Numerical Simulation of Biomass Gasification in a Fluidized Bed
Aiping Shi\textsuperscript{1a}, Yixiang Pang\textsuperscript{2b}, Guanjie Xu\textsuperscript{2c}, Cheng Li\textsuperscript{2d}

1. School of Agricultural Equipment Engineering, Zhenjiang 212013, China; 2. School of Energy and Power Engineering, Zhenjiang 212013, China
\textsuperscript{a}ashap@ujs.edu.cn, \textsuperscript{b}503852295@qq.com, \textsuperscript{c}1329389523@qq.com, \textsuperscript{d}1181099850@qq.com

Keywords: Biomass gasification, simulation, Fluent, fluidized bed

Abstract. In order to study the effects of mass ratio of steam to biomass ($m_\text{S}/m_\text{B}$) and temperature on the gas composition, a model was developed to simulate the biomass-steam gasification process using Fluent in a fluidized bed. The simulated results showed that the volume fraction of H\textsubscript{2} increased firstly and then remained constant with the increase of $m_\text{S}/m_\text{B}$, and that of CO decreased firstly and then got to be stable. The results indicated that the temperature benefited biomass gasification, the volume fraction of H\textsubscript{2} and CO rised. The results of simulation basically agreed with that of experiments. Therefore, the results proved that the dynamical model could be used to simulate the biomass gasification in fluidized bed.

1 Introduction

The development of biomass energy is a research emphasis in the field of energy utilization in the 21st century. Biomass of modern use can be divided into the following basic types: Direct combustion, pyrolysis, gasification, liquefaction and ester exchange\cite{1}. Currently, the development and application of gasification technology research is very valuable all over the world\cite{2,3}. Based on the minimum Gibbs free energy, many scholars simulate the process of fuel gasification using Aspen Plus\cite{4,5}. However, Aspen Plus could not reflect the flow process of reactor and the reactor structure on the influence of the gasification process. Fluent software is one of the widely used CFD software to solve the problems at the aspect of chemical reactions and flow. There are many researchers study biomass gasification technology based on Fluent software\cite{6,7,8}. In dynamic model gasifier, gasification reaction dynamic model, reaction heat and proton transfer model in the process of the gas solid two phase fluid dynamic model phase coupling. Dynamic model involves the mechanism of biomass pyrolysis and gasification, and can simulate the gasification process in different time, different position of reaction conditions, with the development of computational fluid dynamics, dynamics model will become the inevitable trend of model development.

In the presented study, a biomass fluidized bed dynamic model based on Fluent software was established to study the effect of mass ratio of steam to biomass and temperature on the gas composition. This study provides a theoretical basis for biomass gasification process.

2 Mathematical model

Fluent6.3 software is used to establish the model of biomass gasification in this study. Volume reaction of component transport is used to simulate gas homogeneous reaction in the progress of gasification. Limited rate/eddy dissipation model is adopted in rate process model. Standard $k-\varepsilon$ model is adopted in turbulence model. $P1$ radiation model is adopted in radiation heat transfer model.

2.1 Gas-solid fluid dynamics model

CFD modeling of biomass gasification processes describes fluid flow, heat and mass transfer and chemical reaction process. The basic equations include mass, momentum, energy, and transport
equations components are as follows[10]:

\[ \frac{\partial \rho}{\partial t} + \nabla (\rho \vec{u}) = S_p \]  

(1)

\[ \frac{\partial (\rho \vec{u})}{\partial t} + \nabla (\rho \mu \vec{u}) = -\nabla p + \nabla (\mu \nabla \vec{u}) + S_N \]  

(2)

\[ \frac{\partial (\rho H)}{\partial t} + \nabla (\rho u H) = \nabla (\lambda \nabla T) + S_H \]  

(3)

\[ \frac{\partial (\rho Y_f)}{\partial t} + \nabla (\rho u Y_f) = \nabla (D \nabla (\rho Y_f)) + S_y + R_f \]  

(4)

In the formula, \( \rho \) — Density, \( \text{kg/m}^3 \); \( t \) — Time, \( \text{s} \); \( \vec{u} \) — Instantaneous velocity, \( \text{m/s} \); \( p \) — The partial pressure of the gas component, \( \text{Pa} \); \( \mu \) — Fluid dynamic viscosity, \( \text{Pa} \cdot \text{s} \); \( H \) — Fluid specific enthalpy, \( \text{J/kg} \); \( T \) — Temperature, \( \text{K} \); \( \lambda \) — Thermal conductivity of the fluid, \( \text{W/(m-K)} \); \( Y_f \) — Mass fraction of component; \( D \) — Diffusion coefficient of component; \( R_f \) — Production rate per unit volume within the component, \( \text{kg/(s·m}^3 \) \); \( S_p \) — Source term, \( \text{kg/(s·m}^3 \) \); \( S_N \) — Source term, \( \text{N/m}^3 \); \( S_H \) — Source term, \( \text{J/(s·m}^3 \) ; \( S_y \) — Source term, \( \text{kg/(s·m}^3 \) .

2.2 Gasification reaction model

Normally, we consider that Biomass gasification in a fluidized bed are through the following steps: (1) Biomass particles under the environment of high temperature rapid decompose and then become coke, tar and gas; (2) the second reaction occur in gaseous product; (3) the tar crack and coke gasified. Gas-solid product produced by Biomass pyrolysis took complex gas phase and solid complex reaction under the environment of high temperature in gasifier. Main consideration of chemical reaction is as follows:

R1 \[ C + O_2 = CO_2 \]

R2 \[ CO + \frac{1}{2} O_2 = CO_2 \]

R3 \[ CH_4 + 2O_2 = CO_2 + 2H_2O \]

R4 \[ CO_2 + H_2 = CO + H_2O \]

R5 \[ 2H_2 + O_2 = 2H_2O \]

R6 \[ C + H_2O = CO + H_2 \]

R7 \[ C + CO_2 = 2CO \]

R8 \[ CO + H_2O = CO_2 + H_2 \]

R9 \[ CH_4 + H_2O = CO + 3H_2 \]

Model chemical reaction kinetics parameters are shown in Table 1.

In this paper, the Arrhenius model was used to define the reaction process, Arrhenius constant is obtained as follows:

\[ K_i = A e^{-E_i/(RT)} \]  

(5)

where \( K_i \) is Arrhenius constant; \( E_i \) is activation energy, \( \text{kJ/mol} \); \( A \) is pre-exponential factor; \( R \) is molar gas constant, \( 8.314 \text{J/(mol·K)} \); \( T \) is temperature, \( K \).
Table 1 Parameters of chemical dynamics

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Activation energy $E_i$ (J/mol)</th>
<th>Pre-exponential factor $A_i$ (1/s)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>97400</td>
<td>$4.8 \times 10^4$</td>
<td>[9]</td>
</tr>
<tr>
<td>R2</td>
<td>99760</td>
<td>$3.09 \times 10^5$</td>
<td>[9]</td>
</tr>
<tr>
<td>R3</td>
<td>930400</td>
<td>$2.552 \times 10^{14}$</td>
<td>[9]</td>
</tr>
<tr>
<td>R4</td>
<td>398300</td>
<td>$6.245 \times 10^{14}$</td>
<td>[9]</td>
</tr>
<tr>
<td>R5</td>
<td>99760</td>
<td>$8.83 \times 10^8$</td>
<td>[9]</td>
</tr>
<tr>
<td>R6</td>
<td>232000</td>
<td>$1.05 \times 10^7$</td>
<td>[9]</td>
</tr>
<tr>
<td>R7</td>
<td>245000</td>
<td>$1.18 \times 10^7$</td>
<td>[9]</td>
</tr>
<tr>
<td>R8</td>
<td>369000</td>
<td>$2.978 \times 10^{12}$</td>
<td>[9]</td>
</tr>
<tr>
<td>R9</td>
<td>30000</td>
<td>$6.9888 \times 10^3$</td>
<td>[10]</td>
</tr>
</tbody>
</table>

3 Calculation method

3.1 Model hypothesis

Due to the fact that the gasification of biomass gasifier is very complex, we simplified model and put forward the following hypothesis: (1) Biomass is dry ash-free basis, considering only tar and volatile; (2) Volatile of biomass separate out in a moment at high temperature; (3) CO, H2, CH4, CO2, H2O, N2 and O2 are considered during the gasification process.

3.2 Boundary conditions

Boundary conditions of the simulation were set as, the operating pressure was 101325 Pa, the environment temperature was 300 K and the gasifier export was pressure export. Gasifier wall on the infiltration is without velocity slip and quality conditions. Wall temperature is set to 500K.

3.3 The reactor structure and grid

Experiment equipment used is a biomass fluidized bed gasifier. Experiment system is shown in Figure 1. It is mainly composed of gasification device, feeding device, air supply device, separation and purification device and gas storage device. In this study, the diameter of the bottom of the biomass gasifier is 150 mm, top diameter is 300 mm and height is 1600 mm. In the experiment, gasification medium vapor entered the fluidized bed from the bottom. Biomass entered the fluidized bed from biomass inlet the side of the fluidized bed. Gas product discharged from the gasifier outlet at the top of the profile. In the experiment, vinegar residue was used for biomass material of the simulation study. Currently, recycle of vinegar residue is rare. Its material properties and parameters are shown in Table 2. Bed material of the experiment is fluidized bed boiler slag, its average particle diameter is 4mm. Vinegar bad average particle size is 5mm.

The model adopted tetrahedron and hexahedron mesh. It had a total of 39732 mesh. Biomass gasifier simplified mesh diagram is shown in Figure 2.

Fig.1 Simple system diagram of biomass fluidized bed gasification
4 Calculation results and analysis

4.1 gas composition distribution
Simulation of seven conditions were studied. The influence of mS/mB and gasification temperature on biomass gasification was investigated and the simulation value with the experimental value were compared as well. Operating conditions are shown in Table 3. The longitudinal section of Y=0 section was taken to describe the gas volume fraction. Figure 3 shows the gas volume fraction distribution of working condition 2. The volume fraction of H2 rised firstly and then remained constant, and that of CO decreased firstly and then got to be stable. Since the reaction proceeded, the temperature in the gasification furnace decreased, the content of CO2 increased due to reduction reaction of CO2(R7).

Table 3 Parameters for calculation with various mS/mB

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Condition 1</th>
<th>Condition 2</th>
<th>Condition 3</th>
<th>Condition 4</th>
<th>Condition 5</th>
<th>Condition 6</th>
<th>Condition 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>mS/mB</td>
<td>1.23</td>
<td>1.53</td>
<td>1.80</td>
<td>2.47</td>
<td>3.57</td>
<td>1.53</td>
<td>1.53</td>
</tr>
<tr>
<td>Steam (kg/s)</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>Vinegar residue addition rate (kg/s)</td>
<td>0.004075</td>
<td>0.003275</td>
<td>0.002775</td>
<td>0.002025</td>
<td>0.0014</td>
<td>0.003275</td>
<td>0.003275</td>
</tr>
<tr>
<td>Reaction temperature (K)</td>
<td>1225</td>
<td>1225</td>
<td>1225</td>
<td>1225</td>
<td>1225</td>
<td>1175</td>
<td>1275</td>
</tr>
</tbody>
</table>
4.2 Influence of m_s/m_B on volume fraction of gas

Figure 4 shows the volume fraction of the gas components in the different conditions 1~5 (mS/mB = 1.23~3.57). We compared the simulation value with the experimental value. As can be seen from simulation value in Fig. 4, the content of H2 gas was 40.41% ~ 46.67%. The content of CO gas was 20.55%~26.77%. The amount of CH4 gas was 8.03%~11.25%. The content of CO2 gas was 7.76%~10.44%. The content of (H2+CO) gas was 60.96%~73.44%. It indicates that H2 and CO gas is the most important component of the product gas.

Under the constant temperature condition, when mS/mB = 1.23~2.47, water gas reaction (R6) prompted the volume fraction of H2 and CO increasing, but a small amount of water vapor water reaction with CO (R8) which prompted the volume fraction of CO decreased with the increase of mS/mB, the general trend of the volume fraction of H2 increased, however the volume fraction of CO decreased. The content of (H2+CO) gas increased. The content of CH4 gas had trace increace with the increase of mass ratio of steam to biomass. It is observed that, the volume fraction of gas composition changed little since the arrival of saturated steam when mS/mB changed from 2.47 to 3.57. Different results between the simulation value and the experimental value in Figure 4 were due to not taking tar into account in the simulation. And as a result of the existence of tar in experiment, the tar cracked at high temperature, generated CO gas, therefore, the value of the CO in the simulation was slightly lower than that in the experiment.

![Fig. 3 Distribution of mole fraction of gas species in condition 2](image)

![Fig. 4 Effect of m_s/m_B on gas component](image)
4.3 Effects of temperature on volume fraction of gas

Figure 5 shows the volume fraction of gas composition of the condition 2, 6, 7 (temperature = 1175~1275K). The simulation value was compared with the experimental value. Within the scope of the fluidized bed gasification temperature, gasification reaction belonged to control area, when the gasification increased 20K ~ 30K, gasification reaction rate increased nearly one time, so gasification temperature had a decisive influence on thermodynamics and kinetics in gasification process[14]. The influence of temperature on the gas composition is shown in Figure 5. The content of H2 gas was 41.03% ~ 44.80%. The content of CO gas was 23.23%~25.09%. The amount of CH4 gas was 8.71%~10.06%. The content of CO2 gas was 9.33%~9.54%.

Under the same mass ratio of steam and biomass condition, the volume fraction of H2 and CO increased with increase of temperature, while the volume fraction of CH4 and CO2 decreased slightly. Changes in individual components of the gas content were the result of a chemical reaction (R1-R9) together. Wherein reaction R6 and R7 are the two main reactions. The increase of temperature made gasification reaction rate speed, and because the water gas reaction (R6) and hydrocarbon reforming (R9) is an endothermic reaction, so the higher temperature increased the amount of H2 and CO quickly. The content of CH4 is mainly generated by volatile matter of vinegar. As the temperature increases, positive reaction of the methane reforming reaction (R9) speeds, CH4 accelerates the decomposition, which results in the decrease of the content of CH4. The industrial analysis shows that volatile content and oxygen content of vinegar bag is higher, pyrolysis process will release a certain amount of CO2, but with increasing temperature, rate of CO2 and coke reaction (R7) speeds which makes the content of CO2 has a trace of down. Figure 5 reveals that the trend of simulation results and experimental results agree with each other well.

**Summary**

The presented study disclosed that, when mS/mB increased in the range from 1.23 to 2.47, the trend of the volume fraction of H2 increased, however the volume fraction of CO decreased. The content of (H2+CO) gas increased. The content of CH4 gas had trace increase with mass ratio of steam to biomass increasing. When mS/mB increased in the range from 2.47 to 3.57, the volume fraction of gas composition changed slightly since the arrival of saturated steam. The change was gradually stabilized. When temperature increased, the gasification reaction rate speeded, and because the water gas reaction (R6) and hydrocarbon reforming (R9) was an endothermic reaction, so the higher temperature increased the amount of H2 and CO quickly. The methane reforming reaction (R9) led to the decrease of the content of CH4. CO2 and coke reaction (R7) made the content of CO2 has a trace of down.

Coincided basically with the calculated results and experimental results, it shows that the dynamic model can do accurate simulation of fluidized bed gasification.
References


