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Math modeling of heat and mass transfer processes during coal-water fuel gasification

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Abstract. In article the current state of gasification technologies in Russia and in the world is analysed. The perspective directions of development of process – entrained flow gasification of coal-water fuel for the purpose of producing syngas for further catalytic conversion and producing chemicals are defined. The mathematical model of thermophysical characteristics calculation of process is presented. Determination results of design parametrs of a gasifier are given.

Introduction

At present, deep conversion of oil and natural gas is being carried out in Russia to produce energy and various products of chemical synthesis: methanol, ammonia, carbon monoxide, hydrogen, liquid synthetic fuels, etc. At the same time, the use of coal is limited to combustion in boilers. The technologies and plants for solid fuels combustion are morally and physically obsolete, and the process indicators do not meet the requirements of the UN for reducing emissions and technological re-equipment [1].

Based on the "Energy Strategy of Russia until 2035" project, such issues as low share of use of local fuels, development of domestic scientific and technical base of "clean" coal technologies and production of gaseous and liquid fuels, as well as competition in the domestic market through the use of cheaper raw materials require the solution [2]. Experts identify the complex use of coal as the most perspective direction [3]. This technology allows to produce heat and electric energy and various chemical products which are demanded by national economy.

Gasification is one of the most rational, energy efficient and ecologically safe directions of use of coal and coal-water fuel (CWF). Because of a possibility of a variation of syngas composition depending on a type of fuel and operating conditions it can be used in power engineering for combustion in boilers and gas-turbine plants and also as an initial component for producing a wide range of chemical products, on condition of a molar ratio of monoxide of carbon to hydrogen within 0,4-0,6 [5].

The choice of the direction of use syngas depends on its composition and operating conditions of gasification: temperature, pressure, existence and a type of oxidizer and also on reliable method of calculation of gas composition and properties, processes of a heatmass exchange in the reactor, its design. Modeling of gasificationprocess will allow to develop the gasifierunified by the type of fuels.

According to statistical data [6-7] in the world more than 150 plants making syngas which are mainly located in China, the USA and Germany are functioning. On most of it entrained flow gasifiers function that gives the chance to the plants to work on an IGCC cycle, developing electric energy,



pure hydrogen and chemical products [8]. Entrained flow process is carried out at high temperatures 980-1930 °C that provides high (to 99%) conversion of carbon in gas.

Work of entrained flow gasifiers is based on experimental or operational data. At the fundamental level of a research this process is worked still out a little therefore there are no techniques of thermal, thermodynamic and aerodynamic calculation, it complicates design of gas generators when using different types of solid fuels. Thus, line heterogeneous gasification isn't captured by modern methods of modeling and a research on the basis of creation of mathematical models yet.

Math modeling

It is known that process of thermochemical conversion of coals proceeds in 3 stages. At the first stage physically bound water evaporates; at the second stage gas components of coal and the high-carbonaceous coke are formed; at the third stage gas components and the coke react with oxidizer with formation of components of syngas. The third stage is of the greatest scientific and practical interest. At thermochemical interaction of components of steam-gas mix on a surface of the solid coke syngas of various composition at regulation of operating conditions can be formed. As a rule, interaction of a gas and solid phase is described by the generalized equations of reactions between C, O₂, H₂O, CO₂, H₂, CO and CH₄ [6].

Technological parameters of processes: the fuel particle speed, the size, diffusion and heat exchange proceeding in volume of a gasifier influence finally the speed of thermochemical transformations, characteristics syngas and on the possible ways of it use.

Theoretical studies of syngas composition performed earlier by the authors [9] have shown that the optimum composition for further catalytic processing has the syngas obtained in the oxygen-free gasification of water-coal fuel.

The oxygen-free gasification of water-coal fuel is an endothermic process which requires external heat. In the method of gasification proposed by the authors, the CWF drop fall into the hot synthesis gas and, after heating, passes through all the process stages: evaporation of the CWF water, volatilization of gas components, thermal conversion of the mixture components. At each stage, the thermophysical characteristics of the process are calculated, thanks to which it is possible to determine the design parameters of the gasifier.

For determination of the amount of heat which necessary for the thermal conversion of coal-water fuel into syngas and the residence time of the drop of CWF in the gasifier the mathematical model of heat and mass transfer between drop of CWF and the flow of heating gas in the gasifier was developed [10].

$$Q_r = \sum_{i=1}^n (cm(T_0 - T_1))_i \quad (1)$$

$$\sum_{i=1}^b G_{i_inlet} = \sum_{i=1}^k G_{i_exit} \quad (2)$$

$$\frac{dQ_r}{d\tau} = \alpha S_{sur} (T_g - T_d) \quad (3)$$

$$\frac{dm}{d\tau} = \beta S_{sur} (C_{sur} - C_g) \quad (4)$$

$$m \frac{du}{d\tau} = \sum_{i=1}^l F_i + u \frac{dm}{d\tau} \quad (5)$$

$$L = u\tau + \frac{a\tau^2}{2} \quad (6)$$

where Q_r – the required amount of heat to evaporate water of CWF in the first stage of gasification and volatilization of gas components in the second stage, J; n – amount of rated zones of the gasifier, T_0 , T_l , T_d , T_g – temperature of the heating gas at the inlet to the rated zone of gasifier, at the outlet of the rated zone, the drop of CWF and gas, respectively, K; c – specific heat of substances in reaction zones, J/kg·K; m – mass of components, kg; G – components consumption of the mix, kg/s; b – amount of initial substances; k – amount of products; τ – time of the course of certain processes (warming up the drop of CWF, mass transfer, stay of a particle of fuel in a zone), s; α – heat transfer coefficient, W/(m²·K); S_{sur} – surface area of the drop of CWF, m²; l – amount of forces acting on particle of fuel; β – mass transfer coefficient, m/s; C_{sur} , C_g – concentration of evaporating substances at the surface and in heating gas, kg/m³; $\sum F$ – sum of forces acting on a drop of CWF (on particle of fuel), H; u – drop of CWF (particle of fuel) rate, m/s; a – drop of CWF (particle of fuel) acceleration, m/s²; L – zone length, m.

The equations 1 and 2 represent the heat and mass balance of evaporation of water and volatilization of gas components and present the laws of conservation of energy and mass. The equations 3 and 4 describe the value of heat flow and rate of mass loss and represent the equations of heat and mass transfer. The equation 5 is Meshchersky's equation and describes change of drop of CWF (or particle of fuel) rate at a variable mass of particle. The distance which is overcome by variable mass drop of CWF (or particle of fuel) at equally slow driving is determined by the equation 6.

The offered mathematical model of the processes occurring with a drop of CWF at entrained flow gasification considers process that when driving a drop its density and weight changes. At first stage water of CWF evaporates, while the droplet diameter does not change, at the outlet of the first zone drop of CWF represents a coal framework. At the second stage gas components of coal volatilize, and the coal framework turns into coke framework. At the third stage coke is destroyed and, reacting with steam-gas mix, syngas is formed.

At each stage the heat and mass transfer between a particle of fuel and gas phase takes place, at the same time process has to be provided with a necessary amount of heat for evaporation of water and gas component of coal, and for endothermic gasification reactions. Mass transfer between a particle of fuel and gas is characterized by a diffusion coefficient which is defined through change of composition of gas in each gasification zone. To determine the geometric size of the gasifier, the residence time of the fuel particle in the gasifier and the particle rate in each reaction zone are defined.

Assumptions:

- monodisperse composition of CWF drops;
- the temperature of a gas phase in the 1st and 2nd zone of a gasifier is supported at the level of 1150K;
- the produced syngas fills entire volume of a gasifier;
- the movement of the CWF drop along the length of the gasifier is rectilinear;
- the drop of CWF moves equally slowly in each rated zone of the gasifier, drop acceleration is characterized by the rate of diffusion of gas components into the gas phase;
- at the outlet from 1st zone the steam is heated to the temperature in the gasifier, and the carbon particle is reached CWF water evaporation temperature $T_{dl} = T_{evap}$;
- in the 2nd zone the coal particle is heated to the gas components volatilization temperature, and at the outlet from 2nd zone all reaction mix is reached the temperature of the heating syngas $T_{CP2} = T_{volat} = T_{SG}$;
- in the 3rd zone the rate of the coke particle is compared to the gas flow rate $u_{CP} = u_{SG}$;
- due to the heat transfer from the heat pipes in gasifier, the syngas temperature at the inlet to each zone is supported by constant $T_{SG} = const$.

The system of equations 1-6 for each zone corresponds to the heat and mass transfer that take place in the water evaporation and gas components volatilization. The calculation of thermochemical processes in 3rd zone is based on the determination of chemical gasification reactions heat effect and the temperature of the syngas at the outlet.

Results of studies

As a result of calculation of heat transfer in the gasification the following was determined according to the developed mathematical model.

The size of all reaction zones, and the size of the entire gasifier can be influenced by regime and technological factors.

CWF drop sizes, sprayed by the injector, exert the significant impact of the zones of water evaporation and gas components volatilization (fig. 1). It is explained by need of increase in time for course of the processes occurring with particle of fuel in the rated zones.

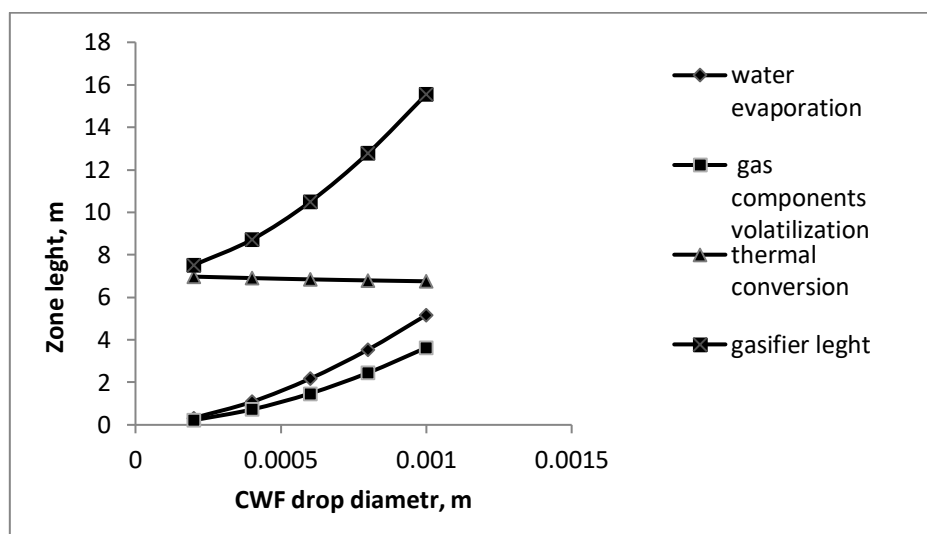


Figure 1. Dependence of length of the conditional zones of a gasifier from CWF drop sizes

At increase in rate of a drop the distance, which is overcome by CWF drop during syngas formation, respectively, and gasifier length increases. At a given gasification temperature, it is necessary to ensure a certain time of the CWF drop in the gasifier to perform its thermal conversion to syngas, regardless of the drop rate. Therefore during mathematical modeling it is necessary to determine the drop rate at which the residence time of the CWF drop in the gasifier at acceptable overall design of the gasification reactor will be provided. At a low drop rate it is required shallow spray coal-water fuel by a injector for providing necessary time for the thermochemical processes in the reactor.

At the same time varying CWF drop rate at the outlet from the injector, it is possible to reach a defined value of length of a gasifier regardless of coal brand, the problem of unification of a gas generator by type of fuel thereby is solved.

Comparison of the received results showed that with a diameter of CWF drop $\sim 0,6$ mm [11] to ensure the calculated time for of processes of water evaporation, gas component volatilization and thermochemical reaction components of the mix it is necessary to provide drop rate at the injector outlet of 14-18 m/s.

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