A COMPUTATIONAL ANALYSIS OF OPERATIONAL PARAMETERS INFLUENCING COAL GASIFICATION IN A LAB-SCALE DROP TUBE GASIFIER

by

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This study uses a numerical simulation for coal gasification operation in a drop tube gasifier to investigate the effects of wall temperature and oxygen-to-coal ratios on gasification. Coal gasification is an efficient approach to electricity generation, offering a cleaner alternative to conventional coal combustion methods. A 2-D CFD model of the gasifier was employed to perform grid sensitivity analysis and subsequently compute the influences of varying wall temperatures (1000 K, 1250 K, and 1500 K) and oxygen-to-coal ratios (0.6, 0.8, 1, and 1.2) on the temperature profile, syngas composition, and velocity within the gasifier. Temperature profiling within the furnace defined a spectrum of maximum and minimum temperatures, with apex values recorded at 2100 K and lowest values at 1300 K for Cases 12 and 1, respectively. High oxygen-to-coal ratios favored the production of CO_2 due to enhanced combustion reactions, whereas lower oxygen-to-coal ratios were conducive to higher yields of CO and H_2 , essential syngas components. Velocity profiles of particles within the gasifier increased with higher temperatures and oxygen-to-coal ratios, and the maximum velocity was 9 m per second. In conclusion, this study offers valuable insights into optimizing operational parameters such as wall temperatures and oxygen-to-coal ratios to enhance the performance and efficiency of coal gasification processes in lab-scale gasifiers.

Key words: coal gasification, oxygen-to-coal ratio, reaction kinetics, CFD, syngas composition

Introduction

Coal gasification is a process that converts coal into a versatile gas called syngas, which can be used to generate electricity and manufacture a range of chemical products. This approach taps into coal potential more efficiently [1]. The escalating electricity demand has historically been met predominantly by oil. However, there has been a noticeable shift towards exploring coal usage in recent research due to depleting oil reserves and the prevalent availability of coal in China [2]. Gasification technology has emerged as a potential avenue for maximizing energy conversion into electricity with minimal hazardous impacts. Researchers' main

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aim is to develop sophisticated gasifiers that exhibit enhanced performance and reduced emissions of pollutants [3-6]. Studies have been conducted to understand the chemical and physical changes occurring during the gasification process to optimize the transformation of coal into gas. Alongside experimental analyses, CFD simulations offer a cost-efficient method to examine factors such as reaction rates, temperature variations, turbulent intensity, the proportions of oxygen and coal, and coal retention time, among others. Nevertheless, CFD modeling of gasification necessitates distinctive mathematical models to analyze and decipher the complexities associated with turbulence, temperature variations, and reaction rates to yield meaningful outcomes.

Numerous researchers have recently undertaken several studies involving CFD simulations in entrained flow coal gasifiers [7-14]. Kim *et al.* [15] used steam as a gasifying agent, evaluated the performance of the IGCC coal gasifier, and also revealed that tangential inflow influences the particle motion. A study by Du *et al.* [16] on the simulation of mixing coal with PET in co-gasification within a fluidized bed discovered that larger particle sizes impede heat flow. Kim *et al.* [17] ran a simulation and found that for coal gasification in a 300 MW IGCC, an oxygen-to-coal (O/C) ratio of 0.7 is ideal. Diba *et al.* [18] found that the optimum airflow for char conversion was 17 kg per hour and that calcination resulted in a higher concentration of CO₂. Sun *et al.* [19] investigate the impact of immersed tubes on gas-particle interactions in fluidization dynamics using CFD simulation, which plays a crucial role in the efficiency and efficacy of biomass gasification. Safeanov *et al.* [20] developed an enhanced analytical model to predict heat transfer in entrained-flow gasifiers. This model specifically accounts for the flow and heat transfer characteristics of the slug layer wall in the reactor during dry-feed coal gasification.

Researchers have experimented with mixed gasification agents with syngas, attaining temperatures of more than 1550 °C through a numerical approach [21]. Wang *et al.* [22] employed discrete-phase and solidification models to perform computational simulations to recover heat from molten slugs and syngas. Euler-Euler [23, 24] and Euler-Lagrangian methods [9, 25-27] have also been applied by researchers to delineate gas and solid flows. Commonly, FR/ED and probability density functions (PDF) have been employed to analyze the chemistry of gasification reactions, with various mediums like air/steam being used for gasification [28-30]. Watanabe and Kurase [31] studied the modeling and simulation of coal gasification in an entrained flow coal gasifier, reviewed the three chemical processes, and discussed the accuracy of the model. In diverse CFD simulations, parameters like gasification reactions, nozzle design, and particle size have been explored [12, 32-36]. A study by Imran *et al.* [37] examines the gasification process for multi-injectors at different O/C ratios, revealing hydrogen composition up to 28% and CO at 52%, indicating that pure oxygen leads to elevated temperatures and enhanced carbon conversion efficiencies.

In our research, a 2-D drop tube gasifier is analyzed, initially focusing on grid sensitivity analysis, followed by an assessment of wall temperature effects at 1000 K, 1250 K, and 1500 K with various O_2 /coal ratios (0.6, 0.8, 1, and 1.2). This approach allows the computation of temperature profiles, syngas compositions, and velocity profiles. The gasification process has been successfully modeled, showing that finite rates significantly influence global chemical reactions.

Simulation model

Gasifier mesh and design

Figure 1 displays the 2-D gasifier drawing: the gasifier operates as a downflow reactor and consists of two parts, with a throat between them, with a height of 3.83 m. The inner diameters of the first and second stages are 0.250 m each. Two levels of injection are incorporated

into the gasifier. The upper level has three coal inlets and two oxygen inlets, as illustrated in fig. 1. Conversely, the lower level contains two opposing coal injections. The gasifier operates at a total dry coal feeding rate of 50 kg per hour, with the lower inlet featuring a surface-type injection situated at 1.910 m. Detailed proximate and ultimate analyses of the coal are presented in tab. 1. Particle size corresponds to the Rosin-Rammler method, with the maximum, minimum, and mean diameters of 0.125 mm, 0.004 mm, and 0.0456 mm, respectively. In the upper stage, pulverized coal undergoes an exothermic reaction with oxygen, resulting in a temperature increase through the devolatilization of coal into char and CO₂. Following this, the second injection stage leverages the generated heat to facilitate an endothermic reaction, primarily yielding carbon monoxide and hydrogen, with a minor CO₂ production. Calcula-



Figure 1. Illustrating the drop tube gasifier furnace

tions for the required oxygen can be based on the O/C ratio of the fixed carbon feeding. While the oxygen injection remains constant at the upper level, coal distribution is evenly split, with 50% at the upper and 50% at the lower.

Proximate [% ad]				$Q_{ m net,ad} [m Jg^{-1}]$	Ultimate [% ad]							
Ash (A)	Moisture (M)	Fix carbon (FC)	Volatile (V)		Hydrogen	Carbon	Oxygen	Sulfur	Nitrogen			
10.30	13.84	47.09	28.77	24,237	3.27	62.03	9.49	0.37	0.70			

Table 1. Ultimate and proximate analyses of coal

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

Governing equation

The numerical analysis in this study involves a 2-D structure and considers both homogeneous and heterogeneous reactions operating under steady and incompressible turbulence conditions. Consequently, species, time-averaged steady-state pressure-based Navier-Stokes, mass momentum, and energy equations have been resolved. The equations that govern the numerical simulation are provided in the following manner [13]:

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

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$$\frac{\partial}{\partial x_i}(\rho c_p u_i T) = \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} - \rho c_p \overline{u_i' T'} \right) + \mu \Phi + S_h$$
(2)

$$\frac{\partial}{\partial x_i}(\rho u_i u_j) = \rho \overline{g}_j - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_i}(\tau_{ij} - \rho \overline{u_i' u_j'}) + S_j$$
(3)

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

The Reynolds stress is denoted by $\rho u'_i u'_j$, and symmetric stress tensor is τ_{ij} . The equation governing turbulent flow was resolved by employing realizable *k*- ε , and the kinematic turbulence viscosity was calculated based on eq. (5). The dissipation rate is denoted as ε , while *k* symbolizes the turbulence kinetic energy, and the viscosity constant is represented as C_{μ} . These values can be determined using the subsequent standards *k*- ε transport equations [38]:

$$\mu_{\rm t} = \frac{\rho C_{\mu} k^2}{\varepsilon} \tag{5}$$

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

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

In the provided model, the turbulence kinetic energy represents the G_k resulting from the mean velocity gradients. The turbulent Prandtl numbers related to the turbulent kinetic energy, k, and its dissipation rate, ε , are symbolically represented by σ_k and σ_{ε} , respectively. Constants such as $C_{1\varepsilon} = 1.44$, $C_{\mu} = 0.009$, $\sigma_k = 1.0$, $C_{2\varepsilon} = 1.92$, and $\sigma_{\varepsilon} = 1.3$ in Launder and Spalding's work [39] were utilized in eqs. (6)-(7). Additionally, turbulence heat conductivity, λ , and the diffusion coefficient, D, were specified in the eqs. (3)-(4):

$$\rho c_p \overline{u_i' T'} = -\lambda \frac{\partial T}{\partial x_i} = c_p \frac{\mu_t}{\Pr_t} \frac{\partial T}{\partial x_i}$$
(8)

$$\rho \overline{u_i' C_j} = -\rho D_i \frac{\partial C_j}{\partial x_i} = -\frac{\mu_t}{\mathrm{Sc}_t} \frac{\partial C_j}{\partial x_i}$$
(9)

The $Sc_t = 0.7$ and $Pr_t = 0.85$ denote the Schmidt numbers and turbulence Prandtl. The discrete phase model (DPM) was employed to determine particles momentum using the Lagrangian method. In the Lagrangian reference frame context, the combined balance force acting on the coal was used to approximate the trajectory of discrete phase particles. This balanced force evaluates the coal inertia against forces acting as substitutes for the coal, as presented in reference [40].

$$\frac{\mathrm{d}u_{\mathrm{p}}}{\mathrm{d}t} = F_D(u - u_{\mathrm{p}}) + g_x \frac{\rho_{\mathrm{p}} - \rho}{\rho_{\mathrm{p}}} + F_x \tag{10}$$

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The formulated equations account for the reduction in particle mass and thermal energy by incorporating source terms that facilitate the exchange between the continuous and discrete phases. The P-1 equation is responsible for determining the interaction of radiation between gas and various particles. Within the P-1 equation, the model mentioned is used to ascertain the radiation intensity.

$$-\nabla q_{\rm r} = \alpha G - 4\alpha G \sigma T^4 \tag{11}$$

where

$$q_{\rm r} = -\frac{1}{3(\alpha + \sigma_{\rm s}) - C\sigma_{\rm s}} \nabla G \tag{12}$$

The symbols G, σ , α , C, and σ_s stand for incident radiation, Stefan-Boltzmann constant, absorption coefficient, linear anisotropic phase function coefficient, and scattering coefficient, respectively.

Gasification primary reaction

Equation (4), the equation for species transport, is useful for identifying key kinetic characteristics and examining the chemical processes inside a gasifier. Nonetheless, because of the intense heat within the gasifier, the coal is converted into char, volatile compounds, and ash [41]. The composition released from the coal is illustrated in eq. (13) [42]. In the zone of intense heat where coal particles are exposed to high temperatures, the introduction of coal from previous sets off a series of chemical and physical variations [34]. These initial processes contain the gasification of char, the burning of any residual char and volatile substances, and the devolatilization of coal. All volatile substances identified in our research were grouped under one category, represented by the formula $C_{1.45}H_{4.64}O_{0.44}$. This categorization was based on the elemental composition of the coal, as revealed in tab. 1. To describe how volatile substances are released, we used a model that breaks down the process into two distinct stages [43] to characterize the release of volatiles, as detailed below:

$$Coal \rightarrow \alpha_1 \text{ volatiles} + \alpha_2 H_2 O + \alpha_3 \text{ char} + \alpha_4 \text{ Ash}$$
(13)

$$\operatorname{Coal} \xrightarrow{\kappa_l} (1 - Y_l) \times \operatorname{Char}_l + Y_l \times \operatorname{Volatile}$$
(14)

$$\operatorname{Coal} \xrightarrow{n} (1 - Y_h) \times \operatorname{Char}_h + Y_h \times \operatorname{Volatile}$$
 (15)

In the equation, Y denotes the stoichiometric coefficient. The lower temperature is depicted in eq. (14), while the 15th equation indicates a faster reaction rate at elevated temperatures. The expression of the kinetic reaction is:

 k_{i}

$$\frac{\mathrm{d}V}{\mathrm{d}t} = (k_l Y_1 + k_h Y_h) \text{Coal}$$
(16)

$$k_h = A_h \exp\left(\frac{-E_h}{\mathbf{R}T_p}\right) \tag{17}$$

$$k_l = A_l \exp \frac{-E_l}{\mathbf{R}T_p} \tag{18}$$

The volatile mass fraction is denoted by *V*, *k* is the pre-exponential factor, the rate constant of the reaction is denoted by the letter *k*, the temperature of the coal particle is denoted by the symbol *TP*, and the reaction activation energy is denoted by the symbol *E*. Data related to values of k_1 , Y_1 , k_h , Y_h , E_h , and E_l were extrapolated from prior research [39, 40], and are tabulated in [44]. The coal devolatilization culminates in the formation of char, which subsequently undergoes gasification to produce CO and H₂. Researchers have employed many reactions to characterize the gasification processes [9, 13, 14, 23, 25-27, 45]. In the present study, various initial reactions were examined to determine the most effective reaction mechanism. Relevant instances are listed in [44].

The heterogeneous reactions were characterized by multiple volatile chemical species involved in the reaction mechanisms, namely H₂O, CO, C_(s), O₂, N₂, CO₂, and H₂. A species transport model was meticulously selected, incorporating particle surface interactions, volumetric reactions, and turbulence-chemistry interactions. These aspects were quantitatively delineated by utilizing the FR/ED model. This computational model facilitated the precise determination of the formation rates of the individual species, allowing for the contemporary updating source term, S_r , as given in eq. (4):

$$S_{r} = M_{j} \sum_{j=1}^{N} w_{j,r}$$
(19)

$$w_{j,r} = (v_{j,r}'' - v_{j,r}')k_{\rm f} \left(\prod_{i=1}^{N_r} [C]^{\eta''} - \frac{1}{K_{\rm eq}} \prod_{i=1}^{N_r} [C]^{\eta'}\right)$$
(20)

$$k_{\rm f} = AT^B {\rm e}^{(-E_a/{\rm R}T)}$$
⁽²¹⁾

Under the principles of the Arrhenius equation, several parameters such as k_f , B, E_a , and A have been delineated to characterize the kinetics of the forward reaction. Here, k_f represents the rate constant of the forward reaction, B – the temperature exponent, E_a – the activation energy requisite for the reaction to proceed, and A – the pre-exponential factor or frequency of collision. References from previous studies [13, 36, 46] have been utilized to ascertain the values of E_a , A, and B pertinent to various reactions, which have subsequently been cataloged and presented in [44] for comprehensive analysis and reference.

Simulation method

Table 1 presents the composition of the coal used. The coal feed rate was maintained at 50 kg per hour across various studies, each employing distinct O/C ratios. The boundary conditions were mass-flow inlets and pressure outlets used for all input/output stream. A fixed wall exhibiting a no-slip condition (meaning that the fluid has zero velocity at the boundary) with a consistent roughness value of 0.5 was modeled. The DPM wall interaction was set to a reflective type for both normal and tangential particle impacts using a polynomial relationship. This setup was examined under different wall temperature conditions: 1500 K, 1250 K, and 1000 K. Temperature plays a key role in the gasification process, making it a primary focus of our grid sensitivity study. Three different densities of mesh have been selected for analysis of temperature and velocity. Figure 2 presents the meshed domain, including a closer view of the nozzles. Furthermore, the initial reaction was determined at various O/C ratios like 0.60, 0.80, 1, and 1.20 at different wall temperatures like 1000 K, 1250 K, and 1500 K, as shown in tab. 2.

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The compositional details of the coal utilized in the experiment are defined in tab. 1. A consistent coal feeding rate of 50 kg per hour was maintained across all case studies, each characterized by varying O₂/coal ratios. Boundary conditions were established for all input and

output streams, incorporating mass-flow inlets and pressure outlets. The walls were considered stationary with a no-slip condition (zero velocity) applied, maintaining a constant roughness of 0.5. Regarding the DPM, the walls were designated as reflective, implementing a polynomial type for both normal and tangent interactions. Wall temperatures were manipulated, applying 1500 K, 1250 K, and 1000 K values to assess their influences. Given its critical influence on gasification processes, temperature was prioritized as a key parameter within the grid sensitivity analysis. A selection of mesh densities, varying across three distinct categories, was applied to facilitate a comprehensive analysis of temperature and velocity parameters. Refer to fig. 2 for a detailed visualization of the meshed domain, including a magnified view featuring the nozzles structural intricacies. Initiating reactions were strategically selected, incorporating varied oxy-



Figure 2. The detailed representation of the 2-D meshed geometry illustrates a zoomed-in view of the upper inlets (right) and the lower inlet (left)

gen/coal ratios such as 0.60, 0.80, 1, and 1.20. These ratios were meticulously paired with diverse wall temperatures, specifically 1000 K, 1250 K, and 1500 K, as systematically categorized in tab. 2.

Case	1	2	3	4	5	6	7	8	9	10	11	12
O/C	0.6	0.6	0.6	0.8	0.8	0.8	1	1	1	1.2	1.2	1.2
Temperature	1000	1250	1500	1000	1250	1500	1000	1250	1500	1000	1250	1500

Table 2. Different scenarios simulated for a range of O/C ratios and wall temperatures

Results and discussion

Evaluation of model validation through grid sensitivity analysis

In the gasification processes, temperature is the paramount parameter influencing outcomes. Consequently, scenarios (Cases A, B, and C) were meticulously chosen for grid sensitivity analysis to scrutinize the variations and impacts associated with temperature fluctuations. Figure 2 illustrates the meshed domain, accompanied by a detailed view of the nozzles. Nonreactive cold flow simulations were conducted using three distinct grid configurations. The subsequent temperature profiles, aligned with the velocity vectors across these grids, are comprehensively shown in figs. 3 and 4, respectively. The grids for cases A, B, and C are 529091, 339027, and 236855, respectively, the grid consists of structured and unstructured mesh. The tetrahedral cells demonstrate a uniform temperature distribution along the central axis, vertical to the height of the gasifier. The velocity profile is almost the same along with height, but minor changes are observed near the top of the gasifier. However, the overall result shows that grid

sensitivity does not influence temperature and velocity profile. The solution demonstrates grid independence for grid sizes exceeding 339027. Consequently, this specific grid size has been adopted for subsequent computations.



Figure 3. Temperature distribution for grid sensitivity analysis (three grid sizes)



Figure 4. Velocity profile for grid sensitivity analysis

Impact of the O/C ratio and wall temperature on synthesis gas generation

Several critical parameters predominantly influence the performance of an oxygenblown drop tube furnace. The oxygen concentration, temperature, and the O/C ratio play pivotal roles in determining the operational efficacy of the gasifier. These variables substantially influence the furnace behavior and overall gasification effectiveness. The combustion reaction influences the generation of CO_2 species, the thermal output requisite for endothermic reactions, and the subsequent formation of CO and H_2 . A series of twelve simulation cases were meticulously analyzed, varying in O/C ratios (0.6, 0.8, 1, and 1.2) and temperatures (1000 K, 1250 K, and 1500 K), as detailed in tab. 2. Figure 5 illustrates how changes in the O/C ratios and temperature levels affect the composition of syngas. Specifically, fig. 5(a) shows the variance in CO composition across different temperatures and O/C ratios, emphasizing a heightened mass fraction of CO composition in the gasifier upper regions. Contrarily, it was discerned that wall temperature exerted minimal influence on the composition. Figure 5(b) shows that the CO₂ composition at the injection site was comparatively reduced. However, a subsequent series of reactions evidenced an amplification in CO₂ formation, with elevated O/C ratios particularly conducive to this increase. A general trend was identified where an ascent in the O/C ratio culminated in an enhanced CO₂ percentage, attributed predominantly to the water-gas shift reaction. Conversely, an elevation in temperature resulted in a diminished CO₂ percentage, substantiated.

Figure 5(c) illustrates an obvious variation in the hydrogen mass fraction under different operational parameters. At an O/C ratio of 0.6, a substantial hydrogen mass fraction is observed predominantly in the upper region. This propensity, however, diminishes when coal is introduced through the second injection point, leading to a reduced hydrogen fraction. A comparative analysis between different cases (1-6 vs. 8-12) reveals a conspicuous disparity in the hydrogen fraction. Cases 1-6 exhibit a more elevated hydrogen fraction than cases 8-12, implying that a higher O/C ratio may not be conducive to optimal hydrogen production. In addition, the investigation elucidates that temperature variations exhibit a nominal influence on the yield of H_2 . The findings suggest that the reaction efficiency was compromised due to a shortage of steam, which is essential for the water-gas shift reaction to proceed. This was because the simulations took place in an environment with plenty of oxygen but without steam.



Impact of O/C ratio and temperature on the temperature profile

In the gasification/combustion reaction, the temperature parameter emerged as a pivotal variable. Increasing the amount of oxygen led to a higher temperature in the top part of the gasifier. A delineation of the temperature profile within the furnace is exhibited in fig. 6, elucidating a conspicuous augmentation in temperature concurrent with increments in the wall temperature and O/C ratio. Extreme temperature values were considered 2100 K and 1300 K for Cases 12 and 1, respectively. A relatively lower temperature gradient characterizes the thermal profile within the upper section of the gasifier. This is attributed to the injection of 50% of the coal feed at this upper injection point, coupled with the spatial limitation due to the upper region's reduced height compared to the gasifier's lower region. Consequently, the lower region





Figure 6. Variation in syngas temperature [K] under different operating conditions of the gasifier

Figure 7. Velocity profile for drop tube gasifier

manifests a heightened temperature profile due to its extended vertical dimension. Factors such as an elevated O/C ratio and increased wall temperatures significantly enhance the gasifier thermal conditions.

Velocity profile for drop tube furnace

Figure 7 depicts the velocity profiles for Cases 1 through 12. It can be discerned from the data that a direct correlation exists between the particle's velocity, the prevailing temperature, and the O/C ratio. The peak velocity registered was 9 m per second, and interestingly, an inverse relationship between the height of the gasifier and the velocity was observed. Due to gravitational force, coal particles drop down without external forces. However, lower injections are side injections that the lower velocity at the inner wall of the gasifier may cause. However, the curve shape between the two also causes the particle to have low velocity. However, the curve shape also helps to increase the velocity of the lower injection particle, which is why the velocity at the lower region of the gasifier is high.

Conclusions

This comprehensive study investigates a 2-D CFD model of a drop tube gasifier, focusing on grid sensitivity and the effects of varying wall temperatures (1000 K to 1500 K) and O_2 /coal ratios (0.6 to 1.2) on gasifier performance. The study finds that the gasifier efficiency is significantly influenced by oxygen concentration, temperature, and the O/C ratio. Notably, the mass fraction of CO is higher in the furnace upper regions, while CO_2 concentration is minimal near the injection zones. Wall temperature appears to have a limited impact on CO composition.

A key observation is the interaction between temperature, O/C ratio, and CO₂ composition. An increase in O/C ratio leads to higher CO₂ levels due to the water-gas shift reaction, whereas higher temperatures decrease CO₂ percentages. Hydrogen fraction analysis shows an optimized presence at an O/C ratio of 0.6, mainly in the upper furnace regions. A decrease in hydrogen fraction is noted with secondary coal injections. Comparative studies between different cases suggest variations in hydrogen presence linked to O/C ratios.

Temperature profiling within the furnace reveals a range of maximum (2100 K) and minimum (1300 K) temperatures, with lower gradients in the upper regions due to operational dynamics. In contrast, the lower regions exhibit higher temperature profiles. Velocity profiling indicates a correlation with temperature and O/C ratios, with a notable increase in particle velocities at higher temperatures and O/C ratios, reaching a maximum of 9 m per second. This study highlights the complex dependencies of operational parameters on the gasifier's performance, providing valuable insights for optimizing gasification processes.

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Nomenclature

- A pre-exponential factor (consistent units)
- temperature constant [-] R
- C coefficient of function for linear-anisotropic phase
- C_{μ} viscosity constant
- C_i mole fraction of species j

- [C] molar concentration of species, $[Kmolm^{-3}]$
- c_p specific heat at constant pressure, [Jkg⁻¹K⁻¹] D_i diffusivity, [m²s⁻¹]
- E_a activation energy for reaction [JK⁻¹mol⁻¹]
- $F_{\rm D}$ drag force, [kgms⁻¹]
- G incident radiation

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- G_k mean velocity gradients
- k kinetic energy for turbulence, [m²s⁻²]
- $k_{\rm f}$ forward reaction rate constant
- M_i molecular weight of specie j
- Prt Prandtl number for turbulence
- q_r heat flux for radiation heat, [Jm²s⁻¹]
- $Sc_t Schmidt$ number for turbulence
- S_{m} , S_{j} , S_{h} , S_{r} source terms for mass, momentum, energy and species
- T - temperature, [K]
- u, u_p velocity, velocity of particles, [ms⁻¹]
- stoichiometric coefficient for reactant i V'i.r in reaction. r
- $v''_{i,r}$ stoichiometric coefficient for product *j* in reaction r

References

- [1] Yamauchi, Y., Akiyama K., Innovative Zero-Emission Coal Gasification Power Generation Project, Energy Proced., 37 (2013), 2013, pp. 6579-6586
- Wang, Q., Li, R., Journey to Burning Half of Global Coal: Trajectory and Drivers of China's Coal Use, Renewable and Sustainable Energy Reviews, 58 (2016), May, pp. 341-346
- [3] Taniguchi, M., et al., A Reduced NOx Reaction Model for Pulverized Coal Combustion under Fuel-Rich Conditions, Fuel, 81 (2002), 3, pp. 363-371
- [4] Taniguchi, M., et al., A Role of Hydrocarbon Reaction for NOx Formation and Reduction in Fuel-Rich Pulverized Coal Combustion, Combustion and Flame, 157 (2010), 8, pp. 1456-1466
- [5] Molina, A., et al., Pathways for Conversion of Char Nitrogen to Nitric Oxide during Pulverized Coal Combustion, Combustion and Flame, 156 (2009), 3, pp. 574-587
- [6] Ampah, J. D, et al., Performance Analysis and Socio-Enviro-Economic Feasibility Study of a New Hybrid Energy System-Based Decarbonization Approach for Coal Mine Sites, Science of the Total Environment, 854 (2023), 158820
- [7] Xu, S., et al., Development of a Novel 2-Stage Entrained Flow Coal Dry Powder Gasifier, Applied Energy, 113 (2014), Jan., pp. 318-323
- [8] Qin, S., et al., Modeling, Thermodynamic and Techno-Economic Analysis of Coal-to-Liquids Process with Different Entrained Flow Coal Gasifiers, Applied Energy, 229 (2018), Nov., pp. 413-432
- [9] Fletcher, D. F., et al., A CFD Based Combustion Model of an Entrained Flow Biomass Gasifier, Applied Mathematical Modelling, 24 (2000), 3, pp. 165-182
- [10] Gharebaghi, M., et al., An Investigation into a Carbon Burnout Kinetic Model for Oxy-Coal Combustion, Fuel Processing Technology, 92 (2011), 12, pp. 2455-2464
- [11] Jeong, H. J., et al., CFD Modeling for Coal Size Effect on Coal Gasification in a Two-Stage Commercial Entrained-Bed Gasifier with an Improved Char Gasification Model, Applied Energy, 123 (2014), June, pp. 29 - 36
- [12] Slezak, A., et al., CFD Simulation of Entrained-Flow Coal Gasification: Coal Particle Density/Sizefraction Effects, Powder Technology, 203 (2010), 1, pp. 98-108
- [13] Silaen, A., Wang, T., Effect of Turbulence and Devolatilization Models on Coal Gasification Simulation in an Entrained-Flow Gasifier, International Journal of Heat and Mass Transfer, 53 (2010), 9-10, pp. 2074-2091
- [14] Gerun, L., et al., Numerical Investigation of the Partial Oxidation in a Two-Stage Downdraft Gasifier, Fuel, 87 (2008), 7, pp. 1383-1393
- [15] Kim, M., et al., Numerical Analysis on the Performance of a 300 MW IGCC Coal Gasifier under Various Operating Conditions, Fuel, 257 (2019), 116063
- [16] Du, S. H., et al., Numerical Investigation of Co-Gasification of Coal and PET in a Fluidized Bed Reactor, Renew Energ., 172 (2021), July, pp. 424-439
- [17] Kim, M., et al., Numerical Analysis on the Performance of a 300 MW IGCC Coal Gasifier under Various Operating Conditions, Fuel, 257 (2019), 116063
- [18] Diba, M. F., et al., CFD Modelling of Coal Gasification in a Fluidized Bed with the Effects of Calcination under Different Operating Conditions, Energy, 239, Part C (2022), 122284

- net production rate of species *i* through Wir chemical reaction, [Kmolm⁻³S⁻¹]

Greek symbols

- absorption coefficient α
- dissipation rate of turbulence, $[m^2s^{-3}]$ ε
- dynamic viscosity, (NSm⁻²] μ
- turbulence viscosity μ_{t}
- rate exponent for product reactant species η'
- η'' - rate exponent for product species λ
 - turbulent thermal conductivity, [Wm⁻¹K⁻¹]
- ρ , ρ_p density, density of particles, [kgm⁻³]
- Stefan-Boltzmann constant σ
- scattering coefficient, [m⁻¹] $\sigma_{\rm s}$
- symmetric stress tensor τii

- [19] Sun, H., et al., Numerical Investigation on the Influence of Immersed Tube Bundles on Biomass Gasification in Industrial-Scale Dual Fluidized Bed Gasifier, Fuel, 357, Part A (2024), 129742
- [20] Safronov, D., et al., Numerical Study on Entrained-Flow Gasification Performance Using Combined Slag Model and Experimental Characterization of Slag Properties, Fuel Processing Technology, 161 (2017), June, pp. 62-75
- [21] Fang, N., et al., Improving Mixing and Gasification Characteristics in an Industrial-Scale Entrained Flow Gasifier with a Novel Burner, J. Clean Prod., 362 (2022), 132157
- [22] Wang, B., et al., Numerical Simulations of Solidification Characteristics of Molten Slag Droplets in Radiant Syngas Coolers for Entrained-Flow Coal Gasification, Acs Omega, 6 (2021), 31, pp. 20388-20397
- [23] Vicente, W., et al., An Eulerian Model for the Simulation of an Entrained Flow Coal Gasifier, Appl. Therm. Eng., 23 (2003), 15, pp. 1993-2008
- [24] Alvarez, L., et al., Numerical Investigation of NO Emissions from an Entrained Flow Reactor under Oxy-Coal Conditions, Fuel Processing Technology, 93 (2012), 1, pp. 53-64
- [25] Choi, Y. C., et al., Numerical Study on the Coal Gasification Characteristics in an Entrained Flow Coal Gasifier, Fuel, 80 (2001), 15, pp. 2193-2201
- [26] Watanabe, H., Otaka, M., Numerical Simulation of Coal Gasification in Entrained Flow Coal Gasifier, Fuel, 85 (2006), 12-13, pp. 1935-1943
- [27] Ajilkumar, A., et al., Numerical Modeling of a Steam-Assisted Tubular Coal Gasifier, International Journal of Thermal Sciences, 48 (2009), 2, pp. 308-321
- [28] Huynh, C. V., Kong, S-C., Performance Characteristics of a Pilot-Scale Biomass Gasifier Using Oxygen-Enriched Air and Steam, *Fuel*, 103 (2013), Jan., pp. 987-996
- [29] Hongtao, L., et al., Method of Oxygen-Enriched Two-Stage Underground Coal Gasification, Mining Science and Technology, 21 (2011), 2, pp. 191-196
- [30] Silva, V. B., Rouboa, A., Using a Two-Stage Equilibrium Model to Simulate Oxygen Air Enriched Gasification of Pine Biomass Residues, *Fuel Processing Technology*, 109 (2013), May, pp. 111-117
- [31] Watanabe, H., Kurose, R., Modeling and Simulation of Coal Gasification on an Entrained Flow Coal Gasifier, Advanced Powder Technology, 31 (2020), 7, pp. 2733-2741
- [32] Kong, X., et al., Compartment Modeling of Coal Gasification in an Entrained Flow Gasifier: A Study on the Influence of Operating Conditions, *Energy Conversion and Management*, 82 (2014), June, pp. 202-211
- [33] Seo, H.-K., et al., Effects of Operating Factors in the Coal Gasification Reaction, Korean Journal of Chemical Engineering, 28 (2011), July, pp. 1851-1858
- [34] Du, S.-W., et al., Performances of Pulverized Coal Injection in Blowpipe and Tuyere at Various Operational Conditions, Energy Conversion and Management, 48 (2007), 7, pp. 2069-2076
- [35] Singer, S., et al., The Influence of Gasification Reactions on Char Consumption under Oxy-Combustion Conditions: Effects of Particle Trajectory and Conversion, Proceedings of the Combustion Institute, 34 (2013), 2, pp. 3471-3478
- [36] Chen, C.-J., et al., Numerical Investigation on Performance of Coal Gasification under Various Injection Patterns in an Entrained Flow Gasifier, Applied Energy, 100 (2012), Dec., pp. 218-228
- [37] Unar, I. N., et al., Numerical Simulations for the Coal/Oxidant Distribution Effects between Two-Stages for Multi Opposite Burners (MOB) Gasifier, Energ. Convers. Manage., 86 (2014), Oct., pp. 670-682
- [38] Jones, W. P., Launder, B. E., The Prediction of Laminarization with a Two-Equation Model of Turbulence, International Journal of Heat and Mass Transfer, 15 (1972), 2, pp. 301-314
- [39] Launder, B. E., Spalding, D. B., The Numerical Computation of Turbulent Flows, Computer Methods in Applied Mechanics and Engineering, 3 (1974), 2, pp. 269-289
- [40] Gonzalo-Tirado, C., et al., Gasification of a Pulverized Sub-Bituminous Coal in CO₂ at Atmospheric Pressure in an Entrained Flow Reactor, Combustion and Flame, 159 (2012), 1, pp. 385-395
- [41] Chen, W.-H., et al., Volatile Release and Particle Formation Characteristics of Injected Pulverized Coal in Blast Furnaces, Energy Conversion and Management, 48 (2007), 7, pp. 2025-2033
- [42] Wen, C. Y., Chaung, T. Z., Entrainment Coal Gasification Modeling, Industrial and Engineering Chemistry Process Design and Development, 18 (1979), 4, pp. 684-695
- [43] Wang, L., et al., Numerical Analysis on the Influential Factors of Coal Gasification Performance in Two-Stage Entrained Flow Gasifier, Applied Thermal Engineering, 112 (2017), Feb., pp. 1601-1611
- [44] Kumar, S., et al., Numerical Analysis for Coal Gasification Performance in a Lab-Scale Gasifier: Effects of the Wall Temperature and Oxygen/Coal Ratio, Energies, 15 (2022), 22, 8645

- [45] Chui, E. H., et al., Simulation of Entrained Flow Coal Gasification, Energy Procedia, 1 (2009), 1, pp. 503-509
- [46] Ubhayakar, S. K., et al., Rapid Devolatilization of Pulverized Coal in Hot Combustion Gases, Symposium (International) on Combustion, 16 (1977), 1, pp. 427-436