Numerical analysis of biomass torrefaction reactor with recirculation of heat carrier

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Abstract. In this paper, results of numerical analysis of the energy-technological complex consisting of the gas piston power plant, the torrefaction reactor with recirculation of gaseous heat carrier and the heat recovery boiler are presented. Calculations of the reactor without recirculation and with recirculation of the heat carrier in torrefaction zone at different frequencies of unloading of torrefied biomass were held. It was shown that in recirculation mode the power of the gas piston power plant, required for providing given reactor productivity, is reduced several times and the consumption of fuel gas, needed for combustion of volatile torrefaction products in the heat recovery boiler, is reduced by an order.

1. Introduction
The purpose of torrefaction is improving of thermotechnical characteristics of solid biofuels [1]. Principal problem encountered in the implementation of torrefaction technology is the utilization of volatile torrefaction products, containing hazardous organic components [2, 3]. One of the possible ways of the volatile products utilization is their incineration in a heat-recovery boiler (HRB) [4–6]. This method is quite effective in reactors with feedstock heating through a wall and in reactors with direct heating, if heating is carried out by volatile products of torrefaction [7]. For a reactor with direct feedstock heating by combustion products of a gas-piston power installation, the problem is complicated by low concentration of combustible components and significant amount of water vapor in vapor–gas mixture of the pyrolysis and flue gases. Due to low concentration of combustible components in the gas mixture leaving the reactor (1.5–2%) the realization of its incineration needs additional fuel for heating the entire volume of gas up to the combustion temperature. The effectiveness of the torrefaction volatile products utilization can be significantly improved by partial recycling of gas mixture in the reactor, which will increase the concentration of combustible components and will facilitate more complete utilization of the thermal potential of gaseous heat carrier. To calculate the operating modes of the reactor with the recirculation of the heat carrier, the mathematical model of the torrefaction reactor applied in [8] was refined. In the article there are presented results of numerical analysis of effectiveness of torrefaction reactor with recirculation of gaseous heat carrier.

2. Mathematical model
The diagram of torrefaction reactor with recycle of heat carrier is shown in figure 1.
As gaseous heat carrier the combustion products of gas-piston power plant (GPU) are used. They are mixed with the gas mixture leaving the reactor in a ratio providing a predetermined constant temperature at the reactor inlet. It is assumed that the mass flow rate of gaseous heat carrier $G_{hg}$ through the reactor is constant and the influence of volatile products of torrefaction on the heat exchange process in the reactor is negligible. At the same time, the heat content of the torrefaction volatile products is taken into account when calculating the heat balance in the mixer, which determines the value of recirculation degree $\beta$. In this case, for a given gas temperature at the reactor inlet $T_3$ the percentage of gas flow $\beta$ used for recycling is determined by the temperature of flue gases $T_1$ at the inlet of mixer, by the temperature of gas at the outlet of reactor $T_2$ and by the amount of volatile products in the gaseous heat carrier. Using the rule of enthalpy mixing $H$ one can write

$$ H_{hg}(T_3) + H_v(T_3) \frac{y}{(1-y)} \beta = H_{hg}(T_1)(1-\beta) + H_{hg}(T_2)\beta + H_v(T_2)\beta \frac{y}{(1-y)}. $$

were

$$ y = \frac{G_v}{G_{hg} + G_v}. $$

The value $G_v$ is determined by the feedstock-mass change as a result of thermal decomposition of its organic components, and can be calculated by using the kinetic equation, describing the process of biomass thermal destruction [9].

Equation for recirculation degree can be easily obtained from equation (1):

$$ \beta = \frac{[H_{hg}(T_3) - H_{hg}(T_1)](1-y)}{[H_{hg}(T_2) - H_{hg}(T_1)](1-y) + [H_v(T_2) - H_v(T_3)]y}. $$
Consider the steady cyclic operation mode of reactor with periodical loading–unloading of pellets. Assume that the loading–unloading time is significantly less than the residence time of pellets in reactor, and moving speed of pellets inside the reactor can be considered equal to zero. When reactor is operated in cyclic mode, the temperature of gas at its outlet changes during pellets heating. To ensure constant temperature of gas at the reactor inlet, the flow of heating gas in recirculation circuit (i.e. recirculation degree $\beta$) should be changed. The change of recirculation degree $\beta$ is also influenced by the change of the volatile products formation rate, which determined by the kinetics of the biomass decomposition process. For a detailed calculation of the reactor with recirculation operated in cyclic mode, a mathematical model of the torrefaction reactor was used [8]. The model was updated with taking into account the heating gas recirculation in the reactor and was supplemented with conservation equation for volatile torrefaction products. Under the assumptions described above, the system of equations describing the distribution of parameters on the length of the reactor, can be written as follows

\[
f \frac{\partial \rho_s}{\partial t} = - \frac{\partial \rho_s u}{\partial x} + V, \tag{4}
\]

\[
f \frac{\partial (\rho_s c_s T)}{\partial t} + \frac{\partial (\rho_s u c_s T)}{\partial x} = \alpha (T_s - T), \tag{5}
\]

\[
(1 - f) \frac{\partial \rho_s}{\partial t} = -V, \tag{6}
\]

\[
(1 - f) c_s \rho_s \frac{\partial T_s}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial x^2} - \alpha (T_s - T), \tag{7}
\]

where $\rho_s$ is the density of volatile torrefaction products; $\rho_{\Sigma}$ and $c_s$—the density and the heat capacity of the mixture of gaseous heat carrier and volatile torrefaction products; $T$—the temperature of gas; $u$—the velocity of gas; $\alpha$—the heat transfer coefficient; $f$—the porosity of a pellets bed; $T_s$—the temperature of pellets; $c_s$—the heat capacity of pellets; $\rho_{s}$—the density of pellets; $\lambda_s$—the thermal conductivity of pellets; $t$—the time; $x$—the coordinate; $V$—the source term.

For numerical solution of equations (4)–(7) their discrete analogue, obtained by integrating the differential equations for the control volume [10], was used. The system of equations is solved numerically by multistep method of Adams with automatic time step choice [11]. In calculating the amount of gas, needed for incineration of volatile torrefaction products, assume that for the boiler operation without significant reduction of its energy efficiency the temperature in the combustion chamber of HRB should not be lower than $T_k$, and the gas–air mixture at the inlet of HRB is at the temperature $T_m$. The fuel gas flow rate $G_g$ supplied to HRB can be calculated from the heat balance equation for stoichiometric combustion of the fuel gas and volatile torrefaction products:

\[
\frac{G_g}{1 - \beta} \left[ Q_g - (S_g + 1) \int_{T_m}^{T_k} c_{gP}^P(T) dt \right] = \int_{T_2}^{T_k} \left[ c_{gP}^P \left( \frac{\delta m}{m_0} ; T \right) \left( S_v \left( \frac{\delta m}{m_0} \right) + 1 \right) G_v + c_{gP}^P(T) G_{hg} \right] dT
\]

\[
+ G_v \left[ S_v \left( \frac{\delta m}{m_0} \right) \int_{T_m}^{T_2} c_{air}(T) dT - Q_v \left( \frac{\delta m}{m_0} \right) \right], \tag{8}
\]

where $G$ is the mass flow rate; $Q$—the combustion heat; $c$—the heat capacity; $S$—the stoichiometry factor (by mass); $T_2$—the temperature at the outlet of torrefaction reactor; subscripts and superscripts: $v$ means volatile torrefaction products; $g$—fuel gas (methane in our case), used in HRB for incineration of volatile torrefaction products; $hg$—gaseous heat carrier; air—air, needed for incineration of volatile products; $cp$—combustion products. While writing the equation (8), it was assumed that $G_{gP}^P = (S_v + 1) G_v$, and heat carrier consists of combustion products, obtained at the excess air ratio equal to 1, therefore $c_{hg} = c_{gP}^P$. 
Figure 2. Temperature dependence of heat capacity of organic compounds belonging to the volatile torrefaction products: 1—acetic acid; 2—lactic acid; 3—furfural; 4—formic acid; 5—acetone; 6—methanol; 7—phenol; lines—calculation, symbols—data [12, 13].

3. Thermophysical properties of volatile torrefaction products

For calculating the operational modes of the mixer, HRB and energy efficiency of the whole energy-technological complex, the data on thermo-physical properties of heat transfer gas and volatile torrefaction products are needed. The calculation of the heat capacity and enthalpy of combustion products was carried out in the approximation of equilibrium thermodynamics [14]. Volatile products of biomass torrefaction are vapor–gas mixture, which in addition to carbon oxide, carbon dioxide and water vapor, includes organic components being liquid in normal conditions. According to the experimental data [3], the liquid fraction consists of water, acids (formic, acetic, lactic), acetone, methanol, furfural, and their content in volatile products depends on the operating parameters of torrefaction process (temperature and exposure time) and the type of wood. To compare thermophysical characteristics of torrefaction volatile products the value of mass loss $m/m_0$ was used as universal parameter, characterizing the torrefaction process. This parameter is equal to the mass yield of volatile products, calculated on dry ash-free state of the feedstock.

In literature there are data on thermal capacity of substances in gaseous form for the following components of volatile torrefaction products: acetic and formic acid, acetone and methanol [12, 13]. To calculate the heat capacity of lactic acid and furfural there was used the method of introducing the corrections to the coefficients of the equation (second-degree polynomial) describing the known temperature dependence of the heat capacity of the substance underlying the homologous series to which belongs the subject compound [12]. After selecting the basic substance, a carbon skeleton analogous to the carbon skeleton of the subject compound is
constructed by consistent replacement hydrogen with CH₃ groups. Then replacing simple linkages by complex ones and introducing instead of one or several CH₃ groups the necessary functional groups (alcohol, acid, carboxyl, etc.), the structural formula of the subject compound is constructed. Each change during the process of construction of the subject compound is followed by introduction of relevant tabulated corrections to coefficients of the equation for the calculation of the heat capacity.

The calculation results for all organic components of the volatile products, are presented in figure 2. The calculated values of heat capacities are in satisfactory agreement with the published data (maximum divergence for methanol is not more than 13%). Assuming additivity, temperature dependences of heat capacity of the volatile torrefaction products corresponding to different mass losses of the feedstock, were calculated. The values of the heat capacity of water vapor, carbon monoxide and carbon dioxide were taken from the reference book [15].

The calculation results are presented in figure 3. Since the maximum difference between the heat capacities of volatile torrefaction products corresponding to different mass losses does not exceed 6%, in further calculations the temperature dependence of heat capacity, obtained by averaging values, calculated for various mass losses, was used

\[ c_p = 1.17 + 9.25 \times 10^{-4}T. \]  

(9)

Figure 3 shows that the heat capacity of volatile torrefaction products substantially exceeds the heat capacity of the combustion products of methane. This difference increases as the temperature rises. Therefore, their contribution to the heat capacity of vapor–gas mixture is to be taken into account when considering operation modes with recycle of heat carrier. The
Figure 4. Changes of the main characteristics of gas mixture supplied to HRB during steady cyclic mode. The frequency unloading–loading of pellets is once every three min.

combustion heat of volatile torrefaction products, depending on the parameter $\delta m/m_0$, was calculated on the basis of composition [3] and the combustion heats of individual components. For the calculation of the latter there were used data on the standard heat of their formation and standard heat of formation of the final products [12]. The difference between the calculated values and data from [16] does not exceed 10%.

4. Results and discussion

The torrefaction reactor calculations for operation modes with and without recirculation of gaseous heat carrier were performed for conditions of experimental reactor of shaft type [16]. The inner diameter of the reactor was 325 mm, the height of the active zone (torrefaction zone) was 1 m. As in [17], direct heating of wood pellets is performed by exhaust gases of a gas piston power plant (GPU), namely the methane combustion products at the stoichiometric air–gas ratio. The calculations used the following values of the main mode parameters: mass flow rate of heat carrier in the reactor is 0.067 kg/s; temperature of gas before the mixer 450 °C and at the entrance to the reactor 250 °C; productivity of reactor 50 kg/h (for untreated pellets). Density of dry wood pellets was assumed to be 1000 kg/m$^3$ and porosity of pellets bed 0.4. As noted above, the calculations were performed for the conditions of reactor operation in a cyclic mode.

The duration of one cycle was determined by the time interval between loading–unloading of pellets. The duration of cycle influences the quality of torrefied pellets and the operation mode of HRB. Reduction of cycle duration and therefore the decrease of the portion of unloaded pellets leads, on the one hand, to reduction of the scatter of density values, i.e. to the improvement
Table 1. Main characteristics of operation modes of the torrefaction reactor.

| Indicators                                      | Cycle duration |
|-------------------------------------------------|----------------|
|                                                  | 180 s | 360 s | 720 s |
| Mass losses of pellets (average)$^a$             | 0.1233 | 0.1167 | 0.1161 |
| Maximum difference of mass losses of pellets$^b$ (%) | 0     | 6.6   | 14.38 |
| Mass concentration of the pyrolysis gases leaving the reactor: |     |      |      |
| cycle beginning                                  | 0.1136 | 0.1097 | 0.1041 |
| end of cycle                                     | 0.1338 | 0.1475 | 0.1773 |
| $1 - \beta$:                                     |       |       |       |
| cycle beginning                                  | 0.1509 | 0.1701 | 0.1998 |
| end of cycle                                     | 0.1255 | 0.1177 | 0.0962 |
| Gas temperature at the reactor outlet (°C):      |       |       |       |
| cycle beginning                                  | 220.2 | 215.5 | 207.4 |
| end of cycle                                     | 226.7 | 228.8 | 233.9 |

$^a$ Average value for unloaded cells.

$^b$ The relative difference between the mass losses in the first and last unloaded cells.

of pellets quality and, on the other hand, to reduction of flow oscillations of heat carrier and volatile torrefaction products entering the recovery boiler during one cycle. In the calculations a uniform computational grid (20 cells for the height of the reactor) was used.

The volume of pellets transported during unloading–loading ranged from 0.05 reactor volume (one computational cell) every 3 min to 0.2 reactor volume (four computational cells) every 12 min. Besides, the total residence time of pellets in the reactor was the same in all modes and amounted to 1 h. The initial temperature of the pellets in the reactor was 100 °C. Stationary temperature cyclic mode of reactor operation was set after 50–100 unloading–loading cycles (depending on mode).

Figure 4 shows typical charts of cyclic changes of volatile products concentration at the reactor outlet ($y$) and share of gas mixture, entering in HRB ($1 - \beta$) calculated for operation mode with 180 s cycle duration (unloading of one cell every 3 min). During one cycle these parameters change in antiphase, which reduces the magnitude of the oscillation amplitude of the energy entering to HRB with gas mixture.

The results of calculation of the main parameters that characterize the operation of the reactor in a steady cyclic mode with various duration of unloading–loading cycle are shown in table 1 and figure 5.

The results of calculations show that the degree of pellets mass losses during torrefaction in schemes with and without recirculation (in case of the same residence time of pellets in reactor) depends only on duration of cycles and is practically independent on recirculation degree. At the same time the thermal power of combustion products of PGU, required for providing given reactor productivity and directly related to power of GPU, is 5–7 times lower for the scheme with recirculation. Generally speaking, by adjusting the degree of recirculation, for example with the help of GRE, energy flows can be flexibly distributed.

The reduction of cycle duration leads to reduction of the difference in density of unloaded torrefied pellets (figure 5), which means improvement of their quality and insignificantly increases
average value of mass losses. Despite the fact that at big duration of cycle the concentration of the volatile products at the outlet of reactor at the beginning and at the end of the cycle differs almost twice, the energy content of the gases entering in HRB during the cycle varies not so much due to reduction of the proportion of the gas mixture fed to the HRB. At the same time the decrease of cycle duration reduces the difference between the values of parameters of operation at the beginning and at the end of the cycle, i.e. contributes to a more stable operation of both the reactor and the heat recovery boiler.

Calculations performed for a mode without recirculation ($\beta = 0$) showed that with an error not exceeding 5%, the concentration of volatile products leaving the reactor for all modes can be considered constant and equal to 0.02, that is significantly less than the concentration of volatile products in operation modes with recirculation of heat carrier.

Characteristics of HRB operation, calculated with using equation (8) for different operation modes of torrefaction reactor, are shown in table 2.

The temperature of combustible mixture (methane–air) $T_m$ supplied to the HRB for combustion of volatile products was assumed to be $20{^{\circ}}C$. It was assumed that to ensure complete combustion of volatile torrefaction products and effective operation of HRB, temperature in the combustion chamber $T_k$ must not be lower than $1600{^{\circ}}C$.

The calculations were performed under the condition of constant heat power of HRB for the selected operation mode of reactor. It follows from the calculation results, that transition to the mode with recirculation of gaseous heat carrier allows usage of HRB with significantly lower thermal power, which respectively decreases energy expenses for the volatile products utilization.
Table 2. Calculated operation modes of HRB.

| Indicators          | Cycle duration With recirculation | Without recirculation |
|---------------------|-----------------------------------|------------------------|
|                     | 180 s    | 360 s    | 720 s    | 180 s    | 360 s    | 720 s    |
| Gas flow rate (kg/s): |          |          |          |          |          |          |
| cycle beginning     | 0.0015   | 0.0017   | 0.0021   | 0.0101   | 0.0102   | 0.0102   |
| end of cycle        | 0.0015   | 0.0018   | 0.0021   | 0.0101   | 0.0102   | 0.0102   |
| Air flow rate (kg/s): |          |          |          |          |          |          |
| cycle beginning     | 0.0290   | 0.0329   | 0.0386   | 0.1775   | 0.1781   | 0.1790   |
| end of cycle        | 0.0291   | 0.0329   | 0.0387   | 0.1775   | 0.1781   | 0.1790   |
| Temperature $T_k$ (°C): |          |          |          |          |          |          |
| cycle beginning     | 1600     | 1600     | 1600     | 1600     | 1600     | 1600     |
| end of cycle        | 1653     | 1702     | 1785     | 1601     | 1603     | 1605     |
| Power (kW):         | 85.59    | 96.57    | 113.39   | 517.39   | 519.10   | 521.75   |

Available energy

- Gas fuel GPU
- Gas fuel HRB
- Pellets

Useful energy

- Electric power GPU
- Heat GPU
- Heat HRB
- Torrefied pellets

Figure 6. Energy balance of the energy-technological complex: GPU—gas-piston power plant; HRB—heat recovery boiler.

As one can see from table 2 the usage of heat carrier recirculation leads to reduction HRB power in 4.6–6 times, depending on cycle duration. The achieved effect is associated with a significant decrease in the flow of ballast gas (heat carrier) into HRB and increasing concentration of volatile products in the reactor volume. The contribution of latter into the energy content of the gas mixture fed to the HRB is about 10%. It should be noted that the decrease of cycle duration also leads to the reduction of HRB power and smoothing over $T_k$ oscillations during one cycle (see table 2).
Table 3. ETC efficiency.

| Operation mode | Without recirculation | With recirculation |
|----------------|------------------------|--------------------|
| K₁             | 0.888                  | 0.991              |
| K₂             | 0.333                  | 0.749              |

Basing on obtained results one can analyze the impact of heat carrier recirculation in the torrefaction reactor on the efficiency of the energy-technological complex (ETC), consisting of a piston gas power plant, torrefaction reactor and heat recovery boiler. Schematic diagram of energy flows of ETC is shown in figure 6.

The effectiveness of ETC can be defined as the ratio of sum of energy produced by the complex and the heat content of the final products (useful energy) to energy content of fuel and feedstock (available energy) (figure 6). It is assumed that the power of GPU is chosen so that it can fully provide the temperature mode of a reactor with specified productivity by heat potential of combustion products from GPU. Two options of ETC operation were considered: thermal energy of HRB is used by consumer (K₁) and HRB is only used for utilization of volatile torrefaction products (K₂). Also it was assumed that the efficiency coefficient of GPU is 0.3; combustion heat of untreated pellets 18 MJ/kg; combustion heat of torrefied pellets 21 MJ/kg; duration of reactor operation cycle 180 s; mass losses of pellets 12%. Calculation results are shown in table 3 and in figure 7.

Figure 7. The distribution of the available energy: a—without recycle; b—with recycle. The distribution of useful energy: c—without recycle; d—with recycle.
The data shown in figure 7 demonstrate that the usage of recirculation significantly changes the ratio of energy flows, by increasing the proportion of initial and torrefied feedstock and, respectively, decreasing the proportion of energy expenses directly related with torrefaction.

In case of supplying the heat of HRB to consumer the usage of recirculation increases the energy efficiency of technology by more than 10% (see table 3). If HRB is used only for combustion of volatile torrefaction products, the energy efficiency is increased more than twice.

5. Conclusions
The studies show that the usage of recirculation of gaseous heat carrier in torrefaction reactor significantly improves the energy indexes of the energy-technological complex and promotes efficient utilization of volatile torrefaction products. In addition, scheme with recirculation allows to control energy flows and to change flexibly the structure of the complex—from production only of torrefied pellets up to technologies of cogeneration and trigeneration.

The developed numerical model allows to determine the optimal ratio of energy and mass flows of the complex (electricity, heat, torrefied pellets) according to the specific conditions and requirements of the consumer.

Acknowledgments
This study has done in the framework of basic research program III.4 of Department of Energy, Engineering, Mechanics and Control Processes RAS. The authors are grateful to J M Faleeva for assistance in carrying out a number of calculations.

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