Simulation of a reactor for thermal processing of coal-water fuel to produce syngas of specified composition

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Abstract. The main physical and chemical regularities for development of a flow gasifier for thermal processing of coal-water fuel (CWF) on condition of the set structure received syngas are presented in this article. Based on the calculations made on the residence time of a CWF drop in the reactor and the time of gasification reactions the gasifier was designed with vertical heating surfaces. Calculation of the main sizes of a gas generator for gas productivity on synthesis gas 500, 1000 and 1500 m³/h is carried out. The results of a constructive calculation show that in order to ensure the required residence time of a CWF particle in the volume of the gasifier it is necessary to ensure a certain length of the reactor, regardless of the gas throughput.

1. The theoretical basis for the development of a gasifier

The using of coal-water fuel (CWF) for the production of energy and chemical products is a promising direction due to the huge reserves of coal which are exceed reserves oil and natural gas the modern industry uses a huge amount of fossil fuels [1]. The thermal processing of CWF is a continuous process that can be implemented in a column type gasifier. Currently, standard designs and methods for calculating these devices are absent, despite the fact that entrained flow gasifier are widespread in the world [2-10]. The largest number of such plants is located in China, where methanol, ammonia, acetic acid, fuel gas, hydrogen, carbon monoxide and other products are produced on their basis.

The scientific works in the field of gasification are mainly aimed at determining the composition of the generating gas, depending on the composition of the initial components and operating parameters of the process [2, 4, 11-15]. But in this work a different approach is used: the composition of the gas is set for the subsequent release of a certain product. For example, for the production of methanol, which is a large-tonnage product, the world production of which is 160-1275 thousand tons per year, it is necessary to produce syngas with a molar ratio of CO / H₂ in the range of 0.4-0.6. The best conditions for the production of such gas are created precisely during the gasification of CWF [11].

1.1. Process mode parameters

The authors earlier determined the temperature at which CWF obtained from coal of various grades decompose with the formation of gas with a molar ratio of CO / H₂ equal to 0.4-0.6 and the minimum content of other components. In the process of oxygen gasification, the reactions of interaction of the components of the fuel with oxygen are exothermic and flow intensively, while the resulting gas contains a significant amount of unreacted vapor. In oxygen-free gasification, steam acts as an oxidizing agent and its amount in the gas decreases. In this case, the reactions of the interaction of the
components of coal with steam are endothermic and heat is required for their flow. The optimum mode of the gasification process was revealed, at which the time to reach equilibrium concentrations during thermal conversion of CWF to syngas at 1150 K is about 3 sec. [16].

1.2. The main calculated dependencies

The main calculated dependences are presented for the process of oxygen-free gasification of coal-water fuel taking into account the processes of heat and mass transfer between a drop of CWF and the flow of hot gas.

In the physical formulation of the problem a CWF drop after spraying by a mechanical injector enters the environment of hot synthesis gas, which is heated due to heat transfer from the beam of flame tubes, inside which the products of combustion of a portion of the produced syngas are circulated. Conventionally, a drop passes through 3 zones of the reactor: evaporation of moisture, extraction of volatile components and reaction of the components of the mixture (Figure 1).

![Figure 1. The scheme of gasification of coal-water fuel.](image)

In each zone heat exchange takes place between the drop of CWF and the environment. To ensure optimum gasification results it is necessary to maintain the temperature in the volume at 1150 K.

In the course of calculation by the mathematical model, the amount of heat transferred from the flame tubes to the gaseous medium was determined in order to maintain the operating conditions at a predetermined level. The estimation of the length of a path that a drop of CWF overcomes in the process of its transformation is carried out on the basis of determining the loss of velocity of a drop due to a change in mass and forces acting on the drop.

The solution of the heat balance equation for the moisture evaporation zone is to determine the amount of heat required to evaporate moisture, warm the fuel particle to the evaporation temperature and heat the steam to the environment temperature:

\[
Q_{req} = rm_{H_2O} + c_{d_0}m_{d_0}(T_{evap} - T_0) + c_{H_2O}m_{H_2O}(T_{SG} - T_{evap}),
\]
where \( m_{d0}, m_{H_2O} \) – is the weight of drop CWF and steam, kg; \( c_{d0} c_{H_2O} \) – is the specific heat capacity of a drop CWF and steam; \( r_{H_2O} \) – is the heat of water vaporization, J / kg. \( T_{evap} \) – is evaporation temperature, K; \( T_0 \) – is environment temperature, K; \( T_{SG} \) – is syngas temperature, K.

For the exit zone of volatile components, the amount of heat needed to evaporate them and heat the particle to ambient temperature is determined:

\[
Q_{eq2} = r_{H_2O} m_{H_2O} volat + r_{CH4} m_{CH4} volat + c_{cokes} m_{cokes}\left(T_{SG} - T_{volat}\right) + c_{volat} m_{volat}\left(T_{SG} - T_{volat}\right)
\]

where \( r_{H2O} \), \( r_{CH4} \), \( m_{H2O} \), \( m_{CH4} \) – is weight of volatile steam, methane, coke particle and volatile compounds, kg; \( c_{cokes}, c_{volat} \) – is specific heat of coke particle, and volatile substances, J / (kg · K); \( r_{H2O} \), \( r_{CH4} \) – heat of water and methane vaporessence, J/kg; \( T_{volat} \) – is temperature of volatile compounds, K.

The equations of heat and mass transfer are solved using the theory of similarity according to known dependencies, taking into account the mechanism for the transformation of a CWF drop.

For the zone of thermochemical reaction of the components of the mixture on the basis of heat balance, the temperature of syngas at the outlet from the gasifier is determined:

\[
T_{SG3} = \frac{c_{SG2} m_{SG2} T_{SG} + c_{volat2} m_{volat2} T_{SG} + c_{cokes} m_{cokes} T_{SG} + Q_{r,c,ld}}{c_{react} m_{react}}
\]

where \( c_{SG2}, c_{react} \) – is specific heat of syngas and reaction mixture, J / (kg · K); \( m_{react}, m_{SG2} \) – is weight of reaction mixture and syngas, kg; \( Q_{r,c,ld} \) – the total thermal effect of gasification reactions on 1 CWF drop, J / kg.

The calculation of the velocity of a drop of variable mass moving in a stream of hot gas which based on the determination of the forces acting on the drop with Meshchersky equation [17]:

\[
m_d \frac{du_d}{d\tau} = \sum F_i + u_d^0 \frac{dm_d}{d\tau},
\]

where \( \sum F_i \) – is as et of forces acting on the drop, N; \( m_d \) – is weight of CWF drop, kg; \( u_d^0 \) – is velocity of a CWF drop, m/s; \( \tau \) – time, s.

As a result of the calculation using the mathematical model it was determined that the length of all reaction zones, and, accordingly, the length of the entire gas generator can be affected by various factors - temperature, size of drops, speed at the nozzle exit. The size of a CWF drop sprayed by a nozzle has a significant effect on the length of the drying zone and the yield of volatile components. This is due with necessity to increase the time for the processes occurring with a moving drop in the respective zones. At a given gasification temperature, it is necessary to ensure a certain time for a CWF drop in the gas generator volume. Therefore in the process of mathematical modeling, the drop rate at the nozzle outlet was determined, at which the required CWF drop time in the gasifier will be provided with acceptable overall dimensions of the gasification reactor.

2. Gasifier design

2.1. Principle of operation

Based on the calculations made on the residence time of a CWF drop in the reactor and the time of gasification reactions the gasifier was designed with vertical heating surfaces. There are made in the form of flue tubes with hot combustion products circulating inside them, which are formed when a certain fraction of syngas is burned obtained by gasification of CWF (Figure 2).

Between the vertical flue pipes and the gaseous medium in the volume of the gasifier the heat transfer occurs which is necessary to ensure the heat of all stages of oxygen-free CWF gasification occurs.
The gasifier works as follows. CWF is supplied through a pipeline to the ring collector 8 and sprayed by nozzles 7 into the environment of synthesis gas at a temperature of 1150 K. Part of the synthesis gas is discharged from the pipe 3, cooled, cleaned and with the air sent through the pipe 10 to the combustion in the flame tube 6. By means of burner 9 a stable supply of the gas-air mixture and its combustion in the flame tube 6 is carried out. The resulting flue gases rise up through the flue tubes 5 and are withdrawn through pipe 11. The syngas which fills the gas generator is heated by means the heat transfer from the hot flue gases passing through the flue tubes 5. As a result the temperature in the gasifier becomes sufficient for gasification of CWF, where the moisture contained in CWF is used as an oxidizer. Formed during the gasification process syngas is discharged through the pipe 3, and the slag through the outlet 4 enters the system of ash and slag removal.

![Figure 2. Entrained flow gasifier: 1 - the case; 2 - lining; 3 - pipe for removal of syngas; 4 - pipe for slag removal; 5 - flue tubes; 6 - flame tube; 7 - CWF nozzles; 8 - ring collector; 9 - burner; 10 - supply of gas-air mixture; 11 - flue gas discharge.](image)

2.2. The determination of basic dimensions

The results of a constructive calculation show that in order to ensure the required residence time of a CWF particle in the volume of the gasifier it is necessary to ensure a certain length of the reactor, regardless of the gas throughput. Table 1 presents the results of a constructive calculation of the gasifier with different gas productivity. Increased productivity is achieved by increasing the number of flame tubes, and, accordingly, the volume of the reactor. At the same time its length remains unchanged.

| Gas productivity, m³/h | Volume gasifier, m³ | Amount of tubes, pcs | Diameter gasifier, m |
|------------------------|--------------------|---------------------|---------------------|
| 500                    | 54.91              | 365                 | 2.28                |
| 1000                   | 112.83             | 750                 | 3.27                |
| 1500                   | 171.5              | 1140                | 4.03                |
In this way the calculation of the gasification process at the design stage of the design parameters of the gas generator makes it possible to achieve unification of the type of fuel when regulating the operating parameters.

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