PHYSICAL MODEL AND BASES OF MATHEMATICAL MODELLING OF ABOVE-SURFACE GASIFICATION OF COAL

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Abstract. A mathematical model describing the heat and mass transfer processes of above-surface gasification of coal with high temperature steam is introduced. Numerical studies have allowed determining the temperature profiles according to the length of the sample and composition of gasification end products. It is found that such parameters as porosity of gasified fuel and oxidant flow have little influence on the composition of the synthesis gas. The main parameter is the temperature of the feed oxidant.

1 Introduction

Gasification of solid fuels is a universal method of its processing. The versatility of the solid fuel gasification techniques can be considered in three ways. Firstly, any solid fuel from organic waste to various anthracitic coal and black coal can be gasified, regardless of their chemical composition, the composition of the cindery part, sulfur impurities, size, moisture content and other properties.
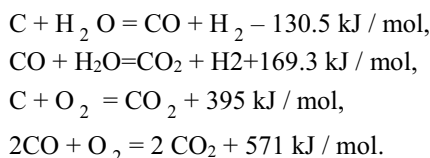
Secondly, the important feature of the solid fuel gasification methods is their wide range of usage. Gas generator can handle with the largest chemical factories, producing millions of tons of ammonia or methanol per year, can supply fuel gas to major CHP plants and at the same time can provide gas to small autonomous power and chemical plants (for example, gas generating systems for cars), towns and villages, small chemical, engineering, or other factories.

2 Formulation of the problem

We consider the work area of the experimental stand [1], created for the high-temperature steam gasification of solid fossil fuels. Work area of the stand has a cylindrical shape, has a thermal insulation on the outside. We fill solid fuel, the water vapor is pumped through it, temperature of the vapor can reach 1473 K. Steam-gas mixture, which is formed at outlet from the cylindrical canister, is supplied to the plant where steam condensation occurs. The gas mixture remaining after the condensation of steam flows into the gas analyzer where its composition is determined. In this research, we propose a mathematical model of the

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process of the solid fuel conversion described above. On the basis of a mathematical model [2] the system of equations averaged over the radius of the working area and describing the researched process is recorded. Based on experimental studies conducted at the Department of the Kuzbass State Technical University [3], we deal with the following chemical reactions:

$$C + H_2O = CO + H_2 - 130.5 \text{ kJ / mol,}$$
$$CO + H_2O = CO_2 + H2 + 169.3 \text{ kJ / mol,}$$
$$C + O_2 = CO_2 + 395 \text{ kJ / mol,}$$
$$2CO + O_2 = 2 CO_2 + 571 \text{ kJ / mol.}$$

The task is to determine the composition of the gas end mixture, non-stationary temperature field in the sample, and outlet from it.

Averaging system of equations over the diameter of the cylindrical part of the working area [1] we obtain following system of equations for a description of the non-stationary mode of solid fuel conversion:

conservation of mass of coke

$$\rho_1 \cdot \frac{\partial \varphi_1}{\partial \tau} = - R_C, \quad R_C = R_{C1} + R_{C2}, \tag{1}$$

if $R_{C1} = s \cdot \rho_4 \cdot \varphi_4 \cdot c_1 \cdot k_{s1} \cdot \varphi_1 \cdot \exp(-E_{C1}/(R \cdot T_S))$,

$R_{C2} = s \cdot \rho_4 \cdot \varphi_4 \cdot c_4 \cdot k_{s2} \cdot \varphi_1 \cdot \exp(-E_{C2}/(R \cdot T_S))$

(we assume that in the process of conversion the mass of condensed water is equal to zero, then volume ratio $\varphi_2 = 0$),

the continuity of the gas phase

$$\frac{\partial \rho_4\varphi_4}{\partial \tau} + v \cdot \frac{\partial \rho_4\varphi_4}{\partial z} = R_C + R_4. \tag{2}$$

where $R_4 = R_{CO}^1 + R_{CO}^2$, $R_{CO}^1 = k_{CO}^1 \cdot c_2 \cdot c_5 \cdot \exp(-E_{CO}^1/(R \cdot T_4))$,

$$R_{CO}^2 = k_{CO}^2 \left(c_1 M / M_{51}\right)^{0.25} \left(c_2 M / M_{52}\right) \cdot T_4^{-2.25} \cdot \exp\left(- E_{CO}/RT_4\right);$$

the continuity of α – component of the gas phase

$$\frac{\partial(\rho_4\varphi_4 \cdot c_\alpha)}{\partial \tau} + v \cdot \frac{\partial(\rho_4\varphi_4 \cdot c_\alpha)}{\partial z} = \frac{\partial}{\partial z}(\rho_4\varphi_4 D_\alpha \frac{\partial c_\alpha}{\partial z}) + R_\alpha, \qquad \alpha = \overline{1.5}; \tag{3}$$

energy conservation of the gas phase and coke

$$\rho_4 \cdot \varphi_4 \cdot c_\alpha \cdot (\frac{\partial T_4}{\partial \tau} + v \cdot \frac{\partial T_4}{\partial z}) = \frac{\partial}{\partial z}((\lambda_4 \cdot \varphi_4 + \lambda_R)\frac{\partial T_4}{\partial z}) - A_s \cdot (T_4 - T_S)$$

$$+ q_{CO}^1 \cdot R_{CO}^1 + q_{CO}^2 \cdot R_{CO}^2 - \frac{2}{r_0} \cdot \alpha_1 \cdot \varphi_4 \cdot (T_4 - T_S), \tag{4}$$

where $\lambda_R = \dfrac{16 \cdot \sigma \cdot T_4^3}{s}$;

$$\sum_{i=1}^{4} \rho_i \cdot \varphi_i \cdot c_{p_i} \cdot \frac{\partial T_S}{\partial \tau} = \frac{\partial}{\partial z}(\lambda_S \cdot \frac{\partial T_s}{\partial z}) + q_{C1} \cdot R_{C1} + q_{C2} \cdot R_{C2} + A_S \cdot (T_4 - T_S) +$$

$$\frac{2 \cdot r_1}{r_0^2} \cdot \alpha_3 \cdot (T_S - T_E) + q_R , \qquad (5)$$

if $\lambda_S = \sum\limits_{i=1}^{2} \lambda_i \cdot \varphi_i$, $c_{p4} = \sum\limits_{\alpha=1}^{4} c_{p\alpha} \cdot c_\alpha$;

gas movement in the pores (in the form of a quadratic law of filtration) and the equation of state

$$v = \frac{k}{\mu + k \cdot \beta \cdot \rho_4 |V|} \cdot (\frac{\partial p}{\partial z}), \quad p = \frac{\rho_4 \cdot R \cdot T}{M_4}, \quad M_4 = 1 / \sum_{\alpha=1}^{4} \frac{c_\alpha}{M_{4\alpha}} . \qquad (6)$$

The system of equations (1) - (6) can be solved with the boundary conditions:

$$\tau = 0: \quad \varphi_i = \varphi_{iH} , \; i = \overline{1.4}; \; c_\alpha = c_{\alpha H} \quad , \; \alpha = \overline{1.5}, \; T = T_S = T_H , \quad p = p_H ; \qquad (7)$$

$$z = 0: \quad T_4 = T_{Pw} , \quad (\rho v)_w = \text{const}, \quad \lambda_S \cdot \frac{\partial T_S}{\partial z} = \alpha_1 \cdot (T_S - T_{Pw}), \quad c_\alpha = c_{\alpha w},$$

$$z = h: \quad \partial c_\alpha / \partial z = \partial T_4 / \partial z = 0, \quad p = p_H , \quad \lambda_S \frac{\partial T_S}{\partial z} = 0. \qquad (8)$$

In equations (3) – (5) we enter a brief notation rates of chemical reactions. Here, V – the filtration rate; M_4 - Molecular weight of the gas phase; 4 index is attributed to the values characterizing the gas, and s – to the condensed phase; k – is a coefficient of permeability of the porous layer; $(\rho v)_H$ – the gas flow rate in the input section; T_S, T_4, T_E – is temperatures of the condensed phase, of the gas in the pores and of the external environment; $E_{L1}, E_{C1}, E_{C2}, k_{L1}, k_{C1}, k_{C2}$ – activation energy and pre-exponential factors of water evaporation reactions, heterogeneous reactions of coke oxidation; R - universal gas constant; $\lambda_{4\alpha}, c_{4\alpha}, M_{4\alpha}$ – thermal conductivity, mass concentration and molecular weight α-constituent, the parameter with an index $\alpha = 1$ corresponds to the oxygen (O_2), $\alpha = 2$ – CO, $\alpha = 3$ – CO_2, $\alpha = 4$ – H_2, $\alpha = 5$ – H_2O; p – is the pressure of the light-end products in the pores; $A_S = \alpha_1 \cdot s$ – is the volumetric heat transfer coefficient; s – is the specific surface area of pores; $q_R = \varepsilon_S \cdot \sigma \cdot T_S^4$ – is the radiative flux from the outer wall of the tube to the environment; ε_S - is the degree of emissivity; τ - is time; z – is the dimensional space coordinate directed along the tube axis; α_1, α_2, α_3 – is the heat transfer coefficients in the input, the output section and on the outer wall of the pipe; r_1, r_0 – inner and outer radii of the tube; $\rho_0, c_{P0}, \lambda_0, \varphi_i$ – is the density, heat capacity, thermal conductivity factor and the volume ratio: coke (i = 1), water (i = 2), fly ash (i = 3) and the gas phase (i = 4); $\lambda_4, \lambda_R, \lambda_S$ – is the coefficients of molecular and radiant thermal conductivity of the gas phase and the thermal conductivity of the condensed phase; σ –

Stefan - Boltzmann constant; μ – Dynamic viscosity coefficient; β – Constant in the quadratic law of filtration.

3 Analysis of the results of numerical calculations

Testing of the mathematical model was used for the future research. As the basis of the test of numerical calculations an experiment with a sample of "Berezovskaya" mine where the temperature in the layer of material is around 1273 K was taken [3].

Numerical calculations were performed for the following parameters:

$\rho_1 = 1500$ kg/m³, $\rho_2 = 1000$ kg/m³, $\rho_3 = 1560$ kg/m³, $\rho_4 = 1.25$ kg/m³, $c_1 = 1630$ J/(kg·K), $c_2 = 4190$ J/(kg·K), $c_3 = 800$ J/(kg·K), $\lambda_1 = 0.4$ W/(m·K), $\lambda_2 = 0.61$ W/(m·K), $\lambda_3 = 0.8$ W/(m·K), $\lambda_4 = 0.0268$ W/(m·K)), $\lambda_{O_2} = 0.0268$ W/(m·K), $\lambda_{CO} = 0.025$ W/(m·K), $\lambda_{CO_2} = 0.038$ W/(m·K), $\lambda_{H_2} = 0.307$ W/(m·K), $\lambda_{H_2O} = 0.029$ W/(m·K), $\lambda_{N_2} = 0.025$ W/(m·K), $E_{S1} = 140$ kJ/mol, $q_{S1} = -1.0875 \cdot 10^7$ J/kg, $E_{S2} = 207$ kJ/mol, $q_{S2} = 9.64 \cdot 10^5$ J/kg, $E_{CO} = 106.5$ kJ/mol, $q_{CO} = -1.08 \cdot 10^6$ J/kg, $k_{S1} = 2.08 \cdot 10^4$ m/s, $k_{S2} = 306$ m/s, $S = 6 \cdot 10^5$ 1/m, $T_H = T_S = 293$ K, $p_H = 1.01 \cdot 10^5$ Pa, $\varphi_{1H} = 0.352$, $\varphi_{2H} = 0$, $\varphi_{3H} = 0$, $\varphi_{4H} = 0.648$.

The testing has shown that there is good agreement on the percentage of gasification products after warming up the sample. The temperature in the sample layer that was found numerically, also consistents with the results of laboratory tests. Thus, the proposed mathematical model can be used to analyze the composition of the gas in the study of organic raw materials conversion processes. During the tests the temperature and the concentrations of gas components relationships that were obtained by numerically solving the mathematical model (1) – (8), were different not more than 5% from the sample conversion process of "Berezovskaja" that was provided in the laboratory.

Thus, the proposed mathematical model can be used to analyze the composition of the gas in the study of organic raw materials conversion processes.
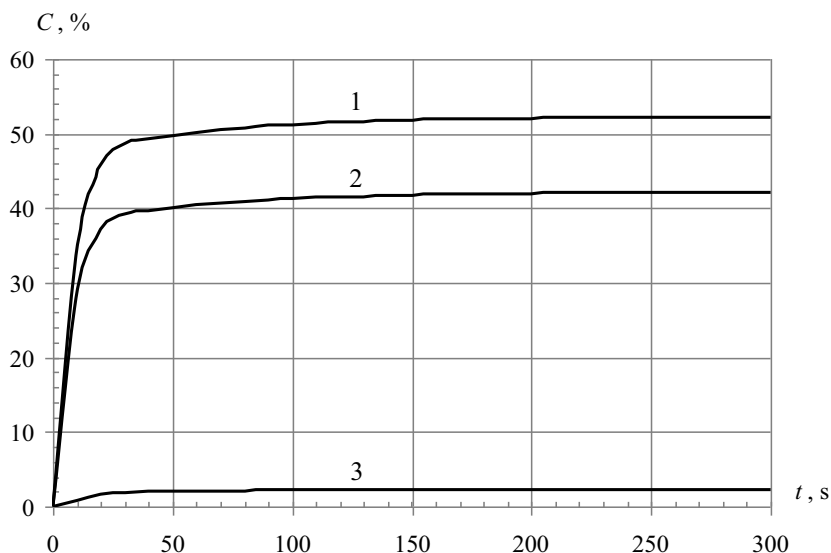
Fig. 1. Percentage of synthesis (water vapor) 873 K: line 1 – H_2 , line 2 – CO, line 3 – CO_2 .

Therefore, based on this model studies of the yield of synthesis gas depending on the temperature of the fed steam, porosity of solid gasified fuel and steam flow have been conducted.

Figures 1 and 2 show the volumes of gas components (in percent) formed by blowing coke with high temperature steam.
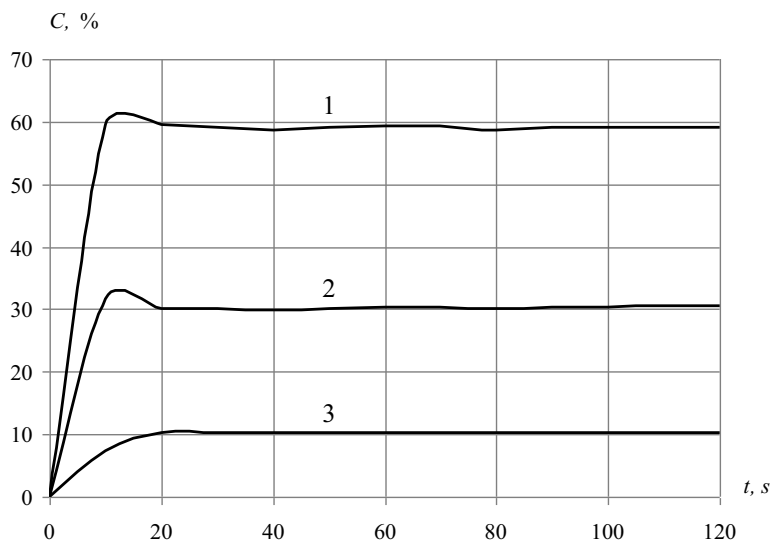
Fig. 2. Percentage of synthesis gas formed during the conversion of coke at a temperature of supplied oxidant (water vapor) 1473 K: line 1 – H_2 , line 2 – CO, line 3 – CO_2 .

Analyzing figures 1 and 2, it can be concluded that the increase in coke gasification temperature alters the composition of the synthesis gas. The proportion of hydrogen and carbon dioxide increases and carbon dioxide concentration decreases. The porosity and oxidant flow rate influence on the composition significantly weaker then the temperature, however, these relationships are not given.

4 Conclusions

On the basis of numerical calculations we can draw the following conclusion: a mathematical model describes the process of a solid fuel conversion with accuracy sufficient for practice, and it can be used to predict the composition of the synthesis gas in the gasification of solid fuels. Changing temperature of oxidant and its rate of supply and the fuel porosity influence on the composition of the resulting combustible gas.

References

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