Effect of Superficial Gas Velocity on the Solid Temperature Distribution in Gas Fluidized Beds with Heat Production

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*Supporting Information

ABSTRACT: The hydrodynamics and heat transfer of cylindrical gas–solid fluidized beds for polyolefin production was investigated with the two-fluid model (TFM) based on the kinetic theory of granular flow (KTGF). It was found that the fluidized bed becomes more isothermal with increasing superficial gas velocity. This is mainly due to the increase of solids circulation and improvement in gas solid contact. It was also found that the average Nusselt number weakly depends on the gas velocity. The TFM results were qualitatively compared with simulation results of computational fluid dynamics combined with the discrete element model (CFD-DEM). The TFM results were in very good agreement with the CFD-DEM outcomes, so the TFM can be a reliable source for further investigations of fluidized beds especially large lab-scale reactors.

1. INTRODUCTION

Polyolefins are one of the important base materials that can be used for various consumer products. Various reactor types can be used for the production of polyolefins. One common type of reactor for this purpose is gas–solid fluidized bed reactor. Gas–solid fluidized beds have several advantages compared to other reactors. Intensive solid mixing, high rate of heat and mass transfer between solid and gas phases, and large heat transfer coefficient between the bed and immersed heating/cooling surfaces are some of the advantages of these reactors. On the other hand, they have some disadvantages too. Attrition of particles and consequently erosion of internals, scale-up difficulty, possibility of defluidization and solid agglomeration are some of their disadvantages.

The very high heat transfer rate in gas fluidized beds is utilized to remove the very large amount of heat produced by the highly exothermic polymerization reactions. A schematic representation of polymer production in gas–solid fluidized beds is presented in Figure 1. In the case that the produced heat is not removed in an effective way, the polymer particles may form hot-spots, become sticky, and form agglomerates. The formation of agglomerates may cause defluidization of the whole process. Thus, it is necessary to have a better understanding of the effect of various parameters on hot-spot formation and solid temperature distribution.

Performing experiments as a parameter study and controlling the experimental conditions is a very costly and challenging job. On the other hand, simulation techniques are a reliable and flexible tool for this purpose as we can systematically control various parameters during simulations and they are relatively cheap. In the past several years, many simulation research efforts were conducted in this area. For example, Kuwagi and Horio used computational fluid dynamics combined with...
discrete element model (CFD-DEM) to investigate the mechanism of agglomeration in fluidized beds with fine particles. Kaneko et al. used the CFD-DEM model to simulate the fluidized beds with gas-phase olefin polymerization at various gas distribution conditions. After that, Limtrakul et al. used a similar model for a catalytic conversion in a spouted fluidized bed and compared the simulation results with the experimental data and they found a good agreement between them. There are also much research about the hydrodynamics and heat and mass transfer in gas solid fluidized beds with the help of CFD-DEM, the two-fluid model (TFM), or other simulation models. In all these works, the researchers tried to understand the behavior of gas solid fluidized beds or mechanisms behind various phenomena at different conditions to optimize or predict these reactors.

Recently, Li et al. investigated the effect of superficial gas velocity and operating pressure on the solid temperature distribution in gas fluidized beds using the CFD-DEM. As the computational time of CFD-DEM is quite long, they only studied small lab-scale pseudo-two-dimensional reactors. In this work, the TFM based on the kinetic theory of granular flow (KTGF) is used. The TFM is suitable for simulating small-to-large lab-scale fluidized beds. Though the TFM requires a shorter computational time compared to CFD-DEM, the simulation of large lab-scale fluidized beds with TFM can still be very long and they may take several months on single processor computers. So, before starting such a time-consuming investigation, it is necessary to gain insight on the accuracy and reliability of the TFM results. Because the TFM requires more assumptions compared to the CFD-DEM, the comparison between these two models gives some indications on the accuracy and reliability of the TFM results. This comparison helps us to analyze the TFM results in a better way too. Hence, the main focus of this work was on the qualitative comparison between the results of these two models. Moreover, the effect of superficial gas velocity on temperature distribution in gas-solid fluidized beds with heat production was explored too. As such, this work provides insight in the predictive capabilities of the TFM with respect to hydrodynamics and heat transfer in gas fluidized beds. In particular, we will focus on systems with heat production with varying superficial gas velocities.

2. GOVERNING EQUATIONS
The TFM has been developed based on the assumption that the particulate phase behaves like a fluid. Thus, the governing equations for both the gas and the solid phases are similar to each other. The governing equations in this model involve the continuity, Navier–Stokes, granular temperature, and thermal energy balance equations. The mathematical representation of these equations is given in Table 1.

Table 1. TFM Governing Equations in Vector Form Based on KTGF

\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g \vec{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{u}_g \rho_g) = 0
\]

(1)

\[
\frac{\partial}{\partial t} (\varepsilon_s \rho_s \vec{u}_s) + \nabla \cdot (\varepsilon_s \rho_s \vec{u}_s \rho_s) = 0
\]

(2)

Equations 1 and 2 are the continuity equations (mass conservation balances) for the gas and the solid phases, respectively. Equations 3 and 4 are the Navier–Stokes equations. These equations represent the conservation of momentum for the gas and the solid phases. Equation 5 is the granular temperature equation that describes the kinetic energy associated with the solid phase fluctuating motion. Finally, eqs 6 and 7 are the thermal energy equations. The governing equations require closure equations. In this work, the closures that have been presented by Nieuwland et al., 1996 were used. These equations are listed in Appendix A of the Supporting Information, Table S1.

3. IMPLEMENTATION AND VERIFICATION
After discretizing of all the aforementioned equations by a finite difference technique, they were implemented in a computer code that was carefully verified and checked. The implementation and verification of the flow solver was previously reported by Verma et al. As a result, only the implementation of thermal energy equations was needed. The implementation and verification of the thermal energy equations is briefly presented by Banai et al. Some additional verification tests are presented and discussed in this work. Here, the verification of the main terms in the energy equations due to conduction, and convection together with interfacial heat transfer between gas and solid phases are presented.

3.1. Verification of Conduction Terms. As a first step, the conduction terms in the energy conservation equations were verified. This verification test was done in a one-dimensional single phase system. As the main purpose of this test was to check the correct implementation of the conduction terms; there was no flow in the system. Consequently, all the convection terms were set to zero. This test was performed for radial and axial directions but only one of them is presented and discussed here for brevity. The simulation settings, simplified governing equation and the general form of the analytical solution of this test case is presented in Table 2.
Table 2. Simulation Conditions, Governing Equation, and the Analytical Solution for Conductive Heat Transfer Verification Test

| parameter      | value | unit | parameter      | value | unit |
|----------------|-------|------|----------------|-------|------|
| \(H_{\text{bed}}\) | 0.5   | m    | \(n_c\)        | 100   |      |
| \(\Delta z\)   | 0.005 | m    | \(\rho\)       | 20.00 | kg/m³|
| \(T_o\)        | 0.0   | K    | \(q\)          | 6.7 \times 10⁶ | J/(m²·s) |
| \(C_p\)        | 1000.0| J/kg·K | \(k\)         | 20.0  | J/(m·K) |
| \(\Delta t\)   | 2 \times 10⁻³ | s | \(t_{\text{sim}}\) | 2.0  | s |

Boundary Conditions:
- at \(z = 0\): \(T = 0.0\) K and at \(z = L\): \(\frac{dT}{dz} = 0\)
- Initial Condition:
  - at \(t = 0\): \(T = a + b \cdot z\)
- Governing Equation:
  \[\rho C_p \frac{dT}{dt} = k \frac{\partial^2 T}{\partial z^2} + q\]
- Analytical Solution:
  \[T = \left(a + \frac{q}{\rho C_p} + \frac{z^2}{2k}\right) \text{erf} \left(\frac{z}{\sqrt{2kt/\rho C_p}}\right)\]
  \[- \frac{q^2z}{k} \left(\frac{1}{\rho C_p}\right)^{1/2} \exp \left(-\frac{z}{4kt}/\rho C_p\right) + bz - \frac{z^2}{2k}\]

After performing the simulation, axial temperature profiles were obtained. The obtained results were compared with the analytical solution as shown in Figure 2. This figure evidently shows the proper implementation of the conduction terms.

![Figure 2. Comparison between the analytical and the numerical results of conductive heat transfer test with heat generation.](image)

### 3.2. Verification of Interfacial Heat Transfer and Convection Terms

The second verification test that is presented here is related to the interfacial heat transfer in a fixed bed. This test was also performed for a one-dimensional system. The simulation conditions and the governing equations for this test case are presented in Table 3.

As there is no analytical solution for this test, a simple 1D model was implemented in MATLAB and the final TFM results were compared with the results of 1D model as shown in Figure 3.

After successful verification of all the implementations, various grid sensitivity analysis tests were performed to find out the suitable computational grid sizes. These analyses are presented in the Supporting Information Appendix B. Then, it was possible to start the investigations on the effect of superficial gas velocity in fluidized beds with heat production. The simulation conditions for this parameter study are presented in the next section.

### 4. SIMULATION SETTINGS

The simulation settings in this work were determined by assuming that a fluidized bed behaves like a continuously stirred tank reactor (CSTR). This strategy can give a good estimation of the thermal steady state temperature in a fluidized bed. This method was used by Li et al.\(^{10}\) and they could estimate the thermal steady state temperature in a reactor without performing time-consuming simulations that would otherwise be required to reach a thermal steady state. This procedure is as follows: first, we found the gas and solid steady state temperature by assuming that the bed behaves like a CSTR reactor. Then, we performed the TFM simulations at the obtained steady state temperature values from the CSTR analyses. Next, we checked if the average temperature of the bed from the TFM simulations increases or decreases with time. In other words, is the system in the thermal steady-state condition or not? If not, we used the obtained temperature evolution from the TFM outcomes and tune the parameters in the CSTR simulations to find our next guesses for the thermal steady state temperatures. We continued this procedure until the average bed temperature does not change significantly with time anymore.

The obtained results are presented in Table S3 in the Supporting Information Appendix C as \(T_{g,0}\) and \(T_{s,0}\). These two parameters are the initial gas and solid temperature, respectively. On the basis of the obtained results from the CSTR analysis, the thermal steady state temperatures change with the gas superficial velocity. For this reason, \(T_{g,0}\) and \(T_{s,0}\) are different for different simulation cases. The evolution of the gas and solids average temperature is presented in Figure 4. This figure clearly shows that the thermal steady state condition was satisfied and the average bed temperature does not change significantly with time. In all the performed simulations, the relative difference between the initial condition and the obtained average solid temperature was less than 0.015%. The other simulation conditions are also presented in Appendix B and Appendix C of the Supporting Information.

It should be noted that, most of the simulation conditions were similar to the simulation conditions of Li et al.\(^{10}\) except the bed size and the bed geometry. In this work, the bed has a cylindrical shape and the simulations were conducted for full 3D systems. On the other hand, the simulations of Li et al.\(^{10}\) were for pseudo-2D rectangular beds. Thus, we could mostly compare our TFM results with the CFD-DEM results of Li et al.\(^{10}\) qualitatively. All the simulations were performed for 10 s and the thermal energy equations were not solved during the first 0.5 s of the simulations to exclude the start-up effect from the final analysis.

After performing the simulations, several parameters were studied. These parameters are the probability distribution function (PDF) of the gas volume fraction and the solid temperature, the bed averaged gas and solid temperatures, the overall Nusselt number in the bed, and the solid flow circulation. All these parameters were calculated at various fluidization velocities and their results were compared with each other. At the same time, the TFM results were compared with the CFD-DEM results of Li et al.\(^{10}\) in a qualitative way too.
5. RESULTS AND DISCUSSIONS

5.1. Gas Volume Fraction Distribution. By increasing the fluidization velocity, it is expected to have more bubble formation in the bed and the bed height increases too. Some simulation snapshots of bubbling gas fluidized beds at various operating gas velocities are presented in Figure 5. These snapshots show the gas volume fraction distribution at one slice in the center of the bed. This figure shows that the number of bubbles and the bed height increases with gas velocity. As the gas velocity increases, the bubbles’ interactions become stronger. As a result, the bed becomes chaotic at high gas velocities and the bubbles lose their distinct boundaries with the emulsion phase. To quantify these effects, the PDF of the gas volume fraction was calculated and the final results are presented in Figure 6, where the definition of PDF for gas volume fraction is given by

\[
\text{PDF} = \frac{\sum_{k \in \text{FRB}} V_k \rho_g k}{\sum_{k \in \text{FRB}} V_k \rho_g k} \quad \epsilon_k \in \left(\epsilon_i - \frac{\Delta \epsilon}{2}, \epsilon_i + \frac{\Delta \epsilon}{2}\right) \quad k \in S_i
\]

where \( V_k \) is the volume of computational cell “\( k \)”. In these calculations, the gas volume fraction from 0 to 1 was divided into 50 equidistant intervals (“bins”) and the free-board was excluded in the calculation of PDF of gas properties.

Figure 6 is divided into three regions (phases) based on the gas volume fraction, that is, emulsion phase (0.4 < \( \epsilon_g \) < 0.55), intermediate phase (0.55 < \( \epsilon_g \) < 0.85), and the bubble phase (0.85 < \( \epsilon_g \) < 1.0). On the basis of this division, this figure clearly shows that the bubble region becomes larger with gas velocity. Furthermore, the division of the emulsion and the bubble phase becomes relatively unclear too. At the same time, the emulsion phase shrinks with increasing the gas velocity. In conclusion, the gas—solid contact becomes more intense with increasing
5.2. Gas and Solid Temperature Distribution. As it is stated in the previous section, the gas and solid have a better contact with increasing the superficial gas velocity. Consequently, it is expected to have a relatively high homogeneity in gas and solid temperature distribution at relatively high superficial gas velocity. This hypothesis will be discussed in this section. For this purpose, probability and cumulative distribution function (CDF) of the solid phase temperature, the maximum gas and solid temperatures during the simulations and the standard deviation of the solid phase temperature distribution were calculated for all cases. The PDF and CDF of the solid temperature were calculated by eq 9 and 10 respectively.

\[
\text{PDF}_{T_s} = \frac{\sum_{k \in S} V_s \cdot \varepsilon_{s,k}}{\sum_{k \in \text{FRB}} V_s \cdot \varepsilon_{s,k}};
\]

\[
T_k \in \left( T_i - \frac{\Delta T}{2}, T_i + \frac{\Delta T}{2} \right) \rightarrow k \in S',
\]

\[
\text{CDF}_{T_s} = \frac{\sum_{k \in S} V_s \cdot \varepsilon_{s,k}}{\sum_{k \in \text{FRB}} V_s \cdot \varepsilon_{s,k}}; T_k \leq T_i \rightarrow k \in S''
\]

Where \(\varepsilon_s\) is solid volume fraction, \(\Delta T\) is the temperature bin size in Kelvin and \(V\) is the volume of the computational cell. After calculation of the aforementioned parameters, the final results are presented in Figures 7-10. It should be noted that the temperature PDF was defined based on 60 equidistance bins in the temperature interval of 324–340 K and the solid superficial gas velocity. This suggests that the solid phase becomes more isothermal too. Whether this is indeed the case, will be discussed in the next section.
phase temperature standard deviation was calculated with eq 11.

\[ \sigma_T = \sqrt{\sum_{i=1}^{N_{\text{bins}}} [(T_i - \bar{T})^2 \cdot \text{PDF}_i]} \]  

(11)

As can be seen from Figure 7a, the solid temperature shifts to lower values with increasing superficial gas velocity. It can also be seen that the PDF of solid temperature is relatively wide and asymmetric at low superficial gas velocities and becomes relatively narrow and symmetric at high superficial gas velocities. This indicates the increase in the homogeneity of solid temperature with gas velocity. The same observation and conclusion can be drawn from the solid temperature CDF (refer to Figure 7b). The slope of solid temperature CDF increases with gas velocity. It can also be observed that the tail of CDF becomes smaller with gas velocity. These two observations show that the solid temperature becomes more uniform in the whole fluidized bed with increasing the gas velocity.

To have a further quantitative analysis on this phenomenon, the solid temperature standard deviation was also calculated and the results are presented in Figure 8. It was found that it decreases with gas velocity. Besides that, the maximum observed solid temperature and average gas and solid temperature in the whole bed decrease with gas velocity too, as can be seen in Figures 9 and 10. All of these results are in very good agreement with the CFD-DEM results that are presented by Li et al.10 Some snapshots of the solid phase temperature distribution in one vertical slice in the center of the bed is presented in Figure 11. These snapshots show the variation of solid temperature distribution at various fluidization velocities.

The solid temperature distribution snapshots are also in fair agreement with the CFD-DEM results, where it was observed that the injected cold gas has a tendency to pass through the bed from bubble to bubble. This leads to finger shaped regions connected to the distributor where the bed is relatively cold. One example of such a situation is presented in Figure 12. This phenomenon was also reported by Li et al.10 from CFD-DEM simulations, but the observations from the TFM are less distinct. This difference is partly due to inevitable numerical diffusion in the convection terms of thermal energy equations in the TFM. Moreover, it should not be forgotten that the TFM can only capture the solid phase temperature on the scale of computational cells. In contrast, the CFD-DEM can capture the temperature for every individual solid particle. For these reasons, it is completely comprehensible to see this difference between the results of the two models.

5.3. Average Nusselt Number. A possible explanation for the more isothermal bed behavior at higher superficial gas
velocities, could be an increase of the average heat transfer coefficient or average Nusselt number. To check this explanation, the average Nusselt number was calculated for all cases. The results show that the average Nusselt number does not increase with superficial gas velocity; in fact, it even slightly decreases. This results are presented in Figure 13. These findings are also in agreement with the CFD-DEM results.\textsuperscript{10} We used the following equations for calculation of the spatially averaged Nusselt number.\textsuperscript{16} After averaging the spatially averaged Nusselt values over time, the overall Nusselt number can be obtained.

\[ N_u = (7 - 10\epsilon_{s, g} + 5\epsilon_{s, g}^2)(1 + 0.7(R_{\epsilon_{s, g}}^2)(Pr^{1/3})) \]

\[ + (1.33 - 2.4\epsilon_{s, g} + 1.2\epsilon_{s, g}^2)(Re_{\epsilon_{s, g}}^{0.7}Pr^{1/3}) \]  

\[ Re_{\epsilon} = \epsilon_{s, g}|\bar{u}_{s} - \bar{u}|/\mu_{g} \]  

\[ Pr = C_{\epsilon,s, g}^{0.5}/k_{g, 0} \]  

\[ Nu_{\text{overall}} = \frac{\sum_{\text{all the cells}} N_u \epsilon_{s, g} V_{\text{cell}}}{\sum_{\text{all the cells}} \epsilon_{s, g} V_{\text{cell}}} \]  

(15)

So, if the overall Nusselt number in the bed decreases with superficial gas velocity, how can the variation of solid temperature homogeneity with gas velocity be explained? In the analysis of simulation results, it was found that the fluctuations in the Nusselt number increase with gas velocity, but the lower average solid temperature and more uniform temperature distribution in the bed cannot be attributed to it. The better uniformity in solid temperature distribution can only be justified by the more intense solid flow circulation and better gas–solid contact with gas velocity. The solid flow circulation patterns at various superficial gas velocities are presented in Figure 14 for more clarification. As the solid flow circulation rate and consequently the mixing rate of the particles increase with gas velocity, all the particles experience similar conditions at relatively high gas velocities. On the other hand, the mixing of particles at low gas velocities is a relatively slow process. Thus, some of the particles may stay at the bottom of the bed much longer than others. Therefore, some of the particles have a very low temperature due to long contact with the cold injected gas and some have a very high temperature. This can also be noticed in the PDF of solid temperature. At low fluidization gas velocities, the solid temperature PDF has a quite long tail and this tail becomes smaller with increasing the gas velocity as the gas–solid contact improves. Accordingly, the more isothermal behavior of the bed and the increase in the average bed temperature with superficial gas velocity are attributed to the two aforementioned changes in fluidization behavior. These results are in agreement with the analysis presented by Kaneko et al.\textsuperscript{4} that the degree of mixing can be a very good indication of hot-spot formation probability.

6. CONCLUSIONS

After verification of the implemented thermal energy equations into an existing two-fluid model code, various simulations were performed to study the thermal behavior in a cylindrical fluidized bed. All simulations were performed for a system with a constant volumetric heat generation in the solid phase and at a thermal steady state condition. The gas and solid physical properties were selected similar to the gas and solid properties in polyolefin production in fluidized beds. In addition, the simulation conditions were selected in a way they could be compared to the CFD-DEM results reported by Li et al.\textsuperscript{10} The effect of the superficial gas velocity on the gas volume fraction distribution, solid temperature distribution, and overall Nusselt number in the bed were investigated. The final TFM results were in very good agreement with CFD-DEM outcomes. It was found that the solid flow circulation rate and the uniformity of the solid temperature distribution increase with superficial gas velocity. At the same time, the overall Nusselt number, average gas temperature, average solid temperature, and maximum observed solid temperature decrease with superficial gas velocity. The relatively high level of uniformity in solid temperature distribution at relatively high superficial gas velocities is mainly due to efficient gas–solid contact and a comparatively high solid flow circulation rate of particles. Furthermore, this work showed the suitability of the TFM for simulation of fluidized beds with heat production. The model can be used for further studies especially in large lab-
scale reactors when CFD-DEM becomes prohibitively costly in terms of computational time.

**ASSOCIATED CONTENT**

* Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.7b00338.

All the closures that have been used in this work and their corresponding references, grid sensitivity analysis, and the conditions for the final set of simulations (PDF)

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Notes
The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

This research forms part of the research programme of Dutch Polymer Institute (DPI), Project No. 751.

**NOMENCLATURE**

\( A \) = area (m\(^2\))

\( AR \) = aspect ratio (—)

\( C_p \) = heat capacity (J/kg·K)

\( d, D \) = diameter (m)

\( E \) = particle–particle restitution coefficient (—)

\( e_w \) = particle-wall restitution coefficient (—)

\( g_0 \) = radial distribution function (—)

\( G \) = gravitational acceleration (m/s\(^2\))

\( H \) = height (m)

\( H \) = heat transfer coefficient (W/m\(^2\)·K)

\( K \) = heat conductivity (W/m·K)

\( L \) = length (m)

\( MW \) = molecular weight (g/mol)

\( n_\phi \) = number of cells in the azimuthal direction (—)

\( n_r \) = number of cells in the radial direction (—)

\( P \) = pressure (Pa)

\( q \) = heat production rate in the solid particles (J/m\(^3\)·s)

\( q_s \) = pseudo-Fourier fluctuating kinetic energy flux (kg/s\(^3\))

\( T \) = temperature (K)

\( t \) = time (s)

\( U \) = velocity (m/s)

\( V \) = volume (m\(^3\))

**Greek Symbols**

\( \alpha_{gs} \) = interfacial heat transfer coefficient (J/m\(^3\)·K·s)

\( \beta \) = interphase momentum transfer coefficient (kg/m\(^3\)·s)

\( \Delta \varepsilon \) = bin size for calculation of gas volume fraction PDF

\( \Delta r \) = computational grid size in the radial direction (m)

\( \Delta T \) = bin size for calculation of solid temperature PDF (K)

\( \Delta t \) = computational time step (s)

\( \Delta z \) = computational grid size in the axial direction (m)

\( \varepsilon \) = volume fraction (—)

\( \rho \) = density (kg/m\(^3\))

\( \sigma_T \) = temperature standard deviation (K)

\( \tau \) = stress tensor (Pa/m)

\( \theta \) = granular temperature (m\(^2\)/s\(^2\))

\( \mu \) = viscosity (Pa·s)

**Subscripts and Superscripts**

\( 0 \) = initial

\( eff \) = effective

\( f \) = frictional

\( G \) = gas

\( r \) = radial direction

\( S \) = solid

\( sim \) = simulation

\( z \) = axial direction

**Greek Subscripts**

\( \phi \) = azimuthal direction

**Abbreviations**

CDF = cumulative distribution function

CFD = computational fluid dynamics

CSTR = continuously stirred tank reactor

DEM = discrete element model
FRB = freeboard
KTGF = kinetic theory of granular flow
PDF = probability distribution function
TFM = two-fluid model

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