CPFD simulation on particle behaviour in an entrained-flow gasifier

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Abstract

A computational particle fluid dynamics simulation model for entrained-flow gasification was established in this study. The simulation results agree with the experimental data. The detailed particle information and residence-time distribution were obtained by injecting particle tracers in the simulation. The results show that the particles in the gasifier can be classified into three flowing zones, i.e. a fast-flowing zone, a recirculation zone and a spreading zone. The criterion for this classification was also provided. The rapid gas expansion caused by the fast reactions plays a significant role in forming the particle stream into these three zones. It accelerates the particles in the centre of the gasifier while pushing the particles near the expansion edge into the gas recirculation. Also, the concentrated oxygen distribution in the gasifier results in the formation of high- and low-temperature regions. The particles in the fast-flowing zone flow directly through the high-temperature region and most of these particles in this zone were fully reacted with a short residence time. Since particles in the recirculation zone are in a relatively low-temperature region, most of these particles are not fully gasified, although with a long residence time. The rest of particles in the spreading zone show moderate properties between the above two zones.

Keywords: CPFD simulation, entrained-flow gasifier, particle behaviour, gasification process

Introduction

Entrained-flow gasification is most widely used in the coal chemical industry. The gasifier can process a large volume of coal at high temperature with high gasification efficiency [1]. However, the hydrodynamics and reactions in the entrained-flow gasifier are quite complex and their mechanisms still are not fully understood. This limits the further optimization of gasifier design. A further investigation
into their mechanisms is of importance. While the characteristics of the hydrodynamics and reactions in the gasifier are difficult to obtain using experimental tests, simulation using computational fluid dynamics is becoming an important tool to investigate these characteristics.

As one of the earliest entrained-flow gasifiers, the one-stage down-fired gasifier has been extensively studied. Wu et al. [2, 3] established a simulation model for a General Electric (GE) gasifier by using the simplified probability density function (PDF) model. The simulation results agree with the industrial data. Bi et al. [4] modelled a Gaskombinat Schwarze Pumpe (GSP) gasifier and obtained its flow field and gas composition by using the same model. Ma and Zitney [1] simulated both one-stage and two-stage gasifiers by using improved physical and chemical submodels. Chen et al. [5] developed a numerical method to predict coal gasification in an entrained-flow gasifier emphasizing the influence of the injection patterns. Vascellari et al. [6, 7] developed advanced submodels for both the pyrolysis process and char reactions. Their simulation results agree with the experimental data. Then, Richter [8] analysed the reacting particles in the entrained-flow gasifier based on their study. Abani and Ghoniem [9] captured the characteristics of the turbulence in a small entrained-flow gasifier through large eddy simulation. Kumar and Ghoniem [10, 11] established a multi-scale model for the entrained-flow gasifier then applied it in both the GE and Mitsubishi Heavy Industries (MHI) gasifiers to investigate the effect of the particle grinding size on carbon conversion [12].

Due to the complexity of the gasification reaction and the limitations of computational power, the geometric models for some of these studies [2–5] were often simplified to 2D or pseudo-3D model. In the pseudo-3D model, only half or one-quarter of the whole gasifier was modelled and a periodic boundary condition was applied. Also, most of these studies [2–5] were based on the steady-state simulation results. Several studies [2–4] assume that the homogeneous reactions in the gasifier are in a chemical equilibrium. Furthermore, the particle trajectories and overall particle properties were discussed in only a few previous studies [1, 8]. Little specific particle information, i.e. temperatures, carbon contents and locations for the discrete particles, was provided.

Recently, computational particle fluid dynamics (CPFD) was developed by Snider [13] and applied in simulations of gas–solid reactors. CPFD is one of the Discrete Element Methods (DEM) [14] based on the Euler-Lagrange model. Being different from the general DEM, CPFD combines the particles with the same properties into one particle parcel, i.e. one computational particle [13]. Also, multiphase particle-in-cell (MP-PIC) is used to simplify the particle–particle interactions in the CPFD model [13, 15]. These two features greatly improve the computing efficiency of CPFD simulation and enable it to model the 3D gas–solid reactors with numerous discrete particles. It has been successfully applied in investigating the gas–solid riser [16, 17] and downer [18, 19], where gas–solid behaviour is similar to that in an entrained-flow reactor. CPFD provides a new way to investigate the entrained-flow gasifier in a transient-state simulation. There are two publications [15, 20] concerning fluidized-bed gasification using CPFD simulation, but none about entrained-flow gasification has been reported. This study will investigate a full-size entrained-flow gasifier by using CPFD simulation. A model for the gasification will be established. Also, the comparison results of experiment and simulation will be shown. Most importantly, the specific particle information will be obtained and a classification of particles in the gasifier will be made based on their hydrodynamics.

### 1 Establishment of the simulation model

The entrained-flow gasifier simulated in this study is the same as the gasifier established by Brown et al. [21] in their experimental study. As shown in Fig. 1, its diameter is 200 mm and its length is 2.0 m. The symbols x and z in Fig. 1 indicate the radial and axial direction, respectively. The Utah Bituminous coal was used and its properties are shown in Table 1. A single burner was mounted at the top of the gasifier in the experiment with two channels, i.e. a primary channel in the centre and an annulus channel. Coal particles and oxygen were injected through the primary channel while the water vapor was injected in the annulus channel. The operating conditions and particle-feed composition are shown in Table 2 and the particle-size distribution for the coal particles is presented in Table 3.

A 3D geometric model (circular cylinder) was established in Solidworks software, then meshed using the mesh generator—a built-in module in Barracuda software. The mesh density in the centre of the gasifier was higher to match the complexity of the hydrodynamics and reactions in this area. Liang et al. [22] indicate that the impact of mesh density on the CPFD-simulation results is limited. The mesh number applied in this study was 15 372. In the CPFD simulation, the number of computational particles is controlled by a parameter named the ‘number density’ [23]. It was set to 200–2000 in most of the simulation cases. Since more computational particles are needed to simulate a dilute gas–solid reactor, the number density in this study was set to 10 000, which corresponds to an injection into the simulated gasifier of 5966 computational particles per second.

There are mainly two kinds of inlet boundary conditions (BCs) in CPFD simulation, i.e. flow BCs and injection BCs. The injection BCs can be used to simulate the injection effect of the nozzle with relatively coarser meshes. So, the primary channel used this kind of BC to save computing power. The initial speeds for both particles and gas were set to 20 m/s. A particle expansion angle of 40° was used. However, the actual expansion angle in the simulation is largely affected by the gas behaviour and it was finally
reshaped to ~20°, as shown in Fig. 4, at 1.018 s in this study. This angle is consistent with that in a down-fired gasifier study simulated by Wu et al. [3]. On the other hand, the annular channel was set with the flow BC, as its area is larger. Also, the annular channel was assumed to be square to reduce the number of Cartesian-coordinate-based meshes in the CPFD simulation, which can further improve the computing efficiency [24]. Besides, an atmospheric-pressure boundary was set at the bottom of the gasifier, where both gas and particles can leave via this exit.

2 The numerical model

2.1 The governing equations

The governing equations for the CPFD simulations are the general ones described by Snider et al. [13, 15].

2.2 Chemical reactions

2.2.1 The devolatilization model

The coal-devolatilization rate is very fast due to the high temperature in the gasifier [4, 9]. The expression for the coal devolatilization [25] is:

\[
\text{Coal} \rightarrow a_1 \text{CH}_x + a_2 \text{CO} + a_3 \text{CO}_2 + a_4 \text{H}_2 + a_5 \text{H}_2\text{O} + a_6 \text{N}_2 + a_7 \text{Char}
\]  

(1)

where \(a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7 = 1\).

Similarly to the simulation method of devolatilization used by Abani and Ghoniem [9], the inert gas during the devolatilization is neglected in this study and the gas products are assumed to be \(\text{CH}_x, \text{CO}, \text{CO}_2, \text{H}_2\) and \(\text{H}_2\text{O}\). A one-step model is used to describe the devolatilization rate [26]:

\[
\frac{dm_v}{dt} = -A_v \exp \left( \frac{E_v}{RT} \right) m_v
\]

(2)

where \(m_v\) is the remaining volatile mass in the particle and \(T\) is the weighted temperature [23] of the particle (0.8) and the gas (0.2). The activation energy, \(E_v\), is \(2.1 \times 10^6 \text{ s}^{-1}\) [2] and the pre-exponential factor, \(A_v\), is \(3.28 \times 10^7 \text{ J.kmol}^{-1}\) [2].

2.2.2 Heterogenous reaction model

After coal devolatilization, the particles mainly consist of char and ash. Three main heterogeneous reactions are used to describe the char reaction [9, 27]:

\[
\text{C} + 0.5\text{O}_2 \rightarrow \text{CO}
\]

(R1)
The studies by Wu et al. [2] and Bi et al. [4] show that the heterogeneous reaction rate is determined by both the intrinsic chemical rate and the diffusion rate. The expression for the heterogeneous reaction rate in this study is introduced from their studies, which is:

\[ R_i = \frac{R_{i,k}}{R_{i,d} + R_{i,k}} \]

where \( R_i \) is the heterogeneous reaction rate for the ith gas with the char particle and \( R_{i,d} \) is the diffusion rate, which can be described as

\[ R_{i,d} = C_i \left( \frac{(T_p + T_i)}{2} \right)^{0.75} \]  

where \( C_i \), the diffusion coefficient, is \( 5 \times 10^{-12} \) s.k m^{-0.75} in this study; \( T_p \) is the particle temperature; \( T_i \) is the gas temperature; and \( d_p \) is the particle diameter. \( R_{i,k} \) is the apparent reaction rate and can be described as

\[ R_{i,k} = A_i \exp \left( - \frac{E_i}{RT_p} \right) \left( \frac{P_i}{10^5} \right)^n \]

where \( n \) is the order of this reaction model; \( A_i \) is the pre-exponential factor; \( E_i \) is the activation energy; and \( P_i \) is the partial pressure for the ith gas. The values [2, 4] for every parameter in this model are listed in Table 4.

### 2.2.3 Homogeneous reactions

Based on the same simulation method of Abani and Ghoniem [9] as well as Anderson et al. [31], the hydrocarbons in this study are expressed as CH\(_4\) and the reaction rates of CH\(_2\) are adopted for CH\(_2\). Six main reactions are used to describe the homogeneous reactions in the gasification [27]:

\[
\begin{align*}
\text{C} + \text{CO}_2 &\rightarrow 2\text{CO} \quad (R2) \\
\text{C} + \text{H}_2\text{O} &\rightarrow \text{CO} + \text{H}_2 \quad (R3)
\end{align*}
\]

\[
\begin{align*}
\text{R1} &\rightarrow 300 \quad 1.3 \times 10^4 \quad 0.65 \\
\text{R2} &\rightarrow 2224 \quad 2.2 \times 10^4 \quad 0.6 \\
\text{R3} &\rightarrow 42.5 \quad 1.42 \times 10^4 \quad 0.4
\end{align*}
\]

Yan et al. [32] established a set of reaction models for the homogeneous reactions of gasification. The expressions of these models are concise, which is beneficial for the computation. These models were introduced for this study and their expressions are listed in Table 5.

### 2.3 The thermal model

The general CPFD thermal model [23] was employed in this study. This model includes the models for both gas–solid and gas–wall heat transfer. The expressions and their explanations are stated in the literature [23]. Also, the heat loss is considerable in the experiment [21] and must be included in the simulation. The wall temperature of the simulated gasifier was set as the same value (1100 K) tested by Brown et al. [21] using a thermocouple on the gasifier wall in their experiment [21]. Besides, the temperature of the wall adjacent to the primary channel was set to the same value as the feeding-particle temperature. Moreover, the built-in radiation model [23] in Barracuda was also applied in this study to further improve the simulation results.

### 2.4 The other models

The drag model used in this study was the Wenyu–Ergun correlation. Its expression is described in the literature [23]. Besides, the model of large eddy simulation (LES) [36] was applied in this study. Its detailed description is stated in the literature [23].

### 3 Simulation results

#### 3.1 Validation of the simulated results

Table 6 shows the comparison between the CPFD-simulation results and the experimental results of Brown et al. [21]. All of the simulation and experimental results were obtained from the central area at a height of 0.23 m above the bottom of the gasifier. The simulation time was 4 s and the simulation results were averaged results in 4 s. As shown in Table 6, the simulation results agree with the experimental data, which validates the CPFD model established in this study.

#### 3.2 The distributions of gas temperature and velocity in the gasifier

Fig. 2a shows the averaged temperature (K) distribution in the simulated gasifier. As shown in Fig. 2a, there are

### Table 4: The values used for parameters of the heterogeneous reaction rates

| Reactions | \( A_i \) (kg.m\(^{-3}\).s\(^{-1}\).Pa\(^{-n}\)) | \( E_i \) (J.kmol\(^{-1}\)) | \( n \) |
|-----------|---------------------------------|-----------------|-----|
| R1 [28]   | 300                             | 1.3 \times 10^4 | 0.65|
| R2 [29]   | 2224                            | 2.2 \times 10^4 | 0.6 |
| R3 [30]   | 42.5                            | 1.42 \times 10^4 | 0.4 |

### Table 5: The expressions for homogeneous reaction rates

| Reactions | Reaction rate (kmol.m\(^{-3}\).s\(^{-1}\)) |
|-----------|------------------------------------------|
| R4 [33]   | \( 1 \times 10^{10} \exp (-15154.25/T_g) \) C\(_{CO2}\)C\(_{CH4}\)C\(_{H2O}\)C\(_{O2}\) |
| R5 [33]   | \( 2.2 \times 10^6 \exp (-13109.63/T_g) \) C\(_{CH4}\)C\(_{O2}\) |
| R6 [34]   | \( 2.119 \times 10^{11} \exp (-24379.1/T_g) \) C\(_{CO2}\)C\(_{CH4}\)C\(_{H2O}\) |
| R7 [35]   | \( 2.5 \times 10^6 \exp (-16597.5/T_g) \) C\(_{CO2}\)C\(_{H2O}\) |
| R8 [35]   | \( 9.43 \times 10^5 \exp (-20563.51/T_g) \) C\(_{CO2}\)C\(_{H2O}\) |
| R9 [25]   | \( 0.312 \exp (-30000/(1.987T_g^2)) \) C\(_{CH4}\) |
two distinct temperature regions in the gasifier: a high-temperature region in the upper half of the central gasifier (red area) and a lower-temperature region near the wall. The general temperature difference for these two regions is more than 1000 K. Fig. 2b shows the averaged gas-velocity (m/s) distribution. As shown in Fig. 2b, there is gas recirculation near the wall at the top of the gasifier. Meanwhile, the central gas gradually turns into the plug flow as it flows downward in the gasifier. These results agree with the reports in the literature [4, 27].

As clearly shown in the amplified picture for Fig. 2b, there exists a rapid gas expansion in the simulated gasifier caused by the fast reactions, where the gas temperature increases sharply from 450 K to >3000 K. The gas expands in both radial and axial directions, with its down-flowing direction being the most prominent. The central gas speed in this expansion is almost four times that on the edge of the expansion. This largely reshapes the particle behaviour in the gasifier and will be discussed in Section 4.4.

Fig. 2c shows the averaged oxygen mole fraction distribution in the simulated gasifier. The oxygen is highly concentrated beneath the burner and is consumed quickly by the fierce oxidation reactions. This forms the high-temperature region shown in Fig. 2a. In other words, the

Table 6: The data comparison between simulation and experiment

| Data       | CO (mol %) | CO₂ (mol %) | H₂O (mol %) | H₂ (mol %) | Carbon conversion % | Outlet gas temperature [K] |
|------------|------------|-------------|-------------|------------|---------------------|---------------------------|
| Simulation | 34.1       | 12.4        | 28.7        | 15.3       | 82.3                | 1453.2                    |
| Experiment [21] | 34        | 16          | 28          | 17         | 82                  | 1350–1400                 |
concentrated oxygen distribution results in the formation of the high- and low-temperature regions discussed above. The high-temperature region can be seen as an excellent reaction area, with a sufficient gas reactant of oxygen and particles flowing through this region to be consumed rapidly. This will be further illustrated in Sections 4.3–4.5.

3.3 The distributions of particle temperature, speed, residence time and carbon content

Fig. 3 shows the sectional views of the simulation results for particles at 4.0 s. As shown in Fig. 3a, the particle-temperature distribution is similar to that for the gas shown in Fig. 2a. The particle temperatures in the central region are becoming lower with particles flowing downward. Meanwhile, the particles near the wall remain at relatively low temperatures (1100 K) as they reach a balance of heat transfer to the wall. The carbon conversion of the particles is highly related to the temperature and will be discussed later.

Fig. 3b and c show the particle residence time and speed distribution at 4.0 s, respectively. As shown in these two figures, the particles in the central region at the upper half gasifier have the lowest residence times due to the highest downward speed, whereas the particles in the wall region have longer residence times with low speed. The particle-residence times are especially longer for particles entrained by the gas recirculation, as they first flow upward then downward with speeds below 5 m.s⁻¹. These results can further illustrate the particle carbon-content distribution shown in Fig. 3d.

Fig. 3d shows the particle carbon content (mass fraction) in the simulated gasifier. As shown in Fig. 3d, the volatile matter was quickly released from the particles. Also, the particle carbon contents are generally lower in the central region and higher in the wall region. The particles in the central region have shorter residence time, but their conversion is higher. This indicates that a long particle-residence time may not always result in a good particle
carbon conversion. The influence of the particle temperature and the gas-reactant distribution should also be included. For a one-stage down-fired gasifier, the particles in the central region have more opportunities to achieve a higher conversion, as they are not only exposed to a high temperature, but also get easier access to the gas reactants like oxygen. The detailed particle-reaction process will be discussed later by injecting particle tracers.

3.4 The detailed particle-reaction process
The detailed particle-reaction process was investigated by particle tracers. Since the gas–solid flow in the gasifier was steady after a simulation time of 1.0 s, the feeding coal particles from simulation time 1.0 to 1.03 s were marked as particle tracers in this study. Note that only the particle identity was changed during this short period of time, while the particle properties and flow rate remained the same throughout the entire simulation. The following results were collected from the particle tracers.

Fig. 4 shows the distribution of carbon contents (mass fraction) for particle tracers at different times. Note that only particle tracers can be seen in Fig. 4, which means that all the other feeding coal particles coexisting in the gasifier were hidden for an easier observation. As shown in Fig. 4, the particle tracers were first centrally injected from the top of the gasifier then \( t = 1.044 \) s distributed as an inverted-cone similar to the gas distribution shown in Fig. 2b. As shown in Fig. 4, at 1.080 s, the axial particle speeds in the central region are much faster than in the other regions. Meanwhile, the particles closer to the gasifier wall are turning back and flowing upward after 1.044 s, entrained by the gas recirculation shown in Fig. 2b. This indicates that the particle tracers quickly spread in both axial and radial directions due to the rapid gas expansion caused by the fast reactions shown in Fig. 2b. This rapid gas expansion is the driving force to push one portion of the particles into the gas recirculation and keep another portion of the particles with a high down-flowing speed. Also, the carbon contents for particles, flowing directly through the high-temperature region, are nearly zero, while the carbon contents for particles closer to the wall are still nearly 80%.

On the other hand, a schematic of the general route for the particles entrained by the gas recirculation is summarized from the simulation results and is shown in Fig. 5. Note that the particle paths shown in Fig. 5 are in a sequential order denoted with numbers from 1 to 5. As shown in Fig. 5, the recirculated particles cannot enter the high-temperature region although they flowed through its edge. This is because their particle speeds are too small (0.9 m·s⁻¹).
shown in Fig. 4 at \( t = 1.518 \) s) while the edge of the central gas speed shown in Fig. 2b is about 10 m s\(^{-1}\). These particles instantly flow downward as soon as they approach the edge of the central gas. As a result, no radial momentum is left for them to enter the central high-temperature region; instead, they flow downward along the edge of the central gas. Afterwards, they are pushed towards the wall surface, driven by the gas expansion, and then flow downward along the wall surface with a temperature of only 1100 K, through the rest of their lifetimes in the simulated gasifier. Consequently, they have the longest particle-residence times but the lowest carbon conversions.

### 3.5 The probability distribution of the particle-residence time

Fig. 6 shows the residence-time probability distribution of the particle tracers by counting the particle numbers in every interval of 0.2 s at the gasifier outlet. As shown in Fig. 6, a considerable number (13%) of particle tracers flew out of the gasifier during 0.4–0.6 s, forming a shortcut particle flow. This result, combined with the results shown in Fig. 4 at 1.518 s, indicates that the shortcut particle flow mainly consists of the fully reacted particles from the central region, whose speeds are much faster due to their much smaller particle masses and the acceleration of the gas expansion.

The ‘long tail’ after 2.0 s shown in Fig. 6 mainly consists of the particles entrained by the gas recirculation, whose flowing route is much longer. However, their conversion is low, since their route provides little access to the high-temperature region. These particles account for 14.8% of all the particles in the gasifier. Besides, the other particles that gradually spread around the entire gasifier contribute to the probability distribution during 0.6–2 s shown in Fig. 6. These particles are the majority, which flow downward with a relatively slow speed and a moderate conversion.
Based on the analysis above, the particles in the gasifier can be classified into three zones: a fast-flowing zone, a recirculation zone and a spreading zone. Fig. 7 shows the schematic of these three zones for particles in the simulated gasifier. The particle distribution in Fig. 7 is based on the results shown in Fig. 4 at 1.198 s. As shown in Fig. 7, the particles with upward axial speed are colored in pink and this is also the criterion for the particles of the recirculation zone. Its corresponding residence-time range is 2.0–3.0 s shown in Fig. 6. On the other hand, based on the first and distinct peak value shown in Fig. 6 (0.4–0.6 s), the fast-flowing zone can be identified and denoted in Fig. 7. Besides, the rest of the particles in the gasifier can be classified as the spread zone (0.6–2.0 s shown in Fig. 6).

4 Conclusion

A CPFD-simulation model for entrained-flow gasification was established in this study. The simulation results agree with the experimental data. The detailed particle information was obtained. The results show that the particles in the gasifier can be classified into three zones, i.e. a fast-flowing zone, a recirculation zone and a spreading zone. The criterion for this classification was also provided. The gas expansion plays a significant role in forming the particle stream into these three zones. It accelerates the axial speed of particles in the centre of the gasifier while it pushes another portion of particles into the gas recirculation.

Also, the concentrated oxygen distribution in the gasifier results in the formation of high- and low-temperature regions, and particles flowing through the high-temperature region will have sufficient time to react with the oxygen. Particles in the fast-flowing zone flow directly through the high-temperature region with a high speed. Most of the particles in this zone are fully reacted, although their residence times are very short. While particles in the recirculation part have little access to the high-temperature region and most of the particles in this zone still have high carbon content, their residence times are very long. The particles in the spreading zone gradually spread throughout the entire gasifier with a moderate residence time, temperature and carbon conversion.

The detailed particle behaviour obtained in this study can deeppen our understanding of the complex reaction process in the gasifier and provide a scientific basis for better gasifier design. Usually, the geometrical model of a simulated gasifier needs to be simplified due to the computing-power constraint. However, some of the non-symmetrically shaped gasifiers are not suitable to be simplified as half-size or 2D geometries. So, CPFD provides a promising way to simulate those gasifiers with complicated geometries.

Nomenclature

| Symbol | Description |
|--------|-------------|
| $A_i$  | Pre-exponential factor $kg.m^{-2}.s^{-1}.Pa^{-n}$ |
| $A_n$  | Pre-exponential factor for coal devolatilization $J.kmol^{-1}$ |
| $a$    | Mass fraction |
| $C_i$  | The diffusion coefficient, $s.k^{-0.75}$ |
| $d_p$  | Particle diameter, $m$ |
| $E_i$  | Activation energy, $J.kmol^{-1}$ |
| $E_c$  | Activation energy for coal devolatilization, $s^{-1}$ |
| $m_r$  | The remaining volatile mass in the particle, $kg$ |
| $n$    | Order of reaction |
| $R$    | Heterogenous reaction rate for the $i$th gas, $kg.m^{-2}.s^{-1}$ |
| $P$    | Partial pressure for the $i$th gas, $Pa$ |
| $T$    | Weighted temperature, $K$ |
| $T_f$  | Fluid temperature, $K$ |
| $T_r$  | Particle temperature, $K$ |
| $t$    | Time, $s$ |

Conflict of Interest

None declared.

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