Application of Numerical Simulation on Biomass Gasification

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Abstract

Biomass gasification is one of the highest thermal efficiency chemical conversion processes. Numerical simulation is an important tool for study on biomass gasification. In this paper, numerical simulation on biomass gasification technology at home and abroad are reviewed. At the same time, two commercial simulation softwares (Aspen Plus and Fluent) applied in chemical process was mainly introduced, and both of them were analyzed and compared. Finally it was put forward that a better simulation result could be achieved for biomass gasification if applying Aspen Plus combined with Fluent.

1. Introduction

Biomass conversion technology is translating biomass into more convenience and cleaner fuel or other energy products through a kind of ways or means [1]. It mainly include direct combustion, methane fermentation, gasification, fuel ethanol, pyrolysis liquefied, indirect liquefied and biological diesel technology, etc [2]. Biomass gasification technology is to use oxidizing substance such as oxygen as gasification agent and to make the carbon of biomass into combustible gas. First the biomass pyrolyzes in gasifier, then production gas takes part in oxidation-reduction reaction in the oxidation and reduction zone. The heat released from oxidation reaction could provide the energy for biomass drying, pyrolysis and reduction reaction. Finally the main composition of combustible gas after removing tar and impurity are H₂, CO, CH₄ and little of unsaturated hydrocarbons CₙHₘ. This technology has changed the form of biomass, improved the energy conversion efficiency and gotten higher grade energy [3].

Numerical simulation is also called computational simulation which could resolve engineering problems and physical problems even the nature phenomena by numerical calculation and image displayed method. Compared with traditional experiment method, numerical simulation has been widely used in many fields, such as mechanical process, large building fire temperature field, hydrogeology, etc. The experimental results can be predicted by simulating the process of actual reaction with appropriated numerical simulation software, greatly saving time and manpower consumption. The pyrolysis gasification process of the biomass is a very complicated thermal and chemical process, which involves flow, heat transfer, mass transfer phenomena, and a series of chemical reactions. Therefore, it is impossible to study...
gasification process only relying on experiment. Numerical simulation as a kind of supplementary tool will accelerate the development and application of biomass gasification technology.

2. mechanism of biomass pyrolysis gasification

The pyrolysis and gasification process of biomass can be divided into the following four stages [4].

1) Drying process: The temperature in drying zone is around 50 ~ 150°C. The free moisture become gas phase and the biomass is translated into dry material.

2) Pyrolysis process: Biomass begins to pyrolysis at temperature above 160°C. The volatile matter separates out from the dry biomass during pyrolysis process. The prevalent pyrolysis product is carbon, hydrogen, carbon monoxide, carbon dioxide and methane, tar and other hydrocarbons. Generally the process can be expressed with chemical reaction equation as follows:

\[
\text{CH}_x\text{O}_y = n_1\text{C} + n_2\text{H}_2 + n_3\text{H}_2\text{O} + n_4\text{CO} + n_5\text{CO}_2 + n_6\text{CH}_4 \tag{1}
\]

In the equation, the formula CH\textsubscript{x}O\textsubscript{y} is the characteristic molecular formula of biomass, and n\textsubscript{1} to n\textsubscript{6} is equilibrium constant decided by specific circumstance of gasification [5].

3) Oxidation reduction: The temperature of the oxidation zone is during 1000°C to 1200°C. The reaction heat produced in this zone can provide heat for biomass drying, pyrolysis, reduction. The chief chemical reaction in the oxidation zone is as following.

\[
\begin{align*}
\text{C} + \text{O}_2 & \rightarrow \text{CO}_2 + 393.51\text{KJ} \tag{2} \\
2\text{C} + \text{O}_2 & \rightarrow 2\text{CO} + 221.34\text{KJ} \tag{3} \\
2\text{CO} + \text{O}_2 & \rightarrow 2\text{CO}_2 + 565.94\text{KJ} \tag{4} \\
2\text{H}_2 + \text{O}_2 & \rightarrow 2\text{H}_2\text{O} + 483.68\text{KJ} \tag{5} \\
\text{CH}_4 + 2\text{O}_2 & \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 890.36\text{KJ} \tag{6}
\end{align*}
\]

4) Reduction reaction: Because the reduction reaction is endothermic, the temperature is lower accordingly, approximately form 600°C to 900°C. The chemical reaction in the reduction zone mainly includes:

\[
\begin{align*}
\text{C} + \text{CO}_2 & \rightarrow 2\text{CO} - 172.43\text{KJ} \tag{7} \\
2\text{H}_2\text{O} + \text{C} & \rightarrow \text{CO}_2 + 2\text{H}_2 - 90.17\text{KJ} \tag{8} \\
\text{H}_2\text{O} + \text{C} & \rightarrow \text{CO} + \text{H}_2 - 131.72\text{KJ} \tag{9} \\
\text{H}_2\text{O} + \text{CO} & \rightarrow \text{CO}_2 + \text{H}_2 - 41.13\text{KJ} \tag{10} \\
3\text{H}_2 + \text{CO} & \rightarrow \text{CH}_4 + \text{H}_2\text{O} - 250.16\text{KJ} \tag{11}
\end{align*}
\]

When the biomass gasification process is simulated, these zones are divided strictly, without considering the interlocking between them. This is one of the reasons resulting in errors between calculated and experimental results.

3. current situation of numerical simulation on biomass gasification

Now, many commercial softwares are developed and widely used for simulating biomass gasification process mainly including stoichiometric calculation software HSC, large-scale general chemical flow simulation software Aspen Plus, and computational fluid dynamics software Fluent etc.
A. Current research abroad

Numerical simulation is applied to energy industry earlier abroad. Philippe Mathieu simulated the gasification process of sawdust around atmospheric on fluidized bed reactor with Aspen Plus, and the sensitivity of the changes of different parameters was analyzed [6]. The simulation result showed that preheating the air could improve the gasification efficiency, while the pressure in gasifier has little influence on gasification efficiency. Wayne Doherty .etc developed a circulation fluidized bed gasification model using Aspen Plus to forecast the performance of gasifier under each kind of operating conditions. The model was based on the Gibbs free energy minimum principle, and was proofread according to the test data with restricted equilibrium. In the model, gasification reaction was controlled through the temperature controlling. The parameters of gas composition, conversion efficiency and gas calorific value forecasted on Aspen Plus coincided with that of experiment very well. Preheating the air can increase the output of H2 and CO, thus increasing the gas calorific value [7]. Nikko, M.B .etc used four Aspen Plus reactor model as well as the built-in FORTRAN subroutine to simulate the hydrodynamics and the reaction kinetic in the gasification process [8]. It is concluded that with temperature increasing, H2 output and carbon conversion rate are all increased, while CO2 output and carbon conversion rate were proportional to the equivalent air directly.

Sofialidis.D simulated the pyrolysis and gasification process of eucalyptus and miscanthus as raw materials in fluidized bed with Fluent [9]. The track of biomass granule in the gasifier and the distributions of temperature and pressure in furnace were simulated, and obtained the pressure and temperature distribution in the gasifier. S.Gerber established 2D mathematic model for bubbling fluidized bed gasifier and simulated the pyrolysis and gasification of wood on Fluent. The influence factors on the gasification product such as initial thickness of bed material, biomass feeding rate and initial thermodynamics boundary condition are analyzed [10]. C. Mandl .etc simulated the thermal decomposition gasification process of sawdust in up-draft fixed bed gasifier on Fluent [11]. In the model, the heat and mass transfer between gas-solid phases was considered for sawdust gasifier. With another large-scale computational hydrodynamics software package CFX4, D.Fletcher.etc simulated the decomposition gasification process of sawdust in entrained-bed [12]. Standard \( K^+ \) \( \epsilon \) model was selected which considered turbulence and displayed the very complex rotate flow of sawdust particle in the gasifier. The results showed that this model could provide a powerful reference to the gasifier's optimization design. Sadaka simulated the gasification process of biomass by air-steam in the circulation fluidized bed using two-phase flow principle. The model had not only considered the quality and energy balance, but also worked out the gas-product rate by the Gibbs free energy minimum method [13].

B. Domestic researches at present

At domestic, the research about biomass gasification technology mainly centralized at universities and research institutions. Huazhong University of Science and Technology State Key Laboratory of Coal Combustion made a great progress in the numerical simulation of gasification technology. Yang Haiping used the HSC chemical packet and PSR reactor model to simulate the thermodynamic equilibrium and dynamic equilibrium of the pyrolysis process of the palm oil wastes. The result showed that the output of H2 and CO increases with pyrolysis temperature increasing. The output will not be steady until the temperature is above 900\(^\circ\)C. By the HSC, only the main gas components, H2, CO, CO2, CH4, H2O and coke could be considered, rather than the small amount gas, such as C2H2, C2H6, C3H8 and so on. Therefore, the PSR was used to introduce detailed dynamics mechanism of reaction--hydrocarbon combustion mechanism (GRI mechanism) to simulate pyrolysis process of biomass [14]. Zhao Xiangfu performed gasification experiments of three kinds of biomass (chips, peanut shells, grass stalk) in a normal atmosphere with air as gasification agent. Then, the biomass gasification model was established using Aspen Plus based on free energy minimization to simulate the influence of different factors on the gas components [15]. The result indicated that the temperature didn’t have significant effect on the production rate of gas. The content of H2 would increase along with the increasement of S/B (the ratio of input velocity of steam to input velocity of biomass) value when air-vapor was used as gasification agent.
steam used as gasification agent, the content of H₂ could reach 55%, and the caloric value was up to 11MJ/m³.

Recently, with the advancement of numerical simulation method and the computer’s performance, the computational fluid dynamics (CFD) is also applied to thermo-chemical conversion. Wang Yiqun established the kinetics 3D model of biomass gasification process with Fluent. The CFD models on biomass gasification or steam gasification for hydrogen and fast pyrolysis for bio-oil are developed. Mathematical governing equations of the fluid flow, heat and mass transfer and chemical reactions in thermochemical systems are considered. Sub-models for turbulence, radiation and other individual processes are also included. The product and temperature distributions of different operation conditions are studied. The model are proved to be sensitive and valid [16]. Biomass pyrolysis model was developed by Zhao Yijun based on the pyrolysis experiments. Biomass gasification model was developed with the simulation results of the pyrolysis model as the entrance conditions of gasification. A model of the cyclone gasifier was developed by Fluent package. Feeding rate of the wood powder of 19.4 kg/h, and ER (equivalence ratio) of 0.23, 0.26, 0.29, 0.32 and 0.35 were simulated. The results show that trends of the axial temperature of the gasifier and the produced gas concentrations simulated agree satisfactorily with the experimental data [17].

4. comparative analysis of Aspen Plus and Fluent

Based on domestic and foreign summarization of numerical simulation technology application in the gasification of biomass, the two frequently-used softwares are the large-scale industry flowsheet simulation software Aspen Plus and the computational fluid dynamics software Fluent. There are many differences between them to simulate gasification process, such as the principle of simulation, the foundation of simulation, the input and output of date and so on.

C. The differences of principle of simulation

The main simulation principle of Aspen Plus is to use the basic property relationship of systemic substance (the balance of mass and energy, velocity coefficient, the reaction, the transfer of mass and heat and all kinds of equilibrium relationship) to simulate and predict the material’s flow rate, composition and property, thus to optimize the condition of operation and structure of reactor and so on. According to the property of thermo chemistry conversion process occurred in gasifier, different unit operation models can be used to simulate the different processes. For example, the RYield block is used to simulate the pyrolysis process of biomass. The Gibbs block, which is based on Gibbs energy minimization principle, is used to simulate the Oxidation-Reduction process. Then all kinds of blocks are connected together with material flow, heat flow or work streams to form a flowsheet, which is showed in figure 1.

Figure 1. The flowsheet of pyrolysis and gasification of biomass
Compared with Aspen Plus, Fluent is to use Gambit to establish the tridimensional spatial model of gasifier firstly. Then the model is messed and its output and input are defined. The mesh document is read into Fluent and then suitable models are chosen, such as turbulence models, gas-solid two-phase flow models, P-1 combustion model etc. Finally iterative computation is processed, and the answer is obtained. The step of simulation using Fluent is showed in figure 2.

**Figure 2. The step of simulation using Fluent**

**D. Difference in the mode of material input**

Before simulating the gasification of biomass using the two softwares, the raw material’s proximate and elemental analysis are performed because there is no data of the raw material in the database of the two softwares. The raw material is defined through the proximate and elemental analysis. The two softwares are the same on this point.

However, the biomass is defined as unconventional component in Aspen Plus, so the data from the proximate and elemental analysis can be input directly. The other gas components produced in the reaction process are defined as conventional components, and they can be found in the database. Compared with Aspen Plus, the non-premixed combustion model is used to define the biomass in Fluent. The model is more complex. Meanwhile because the granule of the raw material is much bigger than coal fines, the simulation of its gasification process is more complex than coal fines.

**E. The difference of output ways for the result**

For Aspen Plus, the simulation outcome is displayed in the form of table. In the table, concentration of each component can be exhibited, even the output components of each block. However, the outcome for Fluent is the concentration cloud map of each component. So the post processing software Tecplot or Origin must be used to process it. Furthermore the details of flow condition of the biomass, granule in the
gasifier, distributions of temperature, pressure and gas composition can be reflected with cloud map, which is conducive to analyse the gasification process.

5. Conclusions

To sum up, the software Aspen Plus and the Fluent cut both ways to perform simulation of biomass gasification. Consequently, hypothesis is put forward that using Aspen Plus together with Fluent to simulate the pyrolysis and gasification process of the biomass. Because pyrolysis process is extremely complex and it is very difficult to be described using reaction equation, using the Fluent to simulate the pyrolysis process is highly inconvenient. However, using the Ryield block of the Aspen Plus to simulate the pyrolysis process is relatively simple. Therefore, the Aspen Plus is used to simulate the pyrolysis process of the biomass. And then the outcome of the Ryield block, as the initial condition, can be used to input the Fluent to simulate the remaining oxidation-reduction reactions. In this way, the final gas components could be obtained, as well as the temperature and pressure distribution in the gasifier.

References


