

# Modeling of a reduction zone of the gasifier installation

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**Abstract.** The development of the mathematical model that describes a reduction zone of the gasifier installation is described in this paper.

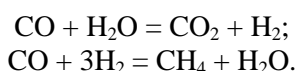
## 1. Introduction

Processes occurring in a reduction zone of the reactor gasification of wood waste, are extremely complex and diverse. They depend on the fractional composition of the processed wood waste and on operating parameters of the recycling process. A recovery zone is the most difficult stage in the gasification process regarding the amount and the quality of substance occurring in chemical reactions. This work considers a stationary layer of material with variable porosity and conventionally constant speed of filtration of a gas phase along the height of the layer.

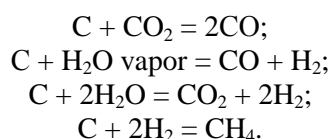
## 2. Subject description and method of solution

Both homogeneous (in volume) and heterogeneous reactions occur in the process of gasification (on the surface of phase separation - solid, liquid or gaseous).

Homogeneous reactions are as follows:



and heterogeneous reactions are:



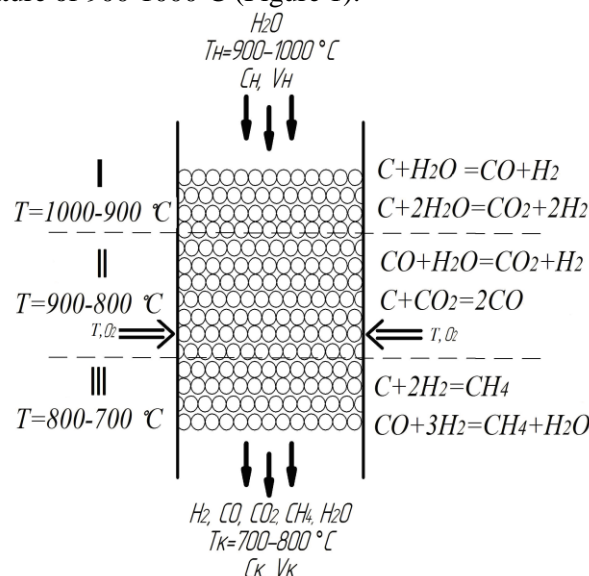
The gasification process can be described by the following main stages: heating, drying, pyrolysis (release of volatiles), combustion of pyrolysis products and the recovery processes of the producer gas formation [1]. The boundaries between these zones are quite conditional and it is almost impossible to specify the exact location of the end of one process and the beginning of the other.

The stage of heating and the yield of volatile matter are less than 15 % of the total time of the gasification process, unlike the recovery stage, which takes most of the time and is one of the main consumers of energy in the gasifier [2]. The recovery phase is a complex set of interrelated physical and chemical processes of heat exchange and mass transfer of reaction products and chemical reactions, as coal is a porous body, which, as a result of heterogeneous reactions, changes its structure and properties.

The modeling process of the restored area starts with the fact that charcoal enters the reactor and forms a dense layer, which defines the height of the recovery zone. It is known that reduction



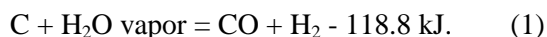
processes occur at temperatures of 800-1100<sup>0</sup>C [3]. In this regard, the layer of charcoal is heated to a temperature of 900 <sup>0</sup>C through the wall of the reactor, then the reactor is fed with a gas agent (H<sub>2</sub>O, CO<sub>2</sub>, H<sub>2</sub>O+O<sub>2</sub>) at a temperature of 900-1000<sup>0</sup>C (Figure 1).



**Figure 1.** Schematic representation of the recovery zone

Let us divide the recovery area conditionally into 3 phases.

In the first section the superheated water vapor is given to the surface of charcoal, heated to 900÷1000 °C. Upon contact of water vapor with the heated layer of charcoal under high temperature (950 °C and above) the following reaction takes place:



Since the reaction (1) is endothermic, the temperature decreases and at a temperature from 900 to 950 °C the following reaction takes place (2):



Both reactions are endothermic and lead to a decrease of the temperature.

In the second plot there is a decrease in the speed of passage of water vapor through the charcoal due to the resistance of the layer. Previously formed CO reacts with water vapor to form carbon dioxide and hydrogen in the reaction:



Also in this plot the reaction of carbon dioxide starts to take place:



In the third phase the hydrogen formed in the reactions (1) – (3) reacts with carbon, forming methane:



The temperature in this zone is about 800-850 °C. The methane content in gas obtained from charcoal is not more than 1%.

Due to the flow of such chemical reactions the charcoal layer decreases.

The reaction (4) goes with the energy consumption due to that fact that the temperature in the reaction zone decreases, and the equilibrium in the reaction shifts towards the formation of carbon dioxide. According to that the heat input either from outside or by internal exothermic reactions is necessary to

maintain the temperature level, providing the formation of CO, for example to supply oxygen to the reaction zone



Also to ensure the conditions for the occurrence of these reactions, it is possible to use catalysts which increase the yield of CO and H by lowering the reaction temperature of 600-700 °C.

The speed of reaction (4) is two times faster than the speed of the reaction (1). The presence of solid carbon limits the reaction zone.

As noted, the stage of heating and the volatile content are less than 15 % of the total time of the gasification process in contrast to the recovery stage, which occupies most of the time and is the primary source and consumer of energy in the gasifier.

The reduction zone is characterized by the occurrence of the following main reactions:



The final composition of producer gas is the following: CO<sub>2</sub>, CO, CH<sub>4</sub>, H<sub>2</sub> and H<sub>2</sub>O [4].

The recovery phase is described by the following equations:

-the equation of coal conservation

$$\frac{dm_y}{d\tau} = -m_y \cdot \sum_{i=1}^z k_i \quad (14)$$

where  $k_i$  - is the rate constant of a chemical reaction,  $m_y$  - is the coal mass

- the equation of mass conservation for each component of the gas flow

$$\pm \frac{dC_i}{d\tau} = -k_i \cdot C_i \quad (15)$$

$C_i$  - is the relative concentration of the i-substance.

The "+" sign is for reactions of CO, H<sub>2</sub>, CH<sub>4</sub> formation.

The sign "-" is for loss reactions of CO<sub>2</sub>, H<sub>2</sub>O.

- the equations of energy conserving for the gas flow and coal

$$\rho_{g-g} \cdot c_{g-g} \cdot \frac{dT_{g-g}}{d\tau} = -\alpha_{g-g} \cdot (T_c - T_{g-g}) \cdot f + \sum_{i=1}^z (q_i \cdot k_i \cdot (C_{i0} - C_i)) \quad (16)$$

$$\rho_c \cdot c_c \cdot \frac{dT_y}{d\tau} = \alpha_{g-g} \cdot (T_c - T_{g-g}) \cdot f - \sum_{i=1}^z (q_i \cdot k_i \cdot (C_{i0} - C_i)) \quad (17)$$

where  $p_c$  and  $p_{g-g}$  are the specific density of coal and gas stream, respectively;  $c_y$  and  $c_{g-g}$  - are heat capacity of coal and gas stream, respectively;  $\alpha_{g-g}$  - is coefficient of convective heat transfer between gas and coal, W/(m<sup>2</sup>·K);  $C_{i0}$  - is initial concentration of the i-substance;  $C_i$  - is the relative concentration of the i-substance;  $z$  - is the number of parallel reactions;  $f$  - is the specific surface area.

The initial conditions for the system of equations (14) – (17)

$$T_{\text{vapor}} = 1000 \text{ °C}, T_y = 900 \text{ °C}$$

$$C_{H_2O} = 100\%,$$

$$m_{y0} = m_{y \text{ entr.}}$$

To solve the system of equations (14) – (17), the following boundary conditions are accepted:

- according to temperature:

$$T_y \Big|_{\tau=0} = T_{entr} = 900^\circ C, \quad (18)$$

- according to weight:

$$C_i \Big|_{\tau=0} = C_{i0}, \quad (19)$$

$$m_y \Big|_{\tau=0} = m_{y0}. \quad (20)$$

The density of the gas flow is determined by the expression

$$\rho_{g-g} = \sum_{i=1}^z M_i \cdot C_i \quad (21)$$

The gas permeability of the layer depends on the layer's porosity and is determined experimentally:  $K = f(\varepsilon)$ .

The calculation of dynamic viscosity of the gas flow is carried out according to the expression

$$\mu_{g-g} = \left( \sum_{i=1}^z v_i \mu_i M_i^{0.5} \right) / \left( \sum_{i=1}^z v_i M_i^{0.5} \right) \quad (22)$$

where  $v_i$  - is the volume fraction of the i-component in the gas mixture;  $\mu_i$  - is the dynamic viscosity of the i-gas, chosen depending on the temperature.

The heat capacity of the gas flow is determined by the expression

$$c_{g-g} = \sum_{i=1}^z v_i \cdot c_i \quad (23)$$

where  $v_i$  - is the volume fraction of the i-component;  $c_i$  - is the heat capacity of the i-component, which is determined depending on the temperature.

The coefficient of convective heat transfer between gas and coal ( $\alpha_g$ ), is calculated using the Nusselt criterion by the formula corresponding to the flow of gases in the layer of a granular material:

$$\alpha_{g-g} = A \cdot \frac{\lambda_{g-g}}{d_2} \cdot Re^{0.6} \cdot Pr^{0.33} \quad (24)$$

where A – is the value depending on the porosity of the layer,  $A = f(\varepsilon)$ .

The thermal conductivity of the gas flow is calculated by the formula

$$\lambda_{g-g} = \frac{\sum_{i=1}^z v_i \lambda_i M_i^{1/3}}{\sum_{i=1}^z v_i M_i^{1/3}} \quad (25)$$

where  $\lambda_i$  is the thermal conductivity of the i-component of the gas mixture, which is taken depending on the temperature.

The Reynolds number is defined by the equation

$$Re = \frac{w_{g-g} \cdot \Delta y \cdot \rho_{g-g}}{\mu_{g-g}} \quad (26)$$

and the Prandtl number according to the equation is

$$Pr = \left( \sum_{i=1}^z c_{pi} C_i \right) \cdot \frac{\mu_{g-g}}{\rho_{g-g} \cdot \lambda_{g-g}} \quad (27)$$

Effective thermal conductivity of the layer depends on the moisture content, porosity and temperature layer:  $\lambda_{eff} = f(U, \varepsilon, T)$ , which complicates its calculation. Therefore it is determined experimentally.

Let us write the speed of chemical reactions for homogeneous and heterogeneous reactions.

Reactions (11) and (12) are homogeneous.

The speed of the reaction (11) has the form

$$\frac{d[\text{CO}]}{dt} = 575RT_g \cdot ([\text{CO}] - [\text{CO}]_{eq}) \cdot (0,5 - p \cdot 10^4 / 253) \exp(-13971/T_g) \quad (28)$$

where  $T_g$  - is the temperature of the components of the gas flow,  $R$  - is the universal gas constant, equal to 8.314 kJ/(kmolK).

The speed of reaction (12) is written as follows:

$$-\frac{d[\text{CH}_4]}{dt} = 312[\text{CH}_4] \exp(-13971/T_g) \quad (29)$$

The speeds of heterogeneous reactions are written as

$$R'_i = \frac{dG_i}{dt} = A'_i(T_c)(c_i - c_{ieq}) \quad (30)$$

where  $dG_i/dt$  is the quantity of  $i$ -gas consumed in a coal wall area of 1 m<sup>2</sup> at the  $m$ -reaction;  $c_{ieq}$  is the equilibrium concentration of  $i$ -gas for this reaction, KMOL/m<sup>3</sup>;  $A_m(T_c)$  is the velocity constant of the reaction, m/s;  $T_c$  - is the temperature of coal, Ph.

The value of  $A'_i(T_c)$  is calculated by the formula

$$\frac{1}{A'_i(T_c)} = \frac{1}{\beta_i} + \frac{1}{k_i} \quad (31)$$

$\beta_i$  is the coefficient of mass transfer for  $i$ -gas.  $\beta_i$  is calculated by the formula

$$\beta_i = Sh \cdot D_i / d_{eff} \quad (32)$$

where  $Sh$  is the Sherwood number;  $D_i$  is the molecular diffusion coefficient of  $i$ -gas, m<sup>2</sup>/s.

The Sherwood number is calculated according to the formula

$$Sh = 0,023Re^{0,8} \cdot Sc^{1/3} \quad (33)$$

This equation conforms to the turbulent gas flow in the pipe.

$Sc$  in equation (33) is the Schmidt number, which is calculated by the formula

$$Sc = \frac{\nu}{D_i} \quad (34)$$

The speed constant for chemical reactions (8-13) can be written as follows:

- for the reaction (8)

$$k_i(T_c) = k_m \exp(-275000/RT_c) \quad (35)$$

$$\log k_m = 0,2 \cdot 10^{-4} \cdot 275000 + 2$$

- for the reaction (9)

$$k_i(T_c) = k_m \exp(-200000/RT_c) \quad (36)$$

$$\log k_m = 0,2 \cdot 10^{-4} \cdot 200000 + 2$$

- for the reaction (10)

$$k_i(T_c) = \frac{k_m \exp(-125000/RT_c)}{1500} \quad (37)$$

$$\log k_m = 0,2 \cdot 10^{-4} \cdot 125000 + 2$$

- for the reaction (13)

$$\begin{aligned}
 k_i(T_c) &= k_m \exp(-200000/RT_c) \\
 \log k_m &= 0,2 \cdot 10^{-4} \cdot 200000 + 2 \\
 \frac{d[\text{CO}]}{dt} &= 575RT_g \cdot ([\text{CO}] - [\text{CO}]_{\text{eq}}) \cdot \\
 &\quad (0,5 - p \cdot 10^4 / 253) \exp(-13971/T_g)
 \end{aligned}
 \tag{38}$$

### 3. Results and discussion:

Due to the fact that in dry charcoal there are cavities and cracks the reaction surface for heterogeneous reactions will differ from the given coal surface. This factor is taken into account in the model by introduction of the enlargement factor of the area, which will vary from 1 to 30 [5].

### 4. Conclusion

The mathematical model allows determining the influence of operating parameters occurring in the reduction zone according to the parameters of the resulting producer gas.

### References

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