Numerical modelling and optimization of pulverized biomass gasification process

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Abstract. Biomass, such as wood, forestry and agricultural wastes, etc., is considered to be a fuel with better environmental characteristics than fossils. The main prospects for the increase in the energy use of biomass are associated with the combustion and gasification in small energy systems, including those being a part of hybrid power plants. One of the ways to improve the efficiency of the gasification process is to increase the temperature by the use of oxygen-enriched gasification agent, as well as grinding the fuel to intensify transfer processes and chemical transformations. Thermodynamic estimates show the possibility of achieving the gasification process efficiency at the level of 80-90%, however, the experimental values rarely exceed 70%. In the present work, by means of mathematical modeling, the possibilities of increasing the efficiency of the biomass gasification process are investigated. The range of optimal conditions is evaluated.

1. Introduction
The replacement of coal and hydrocarbon fuels with renewable sources allows improving the environmental characteristics of energy systems. Among renewables, plant biomass has a significant advantage. Biomass is widely used for energy production (mainly thermal). The current consumption of plant biomass in the energy sector is about 1.3 billion toes [1], and, according to some estimates, will increase by 2-3 times by 2040. In addition to incineration, gasification, and pyrolysis, biomass can be used [2] in combined production of heat and electricity on the basis of small plants, including gas engine [3]. In areas with high prices for imported fuel, the use of local biofuels may be more profitable than the widely used diesel generators [4, 5]. In addition, biomass gasification can be used for chemical production [6]

The overall efficiency of gas engines operating on low-calorific gas rarely exceeds 30% [7]. Therefore, the technical efficiency of biomass gasification plants is largely determined by the efficiency of thermochemical conversion stage (cold gas efficiency, CGE). Cold gas efficiency is influenced by a large number of parameters: the composition of the fuel (proximate, ultimate, fractional), the composition of the gasification agent, process type, gasification plant capacity, gas cleaning conditions, etc. Thermodynamic analysis of biomass gasification [8] gives an upper estimate for cold gas efficiency at 80-90%. However, as the analysis of the available experimental data [9, 10] shows, these values are difficult to achieve in practice. Relatively low temperatures, which are achieved by air gasification of biomass, cause a high yield of tarry products containing a significant portion of the calorific value of the fuel. Tar conversion processes are reviewed in [11]: they are usually associated with high-temperature post-conversion reactors or with expensive catalytic systems. In the papers [12, 13] the options of the staged gasification process were reviewed. In particular, the authors of [14] reported the achievement of CGE values that were close to thermodynamic limits.
In addition to the fluidized- and fixed-bed gasification processes that are appropriate for particles with a size of the order 0.1–1 cm, there are also entrained-flow processes for the gasification of fuel with a particle size of 0.1–1 mm [15]. An oxygen-enriched gasification agent is commonly used to raise the temperature in the combustion zone. In the works [16, 17, 18, 19, 20, 21, 22, 23] these processes were investigated at laboratory-scale units. Experimental reactor with a capacity of 1 MW is described in [24, 25, 26]. Gasification of biomass in a swirling flow was studied in [27, 28]. However, the achieved CGE remains at the same level (about 70%). In order to understand process behavior, it is necessary to investigate the process efficiency using kinetic models.

The authors of [29] proposed a one-dimensional stationary model of gasification process of pulverized biomass in entrained flow, built as a set of submodels for different zones, which are presented as stirred-tank or plug flow reactors (similar to the reduced-order models for coal gasification processes [30, 31]). The paper [32] examines the behavior of biomass particles in a laboratory reactor taking into account the detailed kinetics of pyrolysis processes and gas-phase oxidation. Models of coal and biomass co-gasification processes are proposed in [33, 34, 35]. The CFD-models for biomass particles gasification in the drop tube reactors are proposed in [36, 37, 38].

In the present work, a simplified model is used to study the efficiency of the biomass gasification process in a wide range of conditions, which allows us to find the optimal gasifier operating modes and ways to improve the process characteristics.

2. Input data
Mathematical model described earlier in the previous works of the author [39, 40] was used for calculations. This model is a system of one-dimensional stationary heat and mass transfer equations with a combined kinetic-thermodynamic block describing the processes of pyrolysis and gasification of fuel particles. The reactor is considered to be close to the plug-flow reactor.

The parameters of the reactor are taken from [24]. We consider a cylindrical reactor with fuel consumption of 30–120 kg/h, the working pressure in the reactor is 1–10 bar. Geometrical dimensions of the reactor are as follows: the length of the reaction zone is 2 m; inner diameter is 0.45 m (slightly less than published data; this value was matched for better agreement with residence time). The temperature of the fuel entering the reactor is 25°C; steam temperature is 100°C; the temperature of the gasification agent is 25°C.

The model was verified using [24] data for pressures of 2–7 bar. The results of the comparison between the experimental and calculated data for 28 modes are shown in Fig. 1. Residence time is estimated by the model with good accuracy (using correction for inner diameter). Although the correlation coefficient obtained for all components is 0.91, local errors can reach 50%. Chemical efficiency of gasification is overestimated by an average of 11% (in relative values). The methane content in product gas is underestimated by the model, the content of CO and H2, on the contrary, is higher than the measured ones. Nevertheless, one may conclude that the qualitative correspondence of the modeling results and literature data was observed.

Optimal cold gas efficiency measured in experiments [24] is close to 75%. Gasification agent here is a mixture of O2/N2/H2O with a nitrogen concentration up to 40% vol. Theoretical calculations show the possibility of achieving cold gas efficiency about 87% (for a pressure of 7 bar). It is interesting to find the reasons for this difference.

| Table 1. Fuel composition and properties. |
|------------------------------------------|
| Property | Value |
| W%, %    | 6.7   |
| A%, %    | 0.34  |
\begin{tabular}{|l|c|}
\hline
$V^{\text{daf}}$, % & 82.7 \\
$C^{\text{daf}}$, % & 51 \\
$H^{\text{daf}}$, % & 6.22 \\
$N^{\text{daf}}$, % & 0.1 \\
$S^{\text{daf}}$, % & 0.01 \\
$Q_r$, MJ/kg & 15.96 \\
Density, kg/m$^3$ & 900 \\
Mean particle diameter, $\mu$m & 120-180 \\
\hline
\end{tabular}

\textbf{Fig. 1.} Comparison of measured [24] and calculated values: (a) CGE – cold gas efficiency; $t_c$ – mean residence time, s; (b) dry gas composition, % vol. Solid lines correspond to equation $y = x$.

3. Results of modeling
Further calculations are related to the optimization of the pulverized biomass gasification process in the steam-oxygen entrained flow. The geometrical parameters of the reactor and the fuel reactivity remain the same as for the previous calculations. Fuel consumption is maintained at 50 kg/h. In the calculations, the specific consumption of oxygen and water vapor, as well as the pressure in the reactor (from 1 to 10 bar) varies. Effect of steam consumption within the selected range (0-0.2 mol/mol of carbon) was weak (compared to other parameters). The following results are presented for a fixed steam consumption (0.2 mol/mol of carbon).
Calculations show that the increase of reactor pressure improves the cold gas efficiency, and maximum values of cold gas efficiency are achieved at lower stoichiometric ratios. These effects are associated with heterogeneous kinetics: an increase in pressure leads to an increase of the residence time for fuel particles. As a result, the gas-fuel system is closer to equilibrium state: thermodynamic estimates show that the theoretical value of the stoichiometric ratio for full biomass gasification is within the range of 0.2-0.3. The decrease in the residence time leads to the fact that, with the fixed reactor length, devolatilization is the only completed stage of conversion. In order to gasify the char residue, either high temperature or sufficiently high residence time is required. At low pressures, the first scenario is realized: the maximum cold gas efficiency for 1 bar is achieved at a stoichiometric ratio of 0.41, that corresponds to a combustion zone temperature about of 2250 K (Fig. 2, b). Cold gas efficiency for stoichiometric ratios below 0.3 is obviously determined by the oxidation of pyrogas, which is the main product. With increasing pressure, the gasification reactions complete due to an increase in the particle residence time, as a result, even at low temperatures, the process requires less oxygen.

4. Conclusion
Entrained-flow biomass gasification process was investigated using mathematical modeling. The model was tested on published data and showed good agreement with the experiment. Variant calculations were performed to search for optimal conditions for biomass gasification. Calculations show that different modes of fuel conversion are realized at different pressures. At low pressures, the efficiency of the process is determined by the temperature level. With increasing pressure, the optimum value of specific oxygen consumption decreases due to an increase in particles residence time in the reaction zone.

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