Simulation Research on Temperature and Components’ Concentration Fields of A Moving Bed Gasifier

Long Wu

Dept. Physics and Electromechanical Eng., Sanming University, 25 Jingdong Road, Sanming, 365004, China

Abstract

The briquette oxygen-enriched gasification technology developed with traditional moving bed gasifier is a developing technology in line with our strategic policy of energy. In order to master the flow and reaction states of the existing gasifier, a computational fluid dynamics software was utilized to simulate in this paper. Based on the geometric model with atmospheric pressure gasifier corresponding to the actual operation, the two-way k-\(\varepsilon\) model, the fluid transport model and SIMPLE method was adopted to solve N-S equation and P1 model, so as to simulate internal temperature and components’ concentration fields. The simulation results provide theoretical foundation for further study on combustion in the gasifier, optimization of combustion process and guidance for production process improvement.

Keywords: Moving bed gasifier; temperature field; components’ concentration fields; computational fluid dynamics; briquette oxygen-enriched gasification technology

1. Introduction

Moving bed gasifier is a key gasification equipment in many medium and small sized coal chemical, fertilizer and energy plants. Moving bed gasification technology has been improved in many years and it is showed maturing, but also encountered serious technical bottlenecks, while required further improvement according to our energy saving policy. The briquette oxygen-enriched continuous moving bed coal gasifier is a new gasification technology and has many complex synthesis processes contained many phenomena such as fluid flow, multiphase flow problem, heat transfer, mass transfer and
combustion reaction [1]-[3]. These complex processes are strongly coupled together so as the complex states in the gasifier need to be determined [4][5].

In this paper, the briquette made by a local low-volatile coal resource was combined with the oxygen-enriched continuous gasification technology. Base on existing full and accurate model which could describe many complex processes, the computational fluid dynamics (CFD) software was used to simulate three-dimensional multiphase flow, heat transfer and combustion process in the furnace, so as to obtain temperature and some components concentration fields, in order to find out some key parameters in the process of coal chemical industry and understand the various range of moving bed coal gasification process (for example, oxidation zone, deoxidation zone, etc), various chemical reaction rates and many other nonlinear factors. Numerical simulation has many merits such as low cost, fast master and short period, etc., and can be applied to predict all kinds of data status during the operation of the gasifier. The simulation results can provide theoretical basis and further guidance in design and production for the gasifier.

2. Numerical Simulation Method

The bottom of the gasifier is the entry plane of steam and oxygen-enriched air. A large number of oval-shaped coal briquettes are filled in the gasifier. Considering simplification of the calculation and local coal status, the oval-shaped briquettes were replaced by round briquettes with 50 millimeters of average diameter and properties of low volatile coal was selected in the menu of the computational fluid dynamics software. The products of chemical reactions are discharged through the top plane of the gasifier. The inlet diameter of cone-shaped bottom is 2000 millimeters and the cone angle is 30 degrees. The internal diameter of the gasifier is 3000 millimeters and the height is 6000 millimeters. Consider the symmetry of computational domain, internal flow and chemical reactions, quarter gasifier was acted as model of math region in case heavy simulation load.

It is well known that grid numerical accuracy and convergence speed would be directly influenced by division mesh quality of computing area. In this study, using structured grid, the quarter geometric model of the gasifier was discretized and formed to 477687 individual cells. Fig. 1 is the meshing results automatically of computational domain.

![Fig. 1. Mashing of computational domain](image)

In the simulation process, some mathematical model such as continuity equation, energy equation, momentum equation and component equation should be required. All equations are as follows [6].

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = S_i
\]  

(1)

In above, \( S_i \) is the mass joined from the dispersed secondary phase to the continuous phase.

\[
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho u_i (\rho E + p))}{\partial x_i} = \frac{\partial}{\partial x_i} \left( k_{eff} \frac{\partial T}{\partial x_i} + \sum \gamma J_i + u_i (\tau_{ij})_{eff} \right) + S_i
\]  

(2)
In above, \( k_{\text{eff}} \) is effective thermal conductivity; \( J_j \) is diffusion flux of the component \( j' \); \( S_h \) is chemical reaction heat, and other volume of heat source term user-defined.

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} (\mu \frac{\partial u_i}{\partial x_j}) + \rho u_i F_i
\]  

(3)

\[
\nabla \cdot (\rho \nabla \nu_j) = -\nabla \cdot J_j + R_j
\]  

(4)

In above, \( \nu_j \) is mass fraction of \( i \)-component; \( J_j \) is diffusion fluxes of \( i \)-component; \( R_j \) is net mass production rate caused by chemical reactions of \( i \)-component.

Assume coal porosity is \( \gamma \), component equation in briquette region is as follows.

\[
\nabla \cdot (\gamma \rho \nabla \nu_i) = -\nabla \cdot J_i + R_i
\]  

(5)

In the gasifier, the vapor and oxygen-enriched air act as continuous phase and briquette as the discrete phase. The flow involves numerical simulation of multiphase. In this study, based on Euler/Euler model originated from pseudo-fluid assumption, the briquette owned to discrete phase is now treated as a continuous media and has similar dynamics to gas so as to be describe with same fluid dynamics equations.

The SIMPLE algorithm means that the semi-implicit algorithm of pressure coupled equations built by Patankar and Spalding solution was adopted to solve flow field in the gasifier so as to obtain Neville-Stokes equation. The Internal flow of gasifier is turbulence. The turbulence model uses the two-equation model of realizable \( k-e \) method. The transport equation of \( k \) and \( \varepsilon \) in the model is as follows.

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \left( \mu + \frac{\mu}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) \nabla \cdot F_i - \rho e
\]  

(6)

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \left( \mu + \frac{\mu}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) + \rho C_p E \varepsilon - \rho C_p G \frac{k^{3/2}}{k + \sqrt{\varepsilon}}
\]  

(7)

Before initialization, the entrance rates of turbulent kinetic energy \( k \) and turbulent kinetic energy dissipation \( \varepsilon \) can be estimated based on the following equation.

\[
k = \frac{3}{2} (\bar{u}^\prime T)^2
\]  

(8)

\[
\varepsilon = C_p \frac{k^{1/4}}{0.07 L}
\]  

(9)

In above, \( \bar{u}^\prime T \) is average rate of entrance. \( L \) is characteristic length which can be calculated by hydraulic diameter. \( T \) is turbulence intensity. \( C_p \) equals to 0.09.

The numerical simulation for a gasifier involve some boundary conditions such as velocity inlet, pressure outlet, symmetry and wall boundary, etc. The gas of gasifier inlet is oxygen-enriched air and vapor. The two phases’ velocity and temperature were set to 0.1 m/s and 373K. The nitrogen and the briquette were set as the first and second phases. The gas of gasifier outlet consists mainly of carbon monoxide, carbon dioxide, hydrogen and nitrogen. These phases’ temperature were set to 800K. Because only a quarter gasifier was adopted to simulate, the symmetric boundary conditions would be involved. No-slip wall boundary conditions was selected. The tangential velocity and the turbulent flow of wall surface are all zero. The wall surface is impermeable and insulation. The standard wall function is set in near-wall region. P1 model is selected in the menu of radiation and convection heat transfer. Species Transport is selected in transport model. Simulation involves eight reaction types, as shown in table 1 [7].

Each volume reaction rate \( k_i \) in the gasifier was defined by a given macro of DEFINE_VR_RATE in the UDF definition environment. The magnitude were calculated by following equations, respectively.
Table 1. Reaction type and rate

<table>
<thead>
<tr>
<th>Reaction type</th>
<th>Volume reaction rate ( k_i )</th>
<th>Reaction type</th>
<th>Volume reaction rate ( k_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{C} + \text{O} \rightarrow \text{CO} )</td>
<td>( k_1 )</td>
<td>( \text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O} )</td>
<td>( k_5 )</td>
</tr>
<tr>
<td>( \text{C} + \text{CO} \rightarrow 2\text{CO} )</td>
<td>( k_2 )</td>
<td>( \text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2 )</td>
<td>( k_6 )</td>
</tr>
<tr>
<td>( \text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2 )</td>
<td>( k_3 )</td>
<td>( \text{CO}_2 + \text{H}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} )</td>
<td>( k_7 )</td>
</tr>
<tr>
<td>( \text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2 )</td>
<td>( k_4 )</td>
<td>( \text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2 )</td>
<td>( k_8 )</td>
</tr>
</tbody>
</table>

While a reaction between gas and solid is occurred, volume reaction rate \( k_i \) is as follows [8].

\[
k_i = \frac{1}{k_{di}} + \frac{1}{k_s} + \frac{1}{k_{da}}(Y - 1)\left( p_i - p_i' \right) \quad (i = 1, 2, 3)
\]

In above, \( k_{di} \) is rate constants characterized gas diffusion to the carbon surface. \( k_s \) is chemical reaction rate constant of carbon surface. \( k_{da} \) is diffusion rate constant of gas through the briquette to the outer surface of carbon, and \( k_{da} = k_{da}e^{-2\varepsilon} \). \( \varepsilon \) is porosity of accumulated briquette. \( Y \) is ratio of unreacted briquette and carbon diameter. \( p_i \) is Partial pressure of gas component. \( p_i' \) is effective partial pressure of the reversible reaction.

While a reaction between gas and gas is occurred, volume reaction rate \( k_i \) is as follows.

\[
k_i = k_i \exp\left( -\frac{E}{RT} \right)C_1C_2 \quad (i = 4, 5, 6, 7 \text{ or } 8)
\]

In above, \( k_i \) is frequency factor. \( E \) is Activation energy. \( R \) is universal gas constant. \( T \) is gas temperature. \( C_1 \) and \( C_2 \) are reactant gas concentration.

3. Numerical Analysis

The simulation was carried out in a Hewlett-Packard 6600 workstation, which has four 2.0G CPU and 8.0G memory. In operating, the simulation area was divided into four regions and each region was parallel calculated by a CPU.

It is shown from the temperature distribution of Fig. 2 that high temperature region should be oxidation zone above the slag zone which near the bottom of gasifier. In oxidation zone, mainly oxidation of carbon and oxygen is reacted and a lot of heat is emitted so as to achieve to the temperatures of 1500 K. The deoxidation zone is above the oxidation zone. In deoxidation zone, mainly deoxidation reaction is emerged. The heat is absorbed in deoxidation process and the temperature of top gasifier is decreased gradually.

Fig. 2. Temperature distribution in the gasifier
Fig. 3. Distribution of CO₂ in the gasifier

Fig. 4. Distribution of CO in the gasifier

Fig. 5. Distribution of H₂ in the gasifier
Fig. 3 shows that the magnitude of carbon dioxide has been increased along with carbon oxidation in a high degree in initial stage. The red zone shows the maximum volume fraction is about 79%. With the height of the gasifier is increased, the volume of fraction is reduced gradually because of deoxidation of carbon dioxide.

Fig. 4 and Fig. 5 show that the magnitude of carbon monoxide and hydrogen in bottom and middle of gasifier are lower than the top because adequate oxygen creates oxidation reaction mainly in the region and a small amount of carbon monoxide is produced by incomplete combustion of carbon. To the top of the gasifier, a lot of carbon monoxide and hydrogen are emerged by deoxidation reaction. So the concentration of carbon dioxide and hydrogen are increased rapidly.

4. Conclusion

The simulation results show that oxidation zone in the gasifier is slightly wider than the actual oxidation area compared to the production data. The concentration distribution of hydrogen has an error to the actual distribution of the gasifier. The temperature and concentration distributions of other components are meet current situation basically.

The above analysis of results shows that CFD software utilized to simulate briquette oxidation and combustion in a continuous fixed-bed gasifier is feasible. The results has a certain significance for continuous gasification research and actual production of the fixed bed gasifier.

Based on numerical simulation, the current actual problem of high temperature at gasifier exit can be decreased by adding a certain amount of vapor at the gasifier entrance.

Acknowledgements

Financial support from Education Department of Fujian Province (JA08238, HX200804) and Science and Technology Department of Fujian Province (2010H6020, 2008H0009 ) are highly appreciated. The helpful comments from two anonymous reviewers are also gratefully acknowledged.

References


