CFD-MODELING OF THE MULTISTAGE GASIFIER CAPACITY OF 30 KW

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Abstract. Single-stage fuel gasification processes have been developed and widely studied in Russia and abroad throughout the 20th century. They are fundamental to the creation and design of modern gas generator equipment. Many studies have shown that single-stage gasification process, have already reached the limit of perfection, which was a significant improvement in their performance becomes impossible and unprofitable. The most fully meet modern technical requirements of multistage gasification technology. In the first step of the process, is organized allothermic biomass pyrolysis using heat of exhaust gas and generating power plant. At this stage, the yield of volatile products (gas and tar) of fuel. In the second step, the layer of fuel is, the tar is decomposed by the action of hot air and steam, steam-gas mixture is formed further reacts with the charcoal in the third process stage. The paper presents a model developed by the authors of the multi-stage gasifier for wood chips. The model is made with the use of CFD-modeling software package (COMSOL Multiphysics). To describe the kinetics of wood pyrolysis and gasification of charcoal studies were carried out using a set of simultaneous thermal analysis. For this complex developed original methods of interpretation of measurements, including methods of technical analysis of fuels and determine the parameters of the detailed kinetics and mechanism of pyrolysis.

1. Introduction

In a variety of new directions of thermochemical conversion, the multistage gasification process, which meets modern trends, was left unnoticed for a long time. In a multi-stage process, the exothermic stage of internal combustion proceeds in a separate reactor (or zone), the resulting producer gas is completely or partially burned in the combustion chamber, and the combustion products are used as an air-blasting agent in the second reactor where charcoal from the first reactor enters. Such organization of the process makes it possible to burn resinous products released in the first stage, use their energy to boost the gasification of charcoal and stabilize the composition of the final gas [1, 2].

At present, several plants have been developed and put into operation that implements the principles of multi-stage gasification. For example, two power plants operating on woody biomass, Gussing (4.5 MWth) and Oberwart (1-6 MWth) were put into operation in Austria [3]. Weiss station (1000 kWth) is in Denmark. The thermochemical conversion of wood chips at this station is carried out in the Viking gas generator [4]. This multi-stage gas generator was developed among the first in the Danish Technological University [5]. Also worth noting, is the technology of the three-stage gasification CORTUS-WoodRool, developed in Sweden. In 2011, a demonstration plant with a capacity of 500 kWth was developed. Over the next 12 years, CORTUS plans to increase capacity to 5
MWth [6]. In Russia, a multi-stage gasification system (15 kWth) with a three-stage air supply was also developed based on the UrFU [7].

Despite the large number of demonstration plants and a number of operating power stations, the technology of multi-stage gasification is far from perfect. This is primarily due to the weak controllability of the process due to the large number of control parameters, the number of which reaches 11 (blast flow, moisture and particle size distribution, thermal conditions). In addition, the producer gas quality parameters and intensity of the conversion process are nonlinearly dependent on the thermal regime, the composition of the blowing agent, the degree of clipping (the degree of conversion of fuel at the boundaries of the zones) [8].

Improvement of the technology of multi-stage gasification requires the development of theoretical ideas about the physical processes occurring during the thermochemical conversion of fuels. The modern theory of burning solid fuels was developed in the middle of the last century with regard to quality fossil fuels. The use of this theory in studies of the processes of thermochemical conversion of fuels with a high yield of volatiles is associated with the following difficulties: a) the existing theory is not capable of fully explaining a number of phenomena observed in the combustion of biomass. b) the detailed kinetic description of fuel conversion requires the introduction of a large number of assumptions and the use of a significant amount of empirical data. This circumstance reduces the predictive properties of models. In some cases, the possibility of using a particular model is limited only to the installation for which the model was developed.

In this regard, at present, the evolution of models describing the processes of thermochemical conversion of solid fuels is taking place. This development is facilitated by intensive development of CFD-modeling packages (Ansys Fluent, Thermoflow, Comsol, etc.) [9-11].

The purpose of this paper is to modeling the processes occurring during the pyrolysis of woody biomass in the pyrolysis reactor. The pyrolysis reactor is the first stage of multi-stage gasification. At this stage, volatile substances and tars are released.

2. CFD-modeling of pyrolysis of wood chips

CFD-modeling is performed in COMSOL Multiphysics computational package. The advantage of this package is that it is possible to combine the modules of computational thermodynamics (CFD) and chemical reactions (Chemical Reaction Engineering).

Figure 1 shows a reactor for the pyrolysis of wood chips. This process occurs at 700 °C. In the original installation, the heat of the exhaust gases heats the pyrolyzer. Now realized by zone heating by electric current. In the first stage, at a temperature of 150 °C, the sample is dried, and then at 400 °C the fuel decomposes with the release of predominantly hydrogen-containing compounds and a light tar; in the last stage, at 700 °C, a deep decomposition of the fuel takes place, with the release of predominantly carbon-containing compounds and cracking of the tar. A screw moves the fuel. The length of the pyrolysis reactor is 1.5 m; the internal diameter is 150 mm. The rate of fuel flow through the reactor is 1 mm/sec. As a source of wood chips, a pine is used with the following composition: W - 5%, A - 1.1, C - 54.3, H - 5.2, O - 40.0, N - 0.4 (daf). The chip size is 1x3 cm.
Wood chips
Char, tar and producer gas
heating
150°C 400°C 700°C

Figure 1. A diagram of the screw reactor.

The heat exchange in this reactor was calculated earlier and published in [12]. In this regard, in this paper, we calculated the drying of fuel and the yield of coke at the pyrolysis stage of wood chips.

Several assumptions have been made in the modeling of these processes:

1. The kinetics of drying and devolatilization processes is described by the Arrhenius equation,
2. The kinetics of these processes obey the laws obtained for small samples by the method of thermal analysis,
3. The kinetics of the processes under study is described by the first order.

A general equation describing the kinetics of the processes under study is written in the following form:

\[ r = k \prod_{i=1}^{N} c_i^{r_i} = A^{r_i} T^{r_i} \exp \left( \frac{E_a^{f_i}}{R g T} \right) \prod_{i=1}^{N} c_i^{r_i} \]  

where \( r \) - reaction rate, \( s^{-1} \), \( A \) - pre-exponential factor, \( s^{-1} \), \( E_a \) - activation energy, kJ/mole, \( T \) - temperature, K, \( R_g \) - universal gas constant, kJ/mole K, \( c \) - concentration of formed substances.

To determine the kinetic parameters of the drying and devolatilization stages, thermal analysis methods are used, which is a universally accepted method for studying the kinetics of thermochemical conversion [13].

Thermoanalytical studies were carried out using an integrated complex of synchronous thermal analysis, produced by Netzsch Geratebau (Germany): the weighting system of Netzsch STA 449 F1, quadruple mass-spectrometer QMS 409 C Aeolos and the system of pulse gas supply PulseTA.

The technique for determining the technical characteristics of solid fuels involves the preparation of a representative sample using the standard quarting method. A representative sample of fuel with a mass of 20-30 mg is exposed to a thermal effect from room temperature to 1000 °C in an inert gas stream (argon). The resulting conversion products are recorded by a quadrupole mass spectrometer. A detailed procedure for performing the thermal analysis is given in [14].

In Figure 2 shows a thermogram of drying pine sawdust.
Figure 2. Thermogram drying pine sawdust (5% moisture).

Using the software package NETZSCH Thermokinetics drying study was determined the kinetics of the process. In this case Friedman's isoconversion method was used. Details Friedman kinetic method described in [15].

Table 1 shows the calculated kinetic constants for the drying stage, depending on the moisture content of the fuel used.

| Moisture, % | lg A, s⁻¹ | Ea, kJ/mole |
|------------|-----------|-------------|
| 40         | 3.09      | 40.3        |
| 10         | 2.29      | 34.2        |
| 5          | 1.85      | 31.3        |

The data in Table 1 show that the calculated kinetic coefficients depend on the initial moisture content in the fuel.

Substituting these kinetic coefficients for humidity is 5% in Equation 1 to determine the field change in the concentration of water vapor across the reactor (Figure 3).

Figure 3. The calculated fields of water vapor concentration (kg/m³).
The water vapor formed in the course of drying reaches the highest concentration in the zone of intensive heating, at the beginning of the screw reactor, and, as they move along the reactor, the concentration is equalized over the cross section.

The pyrolysis process is described by a global reaction:

\[ CH_x O_y N_z \rightarrow n_c CHAR + n_{H_2}H_2 + n_{CO}CO + n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{CH_4}CH_4 + n_{TAR}TAR + mN_2 \]

Consider the process of char formation, which is shown in Figure 4. In the temperature range 120 - 900 °C pyrolysis of the fuel under investigation occurs.

![Figure 4. Thermogram of woody biomass pyrolysis.](image)

Using the differential Friedman method, the kinetic coefficients were determined (activation energy - 147 kJ/mole, pre-exponential factor - 9.25·10^{12} s^{-1}).

The obtained kinetic coefficients were used in calculating the formation of char in a screw pyrolyzer (Figure 5).

![Figure 5. Formation of char, %/wt.](image)

As can be seen from Figure 5, the degree of thermal conversion of woody biomass is about 30%.
3. Conclusion

As a result of the work, the heat exchange model for the pyrolysis of wood biomass in a screw reactor is supplemented by the equations of chemical kinetics.

Thermal analysis methods determine the kinetics of the drying and devolatilization stages under the condition of the corresponding first-order reactions.

The calculated kinetic coefficients were used to calculate the fields of the concentrations of water vapor and coke formation over the cross section of the reactor. It is determined that fuel drying takes place on the first 30 cm of the reactor, further formation of water must be limited by introducing macrokinetic constraints.

The degree of thermal conversion of fuel is lower than calculated theoretically, which is about 40%. Consequently, the model underestimates the degree of thermal conversion of fuel.

4. References

[1] Heidenreich S. and Foscolo P.U. (2015) New concepts in biomass gasification Progress in Energy and Combustion Science, 46, 72-95.
[2] Ahrenfeldt J., Egsgaard H., Stelte W., Thomsen T. and Henriksen U.B. (2013) The influence of partial oxidation mechanisms on tar destruction in TwoStage biomass gasification Fuel, 112, 662-680.
[3] Molino A, Chianese S, Musmarra D. (2016) Biomass gasification technology: The state of the art overview Journal of Energy Chemistry, 1, 10-25.
[4] www.eea.dk
[5] Henriksen U., Ahrenfeldt J., Jensen T.K., Gebel B., Bentzen J.D., Hindsgaul C. and Sorensen L. H (2006) The design, construction and operation of a 75kW two-stage gasifier Energy, 31, 1542-1553.
[6] Technologies relevant for gasification and methanation in Denmark (2012) DGC-report, 1-38
[7] Zaitsev A V, Ryzhkov A F at al. 2010. Gas-generating technologies in power engineering, 611
[8] Keiko A.V., Svishecv D.A., Kozlov A.N. and Donskoy I.G. (2012) Studying the controllability of processes for thermochemical conversion of solid fuel in a bed Thermal Engineering 4, 302-309.
[9] http://www.ansys.com
[10] http://thermoflow.com
[11] https://www.comsol.ru
[12] Levin A.A., Shamansky V.A. and Kozlov A.N. (2016) A model of pyrolysis in a staged scheme of low-grade solid fuel gasification Journal of Physics Conference Series, 754, 02206. DOI:10.1088/1742-6596/754/2/022006.
[13] Bridwater A.V. (2004) Progress in thermochemical biomass conversion Oxford: Blackwell Science Ltd., 1693.
[14] Kozlov A.N., Svishchev D.A., Donskoy I.G, Shamansky V. A. and Ryzhkov A.F. (2015) A technique proximate and ultimate analysis of solid fuels and coal tar Journal of Thermal Analysis and Calorimetry, 122, 3, 1213-1220.
[15] Friedman H.L. (1976) New methods for evaluating kinetic parameters from thermal analysis data Journal of Polymer Science: Polymer Letters, 7, 1, 41–46.

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