Mathematical modeling of the fixed-bed staged biomass gasification process

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Abstract
Biomass gasification is a technology suitable for small-scale power plants. This is a well-known and environmentally friendly way to convert biomass (such as forest and agricultural waste) into combustible fuel gas. However there are several disadvantages to overcome. Tarry gases call for a costly gas cleaning system, and the process is often unstable. These drawbacks are typical for widely used single-stage gasification processes. Staged gasification as distinct from the single-stage one allows allothermal and autothermal conversion processes to be separated within the same plant. Separation of the devolatilization and char gasification stages makes tarry volatiles to burn and produce the gasification agent. Such process organization provides both low-tar gas production and better process heat utilization. The plant being studied consists of two fixed-bed reactors and a gas combustion chamber. A mathematical model is developed to predict staged process behavior and to find thermally efficient operation modes. The results outline the control limits within which efficient gasification can be performed.

Keywords: Biomass gasification, staged gasification, fixed bed, equilibrium modeling, diffusion kinetics

Introduction
Biomass gasification has several obvious advantages. It can be implemented at small-capacity energy plants which are opportune to utilize sparsely distributed biomass fuels like forest and agricultural waste. Besides, it allows production of heat and power, pollution reduction, and mitigating climate change [1].

Beside direct combustion there are many biomass-based energy technologies: fixed-bed [2], fluidized bed [3], and entrained-flow gasification [4], pelleting [5] and briquetting followed by co-gasification with coals [6,7], catalytic conversion [8], high-temperature processes [9], etc. The main purpose of them is to convert biomass into a combustible gas to fuel boilers or engines.

A well-known drawback of biomass gasification is rather high content of tars in the producer gas that prevents its combustion in engines without a costly gas cleaning [10,11]. This motivates developing new methods of gasification process organization and control. The staged gasification is among such methods. At the staged gasification fuel pyrolysis and char gasification are separated. A general scheme of staged gasification process is shown in Figure 1. Such process organization has been studied firstly at Technical University of Denmark [12].

In the pyrolysis reactor (the first stage) raw biomass undergoes drying and devolatilization. The pyrolysis gas is combusted in the under-bed space of the gasification reactor (the second stage). The oxidation of pyrolysis products needs not to be complete because high temperatures provide elimination of tar due to secondary pyrolysis. Hot gases serve as a gasification agent at the second stage. The char gasification does not produce tars and fosters tar cracking. Thus, the produced gas is almost tar-free. Endothermic reactions of CO2 and H2O char gasification lessen thermodynamic loses of chemical energy.

To maintain intensive pyrolysis process, an additional heat is needed. At an autonomous plant this heat may be obtained by combustion of raw fuel, pyrolysis gas, char or syngas only. Herein we consider the case when the additional heat is supplied by syngas combustion products from the exhaust of a power unit.

Gasification plants based on the idea of staged process are investigated in several studies, e.g., [12-15], including both fixed-bed and fluidized-bed reactors [16]. In all cases creation of sophisticated process schemes inevitably causes a complicated control to provide proper coordination of mass and heat flows.

Danish researchers developed mathematical models to provide theoretical base for staged gasification process operation and control. In the paper [17] they used one-dimensional diffusion-kinetic model to simulate dynamic behavior of a
gasifier at fixed other parameters. They also used CFD-code to model underbed gas combustion and hydrodynamic flow modes in porous media [18].

In the paper [19] a final-equilibrium thermodynamic model was used to determine the influence of a number of parameters on the thermodynamic limits of coal staged gasification. Among the independent parameters there were specific consumption of air and steam, conversion degree at pyrolysis, and others. In the work [20] a one-dimensional equilibrium model including diffusion-kinetics constraints was applied to obtain thermal stability boundaries for a coal staged gasification process. It was shown that the amount of heat recycled and air excess can be varied within certain ranges to maintain efficient process modes.

A rigorous and precise model of heterophase fuel conversion process still cannot be constructed due to lack of theoretical knowledge on the mechanisms of such reactions, leaving alone the high variability of natural fuels properties. That is why the explanatory potential of mathematical models in this area still dominates their predicting capabilities. This is a fortiori so for low-grade fuels which the biomass belongs to.

It is interesting to investigate staged biomass gasification process using a mathematical model able to predict such phenomena as process extinction (e.g., at insufficient heat recycling). It would help to determine the conditions at which staged gasification can be efficiently operated. Such model and some modeling results are discussed below.

Methods
Model assumptions and structure
The model structure is presented in Figure 2. The input parameters are: reactor sizes (diameters and lengths), raw fuel characteristics and its consumption, heat flow used for raw fuel pyrolysis, oxidizer excess ratio at gas combustion, and kinetic data on heterogeneous brutto-reactions of fuels.

The latter can be obtained experimentally by the means of thermal analysis [21]. The heat flux at the wall of pyrolyzer that is produced by exhaust gases could not be uniform, but we assume it to be so. A detailed study of heat flux distribution in pyrolyzer jacket is yet to be done. Fixed-bed reactors are represented as one-dimensional systems, lateral temperature gradients are neglected. Pyrolysis gas combustion is supposed to reach the complete chemical equilibrium under the conditions of constant pressure and enthalpy. Thus, the key control parameters are the heat consumption in pyrolysis reactor and air stoichiometric ratio at the under-bed pyrolysis gas combustion stage.

The main features of a solid fuel conversion reactor model are discussed in [22]. It is one-dimensional model including two iteratively run submodels. One submodel describes heat transfer in a moving bed. The other one calculates final chemical equilibrium rate-controlled due to diffusion and reaction kinetics.

Model equations describing stationary heat transfer in the fuel bed are following:

\[
\lambda' \frac{d^2 T'}{dz^2} - C_p' \frac{dT'}{dz} + \alpha_s \left( T_s - T' \right) + Q'(z) = 0
\]

\[
\lambda \frac{d^2 T}{dz^2} - C_p \frac{dT}{dz} - \alpha_s \left( T_s - T \right) - \alpha_s \left( T_s - T' \right) + Q(z) = 0
\]

These equations (with corresponding boundary conditions: constant mass flows at bed top) determine gas and fuel
temperatures. To solve them one must define source functions \( Q(\varphi) \). Usually these functions are determined by kinetic equations, but we propose combined kinetic-thermodynamic procedure to obtain them.

Solving the problem numerically, we divide all reactor into a number of small sections. Knowing gas residence time \( \tau \) for every \( i \)-th section (it is equal to \( \Delta V_i / (\rho_i \rho_g) \)), one can write:

\[
Q(z) = -\frac{\Delta H_{r}^i}{\tau_i} = \left( \sum h_j n_j^i - \sum h_j n_j^{\text{out}} \right) \frac{\Delta p}{\tau_i}
\]

Reactions summary heat is found for each small sections using thermochemical database. Chemical composition change is determined by two steps. At first step, heterogeneous processes are considered: drying, pyrolysis and gas-char reactions. Kinetic equations are as follows:

\[
\frac{dn_{H2O}}{V_g dt} = \beta \frac{n_{H2O}}{V_g} \left( 1 - \frac{C_{eq}^{H2O}}{C_{H2O}} \right)
\]

\[
\frac{dn}{dt} = -k_{pyr} n_V
\]

\[
\frac{dn_{CO2}}{dt} = -k_{pyr}^{eff} S_1 \frac{n_{CO2}}{V_g} - k_{CO}^{eff} S_1 \frac{n_{CO}}{V_g} - k_{H2O}^{eff} S_1 \frac{n_{H2O}}{V_g}
\]

where \( k^{eff} \) is obtained from the well-known formula for heterogeneous reactions:

\[
k^{eff} = \frac{1}{\frac{1}{k_1^g} + \frac{1}{k_2^g}}
\]

When quantities of moisture, volatiles and char that turn into gaseous products are determined, gas phase processes are considered. To this end, equilibrium submodel is used:

\[
\mathbf{n}^{g,\text{out}} = \arg \min G(\mathbf{n}^g)
\]

\[
G(\mathbf{n}^g) = \sum n_j^g \mu_j
\]

\[
\mathbf{An}^g = \mathbf{b}^g
\]

The calculation starts from any reasonable closure of axial temperature profile, and the iterations stop when this profile's change becomes negligible, i.e., a steady state is achieved. The transitional states determined during iterations are not physical. The gas composition at each point along the reactor axis is equilibrium under the condition of incomplete fuel conversion derived from kinetic equations for drying, pyrolysis and gas-fuel heterogeneous reactions. Kinetic parameters for these heterogeneous reactions of woody biomass are obtained by thermal analysis and presented in the Table 1. Kinetic constants are of first-order Arrhenius type. They were estimated given one-stage chemical reactions.

| Chemical reaction | Preexponential factor | Activation energy |
|-------------------|----------------------|-------------------|
| Pyrolysis         | 5.4 \(10^5\) s\(^{-1}\) | 96 kJ/mole         |
| Char + CO\(_2\)   | 7.0 \(10^{15}\) m/s  | 259 kJ/mole        |
| Char + H\(_2\)O   | 4.9 \(10^3\) m/s     | 175 kJ/mole        |

There are some works that considers kinetic-controlled or empirically-modified equilibrium modeling of biomass gasifiers. Most of them deal with fluidized bed gasification process [24-29], but fixed bed processes are considered too [30-32]. In the course of presented study, paper [33] should be noted, where dual-bed biomass gasification process was studied with heat recirculation ratio and steam flow as key variables.

For biomass pyrolysis stage produces a large amount of tar, we are to include tar into substances list. The tar produced in biomass pyrolysis is ascribed as a lumped substance with brutto-formula \( \text{CH}_3\text{O}_2 \). Since the combustion of pyrolysis products is implied to reach the final equilibrium the representation of tar is realistic enough.

Results

Modeling results

The reactor sizes chosen in this study are constant: diameter 0.5 m; height 1 m. Raw fuel consumption is taken 100 kg/hr. Fuel proximate analysis data are shown in Table 2.

| Property     | Value |
|--------------|-------|
| C(daf), %    | 49.5  |
| H(daf), %    | 6.3   |
| O(daf), %    | 44.2  |
| V(daf), %    | 85.0  |
| A(d), %      | 1.0   |
| W(r), %      | 20.0  |

The above described model has been applied for a range of gasification regimes. Here we give one of them to provide our colleagues with the material for further discussion. The temperature, gas composition and fuel conversion degree axial profiles are presented at Figure 3. For this case heat flux in pyrolyzer comprises 24 kW; air ratio at pyrolysis gas combustion is 0.4. One can see that at the pyrolysis stage fuel moves in reactor and the most part of fuel does not react (Figures 3a and 3b). Only when the bed temperature rises up to 600 K an intensive pyrolysis starts. A lot of tar is produced during pyrolysis (Figure 3c). At the gasification stage hot gases react with char bed but output gas temperature is still very high (Figure 3f), so this heat may be utilized in pyrolysis reactor. Full regime map is presented at Figure 4.

It can be seen from Figure 4 that the more heat flux at pyrolysis stage the less oxidizer ratio is needed to achieve optimum cold gas efficiency. Pyrolysis starts when the heat...
flux makes up 5-7% of the fuel higher heating value. This is explained by the well-known kinetic feature – the exponential increase in reaction rate with a rise of temperature. At higher heat fluxes raw fuel is completely converted into char, tar and gas. Correspondingly, a larger share of fuel is converted in the pyrolyzer rather than in the gasifier. That is why at higher heat fluxes the gasification stage cannot provide enough combustibles to compensate their combustion in the underbed space. This, in turn, results in oxidation of the most part of biomass and lowers cold gas efficiency of the plant. The optimal values of air ratios range within 0.4-0.5. At lower air ratios the temperature of combustion products is insufficient to promote intensive gasification, and unreacted char leaves reactor with ash. Nevertheless, under very low air ratios unburnt pyrolysis gas has high heating value, so overall cold gas efficiency is near 70%.

There are still many questions to be answered. First of all, optimal distribution of heat flux at the pyrolysis stage is to be investigated. It is also important to improve the description of raw fuel pyrolysis kinetics, as the first-order Arrhenius kinetics is a rough approximation [34]. At last, it does make sense to develop a model that would combine gasification system with the power unit. This would allow a comparison among different sources of additional heat for pyrolysis.

Detailed verification of the model proposed is a problem of future investigations. Nevertheless, it should be noted that experimental cold gas efficiency (for optimal conditions) is about 90% [12]. Our modeling results show that to obtain...
higher values of cold gas efficiency one should increase internal heat flux, but at some point it will decrease efficiency of power plant as a whole.

Conclusion

Process of a staged fixed-bed gasification of biomass is studied using mathematical model. Influence of two major control parameters was studied: pyrolyzing heat flux and air ratio at pyrolysis gas combustion. There is a liminal value of the heat flux in pyrolysis reactor (6% of the fuel higher heating value) that provides efficient fuel conversion. Air ratios have the range of optimal values within 0.4-0.5.

Competing interests

The authors declare that they have no competing interests.

Authors’ contributions

| Authors’ contributions | IGD | AVK | ANK | VAS | DAS |
|------------------------|-----|-----|-----|-----|-----|
| Research concept and design | ✓  | ✓  | --  | --  | --  |
| Collection and/or assembly of data | --  | --  | ✓  | --  | --  |
| Data analysis and interpretation | ✓  | ✓  | --  | ✓  | --  |
| Writing the article | ✓  | ✓  | --  | --  | --  |
| Critical revision of the article | --  | ✓  | --  | ✓  | --  |
| Final approval of article | ✓  | --  | --  | --  | --  |
| Statistical analysis | --  | --  | ✓  | --  | --  |

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