus. In the experiments however, the injected liquid leads to slugging behaviour and gas channeling. Moreover, wet particles often stick to the bed walls. Therefore, the total bed mass per unit cross-section supported by the inflow gas is often lower than in simulations, leading to lower pressure drop. To capture this effect, one would need to include cohesive forces between wet particles and the wall in the model. Introduction of cohesive forces can probably also lead to better agreement regarding the slugging behaviour.

4.4. Time-averaged particle velocity

Fig. 9 displays comparison of the time-averaged horizontal particle velocity profiles obtained from the simulations and the experiments at \( z = 7.8 \) and 12 cm. Both velocity profiles agree fairly well. For both simulations and experiments, intense particle displacements were observed in the spout, with similar particle velocities at \( z = 7.8 \) and 12 cm. Whereas at low bed height (\( z = 7.8 \) cm) the experiments have a bias towards too strong down flow velocities in the annulus. The reason for this is that in case of slugging behaviour velocities in the plugs and slugs are treated equally in the calculation of the velocities, even though there are much fewer particles (with a high negative velocity) in the slugs. To eliminate this bias in the experiments, one would need to apply digital image analysis (DIA) to obtain the local solids volume fraction [26, see].

4.5. Spout fluidized bed without draft plates

Fig. 10 displays a series of snapshots obtained from CFD–DEM simulations for a spout fluidized bed without draft plates. As discussed earlier (in Section 4.2), spout fluidized beds with and without draft plates illustrate similar flow characteristics. Just after liquid injection, a stable spouting was observed where particles near the injection nozzle become wet and accelerate upwards in the centre. However, without draft plates, the particles fall down either in the spout or annulus, with continuous cross-flow from

Fig. 12. Simulation snapshots showing distribution of the moisture in a spout fluidized bed with (a–c) and without (d–f) draft plates.
the spout to the annulus throughout the entire bed height. This leads to enhanced random particle mixing between spout and annulus without clear distinction between the spout and annulus, as can be seen in Fig. 10(c) and (d). Additionally, the spout fluidized bed without draft plates shows a wider distribution of wet particles. This is because of repeated collisions of the wet particles with incoming droplets in the spout, which is less ordered due to the cross flow.

The gas temperature and moisture distribution in the spout fluidized bed with and without draft plates is shown in Figs. 11 and 12. At the beginning of liquid injection at $t < 1 \text{s}$, both arrangements show formation of cold spots (a low temperature and low moisture zones) near the bottom (see Figs. 11(a) and 12(a)). As time progresses ($t = 1.06 \text{s}$), the system with draft plates shows a high temperature gradient and zones with a high mass concentration at a certain distance from the distribution plate in the annulus (see Figs. 11(b) and 12(b)). This is attributed to the clear distinction between the wetting (spout) and drying (annulus) zones.

5. Conclusions

In this work, a novel CFD–DEM model was presented for fluidized systems involving coupled heat and mass transfer in combination with liquid injection. The implementation of the heat and mass transfer was verified by conducting various tests and subsequent comparison of the computational results with analytical solutions, revealing a very good agreement. Hence, the coupled heat and mass transfer effects were successfully implemented. Furthermore, in order to test the model simulations were carried out to analyse the heat and mass transfer aspects in a spout fluidized bed with draft plates in combination with liquid injection for the fluidized bed spouting-with-aeration (dispersed spout) regime. The simulations were done for glass particles and, for the first time, compared with experiments performed through combined visual and an infrared thermometer. The obtained results show a fair agreement in terms of particulate flow pattern, pressure drop and particles velocities. The model could be further improved by including cohesive forces acting between contacting wet particles. Finally, CFD–DEM simulations were performed to analyse the heat and mass transfer phenomena in a spout fluidized bed with and without draft plates in combination with liquid injection. The system with draft plates possesses a unique feature allowing simultaneous co-current (wetting) and counter-current (drying) contact zones.

Acknowledgements

This research is supported by the Dutch Technology Foundation STW, applied science division of NWO and the Technology Program of the Ministry of Economic Affairs in The Netherlands, as well as by the DFG (German Research Foundation) in Germany.

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