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Numerical Analysis for Coal Gasification Performance in a Lab-Scale Gasifier: Effects of the Wall Temperature and Oxygen/Coal Ratio

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Abstract: The optimization of multiple factors for gasification performance using a 3D CFD model with advanced sub-models for single-stage drop tube coal gasification was compared with experimental results. A single-stage down-drop gasifier with multiple coal injectors and a single oxygen injector at the top of the gasifier was investigated at different temperatures and O₂/coal ratios. A finite rate/eddy dissipation (FR/ED) model was employed to define the chemical reactions. Kinetic data for the various reactions were taken from previous work. The realizable k-ε turbulent model and Euler-Lagrangian framework were adopted to solve the turbulence equations and solid-gas interaction. First, various preliminary reactions were simulated to validate the reaction model with experimental data. Furthermore, various cases were simulated at various O/C ratios and wall temperatures to analyze the syngas species, temperature profile in the whole gasifier, exit temperature, carbon conversion, turbulent intensity, and velocity profile. The maximum CO was found to be 75.06% with an oxygen/coal ratio of 0.9 at 1800 °C. The minimum and maximum carbon conversions were found to be 97.5% and 99.8% at O/C 0.9 at 1200 °C and O/C 1.1 at 1800 °C, respectively.

Keywords: CFD simulation; coal gasification performance; single-stage entrained flow gasifier; carbon conversion



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1. Introduction

Coal gasification is one of the cleanest methods of coal utilization to produce syngas, electricity, and additional chemical products [1]. The enormous contribution of oil is helping to satisfy the rising demand for electricity over time. However, in the last few decades, scarcities of oil reservoirs and the accessibility of coal in China shifted the research toward the use of coal [2]. The maximum energy conversion into electricity can be achieved through gasification technology with minimal hazardous effects. The researchers' primary objective is to produce cutting-edge gasifiers with advanced performance and lower pollutant releases [3–6]. The efficient conversion of coal into gas has been widely investigated in terms of the chemical and physical variations that take place during the gasification process. Besides the experimental work, CFD simulation is a cost-effective approach used to investigate the different parameters, such as the rate of reaction, temperature distribution, oxygen and coal ratio, turbulent intensity, and residence time of the coal. However, CFD simulations of coal gasification require a different mathematical model to interpret the complex turbulence, temperature distribution, reaction rate, etc., to achieve valuable results.

Various researchers recently conducted CFD simulation research for an entrained flow coal gasifier [7–14]. Shaohua et al. [15] studied the numerical simulation of the co-gasification of mixing PET with coal in a fluidized bed and found that a larger particle size reduces heat transfer. Kim et al. [16] performed a numerical simulation for a 300 MW IGCC and found that a 0.7 oxygen/coal ratio is optimal for coal gasification. Diba et al. [17] studied the effect of calcination on coal gasification in fluidized bed furnaces. They found that a 17 kg/h airflow has the highest char conversion and the CO₂ composition increased

due to calcination. Some researchers investigated mixing gasification agents with syngas and measured the temperature up to 1550 °C using numerical methods [18]. Wang et al. [19] studied the numerical simulation for heat recovery from molten slug and syngas using the discrete-phase and solidification models. Some other researchers used the Euler–Euler method to elaborate the gas and solid flow [20,21], but some studies used Euler–Lagrangian methods to define the interaction of the gas–solid phase [9,22–24]. Generally, FR/ED and a probability density function (PDF) were used for the chemistry of the gasification reaction. Researchers used various gasification media, such as air/steam and air [25–27]. Some other researchers investigated different parameters through CFD simulation, such as particle size, nozzle design, and gasification reaction [12,28–32]. Imran et al. [33] investigated a two-stage coal gasifier for multi-opposite burners at different oxygen and coal ratios and the result revealed that hydrogen was up to 28%, and CO was 52%; furthermore, it was revealed that pure oxygen produced higher temperatures and maximum carbon conversion efficiencies.

This study used CFD simulations to investigate the influence of different O/C ratios and wall temperatures on parameters such as the temperature distribution, syngas composition, heat generation, and turbulence. First, we investigated different grid densities to determine the grid sensitivity. Having perceptually recognized the independence of the grid sensitivity, we analyzed the effect of the O/C ratio (0.9, 1.0, and 1.1) at different temperatures (1200 °C, 1500 °C, and 1800 °C).

2. Computational Model

2.1. Design and Mesh of the Gasifier

The schematic diagram of the lab-scale gasifier is shown in Figure 1. The height and internal diameter of the gasifier were 4.25 m and 0.3 m, respectively. Pulverized coal and oxygen were inserted into the top of the gasifier, oxygen was inserted into the top of the center, and coal was inserted through six consecutive injectors, as shown in Figure 2. The coal feeder rate was 75 kg/h from the top of the gasifier, and oxygen was injected at various rates. The gasifier was divided into two parts: a combustion zone (upper part) and a reduction zone (lower part). The alternate pattern of coal and oxygen was designed to allow for maximum oxygen utilization in the combustor region and produce a significant amount of heat. The gasifier was a down-drop reactor that consisted of syngas and slug released from the bottom of the furnace. The ultimate and proximate analysis of coal is listed in Table 1. The injection properties were set as a Rosin–Rammmler distribution that was appropriate for the particle size (max diameter: 125 µm, min diameter: 4 µm, and average diameter: 45.6 µm). The total amount of coal and oxygen was injected from the top of the gasifier. The CFD simulations were conducted using the Ansys Fluent platform.

Table 1. Proximate and ultimate analyses of coal samples.

Proximate Analysis (% ad)			FC	$Q_{\text{net,ad}}$ (J/g)	Ultimate Analysis (% ad)				
M	A	V			C	H	N	S	O
13.84	10.30	28.77	47.09	24,237	62.03	3.27	0.70	0.37	9.49

Note: FC, fixed carbon; M, moisture content; ad, air-dry basis; V, volatile content; A, ash content; $Q_{\text{net,ad}}$, lower heating value.

2.2. Governing Equation

In the current work, the numerical study included a three-dimensional design, homogeneous and heterogeneous reactions, and a steady flow with incompressible turbulence. Therefore, the species, energy, mass momentum, and time-averaged steady-state pressure-based Navier–Stokes equations were solved. The governing equations for the simulation are given below [13]:

$$\frac{\partial}{\partial x_i}(\rho u_{ij}) = S_m \quad (1)$$

$$\frac{\partial}{\partial x_i}(\rho u_i u_j) = \rho \bar{g}_j - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_i}(\tau_{ij} - \overline{\rho u'_i u'_j}) + S_j \quad (2)$$

$$\frac{\partial}{\partial x_i}(\rho c_p u_i T) = \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} - \rho c_p \overline{u'_i T'} \right) + \mu \Phi + S_h \quad (3)$$

$$\frac{\partial}{\partial x_i}(\rho u_i C_j) = \frac{\partial}{\partial x_i} \left(\rho D_i \frac{\partial C_j}{\partial x_i} - \rho \overline{u'_i C'_j} \right) + S_j \quad (4)$$

where the symmetric stress tensor is represented by τ_{ij} and the Reynolds stress is represented by $\overline{\rho u'_i u'_j}$. The turbulent flow was solved by using the realizable k - ε turbulence equation, while the kinematic turbulence viscosity was determined from the following equation:

$$\mu_t = \rho C_\mu k^2 / \varepsilon \quad (5)$$

where the viscosity constant is C_μ , and k and ε represent the turbulence kinetic energy and rate of dissipation, respectively, which can be obtained from the subsequent standard k - ε transport equations [34]:

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k - \rho \varepsilon \quad (6)$$

$$\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{1\varepsilon} G_k \frac{\varepsilon}{k} + C_{2\varepsilon} G_k \frac{\varepsilon^2}{k} \quad (7)$$

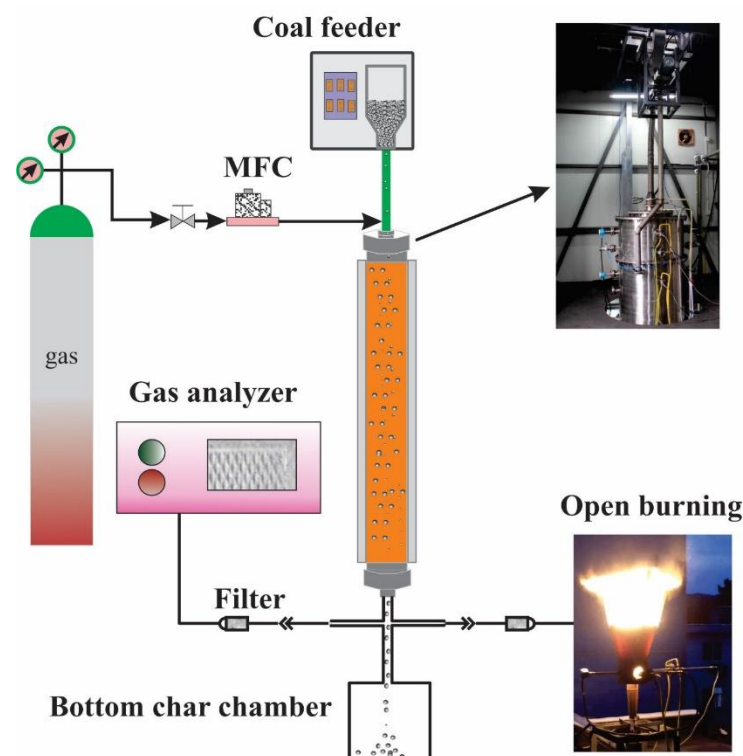


Figure 1. Schematic diagram of the drop tube gasifier.

In the given model, G_k shows the turbulence kinetic energy as a result of the mean velocity gradients. The turbulent Prandtl numbers for k and ε are represented by σ_k and σ_ε , respectively. The constants $C_{1\varepsilon} = 1.44$, $C_\mu = 0.009$, $\sigma_k = 1.0$, $C_{2\varepsilon} = 1.92$, and $\sigma_\varepsilon = 1.3$ in Launder and Spalding's work [35] were used in Equations (6) and (7). The diffusion coefficient (D) and turbulence heat conductivity (λ) in Equations (3) and (4) are given by

$$\rho C_p \overline{u'_i T'} = -\lambda \frac{\partial T}{\partial x_i} = C_p \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \quad (8)$$

$$\rho \overline{u'_i C_j} = -\rho D_i \frac{\partial C_j}{\partial x_i} = -\frac{\mu_t}{Sc_t} \frac{\partial C_j}{\partial x_i} \quad (9)$$

Pr_t ($=0.85$) and Sc_t ($=0.7$) represent the turbulence Prandtl number and the Schmidt number, respectively.

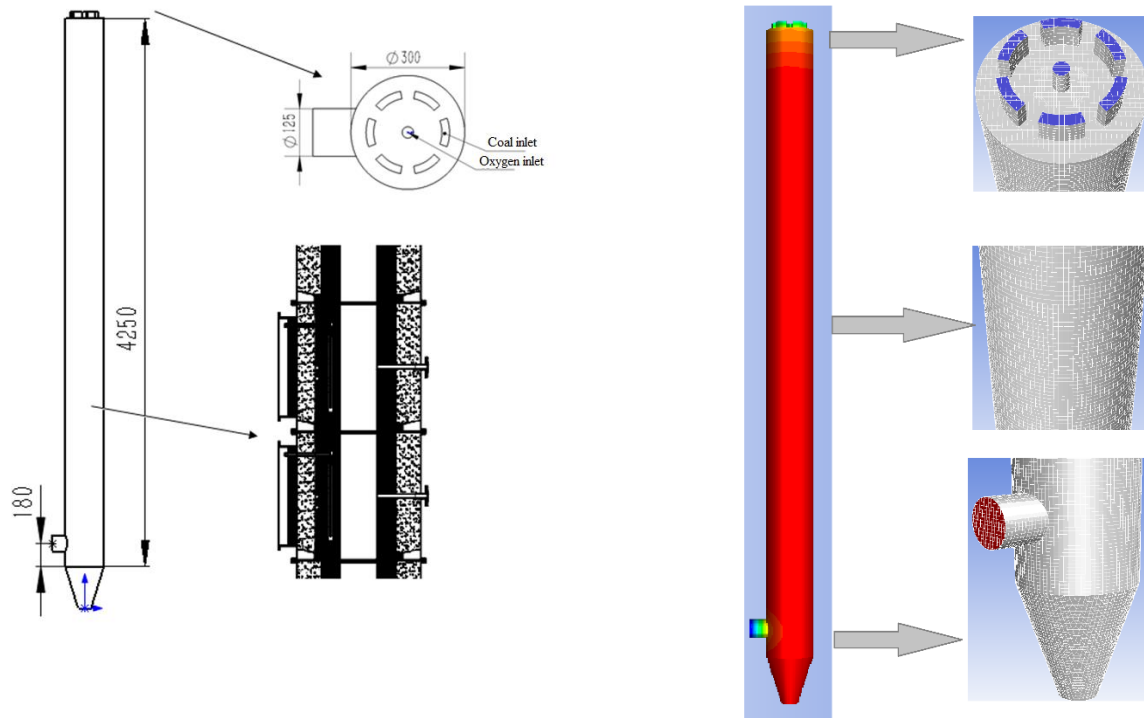


Figure 2. The schematic diagram for the meshed geometry shows a closer view of the inlet and outlet injection.

The discrete phase model (DPM) was used to calculate the motion of the particles in the Lagrangian method. According to the Lagrangian reference frame, the integrated balance force on the coal estimated the discrete phase particle trajectory. The balanced force compares the inertia of coal with the forces as a substitute for the coal and can be represented as follows [36]:

$$\frac{du_p}{dt} = F_D(u - u_p) + g_x \frac{\rho_p - \rho}{\rho_p} + F_x \text{ (for } x \text{ - direction in Cartesian coordinates)} \quad (10)$$

The governing equations consider the mass loss and heat of particles as a source term and consider the interaction between continuous and discrete phases.

The P-1 equation determines the radiation interaction between gas and other particles. In the P-1 equation, the radiation intensity is found using the following model [14]:

$$-\nabla q_r = aG - 4aG\sigma T^4 \quad (11)$$

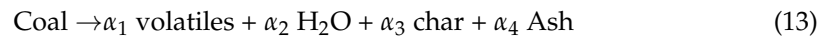
where

$$q_r = -\frac{1}{3(a + \sigma_s) - C\sigma_s} \nabla G \quad (12)$$

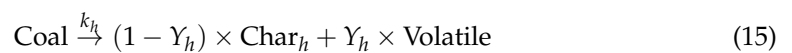
where σ_s , a , σ , C , and G represent the scattering coefficient, absorption coefficient, Stefan–Boltzmann constant, linear anisotropic phase function coefficient, and incident radiation, respectively.

2.3. Main Reaction of Gasification

The species transport equation (Equation (4)) can be utilized for kinetic parameters and chemical reactions inside the gasifier, but due to the high temperature in the gasifier, coal converts into char, volatiles, and ash [37]. The following equation shows the released composition from the coal [38]:



Due to the high temperature near the coal particles, coal inserted from the top in a high heating zone will cause various chemical and physical changes [30]. The main reactions include char gasification, combustion of unburned char and volatiles, and coal devolatilization. In the current work, the volatile species were combined into a single volatile species $\text{C}_{1.45}\text{H}_{4.64}\text{O}_{0.44}$ and determined from the ultimate and proximate analysis of coal in Table 1. The two-step devolatilization model [39] was used to describe the released volatiles and is given as follows:



where Y represents the stoichiometric coefficient. Equation (14) shows the lower temperature and Equation (15) denotes a higher reaction rate at higher temperatures. The kinetic reaction model is represented as

$$\frac{dV}{dt} = (k_l Y_l + k_h Y_h) \text{Coal} \quad (16)$$

$$k_l = A_l \exp(-E_l / RT_p) \quad (17)$$

$$k_h = A_h \exp(-E_h / RT_p) \quad (18)$$

V , A , k , T_p , and E represent the volatile mass fraction, pre-exponential factor, rate constant of reaction, coal particle temperature, and reaction activation energy, respectively. The k_l , Y_l , k_h , Y_h , E_h , and E_l values were obtained from earlier studies [33,34] and are shown in Table 2. The coal devolatilization resulted in char production; therefore, char gasification was the source of CO and H₂ production. Researchers selected different reactions to define the gasification reaction mechanisms [9,13,14,20,22–24,40]. Different preliminary reactions were selected to discover the optimized reaction mechanism between various reactions in the present work; different cases are presented in Table 3.

The different reactions consisted of various chemical volatile species to represent different reaction mechanisms: O₂, C(s), CO, N₂, H₂O, H₂, and CO₂. The species transport model was chosen with the particle surface, volumetric reaction, and turbulence–chemistry interaction defined by the FR/ED model employed to determine the rate of formation of each species and update the source term S_r in Equation (4) as given below:

$$S_r = M_j \sum_{j=1}^N w_{j,r} \quad (19)$$

$$w_{j,r} = (v''_{j,r} - v'_{j,r}) k_f \left(\prod_{i=1}^{N_r} [C]^{\eta''} - \frac{1}{K_{eq}} \prod_{i=1}^{N_r} [C]^{\eta'} \right) \quad (20)$$

$$k_f = AT^B e^{(-E_a / RT)} \quad (21)$$

where k_f , B , E_a , and A represent the rate constant for forward reaction (based on the Arrhenius law), temperature exponent, the activation energy of reaction, and pre-exponential

factor, respectively. The E_a , A , and B values in various reactions were obtained from earlier work [13,32,41] and are listed in Table 2.

Table 2. The kinetic factors for combustion/gasification and devolatilization reactions.

Devolatilization			
Y_h			1
Y_l			0.3
k_h (s ⁻¹)			1.3×10^7
k_l (s ⁻¹)			2×10^5
E_h (kJ mol ⁻¹)			167.4
E_l (kJ mol ⁻¹)			104.6
Gasification or Combustion Reactions		A	B E_a (J Kmol ⁻¹)
Solid–Gas Phase (Heterogeneous Reactions)			
$C(s) + CO_2 \rightarrow 2CO$		242	0 2.75×10^8
$C(s) + 0.5O_2 \rightarrow CO$		0.052	0 6.1×10^7
$C(s) + O_2 \rightarrow CO_2$		0.002	0 7.9×10^7
$C(s) + H_2O \rightarrow CO + H_2$		426	0 3.16×10^8
Gas Phase (Homogeneous Reaction)			
$H_2 + 0.5O_2 \rightarrow H_2O$		6.8×10^{15}	0 1.68×10^8
$CO + H_2O \leftrightarrow CO_2 + H_2$		(1) f 2.75×10^{10}	0 8.38×10^7
		b 2.65×10^{-2}	0 3.96×10^3
$CO + 0.5O_2 \rightarrow CO_2$		2.239×10^{12}	0 1.7×10^8
$C_{1.37}H_{4.58}O_{0.44}$ (volatile) + $2.29O_2 \rightarrow 1.37CO_2 + 2.29H_2O$		(2) 2.119×10^{11}	0 2.119×10^{11}
$C_{1.37}H_{4.58}O_{0.44}$ (volatile) + $1.61O_2 \rightarrow 1.37CO + 2.29H_2O$		(3) 2.119×10^{11}	0 2.027×10^8

Note: 1—WGS reaction, 2—volatile complete combustion, 3—volatile partial combustion.

Table 3. Numerous preliminary models for the evaluation of the best reaction.

Reaction		Simulation Cases					
		A	B	C	D	E	F
$H_2 + 0.5O_2 \rightarrow H_2O$	(1)	γ	γ	γ	γ	γ	γ
$CO + H_2O \leftrightarrow CO_2 + H_2$	(2)	γ	γ	γ	γ	γ	γ
$C(s) + O_2 \rightarrow CO_2$	(3)				γ	γ	γ
$C(s) + 0.5O_2 \rightarrow CO$	(4)	γ	γ	γ			γ
$C(s) + O_2 \rightarrow CO_2$	(5)	γ					
$C(s) + H_2O \rightarrow CO + H_2$	(6)	γ	γ	γ	γ	γ	γ
$C(s) + CO_2 \rightarrow 2CO$	(7)	γ	γ	γ	γ	γ	γ
$Vol + 1.61O_2 \rightarrow 1.37CO + 2.29H_2O$	(8)		γ		γ		
$Vol + 2.29O_2 \rightarrow 1.37CO_2 + 2.29H_2O$	(9)		γ	γ		γ	γ

Reactions: 1—combustion; 2—water gas shift reaction; 3—char complete combustion; 4—char partial combustion; 5—CO combustion; 6—gasification; 7—gasification, Boudouard reaction; 8—volatile partial combustion; 9—volatile complete combustion.

2.4. Simulation Method

The boundary conditions for the input and outlet stream were set as mass flow inlets and pressure outlets, respectively. The coal composition is given in Table 1. The coal feeding rate was constant at 75 kg/h for all case studies. The stationary wall with the no-slip state (zero velocity) at a constant roughness of 0.5 reflected a normal type of wall and the tangent DPM was polynomial. To control the outflow of syngas, the syngas outlet was set as the pressure outlet condition. The energy and momentum equations were decoupled by the implicit pressure, and the steady-state simulation was carried out. The SIMPLE algorithm was employed for coupling the pressure and velocity. Due to the large grid size, parallel processing was used in the numerical calculation. Temperature is the most influential factor in the gasification process, which is why it was chosen for the grid sensitivity analysis.

Figure 2 shows the mesh geometry and a close view of the top nozzles and outlet. First, cold flow simulations were selected for four various grids. Furthermore, temperature contours for all the grid sensitivity analyses are shown in Figure 3. The grid analysis for 490,539 and 747,185 showed a similar temperature around the center of the gasifier. Further simulation results were independent of the grid; therefore, a 917,374 grid size was chosen for other simulations at various O_2 /coal ratios (0.9, 1, and 1.1) and different wall temperatures (1200, 1500, and 1800 °C), as shown in Table 4.

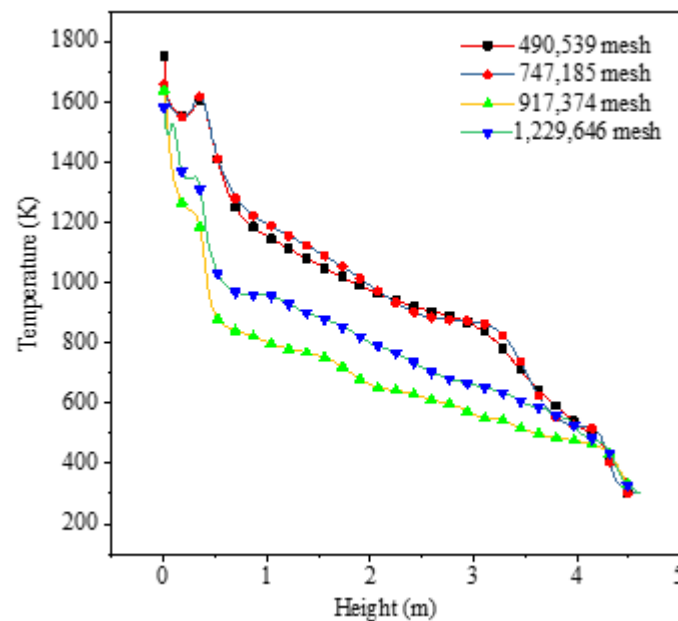


Figure 3. Temperature (K) distribution w.r.t height (m) for the grid sensitivity analysis (four grid sizes).

Table 4. Simulation case for various oxygen/coal ratios and wall temperatures.

Case	O/Coal Ratio	Wall Temperature (K)
1	0.9	1200
2	0.9	1500
3	0.9	1800
4	1	1200
5	1	1500
6	1	1800
7	1.1	1200
8	1.1	1500
9	1.1	1800

3. Results and Discussion

3.1. Various Grid Sensitivity for Validation of the Model

The temperature was the most influential factor in the gasification, and thus, various mesh sizes were employed for the grid sensitivity study. Figure 2 shows the top nozzle (coal and oxygen inlet) and the gasifier outlet. The numerical simulation's cold flow (no reaction) was carried out at various grid sizes (490,539, 747,185, 917,374, and 1,229,646 meshes). Figure 3 shows the temperature contours around the center of the gasifier at various grid sizes. Figure 4a shows the temperature profile of the gasifier along with a close view of the temperature for the 3D fluid domain of the upper and lower parts of the gasifier. Figure 4b shows the temperature at different heights of the experimental gasifier. It is clear from Figure 3 that the fluid domain temperature increased as the gasifier decreased in height, but the temperature at the opposite side of the syngas out was higher than the other side

of the gasifier. The gasifier's temperature trend and the gasifier's height were almost the same, and thus, it can be concluded that the result was independent of the grid; therefore, the 917,374 grids were selected for further simulation.

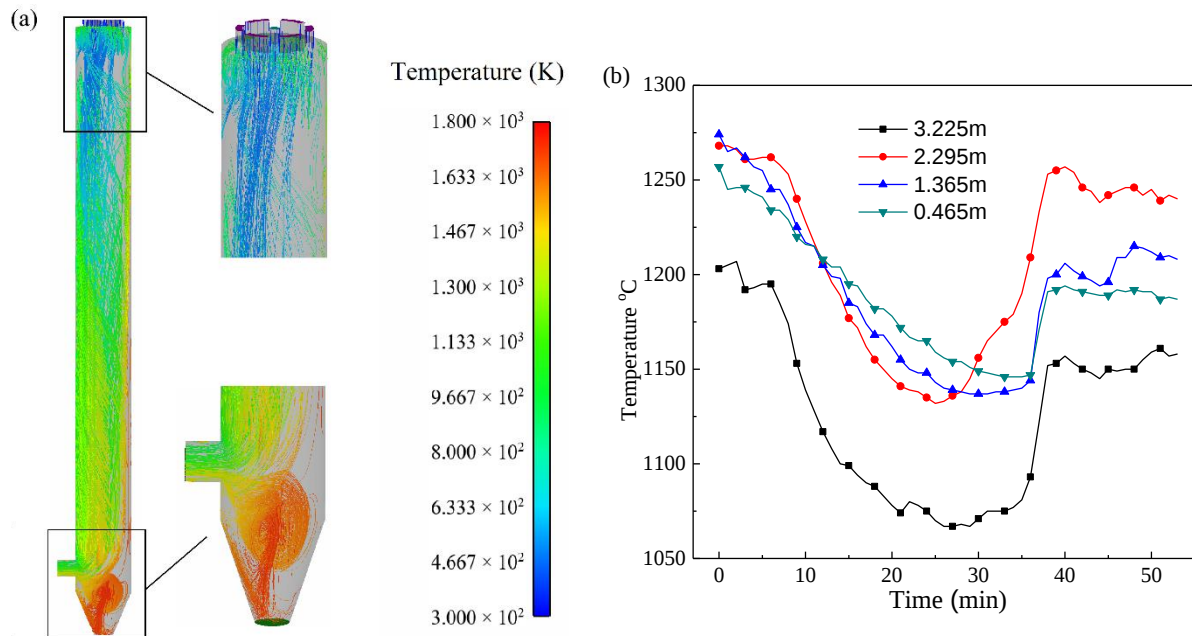


Figure 4. Temperature profiles of the furnace along with a closer view: (a) temperature profile for simulation and (b) temperature profile for experimental gasifier at different heights as a function of time (min).

3.2. Selection of the Reaction Mechanism for Further Simulations

The syngas composition was the best parameter for a comparative study between various reaction mechanisms and experimental results. Figure 5 shows the mol % of CO, H₂, and CO₂ for various preliminary reactions and experimental results at a constant O/C = 1. Figure 5 shows that the maximum CO mol % was 70.51, and the minimum CO was found in the D case at 46.54%, but the CO mol % was 60.4% in the experimental results. LiJun et al. [39] also investigated reaction mechanisms and found that the CO mol % was less than 65%. Compared with the simulation results, the H₂ mol % was higher in the experimental results; indeed, case C had the maximum mol % among the other simulated cases, but the maximum H₂ % in the experimental result was 31.39% and case C had 23.09%, while the minimum mol % was found in case D, which was 18.85%. The CO₂ composition was unsatisfactory in cases A, B, and D, which were 33.39, 22.72, and 34.60%, respectively, but the minimum CO₂ was found to be 6.35% and 8.23% in case C and the experimental results, respectively. Therefore, it is clear from the above discussion that case C showed the best syngas composition regarding the experimental analysis. An ideal reaction mechanism was found in case C, which neglected the oxidation of CO and the proper gasification of char and volatiles was found. Therefore, case C was selected for further simulations.

3.3. Influence of the O/C Ratio and Wall Temperature on the Syngas Production

The temperature and O/C ratio were the key parameters that influenced the gasifier performance because the oxygen-blown drop tube furnace strongly depended on the oxygen concentration. Due to the combustion reaction, CO₂ was produced, along with heat released as an endothermic reaction as a result of CO and H₂ formation. This study simulated nine cases at various O/C values (0.9, 1, and 1.1) and various temperatures (1200, 1500, and 1800 $^{\circ}\text{C}$), as shown in Table 4. Figure 6 shows the effect of O/C and temperature on the syngas composition. Figure 6a shows the effect of an O/C ratio = 0.9 at different temperatures. It is clear from Figure 6a that as the temperature increased from

1200 °C to 1800 °C, the CO mol % also increased from 52.03% to 75.06%, the H₂ % decreased from 29.57% to 5.95% as the temperature increased, and the CO₂ % decreased from 18.39% to 16.76% from 1200 to 1500 °C and then increased slightly up to 18.98% at 1800 °C. Furthermore, Figure 6b,c show the same trend of CO % as in Figure 6a, but the H₂ and CO₂ trends were quite different. In Figure 6b,c, H₂ % was stable at 19% to 20%, but CO₂ % decreased with temperature. In general, CO₂ % increased the O/C ratio because of the water shift reaction, but as the temperature increased, the CO₂ % decreased because a high temperature was not favorable for the water–gas shift reaction. Figure 6b,c show that the temperature and O/C ratio did not have a great impact on the H₂ % yield; the reason for this was the non-availability of steam for the water–gas shift reaction because all the simulations occurred in pure oxygen.

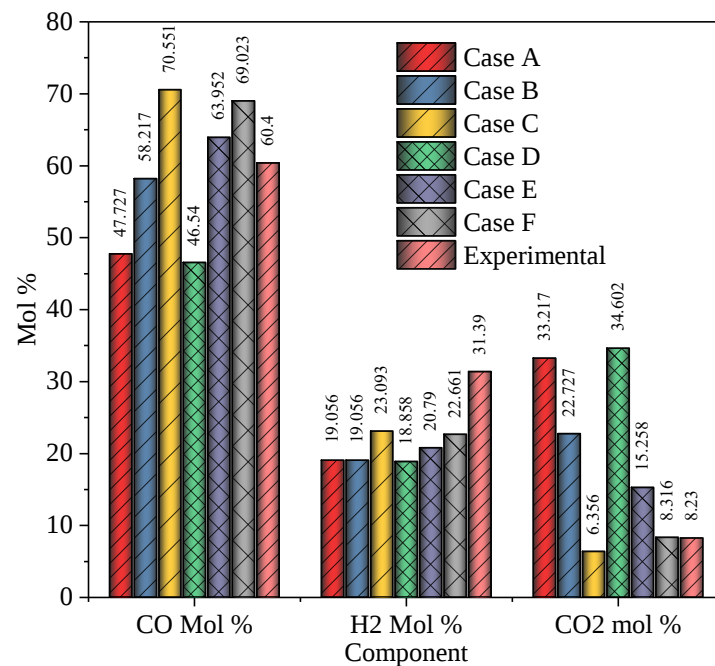


Figure 5. The evaluation of various preliminary reaction results for H₂, CO₂, and CO mol percentages in coal at O/C = 1.

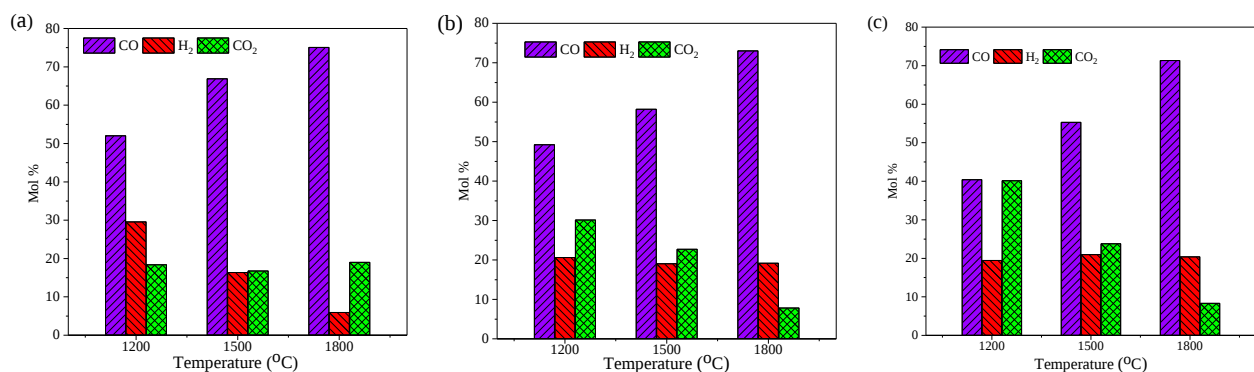


Figure 6. Influence of the wall temperature on the coal gas composition (a) at O/C = 0.9, (b) at O/C = 1, and (c) at O/C = 1.1.

3.4. Effect on the Coal Gas Exit Temperature and Carbon Conversion

The temperature parameter was one of the critical parameters in the gasification/combustion reaction, and increasing the oxygen concentration also raised the temperature profile in an upper section of the gasifier. Figure 7 shows the temperature at the exit of the furnace; it is clearly shown that the temperature at the exit of the furnace increased as the

wall temperature and O/C ratio increased. The maximum and minimum temperatures were found at 1770 °C and 1212 °C for cases 1 and 9, respectively. Further, Figure 8 shows the overall temperature profile in the upper part of the gasifier with increasing wall temperature and O/C. The maximum temperature of 2200 K was observed because a high oxygen concentration resulted in exothermic reactions in the upper part of the gasifier.

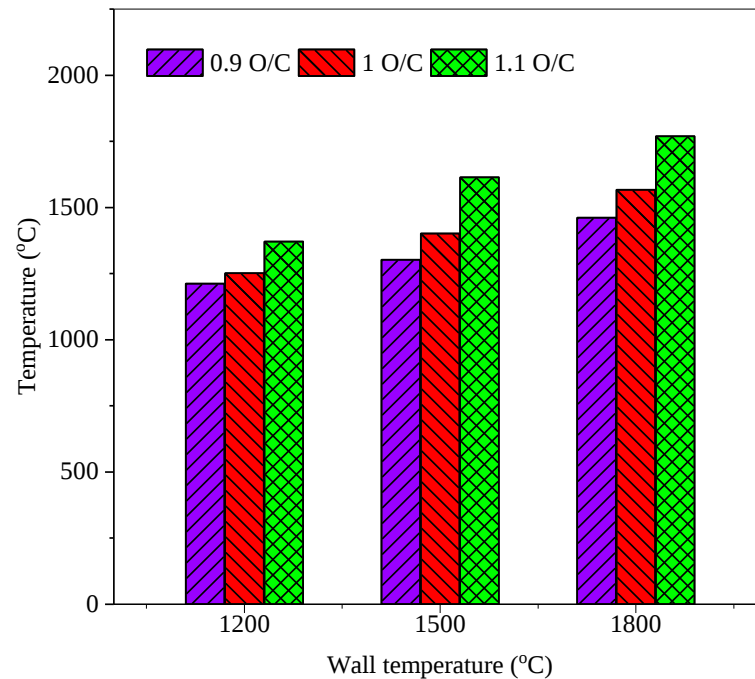


Figure 7. Syngas temperature for numerous cases at the exit of the furnace.

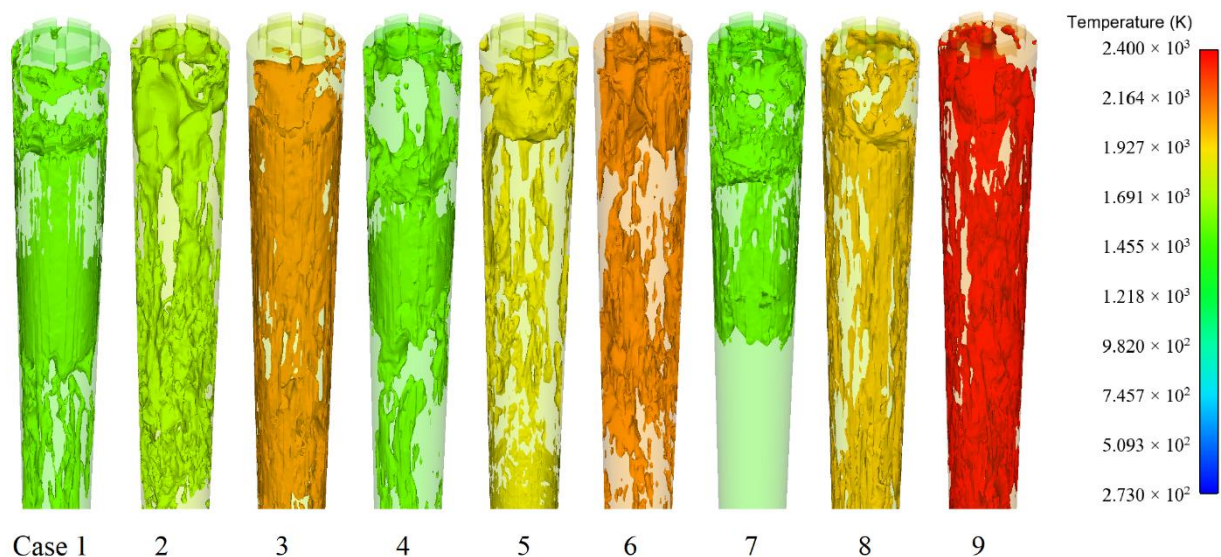


Figure 8. Syngas temperature for various cases at the exit of the gasifier.

The overall variation in the carbon conversion rate shown in Figure 9 was between 97 and 99.8%. It is clear from Figure 9 that the carbon conversion increased with increased wall temperature and O/C ratio. The minimum and maximum carbon conversions were found to be 97.5% and 99.8% in case 1 and case 9, respectively.

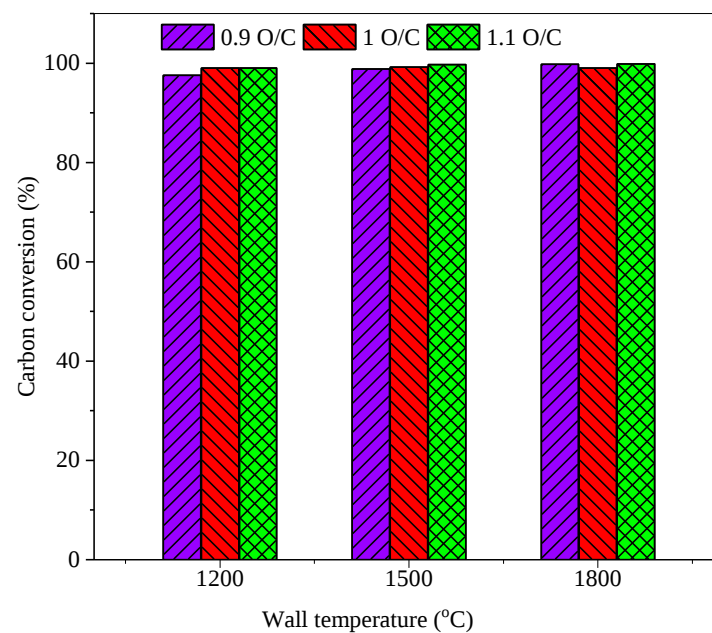


Figure 9. Carbon conversion for various cases.

3.5. Turbulent Intensity and Velocity Profile for Selected Cases

The effect of the turbulence intensity and velocity are shown in Figures 10 and 11. The turbulence intensity was predicted by solving the equation of the reliable $k-\epsilon$ model from Equations (5)–(9). The upper part of the gasifier showed the maximum turbulent intensity range observed at 300–400% because the gasifier's upper part was the main combustion reaction zone. Therefore, it was ensured that a higher mixing rate occurred in the upper part of the gasifier. Furthermore, Figure 11 shows a close view of the velocity profile. The velocity of the particle increased as the temperature and O/C ratio increased. The maximum velocity was observed at 10 m/s and the velocity increased as the height of the gasifier decreased.

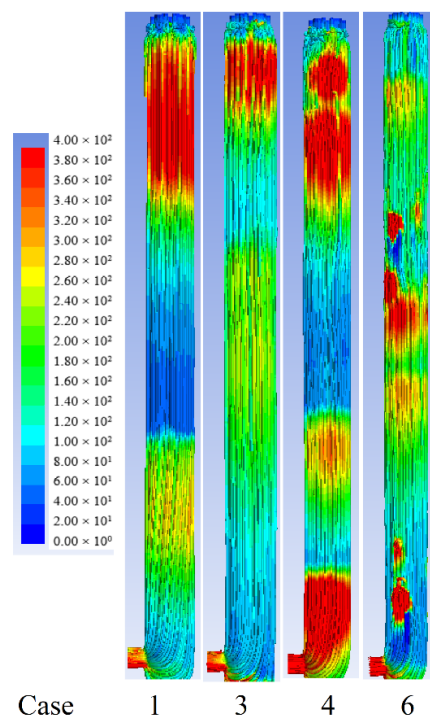


Figure 10. Turbulent intensity for selected cases.

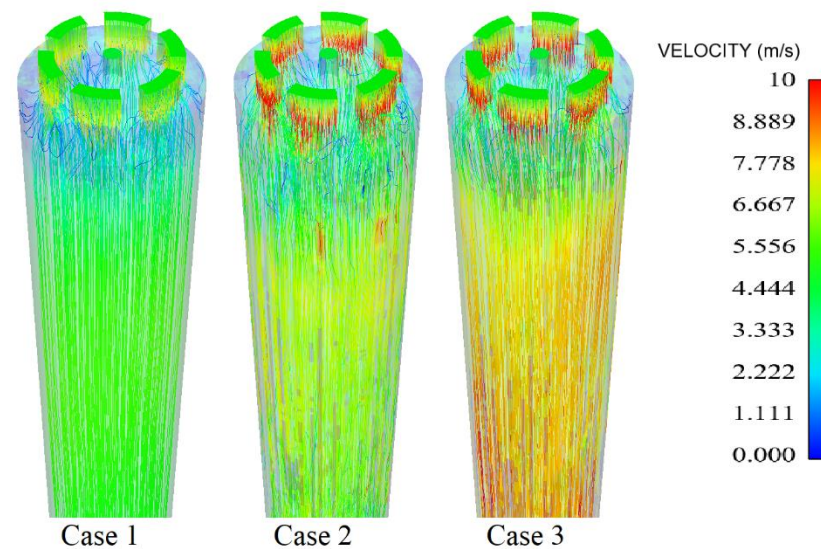


Figure 11. Velocity profile for selected cases.

4. Conclusions

The aim of this work was to investigate multiple factors for a drop tube coal gasifier. First, various preliminary reactions were simulated to validate the reaction model with experimental data. Furthermore, various cases were simulated at various O/C ratios and wall temperatures to analyze the syngas species, temperature profile in the whole gasifier, exit temperature, carbon conversion, turbulent intensity, and velocity profile. The syngas composition was the best parameter for a comparative study between the various reaction mechanisms and the experimental results. The maximum CO mol % was 70.51%, and the minimum CO was found in case D at 46.54%, but the CO mol % was 60.4% in the experimental results. Furthermore, the H₂ mol % was higher in the experimental results at 31.39%, and the maximum mol % was found at 23.09% in case C among the simulated cases. Therefore, case C was selected for further simulations. The various O/C values and wall temperatures have a significant effect on reaction mechanisms. The maximum CO % was found to be 75.06%, with an oxygen/coal ratio of 0.9 at 1800 °C. The maximum H₂ % was found at 1200 °C with an O/C ratio of 0.9, but the trend showed that increasing the wall temperature caused a reduction in the H₂ mol %. The minimum and maximum carbon conversions were found to be 97.5% and 99.8% at an O/C of 0.9 at 1200 °C and an O/C of 1.1 at 1800 °C, respectively. The overall optimized results were found in case C in the preliminary reaction. Furthermore, the best syngas result was obtained in the sixth case. It can be concluded from the results that O/C and the wall temperature had a significant influence on the syngas composition.

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Nomenclature

u, u_p	Velocity, velocity of particles (m/s)
ρ, ρ_p	Density, density of particles (kg/m ³)
S_m, S_j, S_h, S_r	Source terms for mass, momentum, energy, and species
c_p	Specific heat at constant pressure (J/kg K)
τ_{ij}	Symmetric stress tensor
T	Temperature (K)
λ	Turbulent thermal conductivity (W/m K)
C_j	Mole fraction of species j
D_i	Diffusivity (m ² /s)
F_D	Drag force (kg m/s)
μ	Dynamic viscosity (N S/m ²)
k	Kinetic energy of turbulence (m ² /s ²)
ε	Dissipation rate of turbulence (m ² /s ³)
μ_t	Turbulence viscosity
C_μ	Viscosity constant
G_k	Mean velocity gradients
D_t	Diffusion coefficient for turbulence (m ² /s)
Pr_t	Prandtl number for turbulence
Sc_t	Schmidt number for turbulence
q_r	Heat flux for radiation heat (J/m ² s)
G	Incident radiation
C	Coefficient of function for linear anisotropic phase
α	Absorption coefficient
σ_s	Scattering coefficient (m ⁻¹)
σ	Stefan–Boltzmann constant
ε_W	Emissivity
$W_{j,r}$	Net production rate of species i via chemical reactions (K mol/m ³ S)
M_j	Molecular weight of species j
$v''_{j,r}$	Stoichiometric coefficient for product j in reaction r
$v'_{i,r}$	Stoichiometric coefficient for reactant i in reaction r
$[C]$	Molar concentration of species (K mol/m ³)
η''	Rate exponent for product species
η'	Rate exponent for product reactant species
k_f	Forward reaction rate constant
A	Pre-exponential factor (consistent units)
B	Temperature constant (dimensionless)
E_a	Activation energy for reaction (J/K mol)

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