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REGIMES OF GASIFICATION OF LEAN COAL LAYERS

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Based on a generalized volume-average model, the regimes of filtration combustion in gasification of lean coal layers, which are of interest for evaluation of the parameters and realization of underground gasification of brown Belarusian coals, have been analyzed. The existence of two basic regimes — those of cocurrent and countercurrent gasification waves — has been established. Data on the characteristics of the regimes and the conditions of their existence have been obtained.

Introduction. The assumption of underground coal gasification (UCG) was first expressed by the Russian scientist D. I. Mendeleev in 1888. However, industrial UCG technologies were created only in the early 1930s [1–3]. The essence of the method of underground gasification lies in organizing an unusual kind of reactor incorporating channels for feeding of a blast gas and evacuation of a producer gas as well as filtration channels inside the coal seam. Gas formation in the pores and channels of such a reactor is due to the exothermal reactions of oxidation of carbon and thermal decomposition of the coal. The yield, composition, and heat of combustion of the gas produced depend on the composition of the blast fed to the wells (air- or vapor-oxygen type), the grade of coal and its composition, the geological conditions of bedding of a coal seam, its thickness and structure, and other factors. Oxygen-enriched blast is required when the thickness of the coal seams and their water encroachment are small. The calorific value of the product gas does not exceed 4.4 MJ/m^3 for the air blast, 5.0 MJ/m^3 for the vapor-air blast, and 6.7 (65%) for the oxygen-enriched blast.

There is increased worldwide interest in the UCG problem at present; this interest is primarily due to the rise in prices for traditional energy resources: petroleum and natural gas. The topicality of the UCG problem for Belarus is determined by the fact that the low-heat-content brown coals whose open-cut (strip) mining is uneconomical and environmentally unsafe represent most of the coal resources in our Republic.

It is common knowledge that the organization of an efficient and stable UCG process calls for the monitoring of the state of the reactor and adequate simulation modeling of the thermochemical processes in it as well as for a clear idea of possible gasification regimes. Comprehensive numerical UCG investigations based on the modern physicochemical models are absent at present. The available works are concerned with narrow problems. Models and the results of modeling of air and vapor-air gasification of carbon diluted with inert additives, where allowance was made for the dependence of the thermophysical characteristics of phases on the temperature and composition of the solid phase, have been presented in [4, 5]. Three regimes of propagation of a cocurrent gasification wave — normal, inverse, and transition ones — were identified. The weight fraction of carbon in the fill was a determining parameter for distinction between the regimes. However, a number of significant simplifications were made: the reaction-zone thickness was assumed to be small; it was taken that the thermodynamic equilibrium between the components and the thermal equilibrium between the phases are set instantaneously in the reaction zone; the heat loss was disregarded; the stationary problem was solved without allowance for the influence of the initial conditions.

Consideration of the process of propagation of a gasification wave as a stationary one in the reference system tied to the moving front is indeed an adequate approximation for the steady-state regime. However, as has been shown in [6] and in our investigations, the characteristics of the steady-state regime are substantially influenced by the initial conditions, especially the location of the ignition region and the ignition temperature. Furthermore, the chemical-reaction region can occupy a considerable part of the computational domain under certain conditions. In this case, the idea

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TABLE 1. Parameters of the Chemical Model of Air Gasification of Coal

Reaction	z	A, kJ/mole
$C + O_2 = CO_2$	$10.6 \cdot 10^4$ m/sec	120
$CO_2 + C = 2CO$	$6.94 \cdot 10^4$ m/sec	185
$2CO + O_2 = 2CO_2$	$8.5 \cdot 10^{12}/p^{1.5}$ (mole/liter)^2/sec	

of the reaction zone as of the surface of weak discontinuity is incorrect, and it is necessary to consider the structure of the reaction zone in detail.

The present work seeks to investigate the influence of the initial conditions and the parameters of the process on the type and characteristics of the steady-state regime of gasification in lean coals.

Formulation of the Problem. We consider a one-dimensional gas generator with a fixed porous layer, on one side of which (inlet) an air blast is fed, and a product gas is removed on the other (outlet).

The chamber was initially filled with nitrogen. A blast with a composition of 20% oxygen and 80% nitrogen was fed to the inlet. The length and diameter of the computational domain were 0.5 m, the emissivity factor of the solid-phase substance was 0.35, the average diameter of solid-phase particles at the initial instant of time was 2 cm, the density of the solid-phase substance was 1500 kg/m^3, and the specific heat of the solid-phase material was 1000 J/(kg·K). The initial temperature of the gas phase and the temperature of the air blast coincided with the temperature of the walls in all calculations. Heat exchange with the environment was carried out by radiation (gray body) through the inlet and outlet cross sections and was quantitatively determined by the emissivity factor of the ends and lateral walls of the reactor ε_w. The temperature of the fill T_f was prescribed by a step function or was constant throughout the gasifier volume. The initial fill temperature in the cold region was equal to the wall temperature T_w. The settling and falling-down of the porous medium were disregarded.

Since lean coals are characterized by a high ash content and a low heat content, in the model adopted they are determined as a mixture of active carbon and an inert component. The weight fraction of carbon in the solid phase is determined by the relation between the initial and maximum porosities of the system (it is attained when the entire carbon is gasified). It is assumed that the densities of carbon and of the solid-phase material left after gasification are equal. Under such an assumption, the weight fraction of carbon at any instant of time is expressed by the running and maximum porosities as follows:

$$\omega_C = \frac{m_{\max} - m}{1 - m} .$$

Mathematical Model. For the calculations, we use a generalized volume-averaged model of filtration combustion [7]; this model is constructed on the equations of thermal balance in the solid and gas phases, equations of transfer of the gaseous-component mass, and equations of continuity, diffusion hydrodynamics, and state of the gas

$$\frac{\partial (m\rho_g)}{\partial t} = -\nabla\cdot(m\rho_g \mathbf{u}) + m \sum_i R_i ; \tag{1}$$

$$\rho_g \frac{\partial \mathbf{u}}{\partial t} = -\rho_g (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \mathbf{u} \sum_i R_i - \nabla p - \mathbf{f} , \quad \mathbf{f} = \frac{\mu}{k_0}\mathbf{u} + \frac{\rho_g}{k_1} |\mathbf{u}|\, \mathbf{u} ; \tag{2}$$

$$m\rho_g \frac{\partial C_i}{\partial t} = -m\rho_g \mathbf{u}\cdot\nabla C_i - \nabla\cdot(m\mathbf{I}_i) + mR_i - mC_i \sum_j R_j , \quad \mathbf{I}_i = -\rho_g \mathbf{D} \otimes \nabla C_i ; \tag{3}$$

$$m\rho_g c_g \frac{\partial T_g}{\partial t} + m\rho_g c_g \mathbf{u}\cdot\nabla T_g = -\nabla\cdot(m\mathbf{J}) + \alpha\,(T_s - T_g) + Q_g\,, \quad \mathbf{J} = -\mathbf{\Lambda}\otimes\nabla T_g\,; \tag{4}$$

$$\rho_s c_s \frac{\partial\,[(1-m)\,T_s]}{\partial t} = \nabla\cdot(\lambda\nabla T_s) + \alpha\,(T_g - T_s) + Q_s\,; \tag{5}$$

$$\frac{\partial\,[(1-m)\,\rho_s]}{\partial t} = -\rho_s \frac{\partial m}{\partial t} = -m\sum_i R_i\,. \tag{6}$$

To form terms describing the heat and mass sources we write the equations of chemical kinetics of the components in question. The contribution of the chemical reactions to the energy equation is expressed by the heat source, which is equal to $-m\sum_i h_i R_i - m h_C R_C$; the contribution from heterogeneous reactions is involved in Q_s, and that from gas-phase reactions is involved in Q_g.

Chemical Model. We use the following kinetics of combustion and gasification of coal [8]:

$$C + O_2 = CO_2\,, \tag{7}$$

$$CO_2 + C = 2CO\,, \tag{8}$$

$$2CO + O_2 = 2CO_2\,. \tag{9}$$

From the data of [8, 9], at low pressures ($p < 1$ MPa), the heterogeneous reactions (7) and (8) have the first order in the gaseous and surface component, i.e., the rate of decrease in oxygen according to the reaction (7) is determined by the expression

$$\frac{dY_{O_2}}{dt} = -zY_{O_2} S \exp\left(-\frac{A}{R_0 T}\right). \tag{10}$$

We have analogous equations for the rates of formation and decrease in other components of the gas phase. The values of the employed parameters of the reaction-rate constants are given in Table 1. In calculating the rate of the heterogeneous reaction of oxidation of carbon, we assumed that the specific area of the solid-phase surface occupied by carbon was equal to its weight fraction.

Calculation Results. In the computational experiments, we varied the following parameters of the system: initial content of carbon in the solid phase (with a constant maximum porosity) from 0.05 to 0.55, emissivity factor of the walls from 0 to 0.55, maximum porosity of the system (with a constant initial content of carbon in the solid phase) from 0.55 to 0.9, flow rate of the air blast from 0.1 to 90 m^3/h (the flow rate was measured at a temperature of 3000 K and a pressure of 101,325 Pa), initial temperature of the hot region from 500 to 1500 K, and wall temperature from 300 to 1500 K; also, we varied the location and size of the ignition region.

According to the results of the calculations, we revealed three characteristic regimes of gasification: cocurrent and countercurrent gasification waves and slow, low-temperature gasification sustained by the wall temperature throughout the volume of the computational domain.

A cocurrent gasification wave appears in all versions of ignition (location of the heated region) at wall temperatures above 800 K (at an ignition temperature of 1500 K) and is characterized by the complete conversion of coal. This regime is similar to the regime of filtration combustion of an oxidizer-depleted mixture in an inert porous medium. The characteristic temperature profiles of the solid and gas phases for the cocurrent wave are shown in Fig. 1.

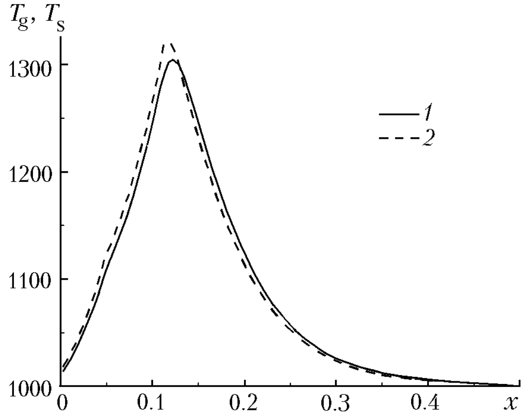

Fig. 1. Temperature profiles of the solid and gas phases in the cocurrent gasification wave: 1) T_g; 2) T_s. $T_w = 1000$ K and $q = 10$ m^3/h. x, m; T_s and T_g, K.

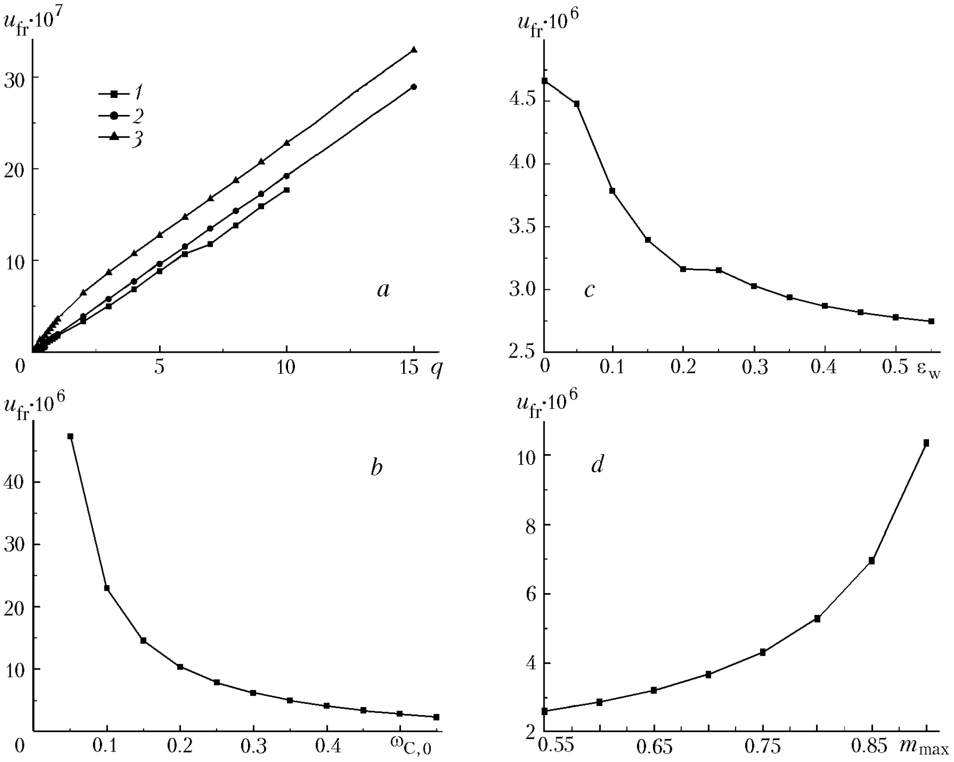

Fig. 2. Velocity of the front of the cocurrent gasification wave u_{fr} vs. flow rate of air q (a) (1) $T_w = 850$; 2) 1200; 3) 1500 K; $\varepsilon_w = 0.45$ and $\omega_{C,0} = 0.56$), initial weight fraction of carbon in the solid phase $\omega_{C,0}$ (b), emissivity factor of the reactor ε_w (c), and maximum porosity of the system m_{max} (d). u_{fr}, m/sec; q, m^3/h.

The velocity of the cocurrent-wave front is approximately proportional to the flow rate of air (Fig. 2a), since the oxygen is consumed completely, decreases with increase in the carbon content (Fig. 2b) and with growth in the emissivity factor of the reactor walls (Fig. 2c), and increases with maximum porosity (Fig. 2d). When the wall temperature is above 850 K, the rate of the front of the cocurrent gasification wave weakly depends on the wall temperature.

A countercurrent gasification wave appears in ignition near the outlet. This occurs for high flow rates of air — from 20 m^3/h at a wall temperature of 800 K and an ignition temperature of 1500 K for nonadiabatic conditions

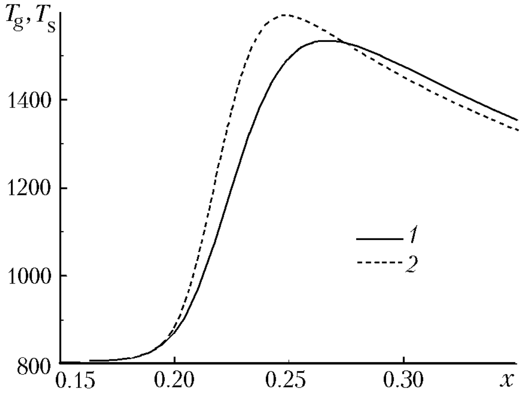

Fig. 3. Temperature profiles of the solid and gas phases in the countercurrent gasification wave: 1) T_g; 2) T_s. T_w = 800 K, q = 50 m^3/h, and ε_w = 0.45. x, m; T_s and T_g, K.

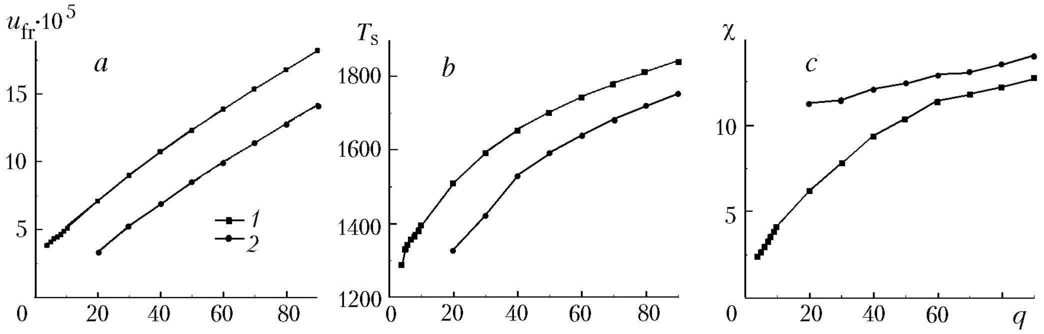

Fig. 4. Velocity of the front of the countercurrent gasification wave (a), peak temperature of the solid phase on the countercurrent-wave front (b), and degree of conversion of carbon after the passage of the countercurrent gasification wave (c) vs. flow rate of air: 1) ε_w = 0; 2) 0.45. T_w = 800 K. u_{fr}, m/sec, T_s, K, χ, %, and q, m^3/h.

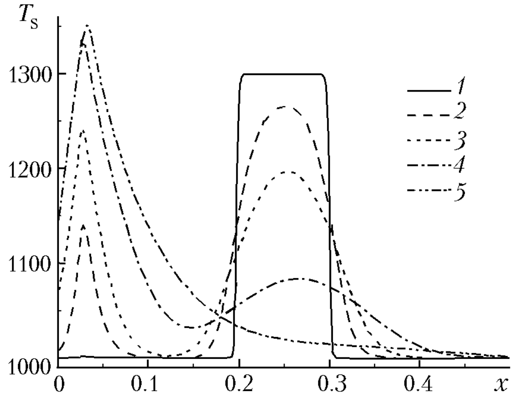

Fig. 5. Evolution of the transition regime of gasification using the coordinate dependence of the solid-phase temperature as an example: 1) t = 1.06; 2) 92; 3) 292; 4) 991; 5) 3332 sec. x, m, and T_s, K.

and for flow rates from 4 m^3/h and a cold-region temperature of 800 K for adiabatic conditions. The wave propagates from the outlet to the inlet of the gasifier; the carbon is gasified incompletely. The higher the flow rate, the narrower the combustion zone, since, when the flow rates are high, we have an increase in the heat release in the reaction zone and consequently in the peak temperature on the front. As the gasifier inlet is approached by the wave, the combustion continues but in the cocurrent gasification wave now. Typical temperature profiles of the solid and gas phases, the dynamic curves, and the dependences of the peak temperature of the solid phase and the degree of conversion of carbon on the flow rate for the countercurrent wave at a wall temperature of 800 K are given in Figs. 3 and 4.

A determining criterion for the appearance of a countercurrent gasification wave is the location of the ignition region and the relation between the heat release and the heat conduction/heat loss. When the flow rates are low, heat released in the hot region is rapidly distributed throughout the reactor length; therefore, the initial location of the hot region does not influence the evolution of the system and the cocurrent gasification wave propagates without a countercurrent gasification wave. A similar situation holds at a fairly high wall temperature (Fig. 5).

Gasification throughout the gasifier volume is observed when the heat released in the reaction is insufficient for sustaining a self-propagating cocurrent gasification wave. Oxygen is consumed incompletely in this regime, but the conversion of carbon is complete, as in the case of a cocurrent wave. A determining factor in the appearance of such a regime is the heat loss. For $\varepsilon_w = 0.45$, this regime is found at wall temperatures below 800 K; for $\varepsilon_w = 0.01$, it manifests itself at lower temperatures, down to 300 K.

Conclusions. Using numerical methods, we have investigated the gasification of lean coal layers in a flow-type reactor. The generalized volume-averaged model modified for solution of this problem has been used for the calculations.

The evolution of the process of gasification has been considered for different values of its parameters. According to the results of the calculations, it has been established that there are two basic regimes: cocurrent and countercurrent gasification waves. Each regime has been investigated in detail and the data on the dependence of the wave velocity, the degree of conversion, and the peak front temperature on the varied parameters of the process have been obtained. Also, the range of parametric values for which each regime is realized has been studied.

The regime of transition from the initial disturbance to a cocurrent gasification wave and the regime of slow gasification (smoldering) throughout the gasifier volume have been identified in addition to the two basic regimes.

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NOTATION

A, activation energy, J/mole; C, weight fraction; c, specific heat, J/(kg·K); $\mathbf{D}$, diffusion-coefficient tensor, $\mathrm{m^2/sec}$; $\mathbf{f}$, volume density of the filtration-resistance force, $\mathrm{N/m^3}$; h, specific enthalpy, J/kg; $\mathbf{I}$, diffusion-flux density, $\mathrm{kg/(m^2 \cdot sec)}$; $\mathbf{J}$, half-flux density in the gas phase, $\mathrm{W/m^2}$; k_0, permeability coefficient, $\mathrm{m^2}$; k_1, Forchheimer coefficient, m; m, porosity; p, pressure, Pa; Q, volume heat-release rate, $\mathrm{W/m^3}$; q, flow rate of the fed gas, $\mathrm{m^3/h}$; R, volume rate of formation of the component, $\mathrm{kg/(m^3 \cdot sec)}$; R_0, universal gas constant, J/(mole·K); S, specific area of the reaction surface, 1/m; t, time, sec; T, temperature, K; $\mathbf{u}$, gas-velocity vector, m/sec; u, velocity, m/sec; x, coordinate, m; Y, molar concentration, $\mathrm{mole/m^3}$; z, preexponential factor whose dimension depends on the reaction order; α, coefficient of interphase heat exchange, $\mathrm{W/(m^3 \cdot K)}$; ε, emissivity factor; Λ, thermal-conductivity tensor in the gas phase, W/(m·K); λ, effective thermal conductivity of the solid phase, W/(m·K); μ, dynamic viscosity of the gas phase, Pa·sec; ρ, density, $\mathrm{kg/m^3}$; χ, degree of conversion, %; ω, weight fraction in the solid phase. Subscripts: C, carbon; f, fill; fr, front; g, gas phase; i, component No.; s, solid phase; w, wall; 0, initial value; max, maximum.

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