Numerical Simulation of an Entrained Flow Gasifier by an Eulerian Model

H.P. Xu, H.B. Zhao, and C.G. Zheng

Abstract

In the present work, the Eulerian–Eulerian method is used to simulate a laboratory-scale coaxial entrained flow gasifier in Brigham Young University. The gas turbulence in the reactor is modeled by the k-ε turbulent model, and the particle phase is modeled with the kinetic theory of granular flow (KTGF). In the simulation of turbulent chemical reaction flow, three heterogeneous reactions and five homogeneous reactions are considered. For thermal energy equilibrium, the P-1 radiation model is coupled with the transport equation of energy. Different from conventional Eulerian model, in this work the gradient-diffusion model is introduced to modify the particle distribution because of turbulent diffusion. Furthermore, it is considered the diameter of solid fuels is changing during the gasification. Therefore, a new variable and its transport equation are implemented to capture the coal particle diameter change in this simulation. All submodels above are integrated and realized in the open-source software MFIX. The simulation results have a good agreement with the experimental measurements, and the carbon conversion in the simulation is 82.8 %.

Keywords

Coal gasification • Numerical simulation • Gradient-diffusion model • Diameter change

With the strict demand of environment protection, more and more attention has been paid to the coal clean technology (CCT). Coal gasification is an important technology of CCT instead of burning coal directly. Many works have been done to study the gasification theory and improve the gasification process. According to research conducted by experiments and numerical simulations, the entrained flow gasifier is the main reactor for coal gasification [1–3].

The syngas composition and temperature distribution can be received based on CFD simulation due to the more affordable and enhanced computation hardwares. Therefore, the CFD simulation is used as a tool for design and optimization of reactor in industries. Chen et al. [4] used the multi-solids process variable method to simulation a pilot-scale gasifier and analyzed the effect of the different operating parameters on gasification results. Watanabe et al. [5] developed the extended model to design and optimize coal gasifiers. Snider et al. [6] conducted the three-dimensional simulation using the computational particle fluid dynamic method and studied the energy transport between phases.

However, the particle mass is changing in the real operation. Many modified submodels are introduced to capture the mass loss in the simulation work. Vascellari et al. [7] investigated the particle diameter changing submodel modeling coal pyrolysis and char conversion, and the results of four different rank coals validated the method. The gas and particles were described by two separate PDF transport equations in the Stoellinger el al. work [8], and the particle diameter change due to pyrolysis and char reaction was modeled with reaction rate. Kumar and Ghoniem [9] introduced the flame model to modify the char reaction model and compared its results with the results of different models. The particles were described with the Lagrangian method in the simulation above. The Eulerian model is another method to simulate the entrained flow coal gasifier and costs less

H.P. Xu · H.B. Zhao (✉) · C.G. Zheng
State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan, 430074, China
e-mail: klinsmannzhb@163.com

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time than the Lagrangian method. Vicente et al. [10] simulated the entrained flow coal gasifier using the Eulerian method, and the results showed a good agreement with the experimental measurements.

In this work, the Eulerian model is integrated with other submodels to simulate the turbulent chemical reaction in the coal gasifier. The model is validated against the laboratory-scale gasifier.

The work is structured as follows: Sect. 2 shows the full numerical model to simulate the turbulent chemical reaction flow. Section 3 provides the simulation case description, and the last two sections compare the results with experimental measurements and then have a conclusion.

1 Numerical Model

1.1 Gas–Solid Turbulent Flow Model

The present model is integrated into the open code software MFIX. Both the gas and particles are described as Eulerian model, the transport equations for both phases. The standard k-ε turbulent model captures the turbulent flow in the gasifier. The equations [11] can be reduced one Eulerian conservation equation as follows:

$$\frac{\partial(\alpha_i\rho_i\Phi_i)}{\partial t}+\frac{\partial(\alpha_i\rho_i\Phi_i V_i)}{\partial x_j}-\frac{\partial(\alpha_j\rho_j\Gamma_j\Phi_j)}{\partial x_i}= S_{\Phi_i}+f_{ij}(\Phi_j-\Phi_i)+m_{i\leftrightarrow j}\Phi \tag{1}$$

where φ represents different variable of gas and particle phases, τ is the diffusion coefficients, S means the source term, f is drag coefficient acting on the particle, and the last term in the right-hand side is the mass transfer for both phases.

The effect of the turbulent fluctuation [12] in the reactor on particle dispersion is included in the present model, and the turbulent correlation is contained in the source term:

$$\overline{\alpha_s' U_s'}=-\frac{\upsilon_t}{\sigma_s}\frac{\partial\alpha_s}{\partial x_i} \tag{2}$$

1.2 The Radiation Model

The radiation heat transfer in the gasifier is important and modeled using the P-1 model [13]. The radiation model is

$$-\nabla q_r=aG-4a\sigma T^4 \tag{3}$$

where

$$q_r=-\frac{1}{3(a+\sigma_s)-C\sigma_s}\nabla G \tag{4}$$

q_r is the radiation heat flux, σ and σ_s are the Stefan–Boltzmann constant and scattering coefficient, and G is the incident radiation. The radiation from the wall to gasifier is expressed as:

$$q_{r,w}=-\frac{4\pi_w\frac{\sigma T_w}{\pi}-(1-\rho_w)G_w}{2(1+\rho_w)} \tag{5}$$

1.3 The Particle Size

During the gasification process, the coal particle mass is decreased. In this work, the particle density keeps constant while a size-calculation method developed by Fueyo et al. [14] is used to capture the particle diameter decreasing. A new variable Φ_s equals to the reverse of solid phase fraction and is determined from the Eulerian transport equation as follows:

$$\frac{\partial}{\partial t}(\alpha_s\rho_s\phi_s)+\frac{\partial}{\partial x_i}(\alpha_s\rho_s U_{i,s}\phi_s)= \frac{\partial}{\partial x_i}(\Gamma_s\phi_s)+S_{\phi_s} \tag{6}$$

and the particle diameter is determined as

$$D_p=D_0\phi^{-1/3} \tag{7}$$

1.4 Coal Pyrolysis

In the process of gasification, the complex turbulent multiphase reaction flow is reduced to different submodels. The coal pyrolysis is modeled with the two-equation method [15].

$$\begin{aligned}&\text{Coal}\xrightarrow{k_1}(1-Z_1)S_1+Z_1V_1\\&\text{Coal}\xrightarrow{k_2}(1-Z_2)S_2+Z_2V_2\\&k_i=A_i\exp(-E_i/RT_p)\end{aligned} \tag{8}$$

The heterogeneous reactions include:

$$\mathrm{C}+1/2\mathrm{O_2}\rightarrow\mathrm{CO} \tag{R1}$$

$$\mathrm{C}+\mathrm{CO_2}\rightarrow 2\mathrm{CO} \tag{R2}$$

Table 1 Kinetic parameters

Index	Kinetic reaction
R1	$k = T_s(-1.68 \times 10^{-2} + 1.32 \times 10^{-5} T_s)$
R2	$k = 4.4T[CO_2]^{0.6} \exp(-1.62 \times 10^5/RT)$
R3	$k = 1.33T[H_2O]^{0.6} \exp(-1.47 \times 10^5/RT)$
R4	$k = 3 \times 10^8[CH_4][H_2O] \exp(-1.25 \times 10^5/RT)$
R5	$k = 6.8 \times 10^{15}T^{-1}[H_2][O_2] \exp(-1.67 \times 10^5/RT)$
R6	$k = 2.24 \times 10^{12}[CO][O_2]^{0.25}[H_2O]^{0.5} \exp(-1.67 \times 10^5/RT)$
R7	$k = 4.4 \times 10^{11}[CH_4][H_2O] \exp(-1.25 \times 10^5/RT)$
R8	$k = 2.75 \times 10^9[CO][H_2O] \exp(-8.37 \times 10^9/RT)$

$$C + H_2O \rightarrow CO + H_2 \quad (R3)$$

The heterogeneous reaction rates are modeled by random core model [16]. In this model, both the particle structure and chemical reaction are included as follows:

$$\begin{aligned} \frac{dx}{dt} &= AP^n(1-x)\exp(-E/RT) \\ &\quad \sqrt{1-\Psi\ln(1-x)} \\ x &= 1 - M_{ci}/M_{c0} \end{aligned} \quad (9)$$

where x is the carbon conversion, A is the frequency factor, E is the activation energy, P is the partial pressure of the reaction gas, and Ψ is the particle structure parameter.

For heterogeneous reaction, the reaction rate is limited due to the bulk diffusion:

$$\frac{dm_{ci}}{dt} = -\frac{\upsilon Sh M_c D_i}{RTd_p} A_p P_i \quad (10)$$

where the v is the stoichiometric coefficient, Sh is the Sherwood number, and T is the mean temperature of the gas and particles.

The homogeneous reactions taken into consideration are as follows:

$$CH_4 + 1/2O_2 \rightarrow CO + 2H_2 \quad (R4)$$

$$H_2 + 1/2O_2 \rightarrow H_2O \quad (R5)$$

$$CO + 1/2O_2 \rightarrow CO_2 \quad (R6)$$

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad (R7)$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (R8)$$

The eddy-dissipation reaction rate is taken as the turbulent effect, and the net rate equals to the minimum between the Arrhenius and eddy-dissipation model [17].

$$\begin{aligned} R_{eff} = \min[&AT^n \exp(\frac{-E}{RT})[X]^a[Y]^b, \\ &C_\mu \rho \frac{k}{\varepsilon} \min(m_{fu}, m_{ox}/\phi)] \end{aligned} \quad (11)$$

All the Arrhenius chemical reaction parameters in the model above are determined from the references [1, 18] (Table 1).

2 Case Description

In the present work, the integrated model above is verified by the gasifier from Brigham Young University (BYU) as shown in Fig. 1. The simulation is done in cylindrical coordinate. The diameter of the primary and second nozzle is 1.3 and 2.85 cm, respectively. The mesh size is refined in the axis of gasifier and near the inject nozzle. The initial condition is given with high temperature with the mixture of CO_2 and H_2O. The heat loss in the wall is negligible. Table 2 shows the proximate and elemental analysis of the coal and the operating condition used in the simulation.

3 Result and Discussion

The contour of temperature in the simulation with the integrated models is displayed in Fig. 2, and the temperature gradient along the axis is high. The high-temperature zone is the combustion zone due to the combustion of the released volatiles, and a large amount of thermal energy is delivered for the gasification; therefore, the temperature drops in the next gasification zone. Figure 3 shows the temperature distribution along the axis. Due to the fast combustion of volatiles, the temperature peak occurs in the initial part of the gasifier. And the simulation temperature has a good agreement with the experimental measurement at the gasifier exit.

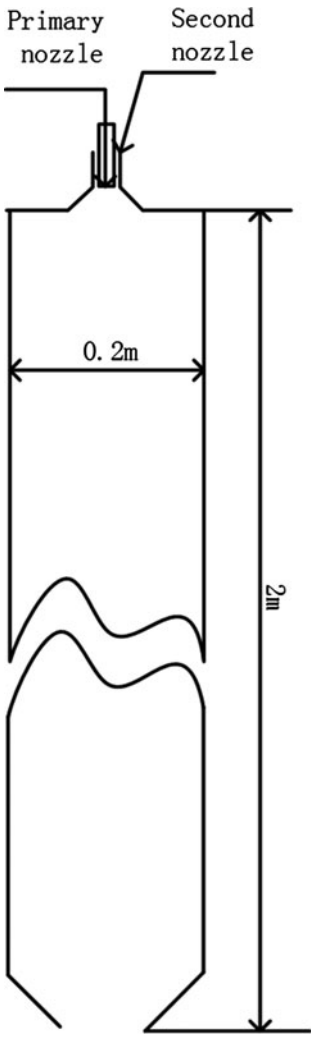

Fig. 1 The simulation sketch of BYU gasifier

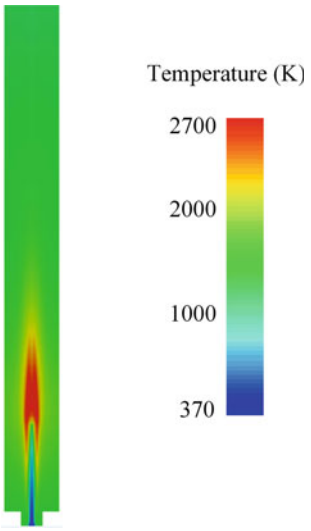

Fig. 2 The temperature contour

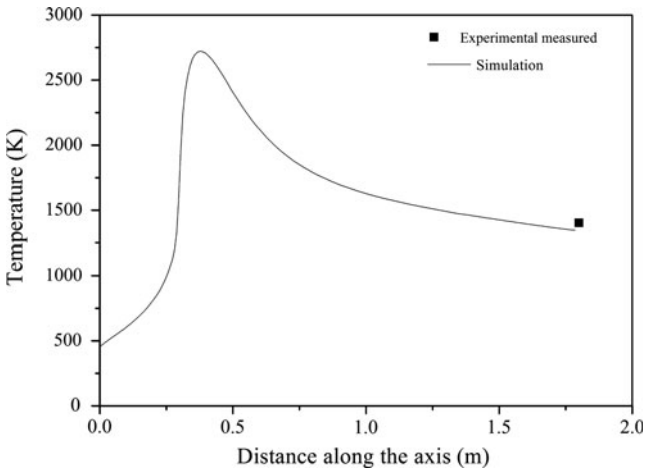

Fig. 3 The temperature along the reactor axis. Symbols mean the experimental measurement at the reactor exit

Table 2 Simulation condition

Utab bituminous		Operating Conditions	
Proximate analysis		Primary flow rate(kg/s)	0.00729
Moisture	2.4	Primary components	
Ash	8.3	O_2	0.85
Volatiles	45.6	Ar	0.126
FC	43.7	H_2O	0.024
Elemental analysis			
Ash	8.5	Sec. flow rate (kg/s)	
C	71	H_2O	0.00184
H	6	Primary particle loading	
O	12.7	0.910	
N	1.3	–	
S	0.5	–	

Figure 4 displays the molar fraction of species in the syngas. Agreement with the experimental measurements is good for the prediction results, although some mismatch exists near the primary nozzle exit. Kumar et al. [9] thought the mismatch was made due to RANS model, because the RANS method may not capture the transient turbulent information detailed. In his work, the RANS method was used to depict the turbulent flow, and the prediction syngas matched with the results in the present work.

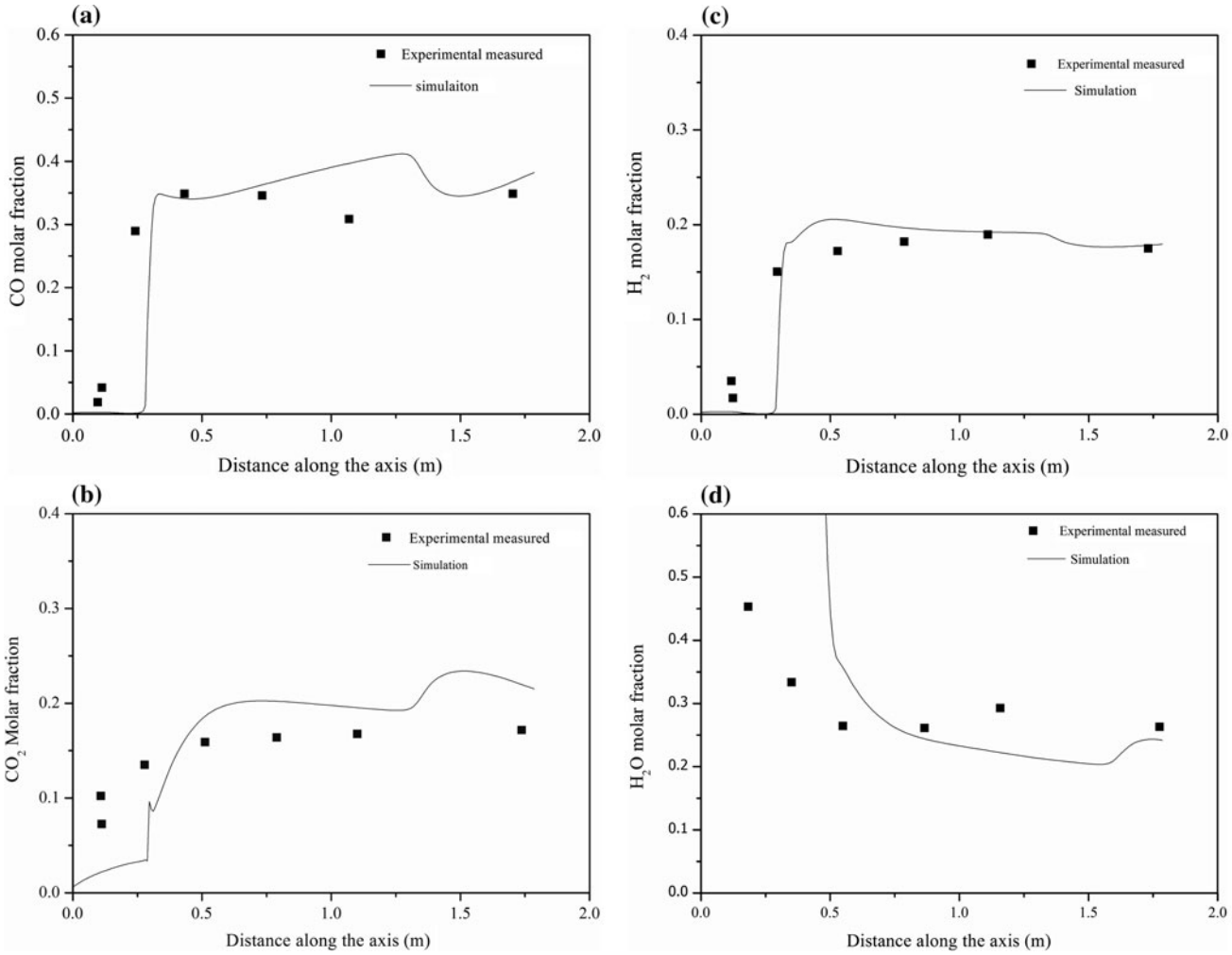

Fig. 4 Composition of species of prediction syngas with experimental measurements along the gasifier axis

4 Conclusion

Compared with the experimental measurements, the Eulerian method is validated to simulate the coal gasification in the entrainedflowgasifier.Inordertocapturetheparticlemotioninthe reactor,thegradientmodelcanimprovetheparticlediffusion.The particle diameter changing is modeled by introducing a new variable. Based on the open-source software, other models referred to multiphase flow and chemical reaction can be incorporated to improve the Eulerian method.

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