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The mathematical description of the gasification process of woody biomass in installations with a plasma heat source for producing synthesis gas

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Abstract. The article presents the scheme of processing of plant biomass in the gasification installation with a plasma heat source to produce synthesis gas suitable for chemical industry. The analyzed physical picture of raw materials' recycling process underlies a mathematical description of the process set out in the form of the basic differential equations with boundary conditions. The received mathematical description allows calculating of the main parameters of equipment for biomass recycling and to determine the optimal modes of its operation.

1. Introduction

Researches in the field of plant biomass' recycling to chemical feedstock for further production of useful products of chemical synthesis has become widespread in recent years and it is accelerating with each year [1, 2]. It should be noted that the high growth of development of scientific activity and application of new developments in this industry has the priority point both for the economy and for the environment. Also the development of research on processing of plant raw materials is of great importance for the development of fundamental areas of knowledge, such as theory heat mass exchange processes, chemical kinetics and others.

One of the developing directions of plant raw materials' recycling is the use of gas-producing installations with a plasma heat source. It is known that various gases can serve as a plasma-forming agent: water vapour, hydrogen, air, oxygen, carbon dioxide (CO₂) and other [3]. Such diversity of gasifying agents leads to the fact that each option requires a separate technical solution, both by the design of the plasma device (plasma torch) and by the method of heat supply.

The article discusses and mathematically describes the process of plant raw materials' recycling - wood biomass on gasification installation with a plasma heat source on the basis of air for the purpose of producing synthesis gas suitable for use in the synthesis of various chemical products. The initial data were used by the source, gasifying agent, the type of plasma gas and the characteristics of the biomass such as biomass type, fractional composition, moisture content.

2. Description and formalization of the process

Considering the purpose of the work, based on the known data and on the processes occurring in gas generators, the physical picture of the process, depicted in Figure 1 has been compiled. The figure



shows that the synthesis gas is formed by multistage biomass recycling in the gasifier. The resulting synthesis gas is subjected to mechanical cleaning, cooling, compressing, and it passes through the stage of catalytic synthesis of chemical products and other related stages.

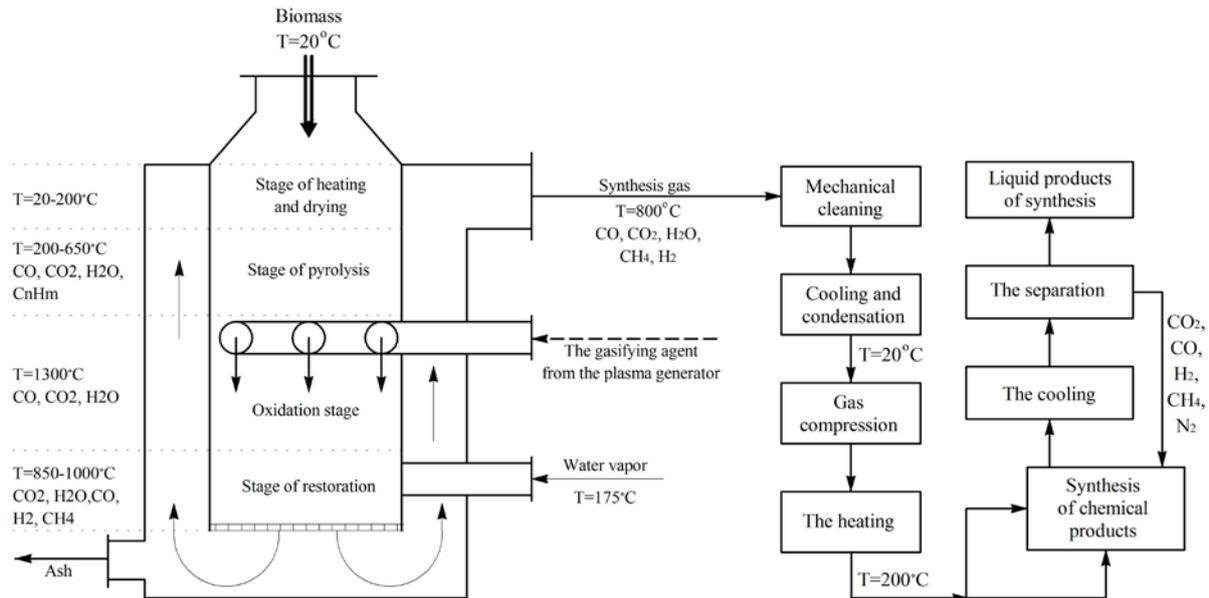
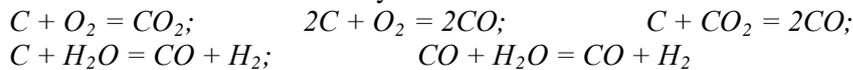


Figure 1. Diagram of the wood biomass' recycling process by the method of gasification and the physical picture of synthesis gas production

Based on the information reviewed and on the process in general, it is possible to conclude that the real picture of the process is complicated and it is imperative to make the following assumptions to receive the constructive mathematical description of the wood biomass recycling process in the gasification installation with a plasma heat source:

- a polydisperse system of particles is conditionally replaced with the equivalent monodisperse system in the form of infinite plates;
- the processes of heating, drying, pyrolysis, combustion, and recovery are discussed by stages, and an overlay of processes in time is not taken into account [4];
- there is a continuous stationary process of heat-mass exchange of the particles with the reactor wall in the area of heating, drying and pyrolysis;
- the change of a particle size during the drying process and pyrolysis is neglected;
- there are no oxidative processes on the heated boundary layer due to lack of oxidizing agents at a temperature equal to the temperature of the end of pyrolysis [5];
- the possible gas-phase chemical reactions between the pyrolysis products are not taken into account [5];
- when considering the stage of pyrolysis it is assumed that the wood consists of two main components - cellulose and lignin in a specific ratio, and the process is taken as a set of processes of thermal decomposition of its main components [4];
- the measures of convective heat transfer in the porous structure of the wood are determined by the mass flow of gaseous products of pyrolysis;
- it should be taken into consideration that there are only homogeneous reactions between gaseous pyrolysis products with an oxidizing agent occurring in the oxidation zone;
- in the reduction zone, the rate of convective transfer in the parallel to the axis reactor direction is much higher than the intensity of molecular diffusion, therefore the latter is neglected;

- the formation of methane (CH_4) in the area of recovery, is not taken into consideration as the rate of formation is significantly lower than that of other reactions [6]. As a result, the reduction zone is defined by the occurrence of the next set of reactions:



- when considering the recovery zone the thermal conductivity and diffusion of gas are negligibly small in comparison with convective heat and mass transfer, so the influence of diffusion and heat conduction is neglected [6];
- the resulting gas-vapor mixture in the reduction zone is subject to the laws of perfect gases due to low pressure and high temperature;
- the particles, a gas-vapor phase and an oxidant at any point in the cross section of the reactor are uniformly distributed;
- the synthesis of chemical compounds on the catalyzer occurs directly from carbon monoxide and hydrogen;
- the change in the chemical composition of the catalyzer under the influence of impurities in the initial mixture is not considered because of its pre-treatment.

Taking into account the accepted assumptions the mathematical description of the process is assuming a classic form from the system of differential equations of thermal and mass conductivity.

3. Description of mathematical model

On the basis of the physical picture (Figure 1), it seems that the stage of heating, drying and pyrolysis all together have an interconnection and in general they can be described by the differential equation of heat transfer [4]

$$c_{layer} \cdot \rho_{layer} \cdot \frac{\partial T_{layer}}{\partial \tau} = \frac{\partial}{\partial x} \left(\lambda_{ef} \cdot \frac{\partial T_{layer}}{\partial x} \right) + q_{layer} \quad (1)$$

where c and ρ – the heat capacity and density, respectively; λ – the coefficient of thermal conductivity; q – heat flow.

For the solution of the differential equation (1) the initial (2) and boundary conditions (3)÷(4) are formulated, shown schematically in Figure 2.

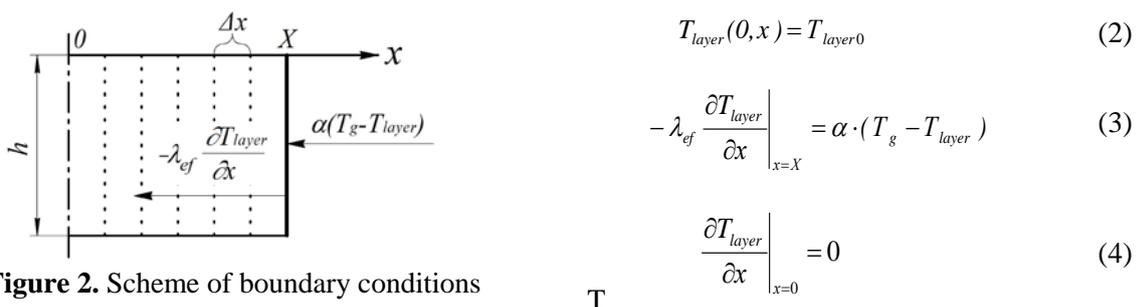


Figure 2. Scheme of boundary conditions

taking into account the accepted assumptions and some transformations the stage of drying is described by the system of equations

$$c_{layer} \cdot \rho_{layer} \cdot \frac{\partial T_{layer}}{\partial \tau} = \frac{\partial}{\partial x} \left(\lambda_{ef} \cdot \frac{\partial T_{layer}}{\partial x} \right) + r \varepsilon \frac{\partial U_{layer}}{\partial \tau} \quad (5)$$

$$\frac{\partial U_{layer}}{\partial \tau} = \frac{k_p}{\rho_0} \left(\frac{\partial^2 P_{layer}}{\partial x^2} \right) + a_m \frac{\partial^2 U_{layer}}{\partial x^2} + a_m \delta \frac{\partial^2 T_{layer}}{\partial x^2} \quad (6)$$

where k_p – is the molar transfer coefficient, a_m – is the coefficient of mass conductivity.

To solve the system of equations (5)÷(6) initial and boundary conditions for temperature, humidity and pressure can be written as follows:

$$U_{layer}(0, x) = U_{layer0} \quad (7) \quad P_{layer}(0, x) = P_{atmos} \quad (9)$$

$$T_{layer}(0, x) = T_{layer0} \quad (8) \quad \left. \frac{\partial U_{layer}}{\partial x} \right|_{x=X} = 0 \quad (10)$$

In its turn, the stage of pyrolysis is significantly different from the pre-heating and drying, as it is accompanied by mass decrease and the formation of the gas phase [1]. Based on the above-mentioned, the stage of pyrolysis can be described by a system of equations of energy conservation

$$c_{layer} \cdot m_{wood} \frac{\partial T_{layer}}{\partial \tau} = \frac{\partial}{\partial x} \left(\lambda_{ef} \cdot \frac{\partial T_{layer}}{\partial x} \right) - m_{wood} \cdot c_{layer} \cdot w_{wood} \cdot \frac{\partial T_{layer}}{\partial x} + q_{chem.reac} \quad (11)$$

and mass change, the assumptions may have the following form:

$$\frac{\partial m_{cell}}{\partial \tau} = -k_{cell} m_{cell} \quad (12)$$

$$\frac{\partial m_{lignin}}{\partial \tau} = -k_{lignin} m_{lignin} \quad (13)$$

$$\frac{\partial m_{coal}}{\partial \tau} = \gamma_{lignin} (-k_{lignin} m_{lignin}) + \gamma_{cell} (-k_{cell} m_{cell}) \quad (14)$$

$$\frac{\partial (m_{vg} \varepsilon)}{\partial \tau} = - \frac{\partial (w_{vg} m_{vg})}{\partial x} + (1 - \gamma_{lignin}) k_{lignin} m_{lignin} + (1 - \gamma_{cell}) k_{cell} m_{cell} \quad (15)$$

where w – the speed; k – the reaction velocity constant; γ – mass fraction of the substance; ε – the porosity of the material, determined from the expression [7]

$$\varepsilon = \left(1 - \frac{m_{wood}}{m_{wood0}} \right) \cdot (1 - \varepsilon_{wood}) \quad (16)$$

The boundary conditions for solving the equation (11) are similar to the stages of pre-heating and drying (Figure 2) and are defined by equations (3)÷(4). To solve the system of equations (12)÷(15) the boundary conditions can be written as (17)÷(20), and the initial conditions take the form (21)÷(25).

$$m_{lignin} \Big|_{x=0} = m_{lignin0} \quad (17) \quad T_{layer}(0, x) = T_{layer0} \quad (21)$$

$$m_{cell} \Big|_{x=0} = m_{cell0} \quad (18) \quad m_{cell}(0, x) = m_{cell0} \quad (22)$$

$$m_{coal} \Big|_{x=0} = m_{coal0} \quad (19) \quad m_{lignin}(0, x) = m_{lignin0} \quad (23)$$

$$m_{vg} \Big|_{x=0} = m_{vg0} \quad (20) \quad m_{coal}(0, x) = 0 \quad (24)$$

$$m_{vg}(0, x) = 0 \quad (25)$$

Consideration of oxidation stage with the accepted assumptions taken into account is reduced to some simple mathematical expressions, in particular the determination of the theoretically required consumption of oxidant, the temperature of the gas mixture combustion and a quantitative yield of combustion products - CO₂ and H₂O.

A theoretically required amount of oxidant to provide the combustion process at the stage of oxidation can be determined by the formula [4]:

$$L_0 = \frac{I}{0,2I} \cdot \left[0,5 \cdot (CO + H_2) + 2CH_4 + \left(n + \frac{m}{4} \right) \cdot C_n H_m - O_2 \right] \quad (26)$$

And the consumption of the theoretical amount of oxidizing agent is calculated from the equations of material and thermal balance

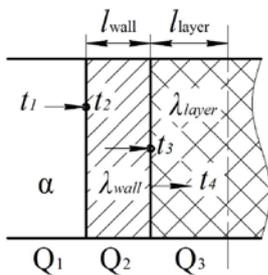
$$\frac{\partial T_{layer}}{\partial \tau} = \sum q_{chem.reac} \cdot k_i (C_{i_0} - C_i) - w_{vg} \frac{\partial T_{layer}}{\partial x} \quad (27)$$

$$\frac{\partial C_i}{\partial \tau} = w_{vg} \frac{\partial C_i}{\partial x} - k_i (C_{i_0} - C_i), \quad (28)$$

where C_i – is the concentration of the i -substance.

Knowing the consumption of the theoretical amount of oxidant and the content of the oxidizing agent in the gasifying agent (plasma gas) it is possible to calculate the total quantity and the required consumption of the gasifying agent supplied to the gasifier. In consequence it is also possible to calculate the amount of heat energy to be carried by a plasma gas for the gasification process and to provide the required operating parameters.

The consumption of the gasifying agent supplied to the gasifier is calculated using the oxidizer (oxygen) provided that the gasifying agent consists of oxygen (O_2), hydrogen (H_2) and water vapor in the percentage ratio by volume of 23÷46÷31 respectively. The heat flow coming together with the gasifying agent is calculated from the law of energy conservation. For clarity, a design scheme is made (Figure 3), according to which the estimated equations have the following form:



$$Q_1 = Q_2 = Q_3 \quad (29)$$

$$Q = c_{wood} \cdot m_{wood} \cdot \Delta t \quad (30)$$

$$Q_1 = -\lambda_{layer} (t_3 - t_4) l_{layer} \quad (31)$$

$$Q_2 = -\lambda_{wall} (t_2 - t_3) l_{wall} \quad (32)$$

$$Q_3 = \alpha (t_1 - t_2) \quad (33)$$

Figure 3. Design scheme of heat flows

where m_{wood} – the mass of the wood; t_1 – the temperature of the gasifying agent, t_2 – the temperature of the outer wall, t_3 – the temperature of the inner wall, t_4 – the temperature of the material.

The recovery phase, taking into account the adopted assumptions, can be written with the system of equations of conservation of matter and energy for a gas stream and carbon residue in the form of

$$w_{stream} \cdot \frac{\partial C_i}{\partial y} = -k_i \cdot C_i \quad (34)$$

$$w_{coal} \cdot \frac{\partial m_{coal}}{\partial y} = -m_{coal} \cdot \sum_{m=1}^z k_i \quad (35)$$

$$\rho_{stream} c_{stream} w_{stream} \frac{\partial T_{stream}}{\partial y} = -\alpha_{stream} (T_{coal} - T_{stream}) f + \sum_{i=1}^z q_i \cdot k_i \cdot (C_{i_0} - C_i) \quad (36)$$

$$\rho_{coal} c_{coal} w_{coal} \cdot \frac{\partial T_{coal}}{\partial y} = \alpha_{stream} \cdot (T_{coal} - T_{stream}) f - \sum_{i=1}^z q_i \cdot k_i \cdot (C_{i_0} - C_i) \quad (37)$$

To solve the system of equations (34)÷(37) the boundary conditions on temperature and mass are taken:

$$T_{coal}|_{y=0} = T_g|_{y=0} \quad (38) \quad C_i|_{y=0} = C_{i0} \quad (39)$$

$$m_{coal}|_{y=0} = m_{coal0} \quad (40)$$

When describing the stage of catalytic synthesis of chemical products the equation of consumption of the components of the synthesis gas can be used, it will have the following form:

$$w \frac{\partial C_i}{\partial y} = -k_i \cdot C_i. \quad (41)$$

And the equation of energy conservation will assume the form

$$w \cdot \rho \cdot c \cdot \frac{\partial T_{syngas}}{\partial y} = \sum_{i=1}^z (q_i \cdot k_i (C_{i0} - C_i)). \quad (42)$$

The time, during which the synthesis gas contacts with the catalyzer (t, sec) at a constant pressure, is calculated according to the formula [8]

$$\tau = \frac{V_k}{V_g} \quad (43)$$

where V_k – the volume of the catalyzer; V_g – the volume of the reaction gas (under normal conditions) passed through the layer of catalyzer per unit time.

4. Conclusions

The mathematical description of the process of wood raw material recycling in the synthesis gas, is presented in the form of the basic differential equations with boundary conditions. Modeling the process according to this mathematical description will allow the following: to calculate the main parameters of the gas generators with plasma heat sources, to determine the optimal modes of their operation and to obtain a synthesis gas suitable for chemical industry.

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