

GENERALIZED VOLUME-AVERAGED FILTRATION COMBUSTION MODEL AND ITS APPLICATION FOR CALCULATING CARBON GASIFIERS

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We have developed a generalized volume-averaged model of filtration combustion of gases taking into account the spatial inhomogeneity of a porous medium and the change in porosity due to the heterogeneous chemical processes. Adequate program codes have been realized. The calculations performed have shown that the gasification rate in a continuous reactor is almost proportional to the oxidizer flow rate and depends on the degree and character of inhomogeneity. It has been found that the CO content at the outlet depends on the degree of inhomogeneity.

Combustion in heterogeneous media under the conditions of gas filtration, or filtration combustion (FC), is widely distributed in natural and technological processes. In the last few years, on this basis technologies of burning up low-calorific gaseous mixtures and cleaning of free-flowing materials and sorbents have been developed, and thermochemical conversion of hydrocarbons has been carried out [1]. The gasification of heterogeneous granular materials that attracts close attention of researchers because of the rising prices for the basic energy carriers and the development of hydrogen power engineering can be considered as an FC process.

To investigate the FC, the volume-averaged (VA) approximation — the model of interpenetrative continua, in which the heterogeneous medium is described by the continuous functions of its averaged parameters, is widely used. This model includes the balance equations of heat in the solid and gas phases, the diffusion of the gaseous components, and the equations of continuity, filtration, and state of the gas [2]

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}) = 0, \quad -\nabla p = \frac{\mu}{k_0} \mathbf{u} + \frac{\rho_g}{k_1} |\mathbf{u}| \mathbf{u}, \quad \rho_g \frac{\partial C_i}{\partial t} + \nabla \cdot (\rho_g \mathbf{u} C_i) - \nabla \cdot (\rho_g \mathbf{D} \otimes \nabla C_i) = R_i,$$

$$\rho_g c_g \frac{\partial T_g}{\partial t} + \rho_g c_g \mathbf{u} \cdot \nabla T_g - \nabla \cdot (\mathbf{\Lambda} \otimes \nabla T_g) = \frac{\alpha}{m} (T_s - T_g) - \sum_i h_i R_i,$$

$$(1 - m) \rho_s c_s \frac{\partial T_s}{\partial t} - \nabla \cdot (\lambda \nabla T_s) = \alpha (T_g - T_s), \quad \rho_g = \frac{pM}{R_0 T_g}.$$

For the terms corresponding to the sources in the heat and mass balance equations, the equations of the chemical kinetics of the gaseous components under consideration are written.

The VA method considerably simplifies the mathematical description of filtration combustion as compared to the detailed consideration of the heterogeneous porous system and makes it available for analytical and numerical studies. However, this leads to a loss of immediate information about the structure of the porous medium and the microstructure of the flows and to a roughening of the data on the temperature and concentration fields.

Systems with spatially inhomogeneous characteristics of the porous medium having several scales of inhomogeneity, as well as systems with time-varying structural parameters, cannot be adequately described from the point of view of the FC model. Therefore, in studying the gasification of polydispersive hydrocarbon materials, one should take

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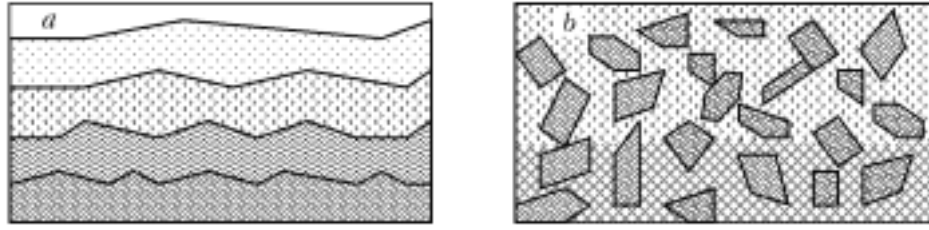


Fig. 1. Schematic representation of the porosity structure in the layer of caked sawdust (a) and charged lump coal (b).

into account the above features. Figure 1 schematically represents the spatially inhomogeneous structure of a porous medium.

Increasing computer powers and the thus-provided possibility of particularization of the computational grid permit partial compensation for the loss of data on the porous-medium structure. Giving the spatial distribution of porosity and other parameters of the porous medium, one can attain the effect of resolution of the solid-phase boundary. If the structural parameters of the frame are given in accordance with the existing inhomogeneities, then the filtration field, the local gasification rate, and other indices of the process will be largely adequate to the real gasification system. We named the model describing the spatial inhomogeneity of the porous medium and the change in these parameters with time the generalized volume-averaged (GVA) model of filtration combustion. Thus, the GVA model is a step on the way to detailed numerical simulation of a porous system. It permits considering more complex objects and processes, in particular, the gasification of media having several scales of inhomogeneity.

Below, the GVA model of FC with spatially inhomogeneous and time-dependent parameters of the porous medium is described. Using the proposed model and the program codes realized on its basis, the influence of the nonuniformity of coal filling on its gasification parameters in a continuous gasifier is investigated. The dependence of the composition of products and the gasification rate on the type and degree of inhomogeneity, the gas flow rate, and the blast and wall temperature is considered.

Mathematical Model. The structure of a porous medium is characterized by many parameters; however, only two of them can be taken as independent ones: porosity m and effective particle size d_0 ; the other parameters, such as specific surface, channel windening, and filtration (permeability) factors, are calculated by m and d_0 .

A generalized volume-averaged model can be derived by averaging the local heat and mass transfer equations without assuming that the local characteristics of the porous medium are constant and homogeneous. In so doing, the mathematical formulation of the model includes the equations of:

continuity

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

motion

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

transfer of individual components of the gas phase

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

energy transfer in the gas phase

$$m\rho_g \frac{\partial E_g}{\partial t} = -m\rho_g \mathbf{u} \cdot \nabla E_g - \nabla \cdot \left(m\rho \mathbf{u} + m\mathbf{J} + m \sum_i h_i \mathbf{I}_i \right) + m\mathbf{f} \cdot \mathbf{u} + \alpha (T_s - T_g). \quad (4)$$

Equation (4), with the aid of (1)–(3), can be written as

$$m\rho_g c_g \frac{\partial T_g}{\partial t} + m\rho_g c_g \mathbf{u} \cdot \nabla T_g = -\nabla \cdot (m\mathbf{J}) + \alpha (T_s - T_g) + Q_g, \quad \mathbf{J} = -\Lambda \otimes \nabla T_g. \quad (5)$$

The model also contains the equations of:
energy transfer in the solid phase

$$\rho_s \frac{\partial [(1-m) E_s]}{\partial t} = \nabla \cdot (\lambda \nabla T_s) + \alpha (T_g - T_s) + Q_s; \quad (6)$$

mass balance of the solid-phase component

$$\frac{\partial [(1-m) \rho_s]}{\partial t} = -\rho_s \frac{\partial m}{\partial t} = -m \sum_i R_i. \quad (7)$$

Note that, compared to the standard VA model in (1), (3), (5)–(7), the value of the medium porosity m has been introduced under the differentiation sign.

Model of the Heterogeneous Chemical Kinetics. In our model, the determination of the types of reactants, reactions, and rules of their description is, on the whole, analogous to that presented in the CHEMKIN package. We took into account thereby the experience of simulating combustion processes and complex chemical transformations (2DBurner package) [3] and the features of gasification of solid hydrocarbon materials.

In the gas–solid phase system, three groups of components are considered: gaseous components, components of the bulk solid phase, and components of the surface solid-phase (sorbates, radicals, molecules, catalytic centers). The bulk solid-phase components fill the internal volume of solid particles, and the surface solid-phase substances occupy an insignificant volume, but, by virtue of their being located at the interface, they can actively interact with other components. A distinguishing feature of this type of substances is the specific value of enthalpy.

The unified representation of the chemical reaction equation is of the form

$$\sum_{(i,g)} s_{i,g} F_{i,g} + \sum_{(i,s)} s_{i,s} F_{i,s} + \sum_{(i,b)} s_{i,b} F_{i,b} = \sum_{(i,g)} s'_{i,g} F_{i,g} + \sum_{(i,s)} s'_{i,s} F_{i,s} + \sum_{(i,b)} s'_{i,b} F_{i,b},$$

where (i, g) , (i, s) , and (i, b) are the indices of the components of the gas, solid, and surface phases. The rate of production of the i th component per unit volume is given by the expression

$$R_i = M_i \sum_k s_{ik} r_k.$$

In the general case, the rate of the k th reaction is given by the relation

$$r_k = -K(T) \prod_{(i,g)} Y_{i,g}^P \prod_{(i,s)} Y_{i,s}^P \prod_{(i,b)} Y_{i,b}^P.$$

The rate constants are calculated by the modified Arrhenius formula

TABLE 1. Parameters of the Elementary Kinetic Model of Air Gasification of Carbon

Reaction	z , m/sec	A , kJ/mole
$C + O_2 \rightarrow CO_2$	$10.6 \cdot 10^4$	120
$CO_2 + C \rightarrow 2CO$	$6.94 \cdot 10^4$	185
$2CO + O_2 \rightarrow 2CO_2$	$8.5 \cdot 10^{12}/p^{1.5}$ (mole/liter) ² /c	87.9

TABLE 2. Parameters of the Kinetic Model of Air Gasification of Carbon [6]

Reaction	A , kJ/mole	z , mole/(m ² ·sec)	ΔH , kJ/mole
$C + O_2 \rightarrow CO_2$	74 ± 3	9.2 ± 0.8	-393.8
$C + 1/2O_2 \rightarrow CO$	179 ± 10	$(37 \pm 5) \cdot 10^3$	-110.6
$C + CO_2 \rightarrow 2CO$	274 ± 8	$(1.8 \pm 0.5) \cdot 10^8$	172.6
$C + 2CO \rightarrow 2C + CO_2$	103 ± 8	0.15 ± 0.05	-172.6

$$K(T) = zT^l \exp \left\{ - \sum_{j=0}^n B_j T^j / T \right\}.$$

The contribution of the chemical reactions to the energy equation is given by a source equal numerically to $-m \sum h_{i,g} R_{i,g} - m \sum h_{i,s} R_{i,s} - m \sum h_{i,b} R_{i,b}$. Depending on the type of specific reaction, the heat released in the reaction can be assigned to the gas (or solid) phase and taken into account in the term Q_g or Q_s , respectively.

Prime Models of the Chemical Kinetics of Carbon Gasification. The simplified kinetics of the carbon gasification process, according to [4], has the following form:



According to the data of [4, 5], at low pressures ($p < 1$ MPa) the heterogeneous reactions (8) and (9) have the first order for the gas and surface components, i.e., the rate of oxygen decay by reaction (8) is given by the following expression:

$$\frac{dY_{O_2}}{dt} = -zY_{O_2}S \exp(-A/(R_0T)). \quad (11)$$

Accordingly, for the decay rate of carbon by reaction (8) we have the kinetic equation

$$\frac{d[(1-m)\rho_{s,C}]}{dt} = zY_{O_2}S \frac{M_C}{N_A} \exp(-A/(R_0T)). \quad (12)$$

The product $(1-m)\rho_{s,C}$ was introduced under the differential sign, since physically the substance decays due to the increase in porosity while the density of the solid-phase material remains constant. The numerical values of the parameters of the rate constants of the reaction are given in Table 1. The kinetic parameters of carbon gasification reactions, according to the data of [6], are given in Table 2.

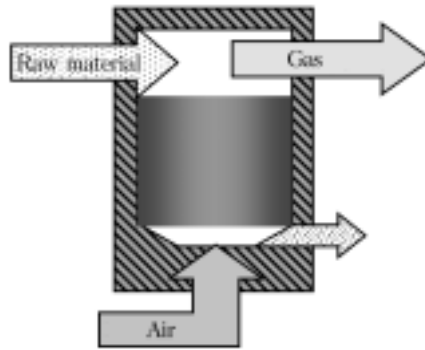


Fig. 2. Scheme of the forward-type gasifier.

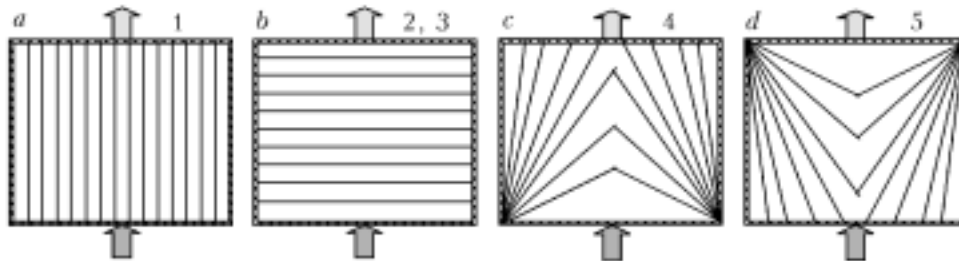


Fig. 3. Types of inhomogeneity of the gasifier fill: 1-5) geometries.

Problem Formulation. Depending on the type of fuel used in the gasifier and the requirements placed upon the process, various types of gasifiers are used. One of the most widely used gasifier schemes is the forward one (Fig. 2). In the present paper, a gas generator with a static layer with a different initial character of inhomogeneity has been considered. The most important quantitative characteristics of the gasifier operation are the time of going to the quasi-stationary regime, the mass rate of gasification, and the composition of the generator gas. Using the GVA model, we have made numerical studies of these characteristics depending on the blast temperature (the wall temperature was assumed to be equal to the blast temperature), the air flow rate, and the degree and configuration of the initial inhomogeneity of the raw-material filling.

The height and diameter of the gasifier chamber were equal to 0.5 m. In the calculations, we used five types of geometry of the initial inhomogeneity configuration, for which the schemes of the porosity isolines of the gasifier filling are depicted in Fig. 3: vertical geometry (Fig. 3a, geometry 1); horizontal geometry with an increase (geometry 2) and a decrease (geometry 3) in the flow porosity (Fig. 3b); axially symmetric conical geometry with a decrease (Fig. 3c, geometry 4) and an increase (Fig. 3d, geometry 5) in the flow porosity. Geometries 3 and 4 correspond to the reversed scheme of the gasifier.

In the calculations, uniform coordinate dependences of porosity were used. In so doing, in all cases the mean-volume porosity and the root-mean-square deviation from the mean values (except for the calculations of the influence of the degree of porosity) remained constant. The porosity values were varied over the range from 0.15 to 0.65. The granular carbon load mass was 100 kg at a material density of 1500 kg/m^3 . The size (effective diameter) of filling particles at the initial instant of time $d_0 = 2 \text{ cm}$. Because of the lack of data on kinetic models of gasifications, we took the elementary case — air gasification of carbon. The calculations were performed in the range of air flow rates $G = 0.3\text{--}20 \text{ m}^3/\text{h}$ under normal conditions. The following initial and boundary conditions were used: the filling temperature is T_f ; the chamber is initially filled with nitrogen; air is fed into the chamber at temperature T_0 ; the temperature of the chamber walls is T_w . The calculations by an analogous model [7] have shown that for a fairly large heat content of the gasification product (predominance of CO over CO_2 in the product) it is necessary to hold the wall and blast temperature at a high value of $T_w > 1200 \text{ K}$. Therefore, we used temperatures in the 1200–1500 K range. In all calculations, the initial filling temperature $T_f = 1500 \text{ K}$.

Results of the Calculations. We can distinguish two stages in the development of the gasification process: initial establishment of concentration fields that lasts for about 100 sec (during this time the CO wave reaches the exit

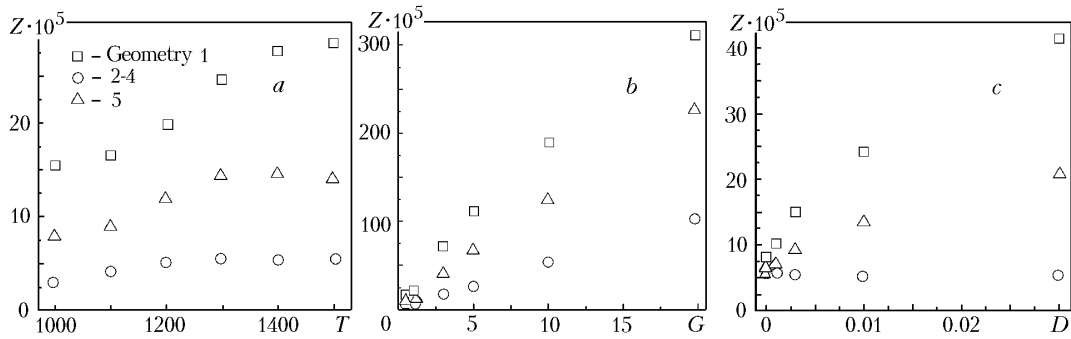


Fig. 4. Gasification rate Z versus temperature T_0 (for different types of inhomogeneities at temperatures from 1000 to 1500 K (a); air flow rate G (b); porosity dispersion D (c); Z , kg/sec; T_0 , K; G , m³/h.

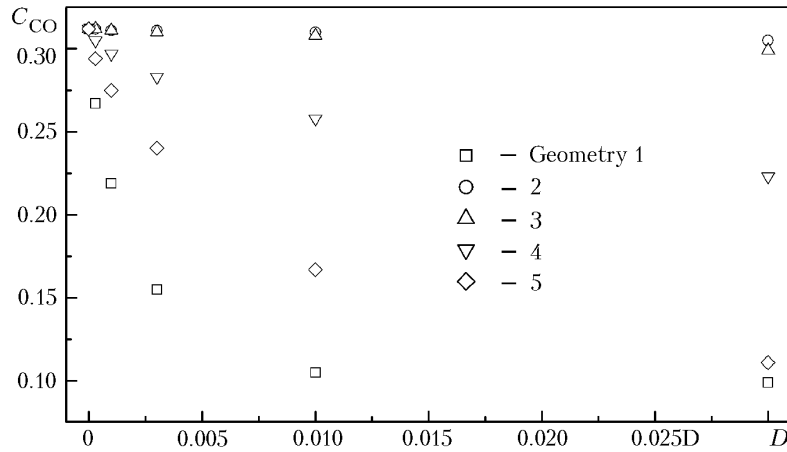


Fig. 5. Mass concentration of carbon monoxide at the gasifier outlet C_{CO} (at time $t = 600$ sec) versus the degree of inhomogeneity (dispersion D) for several types of configuration.

from the gasifier) and establishment of the steady state of heat beginning at 500–1000 sec. During the first stage, the mass concentration of CO at the outlet reaches its maximum value, and the blast and wall temperature turns out to be immaterial. During the second stage, the CO concentration begins to decrease because of the chamber cooling due to the walls and the blast.

The blast and wall temperature practically does not influence the proceeding of the first stage of the process. The mass concentration of CO at the outlet reaches its maximum value, equal to about 0.33 over the course of 1–100 sec (depending on the flow rate and the degree and type of inhomogeneity), after which it begins to decrease. At a higher temperature of the blast and walls, the decrease in the CO concentration is markedly retarded.

As the blast and wall temperature increases from 1200 to 1400 K at an equal air flow rate, the mass rate of gasification changes but slightly (Fig. 4a): as the temperature increases from 1200 to 1300 K, it increases by 7%, and with increasing temperature from 1300 to 1400 K — by 0.6%. This is due to the fact that, under such conditions, the whole of the inflowing oxygen enters into the reaction and the end product of the gasification is CO. At lower temperatures, as the calculations of [7] show, the mass rate of gasification is temperature-dependent. This is attributed to the fact at the outlet CO₂ prevails and for each molecule of oxygen there is one carbon atom rather than two as in the case of CO. At even lower temperatures, not all oxygen enters into the reaction.

The calculations have shown that the mass rates of gasification at horizontal (Fig. 3b, geometries 2 and 3) and conical (reversed scheme of the gasifier, Fig. 3c, geometry 4) inhomogeneities differ insignificantly, while at conical inhomogeneity in the forward scheme of the gasifier (Fig. 3d, geometry 5) the rate is about 2.5 times higher, and with the use of vertical inhomogeneity (Fig. 3a, geometry 1) it is 5 times higher.

An increase in the degree of inhomogeneity of the material being gasified leads to an increase in the mass rate of gasification (see Fig. 4c). With increasing degree of inhomogeneity the mass concentration of CO at the outlet C_{CO} decreases (Fig. 5). In the case of horizontal inhomogeneity of a porous medium, the maximum value of C_{CO} and in the case of vertical inhomogeneity the minimum value of C_{CO} is reached.

CONCLUSIONS

1. A generalized volume-averaged model of filtration combustion of gases has been described. This model has been used to simulate the gasification process in a gasifier.
2. Dependences of the mass rate of gasification on the air flow rate, the temperature, and the degree of inhomogeneity of the fill for several types of geometries have been plotted.
3. It has been shown that the gasification rate is approximately proportional to the flow rate, increases with increasing temperature, reaching saturation at temperatures of the order of 1500 K, and increases with increasing degree of inhomogeneity of the fill.
4. The time dependence of the mass concentration of CO at the gasifier outlet has been obtained. It has been found that the mass concentration at the outlet decreases with increasing degree of inhomogeneity.
5. It has been found that the mass rate of gasification and the mass concentration of CO at the outlet, all other parameters being equal, depend on the type of inhomogeneity. The largest value of the gasification rate at the least content of CO is attained at vertical inhomogeneity.

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NOTATION

A , activation energy, J/mole; B , power-series coefficients, whose dimensionality depends on the ordinal number; C , mass concentration; c , specific heat capacity, J/(kg·K); \mathbf{D} , diffusion coefficient tensor, m²/sec; D , statistical variance of porosity; d_0 , particle size of the fill, m; E , specific inertial energy, J/kg; \mathbf{f} , volume density of the filtration drag force, N/m³; F , chemical formula of the component; G , inflowing gas-flow rate, m³/h; h , specific enthalpy, J/kg; H , molar enthalpy, J/mole; \mathbf{I} , diffusion flow density, kg/(m²·sec); \mathbf{J} , thermal flow density in the gas phase, W/m²; k_0 , permeability coefficient, m²; k_1 , Forchheimer coefficient, m; K , reaction-rate constant whose dimension depends on the order of the reaction; l , power parameter in the Arrhenius formula; m , porosity; M , molar mass, kg/mole; n , number of terms of the power series; N_A , Avogadro constant, mole⁻¹; p , pressure, Pa; P_i , order of reaction for the i th component; Q , volume heat-release rate, J/(m³·sec); R , volume rate of component formation, kg/(m³·sec); R_0 , universal gas constant, J/(mole·K); r , chemical reaction rate, mole/(m³·sec); s , stoichiometric coefficients of reagents; s' , stoichiometric coefficients of reaction products; S , specific area of the reaction surface, 1/m; t , time, sec; T , temperature, K; T_0 , inflowing gas temperature, K; \mathbf{u} , velocity vector, m/sec; Y , molar concentration, mole/m³; z , pre-exponential factor, whose dimension depends on the order of the reaction; Z , mass rate of gasification throughout the reactor volume, kg/sec; α , interphase heat-transfer coefficient, J/(m²·sec·K); Λ , heat-conductivity coefficient tensor in the gas phase, W/(m·K); λ , effective heat conductivity of the solid phase, W/(m·K); μ , dynamic viscosity of the gas phase, Pa·sec; ρ , density, kg/m³. Subscripts: b, bulk solid phase; C, carbon; f, fill; g, gas phase, i , component number; j , power-series term number; k , chemical reaction number; P , order of reaction for the component or temperature; s, solid-phase surface; w, wall.

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