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Calculation of the Fixed Bed Coal Gasification Regimes by the Use of Thermodynamic Model with Macrokinetic Constraints

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Abstract—We discuss an equilibrium model of a fixed-bed solid fuel gasification process that takes into account macrokinetic constraints imposed on the rates of heterophase processes and allows the pyrolysis and gasification processes to be described in a fairly simple manner with the use of thermal analysis data. The results of calculations are compared with the measured parameters characterizing the Azeisk coal steam–air gasification process that were obtained in experiments on a laboratory setup.

Keywords: fixed-bed gasification, thermodynamic modeling, models of extreme intermediate states, thermal analysis

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Gasification holds promise as a basic component of technologies for processing low-grade fuels such as brown coal and biomass. Those who design gas generators must know how to calculate the fuel exhaustion intensity (the mass rate at which fuel is converted into gaseous products), as well as the composition and calorific value of producer gas. Reliable engineering procedures for carrying out such calculations are not available as yet, which is due to the fact that such processes involve a large number of independent parameters as compared with direct combustion of fuel. Attempts to develop gas generator technologies using an empirical approach would take much time and involve excessively high costs. Therefore, it is expedient to develop mathematical models that would allow the characteristic parameters of the process to be calculated proceeding from general physicochemical concepts.

The main avenue in which models describing gasification of solid fuel are constructed consists in the use of diffusion-kinetic modeling. For being applied to low-grade fuels, the classic diffusion-kinetic carbon combustion theory has to be supplemented with kinetic equations describing the release of volatiles and tars and their thermochemical conversions [1]. The physicochemistry of elementary solid fuel decomposition processes has not been worked out to sufficient detail; therefore, simplifications and assumptions have to be used in developing such models, the validity limits of which is difficult to estimate.

We propose a method for describing chemical conversions of fuel central to which is the methodology for constructing models of extreme intermediate states (MEISs) [2, 3]. Extreme thermodynamic models are convenient for describing processes the detailed mechanism of which is unknown. For constructing them, it is sufficient to specify the set of substances that participate in the chemical reactions.

MEISs differ from the classic thermodynamic models in that the system equilibrium conditions can be supplemented with constraints that make the set of attainable states fewer in number while not allowing the reaching of full equilibrium. Such constraints are connected with chemical kinetics and transfer processes. Similar models were used in [4–7], the constraints in which were formulated on the basis of empirical information on the composition of producer gas.

Models of extreme intermediate states were used in [8, 9] for simulating gasification of fuels, where the fuel conversion ratio vs. the bed height was specified using experimental data. In this article, we present a spatially-1D MEIS of a fixed-bed gasifier the equilibrium conditions in which are supplemented with constraints obtained from the diffusion-kinetic theory. The operating parameters characterizing steam–air gasification of Azeisk coal were determined using this model, which are then compared with the data of a physical experiment.

DESCRIPTION OF THE MODEL

The model of thermodynamic equilibrium is written in the form of a mathematical programming problem as follows.