Numerical Simulation on the Effect of Burner Bias Angles on the Performance of a Two-Stage Entrained-Flow Gasifier

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ABSTRACT: A 2000 t/day HNCERI (Huaneng Clean Energy Research Institute) entrained-flow pulverized coal gasifier suffers from the problem of a high ash–slag ratio. An appropriate bias angle of the burners is the key to solve this issue for the gasifier with a specific structure. A random pore model considering bulk and pore diffusion effects was extended by user-defined function to describe the gasification reactions. The simulation of the gas flow and char gasification characteristics under different bias angles (0, 1.5, 2.5, 3.5, and 4.5°) of the four burners in the first stage was conducted. The simulation results showed favorable agreement with the industrial data. The evaporation, devolatilization, and char oxidation mainly occurred in the first-stage jet zone, and the upflow and downflow zones are dominated by the gasification reactions. The bias angles of the burners mainly affect the scale of gasification reaction zones. As the bias angles increased from 0 to 4.5°, the gas temperature at the slag tap hole decreased from 1880 to 1500 K. The carbon conversion efficiency of the first stage decreases and that of the second stage increases with the bias angle increasing. An optimal bias angle of 2.5° is recommended for the HNCERI gasifier with a total carbon conversion efficiency of 98.16%.

1. INTRODUCTION

The entrained-flow coal gasification technology can realize the cleanest and most efficient utilization of coal by converting the entire non-ash fraction in coal into clean syngas, which can be used for chemical production and power generation.1 It has the advantages of large processing capacity, high carbon conversion, tar-free products in syngas, and wide adaptability for coals.2,3 Integrated gasification combined cycle (IGCC) power generation is commonly treated as one of the most extensive and important applications of the entrained-flow gasification technology. It can integrate the advantages of the chemical industry and the power industry to achieve clean coal-fired power generation. As the plan for carbon neutrality is put forward by the Chinese government, the coal gasification technology draws more attention due to its convenient and efficient implementation of CO₂ capture.4 HNCERI has established an advanced two-stage pressurized entrained-flow gasifier in Tianjin, which acts as one key part of China’s first IGCC power generation system and has been operated stably since 2012.5 The processing capacity of this gasifier has reached 2000 t/day with a high carbon conversion rate of 98.9% and a cold syngas efficiency of 83.2%. Moreover, the precombustion CO₂ capture technology has been successfully implemented in this system, which has achieved a CO₂ capture rate of over 90% and a capacity of 100,000 tons/year.

In the first stage of the HNCERI gasifier, four burners are operated at the impinging mode. However, a high ash–slag ratio induced by such a pattern easily shortens the service life of the ceramic filter in the syngas purification process. The
emission of fly ash also puts tremendous pressure on the environment, which needs to be urgently resolved. Altering the bias angles of the four burners would promote the formation of a swirling-flow field, which generates a centrifugal force accelerating the movement of coal particles toward the wall.\textsuperscript{6,7} Under swirling-flow conditions, more particles are trapped easily by the molten slag wall in the first stage. However, an appropriate bias angle of the burners in the HNCERI gasifier is still a big technical challenge. It has to be noted that the variation of bias angles of four diametrically opposed burners will change the fields of the temperature, velocity vector, and particle concentration as well as the controlling mechanisms of the gasification reactions in different regions of the gasifier. It is well-known that the temperature distribution significantly affects the thickness and flow characteristics of the slag, which is crucial to the safe operation of the gasifier.\textsuperscript{8–11} Therefore, it is necessary to study the effect of the bias angles of the four burners installed in the first stage on the gasifier performance. During the actual process, more detailed information cannot be achieved because of the high operating pressure and temperature easily causing the explosion and leakage of the combustible gas when opening holes on the wall.\textsuperscript{12} CFD (computational fluid dynamics) simulation methods as one of the most popular tools provide a great possibility for studying the effect of different factors and predicting the retrofitting effectiveness for industrial gasifiers. On the other hand, it also has the advantages of low cost and high flexibility.

Many researchers have proven that the swirl number of the burner of a gasifier has a significant influence on the gasification performance and equipment failure. Xu et al.\textsuperscript{13} recommended that the swirl number of the burner of a GSP gasifier should be between 0.66 and 0.9 in consideration of the membrane safety. A similar result on the swirl number was also obtained by Bi et al.\textsuperscript{14} Chen et al.\textsuperscript{6} found that the adhesion behavior of molten slag was mainly controlled by the swirl ratios of burners and the throat diameter in a 200 t/day two-stage air-blown gasifier. Cao et al.\textsuperscript{15} confirmed that the optimal bias angle of the burners was $5.0 \times (\pi/180)$ rad for a Shell gasifier. Refractory failure in a multinozzle OMB (opposed multiburner) gasifier was systematically studied by Gong et al.\textsuperscript{16} through numerical simulation methods. For the HNCERI gasifier, Peralta et al.\textsuperscript{17} and Wang et al.\textsuperscript{18} used a high-pressure wire-mesh reactor and a thermogravimetric analyzer to study the pyrolysis and gasification reactivity of coal, which is used in the HNCERI gasifier. Ren et al.\textsuperscript{19} and Li et al.\textsuperscript{20} studied the gasification performance under different operational conditions including varying gasifying agent concentrations, coal input rates, and single- and two-stage operational modes. Zhang et al.\textsuperscript{21} used CFD coupled with the reduced order model (ROM) approach to analyze the pollutant emission of the HNCERI gasifier. The above studies on the HNCERI gasifier mainly focus on the basis of the existing four-burner impinging flow field structure. However, the study on the burner bias angles influencing the performance of a two-stage dry-powder pressurized pure oxygen gasifier is still rare.

Figure 1. (a–d) Schematic diagram of the HNCERI gasifier.
The main objective of this work is to comprehensively study the gas–solid flow, the reaction behavior, and detailed information inside the HNCERI gasifier. Also, the influence of bias angles of the four burners in the first stage of the HNCERI gasifier on the fields of the temperature, species, velocity, particle concentration, and the controlling mechanisms of the gasification reactions in different regions is analyzed. The aim is to formulate a control strategy for the high ratio of ash–slag in the HNCERI gasifier by adopting rotation of the bias angles of the burners. Furthermore, the present work can also provide some guidance for the new design of gasifiers and a reliable theoretical basis for the subsequent transformation of the gasifier to solve the existing problems.

2. MODEL FORMULATION AND SIMULATION SETTINGS

2.1. Physical Model of the HNCERI Gasifier. Figure 1 presents the schematic diagram of the HNCERI two-stage pressurized entrained-flow gasifier. The lower cylindrical chamber is a combustor (in the first stage), and the upper chamber is a reductor (in the second stage), as shown in Figure 1a. There are four diametrically opposed burners (α = 0°) installed at the same height of the side wall of the lower combustor, and two opposite burners are installed at the bottom of the reductor chamber, as shown in Figure 1b,c. As shown in Figure 1d, each burner has a central channel and an annulus channel.

2.2. Simulation Settings. When the gasifier is operating on the existing four-burner impinging mode, the ash–slag ratio, which is the ratio of the mass of fly ash taken away by the syngas at the upper outlet of the gasifier to the mass of the liquid slag flowing out of the slag tap hole at the bottom of the gasifier, is about 2–2.2. In order to reduce the fly ash in the syngas and the burden of the purification process, the bias angles of the four burners in the combustor were adjusted from α = 0° to α = 1.5°, as shown in Figure 1. During the operation under this condition, the ash–slag ratio reduced to 1–1.2, which greatly reduces the burden of the subsequent purification process. However, the temperature field, particle trajectory, and main reaction zone distribution in the gasifier will also change with the burners’ bias angle increasing. A better understanding of the laws of these changes is crucial to the next transformation of the gasifier and the design of new gasifiers. In this study, the changes in the temperature and gasification performance of the gasifier after increasing the bias angle to 1.5° were investigated. Moreover, the bias angles were adjusted from 2.5 to 4.5° with an interval of 1° to further study the effect of the burners’ bias angles on the gasifier performance to provide guidance for the future transformation of the gasifier.

Based on the above, five cases were considered, as shown in Table 1. Case 1 (base case) is the verification of the numerical simulation method representing the original design condition. The properties of coal are given in Table 2. The distribution of coal particle diameters is shown in Table 3. During pulverized coal gasification, the conventional pulverized coal diameter is 70 μm, when the diameter smaller than 40 μm is considered to be micropulverized coal.22 It can be found that 65.9% of pulverized coal used in the HNCERI gasifier has a diameter of smaller than 35 μm, which reaches the standard of micro-pulverized coal.

2.3. Temperature of Critical Viscosity. The temperature of critical viscosity (Tcv) that is a key parameter for the normal operation of the gasifier represents the slag flowability in relation to the syngas temperature. It is considered as a key characteristic that affects the behavior of liquid slag on the gasifier wall.23 The critical viscosity varies depending on the coal types, but the typical value of 25 Pa s is widely used.24 A high-temperature rotational viscometer for the RV DVIII system (Theta Industries, Port Washington, NY) was used to measure the viscosity of coal slag, and the relationship between viscosity and temperature is shown in Figure 2. Therefore, the typical value of 25 Pa s is used to define Tcv, which is 1583 K in this study. Generally, the operating temperature of the gasifier should be higher than Tcv, about 50–150 K. It is important to keep the temperature at the slag hole within a certain value because the flow characteristics of the slag near the slag hole are very sensitive to the temperature range. In this study, 1683 K is selected as the standard temperature for safe slag discharge at the slag tap hole of the gasifier.

3. NUMERICAL SIMULATION METHODS

During the coal gasification process, a series of complicated physical and chemical processes almost simultaneously occur,

| items               | unit | case 1 | case 2 | case 3 | case 4 | case 5 |
|---------------------|------|--------|--------|--------|--------|--------|
| bias angle          | °    | 0      | 1.5    | 2.5    | 3.5    | 4.5    |
| combustor coal      | kg/h | 58,802 | 58,802 | 58,802 | 58,802 | 58,802 |
| combustor oxygen    | kg/h | 51,030 | 51,030 | 51,030 | 51,030 | 51,030 |
| combustor steam     | kg/h | 1975   | 1975   | 1975   | 1975   | 1975   |
| reductor coal       | kg/h | 3817   | 3817   | 3817   | 3817   | 3817   |
| reductor steam      | kg/h | 590    | 590    | 590    | 590    | 590    |
| reactor pressure    | MPa  | 3.0    | 3.0    | 3.0    | 3.0    | 3.0    |

| proximate analysis (wt %, ad) | ultimate analysis (wt %, ad) | LHV (MJ/kg) |
|------------------------------|------------------------------|-------------|
| moisture                     | ash                          | volatile    | fixed carbon | C | H | O | N | S | LHV (MJ/kg) |
| 1.2                          | 13                           | 31.2        | 54.6         | 69.1 | 4.1 | 11.2 | 0.8 | 0.6 | 25.6         |

Table 2. Chemical Compositions of Coal

Table 3. The Distribution of Coal Particle Diameters

| min/max diameters (μm) | 0/5 | 5/10 | 10/35 | 35/45 | 45/70 | 70/90 | >90 |
|------------------------|-----|------|-------|-------|-------|-------|-----|
| mass fraction (%)      | 12.1| 11.8 | 32.8  | 9.2   | 17.8  | 8.4   | 8.0 |
3.2. Homogeneous Reactions. The chemical reactions of the gas phase usually take place in a turbulent flow. Therefore, the chemistry–turbulence interactions require special considerations in modeling the entrained-flow gasification. In this study, the finite-rate/eddy-dissipation model is used to calculate the chemical reaction rate. In this approach, the Arrhenius rate calculated by the finite-rate model and the mixing rate calculated by the eddy-dissipation model are compared, and the smaller one is adopted. Thirteen homogeneous reactions shown in Table 4 are considered, and the net source of species is due to the reaction is calculated by the sum of the Arrhenius reaction sources over reactions that the species participate in:

\[
R_i = M_{w,i} \sum_{r=1}^{N} \Gamma(v_{r}^m - v_{r}^e) \left( k_{f,i} \prod_{j=1}^{N} \left[ C_{r,j} Y_{p,j}^{v_{j}^m} + v_{j}^e \right] \right)
\]  

(6)

The kinetic reaction rate constant is defined as follows:

\[
k_{j,r} = A \tau^\delta \exp(-E/RT)
\]  

(7)

With the eddy-dissipation model, the net rate of production of species is due to reaction is calculated by the following two expressions, and the smaller one is used.

\[
R_{i,r} = v_{p}^e M_{w,i} A_{eddy} \beta \epsilon \frac{\sum_{p} Y_{p}^{v_{p}^e} M_{w,p}^{v_{p}^m}}{k \sum_{j} v_{j}^{v_{j}^m} M_{w,j}^{v_{j}^e}}
\]  

(8)

\[
R_{i,r} = v_{p}^e M_{w,i} A_{eddy} \beta \epsilon \frac{\sum_{p} Y_{p}^{v_{p}^e} M_{w,p}^{v_{p}^m}}{k \sum_{j} v_{j}^{v_{j}^m} M_{w,j}^{v_{j}^e}}
\]  

(9)

3.3. Heterogeneous Reactions. The char coal pore structure changes during the release of volatile components and the coal gasification. In this work, the multiphase surface reaction model is adopted to describe the reaction rates of char combustion (R14) and gasification (R15 and R16). The random pore model, which considers the char gasification on the internal surfaces of the char coupled with an effectiveness factor, is used to improve the char gasification model. The kinetic parameters of heterogeneous reactions are listed in Table 5. The gasification reaction rate equation for each gasifying agent in the random pore model is given as follows:

Table 4. Homogeneous Reactions

| homogeneous reactions | \( A_i \) (kg/m²-s·Pa) | \( E_i \) (J/mol) |
|-----------------------|-----------------|-----------------|
| R1 vol + 0.08C,H₄ + 0.67CO + 1.657H₂ + 0.02745N₂ + 0.0179H₂S | 4.26 \times 10^6 | 1.08 \times 10^8 |
| R2 vol + 1.2135SO₂ + 1.16CO + 1.9371H₂O + 0.02745N₂ + 0.0179H₂S | 9.2 \times 10^6 | 8.02 \times 10^7 |
| R3 C₇H₈ + 9O₂ → 7CO₂ + 4H₂O | 1.6 \times 10^6 | 1.26 \times 10^8 |
| R4 C₇H₈ + H₂ → C₇H₆ + CH₄ | 1.04 \times 10^7 | 2.47 \times 10^8 |
| R5 CO + 0.5O₂ → CO₂ | 2.24 \times 10^7 | 1.67 \times 10^8 |
| R6 H₂ + 0.5O₂ → H₂O | 6.8 \times 10^{13} (β = 1) | 1.68 \times 10^8 |
| R7 CH₄ + 0.5O₂ → 2H₂ + CO | 4.4 \times 10^{13} | 1.25 \times 10^8 |
| R8 CO + H₂O → CO₂ + H₂ | 2.75 \times 10^{10} | 8.37 \times 10^7 |
| R9 CO₂ + H₂ → CO + H₂O | 2.2 \times 10^7 | 1.98 \times 10^8 |
| R10 CH₄ + H₂O → CO + 3H₂ | 3 \times 10^8 | 1.25 \times 10^8 |
| R11 C₇H₈ + 7.5O₂ → 6CO₂ + 3H₂O | 1.13 \times 10^9 | 1.26 \times 10^8 |
| R12 C₇H₈ + 6H₂O → 6CO + 9H₂ | 3.0 \times 10^8 | 1.26 \times 10^8 |
| R13 C₇H₈ + 3O₂ → 6CO + 3H₂ | 1.58 \times 10^{15} | 2.21 \times 10^8 |
Table 5. Heterogeneous Reactions

| reactions          | \(n_i\) | \(\psi_i\) | \(A_i\) | \(E_{p,i}\) (J/mol) |
|-------------------|--------|--------|--------|------------------|
| R14 \(\text{C} + 0.5\text{SO}_2 \rightarrow \text{CO}\) | 0.68   | 14     | 1.13 \(\times 10^7\) (1/\(P_a^{0.68}\)s) | 1.3 \(\times 10^4\) |
| R15 \(\text{C} + \text{CO}_2 \rightarrow 2\text{CO}\) | 0.54   | 3      | 6.27 \(\times 10^7\) (1/\(P_a^{0.64}\)s) | 2.83 \(\times 10^4\) |
| R16 \(\text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2\) | 0.64   | 3      | 4.18 \(\times 10^6\) (1/\(P_a^{0.64}\)s) | 2.52 \(\times 10^8\) |

\[
\frac{dm_{p,i}}{dt} = -m_{p,i}D_{eff,i}e^{-E_{p,i}/RT_{0}}(1 - x)
\times \sqrt{1 - \psi_i\ln(1 - x)}
\]

\[
\eta_i = \frac{3}{\phi_i} \left[ \frac{1}{\tanh \phi_i} - 1 \right]
\]

\[
\phi_i = \frac{d_{p,i}}{6} \left[ \frac{n_i + A_i e^{-\psi_i/R_{0}}(1 - x)\sqrt{1 - \psi_i\ln(1 - x)}RT_{0}P_{0}^{1/3}}{M_i\rho_{i}} \right]
\]

The model parameters are listed as follows: \(\tau = \frac{1}{\phi_i}\), \(D_{eff,i} = \frac{\theta}{\tau} \left[ \frac{1}{\phi_{i,0}} + \frac{1}{\phi_{i}} \right]^{-1}\), \(D_{KN,i} = 97.0\rho_{i} \tau_{i}^{0.5} \), \(D_{O,i} = \frac{T_{i}^{0.5}}{p_{i}(V_{i})^{0.5} + (V_{i})^{0.5}} \times 10^{-7}\), and \(\tau_{f} = \frac{2\rho_{f}^{0.5}}{S_{f}}\).

When the char gasification rate is controlled by a bulk diffusion limitation, the following expression is used:

\[
\frac{dm_{p,i}}{dt} = -2\pi d_{p,i}D_{O,i} \rho_{f} \frac{M_{c}}{\rho_{i} \sqrt{\phi_{i}} \tau_{f}}
\]

3.4. Model for Changing the Particle Sizes and Density. When the pulverized coal particles enter the gasifier, their size will undergo a series of complex changes such as swelling, breakage, and agglomeration. Zeng et al. found that the particle diameter will increase during devolatilization. Smith's research reported that the particle diameter decreases as the degree of coal particle burnout increases. After the process of devolatilization is completed, the particle size is considered to no longer change when the multiphase surface reaction model is used to calculate the gasification and combustion of char particles in Fluent. It is very complicated to simulate the breakage and agglomeration of coal particles. In this paper, the particle diameter and density changes during the gasification process are calculated by the empirical correlation equations obtained by Smith. The empirical correlation equations are shown as follows. As shown in Figure 4, the particle size and density are updated before and after the surface combustion model.

\[
\frac{d_{p}}{d_{p,0}} = \left( \frac{m_{p}}{m_{p,0}} \right)^{0.25}
\]

\[
\frac{\rho_{p}}{\rho_{p,0}} = \left( \frac{m_{p}}{m_{p,0}} \right)^{0.25}
\]

3.5. Grid Meshing and Other Boundary Conditions. The ANSYS ICEM (2014) was used to mesh the three-dimensional geometric model of the HNCERI gasifier. The detailed grid and the boundary conditions are shown in Figure 3. The hexahedral structured grid was used in this work. The maximum aspect ratio of the grid is controlled within 40 due to the large size of the gasifier. The grid near the burner was refined due to the large gradients of velocity in those regions, as shown in Figure 3 (A–A, B–B, and C).

The wall boundary condition of the particles in the first stage was set to “trap” to simulate the wall slagging model. After the unburned coal particle sticks to the slag film, it continues to burn out for some time, but the simulation proved that it is a little amount. Therefore, it is ignored in this simulation. The second stage of the gasifier was set to “reflect”. The thermal conditions of the wall were set as “convection” with an equivalent convective heat transfer coefficient of 169 W/m² K in the first stage and 121 W/m² K in the second stage, assuming a free stream temperature of 473 K. The internal emissivity of the refractory brick was set to be 0.6. The discrete ordinate (DO) radiation model coupled with the weighted-sum-of-gray-gases model (WSGGM) was adopted to calculate radiative heat transfer. The PRESTO scheme was adopted for the pressure discretization. The equations of the momentum, turbulence, species, energy, and radiation were solved by the second-order upwind scheme. All the equations of the heterogeneous reactions were extended via UDF into Fluent.

4. RESULTS AND DISCUSSION

4.1. Grid Independence. In this work, the grid numbers of 1,226,948, 1,623,820, and 2,264,076 were used to study the independence of the grid based on case 1. By comparing the gas temperature profile along the central axis of the gasifier under different grid numbers, the number of grids is independent of the simulation results when the number of grids exceeds 1,623,820. In consideration of the required calculating time, here the grid number of 1,623,820 is chosen for all the cases.

4.2. Reference Case. To verify the accuracy of the numerical models, the simulation results including the gas
composition and carbon conversion efficiency are compared with the industrial data. Fan et al.’s simulation results, which used a simplified PDF model to describe the interaction of turbulence and gas-phase chemical reactions, are also compared. As presented in Table 6, the predictions presented in this work show favorable agreement with the industrial data. Fan et al.’s simulation result represents the mole fraction of each component at the outlet of the gasifier under the thermodynamic equilibrium state. It can be seen from Table 4 that the gas components at the outlet of the gasifier have basically reached the thermodynamic equilibrium state.

|          | CO (%) | H₂ (%) | CO₂ (%) | CH₄ (ppm) | carbon conversion efficiency (%) |
|----------|--------|--------|---------|-----------|----------------------------------|
| industrial data | 57.52  | 23.93  | 3.32    | 820       | 99.42 97.73                     |
| our simulation  | 57.64  | 23.54  | 3.90    | 711       | 99.72 98.12                     |
| fan simulation  | 59.05  | 23.20  | 3.13    |           | 98.98                           |

Figure 4. Grid independence verification.

Table 6. Comparison of Simulation Results and Industrial Data

Figure 5 shows the velocity vector field on the center plane. As shown in Figure 5b, after flowing into the gasifier, the pulverized coal is entrained by the high-speed jets of the oxidant to expand and form the first-stage jet zone. The maximum velocity of the first-stage jet zone can reach above 90 m/s, while the velocity of the areas around the first-stage jet zones is less than 5 m/s. Such a large velocity gradient can continuously promote the formation of large eddies and then break them into small eddies around the edge regions of the jet. It promotes the high-temperature syngas (CO and H₂) and active radicals to be quickly entrained by the oxidant jet and oxidized by oxygen releasing a large amount of heat, which is beneficial to quickly heating the pulverized coal and promoting the gasification reactions. However, the high temperature near the burner would shorten the lifetime of the burner and may cause water leakage of the burner cover. The adverse pressure gradient formed by the jets promotes the formation of the up-recirculation zone and the down-recirculation zone above and below the burner plane, which can prolong the particles’ residence time with particles circulating in them. Four jets in the first stage collide with each other forming a first-stage impinging zone. The particles will oscillate back and forth in the first-stage impinging zone due to inertia, which would increase the residence time of the particles in the high-temperature reaction zone, thereby promoting carbon conversion. The gas flow after impinging flows up and down along the axial direction forming an upflow zone, which flows to the second stage, and a downflow zone, which flows to the bottom of the gasifier, respectively. The distribution of the upflow and downflow is trumpet-shaped. Figure 5c,d shows two jets forming two second-stage jet zones and one second-stage impinging zone. In the second stage, no recirculation zone is formed because the jet velocity is too small. The gas flows up to the outlet of the gasifier in the form of a plug flow. The second-stage reaction zone is very long, which can prolong the particles’ residence time to promote carbon conversion efficiency and cool the syngas.

The distributions of gas temperature and species mole fractions on the center plane are shown in Figure 6. It can be seen from Figure 6a that the gas temperature at the edge of the first-stage jet zone is the highest, which can reach more than 2200 K. The pulverized coal is heated rapidly and then undergoes the process of drying, devolatilization, and combustion reactions in the first-stage jet zone. The gas temperature in the impinging zone is lower than its surrounding area due to the high particle concentration resulting in more heat absorbed by gasification reactions.

Figure 5. (a–d) Velocity vector field on the center plane.
The upflow and downflow zones are also the high-temperature zones where the temperature is about 1900 K. Because the oxygen is consumed rapidly in the jet zone by the combustion reaction, the gasification reaction mainly occurs in the upflow and downflow zones, so the temperature drops quickly. As can be seen in Figure 6a, the high-temperature zone is large enough in the HNCERI gasifier, which would result in a fast gasification reaction rate promoting the carbon conversion. It is interesting that the gas temperature below the burner plane is higher than that above the burner plane. This is because the zones below the burner plane are a dead zone where high-temperature gas cannot flow out from the bottom outlet of the gasifier and circulates inside it. The temperature near the slag tap hole can reach to 1800 K, which is much higher than the $T_{cv}$ of the coal ash, which is beneficial to the slag discharge. It is shown in Figure 6b–d that the regions where the mole fractions of CO$_2$, H$_2$, and CO changed obviously are in first-stage jet, upflow and downflow zones and the second-stage jet zone, which also illustrates that the gasification reactions R15 and R16 are very strong. The mole fraction of CO$_2$ is high in the first-stage jet zone, which is mainly caused by the oxidation of CO. It can promote the reaction of C+CO$_2$ resulting in the rapid conversion of char. This will be analyzed below. In the second stage, the gas temperature significantly decreases from 1510 to 1100 °C after second-stage coal injection.$^{41}$

4.3. Influence of the Bias Angle. 4.3.1. Effect on the Velocity Vector. To explore the influence of the bias angle on the fields of the velocity vector, temperature, and particle concentration, the bias angles increasing from 1.5 to 4.5° with an interval of 1° are further studied. Figures 7 and 8 show the velocity vector distributions on the center plane of the first stage and the gas axial velocity distributions along the central axis under different bias angles, respectively. It can be seen from Figure 7 that the recirculation zones are formed both above and below the burner plane under all cases. With increasing bias angle from 1.5 to 4.5°, the size of the up-recirculation zone gradually decreases, which results in the particle circulation area decreasing, but the size of the down-recirculation zone almost remains unchanged. The radial velocity gradually increases around the impinging zone with the bias angle increasing. This may cause the high-temperature gas to flush the refractory brick wall directly. It is interesting that when the bias angle is higher than 3.5°, two new recirculation zones are formed near the slag tap hole due to the adverse pressure gradient, which are not conducive to the transport of the high-temperature gas to the slag tap hole. It can be seen from Figure 8 that the maximum axis velocity in upflow and downflow zones decreases from 22 to 5 m/s with

![Figure 6.](image1)

(a) Temperature (b) CO$_2$ (c) CO (d) H$_2$

Figure 6. (a–d) Temperature and species mole fraction distributions.

![Figure 7.](image2)

(a) $\alpha = 0^\circ$ (b) $\alpha = 1.5^\circ$ (c) $\alpha = 2.5^\circ$ (d) $\alpha = 3.5^\circ$ (e) $\alpha = 4.5^\circ$

Figure 7. (a–e) Effect of the gas velocity vector on the center plane.

![Figure 8.](image3)

Figure 8. Axial velocity along the central axis.
the bias angles increasing from 1.5 to 4.5°. This will reduce the drag force on particles in the axial direction resulting in more particles entrained to the bottom of the gasifier. In a word, as the bias angle increases, the axial gas velocity decreases in upflow and downflow zones resulting in axial mixing and transport capacity to become weaker, while the radial gas velocity increases near the impinging zone causing radial mixing and transport capacity to become stronger.

Figure 9. (a–e) Effect of the particle concentration on the center plane.

Figure 10. (a–e) Effect of the char concentration on the center plane.

Figure 11. (a–e) Effect of the characteristic timescale of large eddies.

4.3.2. Effect on the Particle and Char Concentration. Figures 9 and 10 show the distributions of the particle and char concentrations under different bias angles, respectively. The particle and char concentrations are evenly distributed above and below the burner plane when the bias angle is 0°. With increasing bias angle from 0 to 4.5°, the particle concentration gradually decreases above the burner plane and increases below the burner plane due to the change in the drag force
between the gas and particles. It can be seen from Figure 10 that the char consumption rate becomes slower below the burner plane and faster above the burner plane. The reason is that the increase in the particle concentration below the burner plane leads to an increase in the heat absorption by the gasification reaction. It would cause the decrease in gas temperature below the burner plane. The decrease in gas temperature would reduce the gasification reaction rate in turn.

It is interesting that the particle and char concentrations under the burner plane are distributed in the form of an inverted "V" when the bias angle is 4.5° due to the large bias angle resulting in the jet separation after impinging. It can be inferred that α = 4.5° is the critical angle for the separation of the particle concentration field.

4.3.3. Effect on Char Reactions. In an entrained-flow gasifier, gas–solid heterogeneous gasification reactions are very important to the performance of the gasifier. The gas–solid mixing is an important factor in gas–solid reactions. In general, the gas–solid mixing is controlled by the turbulent fluctuations, which can be considered in the continuous formation and breaking of eddies. In this work, the integral time of large eddies \( \tau_{\eta} \), which is defined as \( k/\varepsilon \), is used to evaluate the frequency of the turbulent fluctuations in the macroscale. The timescale of heterogeneous reactions, \( \tau_{c,i} \), is the period where the char concentration in the unit volume at a certain spatial position of the gasifier drops to \( 1/e \) of its original value. It is used to evaluate the characteristic timescale and reaction intensity for the \( i \)th heterogeneous reaction.\(^{42}\)

Figure 12. (a–e) Effect of \( \tau_{c,i} \) of R14.

Figure 13. (a–e) Effect of \( \tau_{c,i} \) of R15.

\(^{42}\) Figures 11–14 show \( \tau_{\eta} \) and \( \tau_{c,i} \) of R14–R16 on the center plane (\( y = 0 \text{ mm} \)) and the burner plane in the first stage of the gasifier under different bias angles, respectively. Figure 11 shows that the highest frequency of the turbulent fluctuations appears in the jet zone due to the high-speed jet of the oxidant. The frequencies of the turbulent fluctuations in the impinging, upflow, and downflow zones are also high due to the large gradient of the local velocity. It proves that there are the
strongest mixing processes in the jet, impinging, upflow, and downflow zones because $\tau_\eta$ is inversely proportional to the local stretch rate. The flow is steady in the zone near the wall, which can be proven by the low frequency of turbulent fluctuations. Figures 12−14 show that the zones with strong turbulent fluctuations are also the zones with strong gas−solid heterogeneous reactions. However, the combustion reaction R14 only occurs in first-stage jet zone due to the rapid consumption of O$_2$. It can be seen from Figures 11−14 that the magnitude of $\tau_\eta$ in the first-stage jet zone is about $10^{-2}$−$10^{-3}$, which is the same as the $\tau_\eta$ of R14−R16. This means that the macroscale turbulent fluctuations have a strong effect on heterogeneous reactions R14−R16 in the jet zone. This is not affected by the bias angles of the burners. In the impinging zone, the $\tau_\eta$ of R15 and R16 are larger due to the high char concentration and low temperature. In the upflow and downflow zones close to the burner plane, the magnitude of $\tau_\eta$ is $10^{-2}$−$10^{-1}$, which is the same as the $\tau_\eta$ of R15 and R16. It means that the macroscale turbulent fluctuations still have a strong effect on the heterogeneous gasification reactions. In other zones, the magnitude of $\tau_\eta$ is larger than $10^0$, and $\tau_\eta$ is about $10^{-1}$, which means that gasification reactions are very weak and the turbulent fluctuations have little effect on the heterogeneous gasification reactions. Thus, the regions in the gasifier can be divided into two regions: the flame regions and nonflame regions. In flame regions (the jet, upflow, downflow, and impinging zones), both the gas temperature and the velocity gradient are very high, and the mixing rate is strong. In nonflame regions (the zones near the wall), the fluctuations and mixing rate are weak, and the gasification reactions are slow. With increasing the bias angle from 0 to 4.5°, the strong turbulent fluctuation zones where the magnitude of $\tau_\eta$ is smaller than $10^{-1}$ gradually become bigger in the radial direction and smaller in the axial direction in upflow and downflow zones, as shown in Figure 11. Combining Figures 13 and 14, it can be inferred that the main gasification areas gradually approach to the burner plane with the increase in the bias angles. The reaction intensity of R15 and R16 becomes weaker near the slag tap hole with the bias angle increasing. Especially, when the bias angle of the burners is 4.5°, the gasification reaction $\tau_\eta$ is greater than 1 in a large area close to the slag tap hole. It means that the intensity of the gasification reaction in this area is very weak.

Figure 15 shows the value of $\ln(10^{-15} + S_m)^{42}$ on the center plane of the first stage. When coal particles are entrained into the gasifier, the processes of evaporation and devolatilization
occur in sequence near the burner regions. This makes the mass source yield a lot in the jet zones. These processes are not affected by increasing the bias angles of the burners because they have been completed before the impinging of four jets. Most of the mass sources yield in the regions of impinging, upflow, and downflow, which is mainly caused by the gasification reactions R15 and R16, as shown in Figures 13 and 14. The particle mass source is very low in the upper region of the first stage and the region near the wall. As shown in Figure 10, it can be inferred that most of the char is converted through the endothermic gasification reactions $C + CO_2$ and $C + H_2O \rightarrow CO + H_2$ in the regions of upflow and downflow.

4.3.4. Effect on Temperature Distribution. Figure 16 shows the gas temperature distributions of the first stage under different bias angles. In the regions of the jet, volatile components, CO, and H$_2$ are quickly mixed and reacted with O$_2$, making the gas temperature distribution similar. As the bias angle increases, the gas temperature below the burner plane gradually decreases and above the burner plane gradually increases. In particular, the decrease in the gas temperature near the slag tap hole is the most obvious. As discussed above, the increase in the bias angle causes the radial transport and mixing ability of the gas flow near the impinging zone to increase while the axial transport and mixing ability decrease, resulting in the high-temperature gas that cannot be transported to the bottom of the gasifier. At the same time, the particle concentration below the burner plane increases with the bias angle increasing, as shown in Figure 9, which means that the heat absorption by gasification reactions R15 and R16 increases. In general, the decrease in temperature near the slag tap hole is not conducive to the slag discharge. As can be seen in Figure 16a–c, the flame near the center line of the gasifier

**Figure 16.** (a–e) Gas temperature on the center plane under different bias angles.

**Figure 17.** (a–c) Gas temperature along the axial and radial directions of the gasifier.
formed by the four jets gathers together. As the bias angle increases to 3.5°, the flame in the upflow and downflow zones starts to separate. When $\alpha = 4.5^\circ$, the flame in the upflow and downflow zones has detached from each other and washed to the wall.

Figure 17 shows the gas temperature along the central axis of the gasifier and the radial temperature at the height of $z = 360$ mm and $z = 3870$ mm. As can be seen in Figure 17a, the distribution trend of temperature under different bias angles is similar to the base case. When the bias angle is 4.5°, the peak temperature in the central axis above the burner plane is much lower than those of other cases due to flame separation. This means that $\alpha = 4.5^\circ$ is the critical bias angle of the flame to separate. Comparing Figure 17a and b, it can be seen that the gas temperature at the slag tap hole ($z = 360$ mm) decreases from 1880 to 1500 K as the bias angle increases from 0 to 4.5°. It means that the temperature at the slag tap hole would decrease by approximately 95 K for increasing 1°. When the bias angle is 3.5°, the temperature at the slag tap hole is 1610 K, which is lower than 1683 K. This means that $\alpha \geq 2.5^\circ$ is inappropriate for the HNCERI gasifier under the current $O_2$/coal ratio. By the way, Figure 17c shows that the gas temperature near the wall increases as the bias angle increases. When $\alpha = 4.5^\circ$, the gas temperature near the wall increases to 1950 K, which may burn out the refractory bricks before the slag film is formed.

By increasing the $O_2$/coal ratio, the temperature near the slag hole can be increased, but the CGE (cold gas efficiency) will be decreased. It should be known that the bias angle of the Shell gasifier is 4.5°15,44 but the distance between the burner plane and the slag tap hole is smaller than that of the HNCERI gasifier. Therefore, on the premise of ensuring the performance of the gasifier and reducing the ash–slag ratio, it is important to select an appropriate bias angle to ensure the smooth slag discharge of the gasifier. In general, as the bias angle increases, more ash particles would be captured by the slag wall, so as to reduce the ash–slag ratio. To obtain an ideal ash–slag ratio and a suitable distribution of temperature, it is important to choose an appropriate bias angle and a suitable distance between the burner plane and the slag tap hole to discharge the slag smoothly when designing a new gasifier. It can be inferred that the larger the bias angles of the burners are, the smaller the distance between the slag tap hole and the burner plane should be.

4.3.5. Effect on Carbon Conversion. Figure 18 shows the effect of the bias angle on the carbon conversion, residence time, temperature, and wall heat loss of the gasifier. It can be seen from Figure 18 that the carbon conversion efficiency of the first stage decreases slightly as the bias angle increases from 0 to 3.5°. As the bias angle increases from 3.5 to 4.5°, the carbon conversion efficiency of the first stage significantly decreases from 99.5 to 98.99%. This is because the gasification rates of R15 and R16 near the slag tap hole gradually decrease with the increase in the bias angle. When the bias angle is 4.5°, the char concentration is still high and the gasification reaction rate is very slow near the bottom slope wall of the gasifier. The simulation result shows that the char particle with low carbon conversion is mainly captured by the bottom slope wall. The residence time of those particles under different bias angles is shown in Figure 18b. It can be seen that the residence time of those particles increases with the bias angle increasing.

Therefore, it can be inferred that the carbon conversion efficiency in the first stage is mainly controlled by the intrinsic gasification reaction rate. In fact, temperature is an important factor that affects the gasification process. As the temperature increases, the gasification reaction rate increases, which leads to a higher carbon conversion efficiency. However, if the temperature is too high, it may cause the slag to melt and then form a slag film, which will affect the gasification efficiency. Therefore, it is necessary to balance the temperature and the gasification reaction rate to achieve a good gasification efficiency.

By increasing the $O_2$/coal ratio, the temperature near the slag hole can be increased, but the CGE (cold gas efficiency) will be decreased. It should be known that the bias angle of the Shell gasifier is 4.5°, but the distance between the burner plane and the slag tap hole is smaller than that of the HNCERI gasifier. Therefore, on the premise of ensuring the performance of the gasifier and reducing the ash–slag ratio, it is important to select an appropriate bias angle to ensure the smooth slag discharge of the gasifier. In general, as the bias angle increases, more ash particles would be captured by the slag wall, so as to reduce the ash–slag ratio. To obtain an ideal ash–slag ratio and a suitable distribution of temperature, it is important to choose an appropriate bias angle and a suitable distance between the burner plane and the slag tap hole to discharge the slag smoothly when designing a new gasifier. It can be inferred that the larger the bias angles of the burners are, the smaller the distance between the slag tap hole and the burner plane should be.

4.3.5. Effect on Carbon Conversion. Figure 18 shows the effect of the bias angle on the carbon conversion, residence time, temperature, and wall heat loss of the gasifier. It can be seen from Figure 18 that the carbon conversion efficiency of the first stage decreases slightly as the bias angle increases from 0 to 3.5°. As the bias angle increases from 3.5 to 4.5°, the carbon conversion efficiency of the first stage significantly decreases from 99.5 to 98.99%. This is because the gasification rates of R15 and R16 near the slag tap hole gradually decrease with the increase in the bias angle. When the bias angle is 4.5°, the char concentration is still high and the gasification reaction rate is very slow near the bottom slope wall of the gasifier. The simulation result shows that the char particle with low carbon conversion is mainly captured by the bottom slope wall. The residence time of those particles under different bias angles is shown in Figure 18b. It can be seen that the residence time of those particles increases with the bias angle increasing.

Therefore, it can be inferred that the carbon conversion efficiency in the first stage is mainly controlled by the intrinsic gasification reaction rate. In fact, temperature is an important factor that affects the gasification process. As the temperature increases, the gasification reaction rate increases, which leads to a higher carbon conversion efficiency. However, if the temperature is too high, it may cause the slag to melt and then form a slag film, which will affect the gasification efficiency. Therefore, it is necessary to balance the temperature and the gasification reaction rate to achieve a good gasification efficiency.
factor affecting the gasification reaction rate. It is interesting that the carbon conversion efficiency of the second stage increases with the bias angle increasing, as shown in Figure 18a. It can be seen in Figure 18c that the gas temperature at the outlet of the first stage and the second stage increases with the bias angle increasing, which is conducive to improving the gasification reaction rate of the second stage. There are two main reasons for this. One is that the decrease in the carbon conversion efficiency in the first stage causes the heat absorption of the endothermic gasification reaction to decrease. The other is that as the bias angle increases, the inner wall average temperature of the first stage and the second stage decreases, which causes the heat loss through the wall to decrease, as shown in Figure 18d. It can be inferred that the carbon conversion efficiency of the second stage is sensitive to the gas temperature at the outlet of the first stage and the wall heat loss of the second stage. Increasing the outlet temperature of the first stage and reducing the heat loss of the second stage can increase the carbon conversion efficiency of the second stage. It can also be seen from Figure 18 that when the bias angle is 2.5°, the carbon conversion efficiencies of the first stage, the second stage, and the total are 99.54%, 76.79%, and 98.16%, respectively.

5. CONCLUSIONS

The gas–solid flow and reaction behavior in the HNCERI gasifier were comprehensively studied by CFD simulation. The influence of burners’ bias angles increasing from 0 to 4.5° with an interval of 1° on the fields of the velocity vector, temperature, particle concentration, and gasification reactions was systematically studied. The main conclusions are drawn as follows:

1. The main gas composition (CO and H₂) and carbon conversion efficiency obtained by CFD simulation well agreed with the industrial data. In the HNCERI gasifier, the evaporation, devolatilization, and char oxidation mainly occur in the first-stage jet zone, while the upflow and downflow zones are dominated by the endothermic gasification reactions.

2. With the bias angles increasing, the particle and char concentrations below the burner plane increase, which leads to the increase in heat absorption by gasification reactions. At the same time, the gas axial velocity in the upflow and downflow zones becomes smaller, which makes the transport of the high-temperature gas to the bottom of the gasifier more difficult. The above two reasons would well explain the decreasing trend of the gas temperature at the slag tap hole.

3. The effect of turbulent fluctuations on gasification reactions in the first-stage jet, upflow and downflow regions is stronger than that in other regions. The bias angles of the burners mainly affect the distribution of gasification reaction zones in the first stage but have little effect on the intensity of gasification reactions. Most of the particle mass sources yield in the regions of the jet by the processes of evaporation and devolatilization and in the regions of upflow and downflow by gasification reactions. With the bias angle increasing, the carbon conversion efficiency in the first stage decreases, while in the second stage, it increases.

4. When the bias angle is 2.5°, the carbon conversion efficiencies of the first stage, the second stage, and the total are 99.54%, 76.79%, and 98.16%, respectively. In consideration of guaranteeing the safety of the slag discharge and improving the carbon conversion efficiency, an optimal bias angle of 2.5° is recommended for the HNCERI gasifier.

5. When the bias angle increases to obtain a smaller ash–slag ratio, the distance between the burner plane and the slag tap hole should be decreased to ensure the stable discharge of the slag when designing a new gasifier.

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### Author Contributions

X.W. performed the methodology, investigation, and formal analysis and wrote the manuscript. S.X. performed the methodology and reviewed and edited the manuscript. Y.W. and H.T. performed the investigation and reviewed and edited the manuscript. G.L. performed the methodology and funding acquisition. X.L. and Y.R. acquired resources and reviewed and edited the manuscript. X.X. reviewed and edited the manuscript.

### Notes

The authors declare no competing financial interest.

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### NOMENCLATURE

- $A$: pre-exponential factor
- $A_{1}, A_{2}$: $2 \times 10^{4}, 1.3 \times 10^{5}$
- $A_{\text{eddys}} B_{\text{eddys}}$: 4.0, 0.5
- $A_{p}$: particle surface area
- $B_{m}$: spalling mass number
- $C_{j}$: molar concentration of $j$
- $d_{p}$: current particle diameter
- $d_{p,0}$: initial particle diameter
- $D_{\text{eff,ij}}$: effective diffusivity coefficient
- $D_{\text{KN,ij}}$: Knudsen diffusion coefficient
- $D_{\text{ij}}$: molecular diffusion coefficient
- $E$: activation energy.
- $E_{1,2}$: $1.05 \times 10^{5}, 1.67 \times 10^{8}$ J/kg mol
- $f_{w,0}$: mass fraction of the evaporating/boiling material
- $k_{i}$: mass transfer coefficient
- $k_{f,i}$: forward kinetic reaction rate constant
- $m_{p}$: current particle mass
- $m_{p,0}$: initial particle mass
- $m_{i}$: devolatilized mass
- $m_{a}$: ash mass
- $M_{i}$: molecular weight of species $i$
- $M_{\text{dev},ij}$: molecular weight of species $i$
- $N$: number of reactions
- $n$: reaction order
- $n_{i}$: constant
- $P$: pressure
- $R_{p}$, $R_{2}$: volatilization rates
- $S_{I}$: current surface area of char particles
- $S_{m}$: particle mass source term
- $t$: time
- $T$: gas temperature
- $T_{s}$: particle temperature
- $V_{i}$: binary diffusion volume
- $V_{\text{CO}}$: diffusion volume for CO
- $x$: total carbon conversion
- $Y_{p}$: mass fraction of product species
- $Y_{R}$: mass fraction of reactants
- $Y_{i}$: mass fraction of species $i$
- $\alpha_{i}$: constant
- $\beta$: temperature exponent
- $\beta_{1}, \beta_{2}$: yield factors
- $\theta$: porosity of the char particles
- $\rho_{s}$: gas density
- $\rho_{p}$, $\rho_{p,0}$: current particle density, initial particle density
- $I$: net effect of third bodies
- $k_{i}$, $\psi$: kinetic energy, dissipation rate
- $\eta_{i}$: effectiveness factor
- $\psi$: pore structure parameter
- $\phi$: Thiele modulus
- $\tau$: tortuosity of the pores
- $r_{p}$: mean pore radius
- $v_{p,1}$, $v_{p,1}$: stoichiometric coefficient of product $i$ and reactant $j$
- $\eta_{i,1}$, $\eta_{i,1}$: stoichiometric factor of each gasifying agent for each mole of carbon consumed

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