Simulation and Optimization of Entrained-Flow Air-Steam Gasification of Brown Coals

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***Abstract* — A mathematical model was used to estimate the achievable efficiency of brown coals gasification in air-steam atmosphere. The optimal conditions for gasification were determined, the values of the cold gas efficiency and the produced gas composition were obtained. The dependence of the incompletely burned carbon yield on the conversion conditions was established. The results obtained can be used to evaluate the engineering and economic performance of thermal power plants with integrated gasification combined cycle (IGCC) fed by brown coals.**

***Index Terms*: gasification, brown coal, mathematical modelling, optimization.**

I. Introduction

Prospects for the use of coal in the energy sector are currently ambiguous. On the one hand, coal is considered as a «fuel of the past» (due to its high specific emissions), and the recent energy projections indicate its gradual replacement with more environmentally friendly fuels [1, 2]. On the other hand, despite the decline in the share of total energy consumption, the coal consumption is still huge. The advantages of coal as a fuel are large reserves and low cost. Reducing fuel costs will make it possible to use power equipment to improve the efficiency of energy production and purification of combustion products. In this case, coal may be more attractive than fossil hydrocarbons (especially under the current circumstances of political and economic turbulence).

Clean coal technologies traditionally include combustion technologies (low-temperature combustion, Rankine cycle with higher values of parameters) and gasification technologies (combined cycle, CO_2 capture). In this paper, we address the latter way to improve the efficiency of coal fuel use. Until now, coal gasification has been used mainly in chemical technology (primarily for the production of cheap hydrogen). There have been several major projects aimed at the energy application of coal gasification but most of them were closed or put on hold after government subsidies were used up (e.g., the Wabash River) or for economic or technological reasons (e.g., the Kemper power plant). Few of them are currently operating (e.g, Nakoso IGCC [3] and Taean IGCC [4] plants). The slow development of gasification-based energy technologies in the area of high-capacities is primarily due to competition with coal combustion technologies, for which average efficiency of power production has increased almost to the level of IGCC [5]. The specific capital costs for the construction of IGCC plants are high, and their reliability is lower than that of conventional plants [6]. The advantages of coal-fired IGCCs are their values of environmental metrics: low nitrogen and sulfur oxides emission, lower costs for CO_2 removal [7, 8], and the possibility of combining the production of energy and chemical products [9]. The increase in gasification capacities is mainly concerned with the chemical industry, where coal is a source of cheap hydrogen and synthesis gases.

The reserves of brown coals exceed those of black coals but the thermochemical conversion of brown coals is, as a rule, more complicated from the technological standpoint. This is due to the lower calorific value of brown coal (low carbon content and higher moisture content) and the peculiarities of the physicochemical transformations of the organic and mineral parts under high-temperature conditions. The process of brown coal gasification discussed in this work is not considered from the point of view of the transformation of the mineral part (slagging and fly ash formation). The aim of the work is to assess the energy characteristics of the gasification process, which are determined by the composition of the organic part and moisture content.

For a reliable evaluation of the engineering and economic performance of IGGC plants, a method for calculating the characteristics of the gasification process is needed. The cold gas efficiency largely determines the

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thermal efficiency of the plant as a whole, as well as the choice of equipment for gas treatment and cooling. In some cases, experimental data are available [10]. However, that is not the case for new processes which have not been used in industry. In this regard, mathematical models of different levels of detail are also employed: from semi-empirical schemes and equilibrium approximations [11, 12] to complex multidimensional thermohydrodynamic codes [13]. When choosing the level of detail, first of all, it is necessary to take into account the application of simulation results: the optimization of the flow and heat transfer features requires the use of computational fluid dynamics models but the optimization of the gasifier operation modes as part of a power plant inevitably leads to the use of the simplest (empirical and thermodynamic) models.

In this work we study the single-stage process of pulverized coal gasification in air-steam mixtures numerically. To this end, a one-dimensional stationary fuel conversion process model is used. Despite simplifications and assumptions made, this model allows one to obtain more reliable estimates of the gasification process efficiency than the widely used chemical equilibrium models, while achieving it at a much lower computational cost than detailed thermohydrodynamic models. The proposed model can be used for a full-fledged engineering and economic optimization of the gasifier operation modes as part of an IGCC plant.

II. Mathematical Model and Input Parameters

A detailed description of the mathematical model and the results of its partial validation can be found in [14, 15]. The model was used earlier in the computational optimization of the parameters of entrained-flow gasification of various fuels with various gasifying agents [16, 17].

$$Uc_p \frac{d\left(m_p T_p\right)}{dz} = \alpha S_p \left(T_g - T_p\right) + \varepsilon\sigma S_p \left(T_w^4 - T_p^4\right) + \sum_j Q_j r_j . \qquad (1)$$

Eq. (1) includes the spatial coordinate z (reaction zone length), m; particles velocity U, m/s; particle mass m_p, kg; particle temperature T_p, K; particle heat capacity c_p, J/(kg·K); heat transfer coefficient α, W/(m^2·K); particle surface S_p, m^2; particle emissivity ε; Stefan-Boltzmann constant σ, W/(m^2·K^4); gas temperature T_g, K; wall temperature T_w, K; physicochemical processes rates r_j, kg/s (drying, pyrolysis, heterogeneous reactions); their thermal effects Q_j, J/kg.

Drying rate r_{dr} depends on the temperature range:

$$r_{dr} = \begin{cases} \dfrac{\beta S_p M_{H_2O}}{R_g T}\left(P_{H_2O}^{eq} - P_{H_2O}\right),\ T_p \le T_b, \\ \dfrac{\alpha S_p \left(T_g - T_p\right) + \varepsilon\sigma S_p \left(T_w^4 - T_p^4\right)}{\left|Q_{dr}\right|}, T_p > T_b. \end{cases} \qquad (2)$$

Here T_b is water boiling point, K; β is mass transfer coefficient, m/s; P_{H_2O} is partial water vapors pressure, Pa; R_g is gas constant, J/(mol·K).

Pyrolysis rate r_{pyr} depends on the temperature in Arrhenius law:

$$r_{pyr} = k_{pyr} \exp\left(-\frac{E_{pyr}}{R_g T_p}\right) m_V . \qquad (3)$$

Here k_{pyr} is a preexponential factor, 1/s; E_{pyr} is activation energy, J/mol; m_V is volatile matter content in particle, kg.

The heterogeneous reactions rate is determined by the diffusional kinetics equation:

$$r_g = \frac{S_p C_g}{\dfrac{1}{k_g e^{-\frac{E_g}{R_g T}}} + \dfrac{d_p}{Nu_D D_g}} . \qquad (4)$$

Here C_g is gasification agent concentration (O_2, CO_2, H_2O); k_g is a preexponential factor, m/s; E_g is activation energy, J/mol; Nu_D is diffusional Nusselt number; D_g is diffusivity, m^2/s; d_p is average particle diameter, m. Reaction heat Q_j was calculated from thermochemical data [18]. Arrhenius parameters of heterogeneous reactions were estimated using correlations proposed in [19]. The particle velocity is considered equal to the gas velocity as determined by the continuity equation. The gas composition in each section is at equilibrium given a fixed degree of fuel conversion (i.e., the equilibrium problem is solved for the gas phase). An iterative scheme is used to search for a stationary solution: the fuel conversion rate is calculated using a system of ordinary differential equations for changing the mass of particles at a given temperature distribution; using the thermodynamic model, the heat release and the composition of the gas phase in each calculation element are calculated; then the stationary problem of heat transfer is solved under fixed heat sources. The iterations are completed when the temperature distribution ceases to change perceptibly.

The gas phase equilibrium problem is as follows [20]: find

$$\mathbf{n}^{eq} = \operatorname{argmin} G(\mathbf{n},T)$$

subject to constraints:

$$G(\mathbf{n},T) = \sum_{j=1}^{N_g} n_j^g \left(\mu_j^g\left(T\right) + R_g T \ln \frac{n_j^g}{\sigma^g}\right) + \sum_{k=1}^{N_c} n_j^c \mu_j^c\left(T\right),$$

$$\mathbf{A}(\mathbf{n} - \mathbf{n}^{in}) = 0,$$

$$\mathbf{n} \ge 0.$$

Here G is Gibbs free energy, J/K; $\mathbf{n}$ is composition vector, mol ($\mathbf{n}^{in}$ is a vector of initial composition, $\mathbf{n}^{eq}$ is equilibrium composition), indices g and c correspond to gaseous and condensed phases; μ_j is the chemical potential of j-th component, J/mol; σ^g is gas phase molar sum, mol; $\mathbf{A}$ is element balance matrix. The enthalpy of coals is determined through the calorific value and enthalpies of combustion products. Properties of coal matter are modelled by pure carbon. The solution to the equilibrium problem in this form exists and is unique, which follows from the convexity of the thermodynamic functions for such systems [21, 22].

Table 1. Characteristics of coals.

	Berezosvky	Mugunsky	Urtuysky
C^{daf}, %	70.95	73.72	76.01
H^{daf}, %	4.98	5.61	4.86
O^{daf}, %	23.11	17.63	17.83
N^{daf}, %	0.64	1.44	0.81
S^{daf}, %	0.32	1.44	0.49
W^{r}, %	33	22	29.5
V^{daf}, %	48.0	56.4	39.1
A^{d}, %	7.0	20.0	8.8
HHV, MJ/kg	16.01	16.84	17.81
m_{air}, kg/kg	5.59	6.12	6.27

The composition of the coals used in the calculations is given in the table (data originate from the handbook [23]). These three coals are quite similar in composition: Mugunsky coal contains 2–3 times more ash and less moisture; Urtuysky coal contains more carbon in the organic mass and therefore has a higher calorific value. The stoichiometric amount of air required for complete combustion varies for the coals in the range of 5.5–6.3 kg/kg. The moisture content of coals is 22–33%, which does not quite correspond to the fuel milling and transport conditions (moisture content of pulverized coal can hardly exceed 10%): we use this assumption to simplify the calculations and partially take into account the costs of drying.

Calculations are carried out for a cylindrical reactor with a diameter of 3 m and a length of 9 m. The operating pressure is about 15 atm. The fuel consumption is about 50 kg/s. The average particle size is 0.1 mm. The gasification agent is a mixture of air and water vapor (initial temperature is 655 K). Variable parameters are specific air consumption (1–6 kg/kg of fuel), specific steam consumption (0–0.1 kg/kg of fuel), and fuel load (from 80 to 120% of the nominal flow rate). The characteristics of the gasification process are the temperature and composition of the produced gas, the incompletely burned carbonyield and the cold gas efficiency, which is equal to the ratio of the heating values of the produced gas and raw fuel:

$$\eta = \frac{q_{CO}n_{CO} + q_{H_2}n_{H_2} + q_{CH_4}n_{CH_4}}{Q_f}100\%.$$

Here Q_f is coal heating value, q_j is heating value of j-th gaseous component, n_j is the yield of j-th component, kg/kg$_{fuel}$. Produced gas heating value is calculated based on the main combustible components: CO, H_2 и CH_4. Cold gas efficiency is usually a function of stoichiometric parameters and temperature. In the present paper, we study the effect of fuel composition and air/fuel ratio.

III. Calculations Results and Discussion

A typical dependence of the produced gas composition on the air/fuel ratio is shown in fig. 1a. In the range of air-fuel ratios up to 2.5 kg/kg, the fraction of combustible components (CO and H_2) increases and the concentration of gasification agents (CO_2 and H_2O) decreases. Fig. 1b shows the corresponding growth of cold gas efficiency (Fig. 1b). With a further increase in the air/fuel ratio, combustible components are oxidized, and the cold gas efficiency decreases. In qualitative terms, this dependence is the same for all coals (Fig. 2), with slight deviations, which are explained away by the differences in the chemical and proximate composition. The curve shown in Fig. 1b has its extremum, approximately at the same level for all selected coals (corresponding cold gas efficiency is 67–69%). Unreacted oxygen appears in the reaction products below the stoichiometric air/fuel ratio. This is because an increase in air-fuel ratio (given a constant reaction zone length) reduces the dwell time of fuel particles in the reactor. At an air/fuel ratio of about 5 kg/kg, a significant incompletely burned carbon yield and a sharp temperature decrease are observed (Fig. 3). Interestingly, the maximum cold gas efficiency and the minimum incompletely burned carbon yield do not coincide: for a more complete conversion of the fuel, a small excess of air above the optimum is required. Commonly used thermodynamic models tend to make these extrema equal.

The fuel load slightly affects the per-unit indicators. Figure 4 shows the dependencies of the main combustible components yield (CO and H_2) in absolute units (mass flow rates) and below – in relative units (per-unit mass of the fuel from which they were obtained). Fuel consumption fluctuates within the 20% range, either above or below. As can be seen, the dependencies of the specific yields of the components practically coincide, at least in the region most interesting from a practical point of view (near the efficiency maxima).

Calculations were carried out to assess the effect of the fuel load and steam-fuel ratio on gasification efficiency. As expected, an increase in the steam-fuel ratio leads to a decrease in the incompletely burned carbon yield and a slight decrease in cold gas efficiency. Note that gasification reactions also involve moisture evaporating from the fuel and forming during the oxidation of volatile substances. An increase in fuel consumption leads to both an increase in incompletely burned carbon and a decrease in cold gas efficiency by 2–3 percentage points (Fig. 5).

Thermodynamic models of gasification processes usually underestimate the final equilibrium temperature, which is due to an overestimation of the fuel conversion [20]. Long dwell times are needed to achieve final equilibrium at temperatures below 900–1000°C. Therefore, in practice, the gasification reactions occur, as a rule, above the thermodynamically optimal temperature. The model used in this work takes into account the kinetic features of heterogeneous reactions; therefore, the estimates obtained with its help will be more realistic than the equilibrium approximation. The heating value of brown coal, as can be seen in Table 1, is 16–18 MJ/kg. Therefore, to maintain

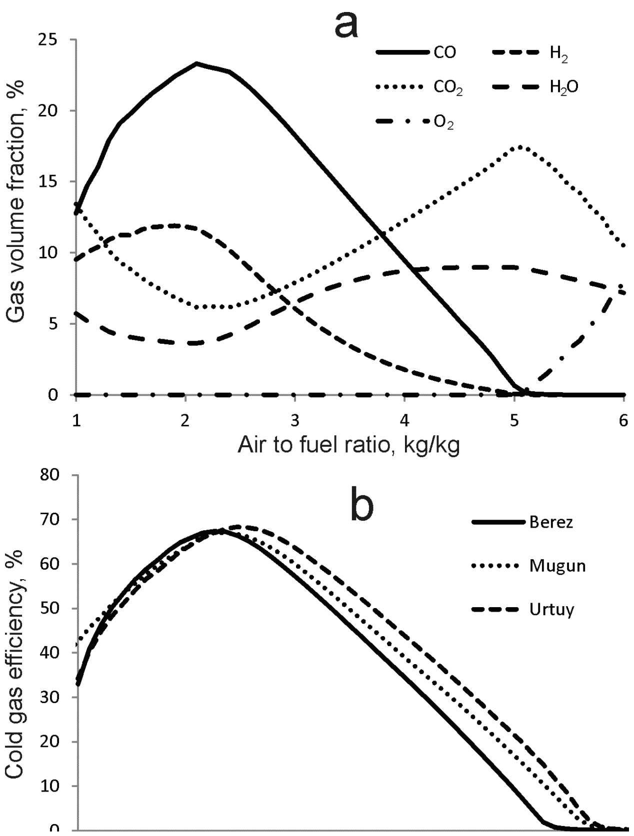

Fig. 1. (a) Dependence of the produced gas composition on the air-fuel ratio (Berezovsky coal, steam-fuel ratio 0.05 kg/kg); (b) Dependence of the cold gas efficiency on the air-fuel ratio and coal composition.

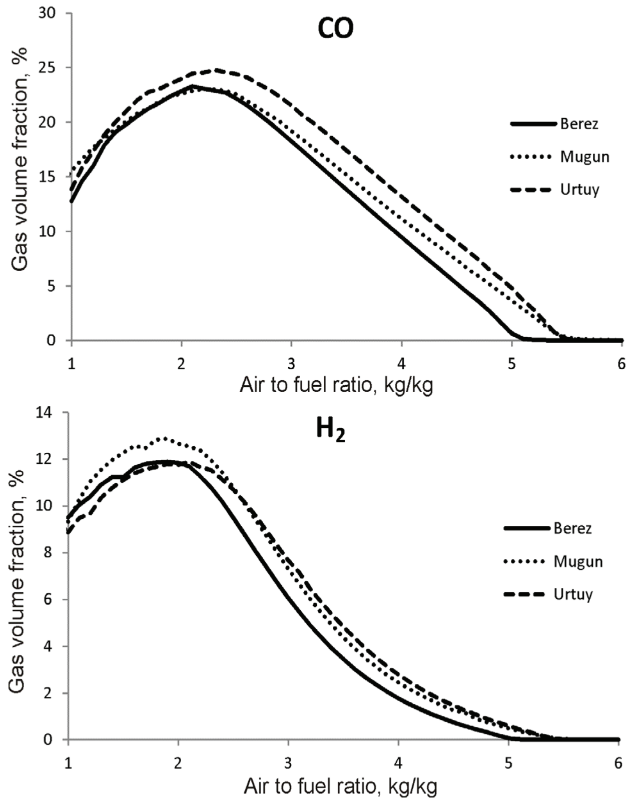

Fig. 2. Dependence of the volume fraction of CO and H_2 in produced gas on the air-fuel ratio and coal composition (steam-fuel ratio 0.05 kg/kg).

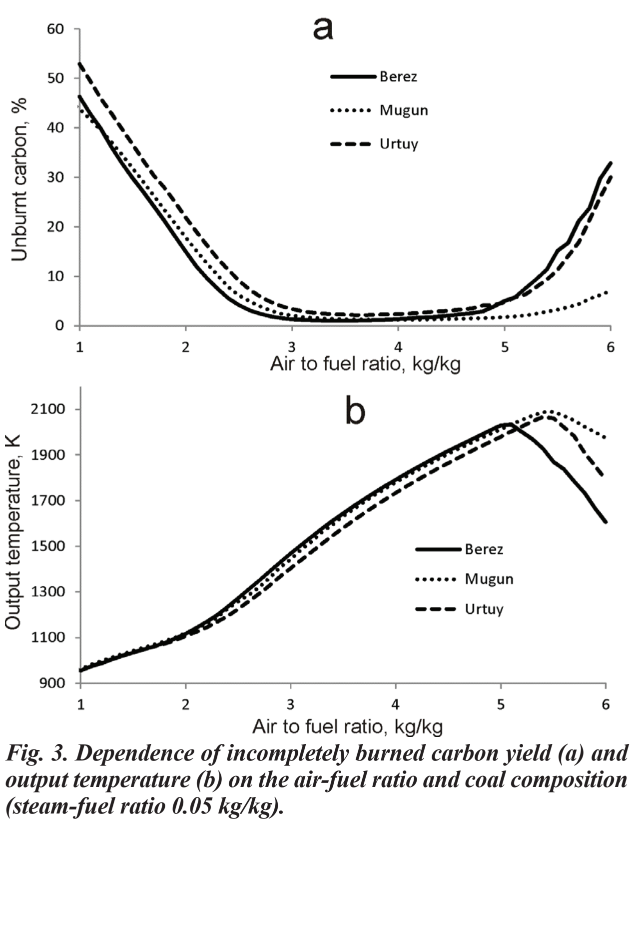

Fig. 3. Dependence of incompletely burned carbon yield (a) and output temperature (b) on the air-fuel ratio and coal composition (steam-fuel ratio 0.05 kg/kg).

a stable process, it is necessary to spend about 25% of this heating value to achieve a temperature at which gasification reactions will proceed at a sufficient rate. These losses along with incompletely burned carbon lead to low cold gas efficiency (60–70%). They can be reduced, for example, by heating the air [24].

As mentioned above, the relationship between the cold gas efficiency and the fuel conversion degree is, in general, non-monotonic. Figure 7 shows the calculated dependencies: the air-fuel ratio there increases from right to left. It can be seen that the higher values of the cold gas efficiency correspond to a rather high level of incompletely burned carbon yield. To reduce incomplete combustion to an acceptable level, it is necessary to increase the air-fuel ratio, reducing the cold gas efficiency. Similar problems in choosing the parameters of the gasification process were considered earlier, for example, in [16], where an increase in temperature was required to ensure conditions for liquid ash removal.

Gasification of Urtuysky coal has the highest cold gas efficiency due to its higher heating value. It is followed by Berezovsky coal and, finally, Mugunsky coal. The last two coal blends, however, differ little, and given the assumptions made, the characteristics of their gasification can be considered almost identical.

In total, 300 regimes were obtained for each coal

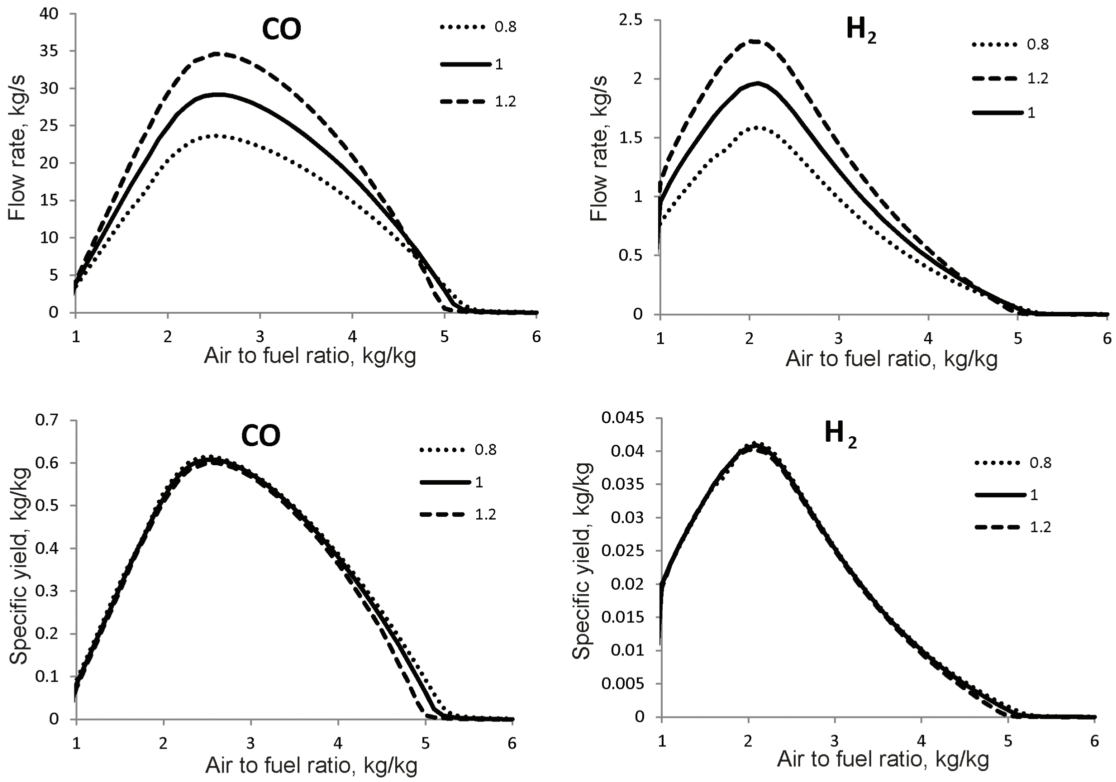

Fig. 4. Dependence of the output flow rates and specific yields of the main combustible gases on the air-fuel ratio and coal composition.

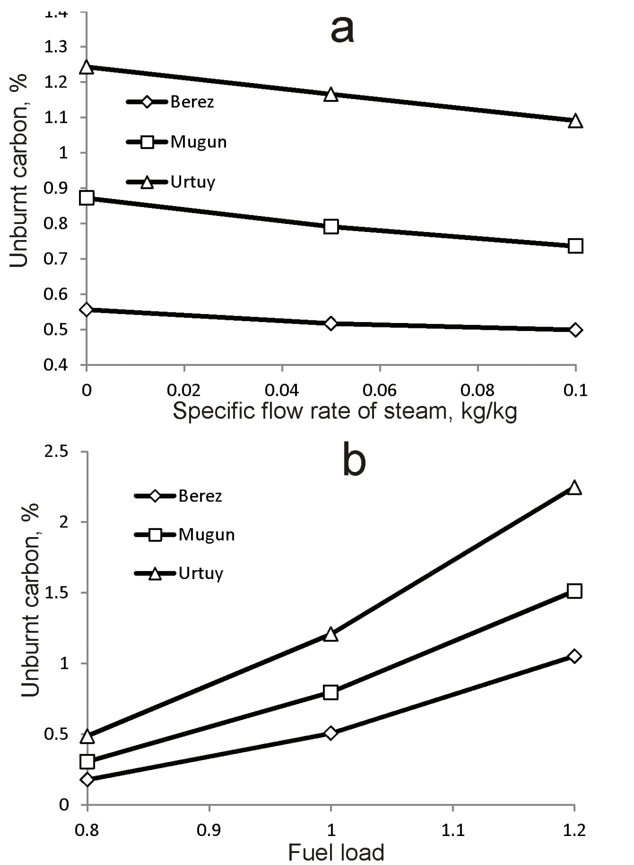

Fig. 5. Dependence of the minimum incompletely burned carbon yield on the steam-fuel ratio (a) and fuel load (b).

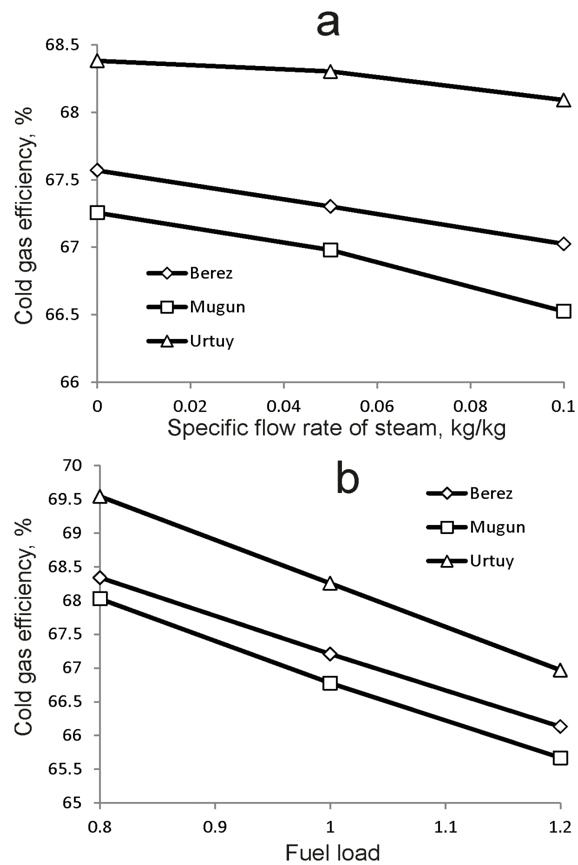

Fig. 6. Dependence of the maximum cold gas efficiency on the steam-fuel ratio (a) and fuel load (b).

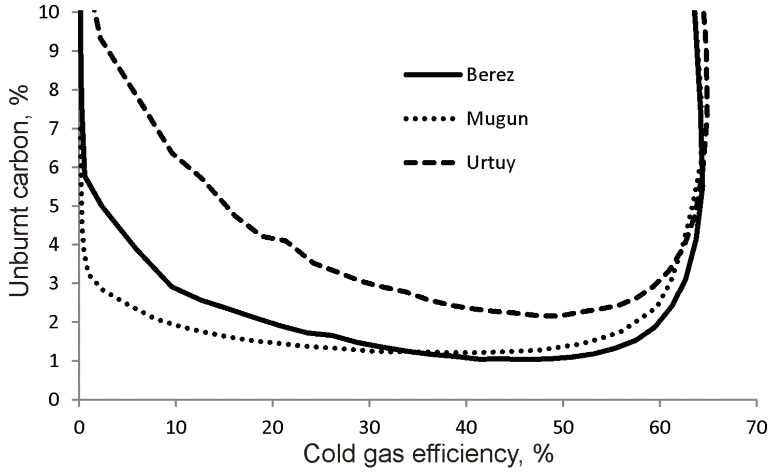

Fig. 7. Relationship between the incompletely burned carbon yield and the cold gas efficiency for different coals.

composition with varying fuel, air and steam flow rates. The results of calculations presented in the form of tables can be used to optimize parameters of power and chemical plants with brown coal gasification. In this case, numerical tables can be used to evaluate the characteristics of the gasification process with a discrete range variables but estimates show that interpolation between nodes allows one to transition to continuous variables.

In future studies, it will be possible to further reduce the computational costs in several ways: (1) to narrow down the intervals for air-fuel ratios; (2) to sparse the grid of parameters in areas where the change in efficiency and product yield is sufficiently close to linear; (3) to use the dependence of the incompletely burned carbon yield on temperature as a constraint in the thermodynamic model.

Conclusion

The paper presents the findings of a computational study of entrained-flow air-blown gasification process characteristics for different brown coals. Constraints imposed on the process efficiency that are due to the reactivity and fuel heating value are shown. The maximum values of the cold efficiency for the selected coals reach 66–68%. However, to achieve sufficiently deep fuel conversion, it is necessary to increase the air-fuel ratio and to reduce cold gas efficiency. The results of the calculations will be used to conduct optimization studies of combined-cycle plants with integrated gasification of brown coals.

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