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A MATHEMATICAL MODEL OF THERMAL DECOMPOSITION OF WOOD IN CONDITIONS OF FLUIDIZED BED

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ABSTRACT

The mathematical model of thermal decomposition of wood in the conditions of fluidized bed is developed. The estimation of the temperature distribution along the radius of the particle, the influence of the temperature of reactor on kinetics of the process, as well as the influence of the temperature and length of the reactor on the product yield are made in the course of the mathematical modeling.

Key words: thermal decomposition, pyrolysis in fluidized bed, liquid products of pyrolysis, mathematical model, ecologically pure technology.

INTRODUCTION

There is a constant decrease in the world oil and gas reserves, resulting transition to renewable resources is one of urgent problems of economy and industry. This circumstance forces researchers to look for the most practically feasible renewable materials and cheap energy sources, one of which is the plant biomass. However, using biomass as a fuel and chemical feedstock is ineffective in some cases due to the fact, that it is disseminated on the territory of, has a small transport density and practically is not adapted to the existing production infrastructure, oriented on consumption of fossil resources (TUNTSEV et al. 2013). Minimizing of the negative influence of these factors is possible with the help of the provisional decentralized processing of plant biomass in intermediate products with higher density, which could then be processed in the large industrial centers and traditional petrochemical products could be obtained. Thermochemical treatment is one of the nonselective methods of processing of plant biomass in the solid, liquid and gaseous products (BRIDGWATER 2004), and the liquid products are of greatest interest of in involving plant biomass in the existing industrial infrastructure. Maximizing the yield of liquid products during the thermal decomposition of wood can be achieved by the increasing heating rate and the reduction of the duration of stay products in the reaction zone, by reducing the dimension of processed raw materials and the rate of cooling of vapor-gas mixture (DIEBOLD et al. 1997). High heating rate combined with low duration of stay of the products is achieved in the fluidized bed reactors in practice. Therefore the study of the process taking place during the thermal decomposition of wood in fluidized bed is an urgent problem of the modern science.

MATERIAL AND METHODS

The process of thermal decomposition of wood in the conditions of fluidized bed is a problem of heat and mass transfer in the particle in the presence of chemical transformations. Thus the mathematical model provides for the energy transfer in a solid porous medium, the chemical reactions of thermal decomposition and the transfer of energy and mass in gasvapor phase (Fig. 1) (DI BLASI 1993; TIMERBAEV 2014).

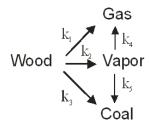


Fig. 1 The two-stage mechanism of reactions of thermal decomposition.

When developing a mathematical model the assumption that thermal decomposition of wood is realized in form of two-stage process with competing reactions and with the formation of three main groups of products of thermal decomposition (gas, liquid and coal) was made. The kinetic constants for the selected mechanism are made on the basis of works of DI BLASI (1996). It is also supposed that the processes of diffusion and filter of vapor-gas mixture in the wood particle, due to the smallness of its size, in terms of the fluidized bed have no significant influence on the yield of products of thermal decomposition. The solid phase is described by the model of ideal mixing in view of intensive mixing, and the gas phase is obeys the law of ideal displacement.

Stationary fluidized bed during thermal decomposition of wood can exist in a limited interval of flow rates in accordance with

$$\mathcal{G}_{cr}\langle \mathcal{G}\langle \mathcal{G}_{abl}.$$
 (1)

where \mathcal{G}_{cr} - critical speed;

 \mathcal{G} - flow rate;

 \mathcal{G}_{abl} - rate of ablation

The flow rate should be higher than the critical one for inert filler, characterizing the beginning of fluidization, and lower than the rate of ablation for wood particles, characterizing the removal of particles from the reactor.

The height of fluidized bed can be defined by correlation

$$l = \frac{l^0 (1 - \varepsilon_0)}{(1 - \varepsilon)} \tag{2}$$

where l^0 - a fixed layer thickness, m;

 ε_0 - fenestration of layer;

 ε_0 - a fixed layer fenestration

Mass capacity of the reactor can be defined by expression

$$P = V_{reactor} \rho_{m} / \tau_{t.d.}, \tag{3}$$

where $V_{reactor}$ - reactor volume, m³;

 $ho_{\rm m}$ - material density, kg/m³;

 $\tau_{t,d}$ - time of thermal decomposition, s

Taking into account the accepted assumptions on the mechanism of chemical reactions equation of formal chemical kinetics for local volume of a solid phase is represented as:

$$\frac{\partial \rho_{\mathbf{w}}}{\partial \tau} = -(K_1 + K_2 + K_3)\rho_{\mathbf{w}} \tag{4}$$

where K_i - reaction rate constant, s⁻¹;

 $\rho_{\rm w}$ - wood density, kg/m³

for carbonaceous substances

$$\frac{\partial \rho_c}{\partial \tau} = K_3 \rho_w \tag{5}$$

Differential equations for defining the change of the concentration of vapors and gases generated in a primary decomposition of wood inside wood particles can be written, respectively, for steam

$$\frac{\partial \rho_{v}}{\partial \tau} = K_{2} \rho_{w},\tag{6}$$

and for coal

$$\frac{\partial \rho_g}{\partial \tau} = K_1 \rho_w, \tag{7}$$

The heat equation in the case of thermal decomposition of wood for a one-dimensional spherical particles can be written as:

$$\left(\rho_{_{W}}c_{_{W}}\right)\frac{\partial T}{\partial \tau} = \frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\lambda\frac{\partial T}{\partial r}\right) + Q_{\text{react.}},$$
(8)

where r - radius, m

where the left part of the equation represents the total energy change for local volume of time, and the first term in the right part - the change in internal energy due to the molecular thermal conductivity.

The second member of the right side of the expression Q_{react} characterizes the change in the internal energy of local volume of the frame due to thermal effects of chemical reactions of thermal decomposition of biomass. Coefficients of thermal conductivity are determined on the assumption of the linear change of thermo-physical characteristics depending on the share of reacted wood χ .

$$\lambda = (1 - \chi)\lambda_w + \chi\lambda_c + \lambda_{radiat} \tag{9}$$

where λ_w - heat transfer coefficient of wood, W/(m · K);

 λ_c - heat transfer coefficient of coal, W/(m · K)

where the coefficient of thermal conductivity by radiation can be determined from the equation:

$$\lambda_{radiat} = \frac{13.5\sigma T^3 d}{e} \tag{10}$$

where σ - Boltzmann constant;

e - emissivity

The change of concentration of the components of the mixture of vapor throughout the height of the reactor may be determined by the ratio

$$\frac{\partial \rho_{\nu}}{\partial l} = \frac{1}{9} \left(\overline{j_{\nu}} f - \left(k_4 \rho_{\nu} + k_5 \rho_{\nu} \right) \right) \tag{11}$$

where ρ_{y} - vapor density, kg/m³;

f - specific surface, m^2/m^3 ;

j - mass flow kg/m²;

 \mathcal{G} - speed m/s

and the change of concentration of the incondensable gas is determined by an expression

$$\frac{\partial \rho_g}{\partial l} = \frac{1}{9} \left(\overline{j_g} f + k_4 \rho_v \right) \tag{12}$$

The change in the concentration of coal in the gas phase reactor due to the secondary cracking of gas-vapor mixture throughout the height of the reactor is determined by the expression

$$\frac{\partial \rho_c}{\partial l} = \frac{1}{9} (k_5 \rho_v) \tag{13}$$

It is supposed that applicable model of ideal mixing is applicable for a solid phase, so the value of distributed stream of gas mixture caused by thermal decomposition throughout the height of the reactor will be permanent. Average value of flow can be determined using the medium-integral value for duration of stay of particle in a layer

$$\overline{j_i} = \frac{1}{\tau_{t,d}} \int_0^{\tau_{t,d}} j_i d\tau \tag{14}$$

where the value of the instantaneous flow can be determined by the expression

$$j_{i} = \frac{1}{R_{part}^{2}} \int_{0}^{R_{x}} \frac{\partial(\rho_{i})}{\partial \tau} r^{2} dr$$
(15)

where R_{part} - particle radius, m

For solving the task it is necessary to formulate initial and boundary conditions for equations. Initial conditions are recorded as:

$$\rho_{\scriptscriptstyle W}(r,\tau=0) = \rho_{\scriptscriptstyle \scriptscriptstyle W}^{0} \tag{16}$$

$$T(r,\tau=0) = T_0 \tag{17}$$

$$\rho_{g}(l=0) = \rho_{g}^{0} \tag{18}$$

$$\rho_{\nu}(l=0) = 0 \tag{19}$$

Boundary conditions, taking into account the target setting, are determined by the expression

$$\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0, \tag{20}$$

$$-\lambda^* \frac{\partial T}{\partial r}\Big|_{r=R} = \alpha (T_r - T) + \sigma e (T_r^4 - T^4), \tag{21}$$

Moreover, the heat transfer coefficient for the conditions of the boiling layer can be identified using the criteria equations of the Rants-Marshal (NAVALOV 1968)

$$\alpha = \frac{\lambda_g}{d_{part}} \left(2 + 0.6 \,\text{Re}^{1/2} \,\text{Pr}^{1/3} \right). \tag{22}$$

where d_{part} - particle radius, m;

 λ_g - gas heat transfer coefficient, W/(m·K)

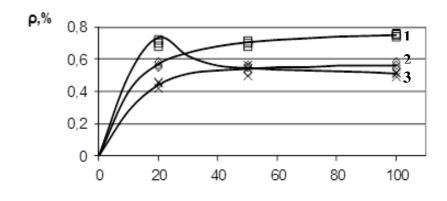
Thus, the mathematical model allows simulating the processes of thermal decomposition in a boiling layer with appropriate boundary and initial conditions.

RESULTS AND DISCUSSION

Experimental and theoretical researches of the processes of thermal decomposition of wood in the conditions of fluidized bed have been performed in the course of this work. The results in the form of graphic dependences are presented, where dots are experimental data and lines are the calculated values.

The basic studies of thermal decomposition have been performed on wood flour brand of softwood No. 560 with an average particle size of 0.3 mm.

Fig. 2 shows the dependences of the relative concentration of vapors to the mass of the raw materials throughout the height of the reactor at different temperatures. As may be seen from the dependencies, the concentration of vapors increases throughout the height of the reactor the faster, the higher the temperature. However, at higher temperatures (700 °C) in height of 20 cm the concentration of primary vapor is decreased due to their secondary thermal decomposition.



L, sm

Fig. 2 Changes in the concentration of vapors throughout the height of the reactor at different temperatures: $1-500^{\circ}\text{C}$; $2-400^{\circ}\text{C}$; $3-700^{\circ}\text{C}$: ρ -vapor concentration, %; L - the height of the reactor, sm.

Vapor samples were taken at different points (20, 50, 100 cm) of the reactor of fluidized bed by the sampler. The comparison of the calculated and experimental data shows satisfactory convergence of the concentrations along the length of reactor at different temperatures. The difference between the values is not more than 18%, indicating the adequacy of the developed mathematical description.

The temperature distribution along the radius of wood particle (Fig. 3) shows that the temperature in the particle rises almost instantly to the level of decomposition temperatures. It should be noted, that the temperature profile has no significant temperature drop at the size of particle of the order of 0,0001 m, that is warming up and response in the particle occur almost immediately on the surface and in the center of it in contrast to great temperature drops during the pyrolysis of large particles. The temperature profile is stabilized at the duration of thermal decomposition 1sec. Volumetric response on the thickness of the particle takes place. With increase of diameter of the particle the irregularity of warming increases, as well as the duration of thermal decomposition and the duration of particles in the reaction zone. These circumstances lead to a greater probability of passing of secondary reactions of thermal decomposition and, as consequence, to decrease in the output of pyrolysis liquid products.

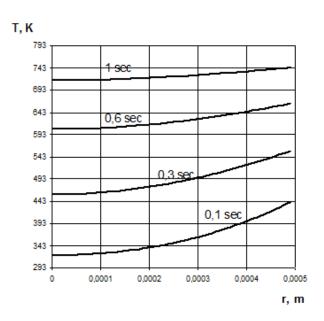


Fig. 3 The temperature distribution along the radius of the particle in the process of thermal decomposition: r - particle radius, m; T - temperature, K.

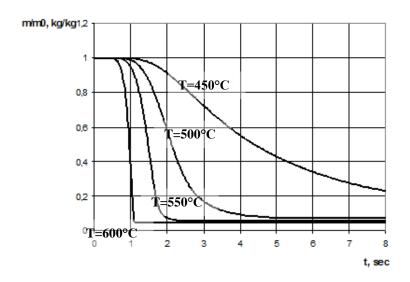


Fig. 4. Kinetic dependence of the relative masses of the particle in the process of thermal decomposition at different temperatures of reactor: m/m0 - relative mass of particles, kg/kg; t – time, sec.

The temperature of fluidized-bed reactor provides the strongest influence on the process of thermal decomposition. Kinetic dependence of the mass of particles at different temperatures of the reactor is presented in Fig. 4. It shows that with increase of the temperature the duration of thermal decomposition is significantly reduced. Thus, the rise in temperature in the reactor allows to intensify the process under other equal conditions. However, while increasing the temperature in the reaction zone output of pyrolysis liquid decreases and output of gaseous products increases. It is therefore necessary to determine the optimum temperature regimes of the process in each specific situation (TUNTSEV 2011).

Deep study of thermal decomposition in a boiling layer gives the more detailed understanding of the mechanisms taking place in the pyrolysis process. The developed mathematical model allows to define the main characteristics of instrumentation of the process and to find the optimal parameters of the process, with the aim of obtaining liquid product of thermal decomposition. The liquid product of thermal decomposition is valuable in mind the possibility of its use as an alternative fuel (biofuel) or raw materials for chemical production (SADRTDINOV *et al.* 2015). The carried out researches allow involving unclaimed vegetable raw material in the treatment with the purpose of obtaining new or cheaper existing products (Tuntsev *et al.* 2014).

CONCLUSION

In the course of research work the mathematical model of thermal decomposition in the conditions of a boiling layer was developed. An assessment of the temperature distribution along the radius of the particle, the influence of temperature of reactor on kinetics of the process, as well as the influence of the temperature and length of the reactor on the product yield were made at the stage of mathematical modelling of the process of thermal decomposition.

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