

# The Mathematical Model of the Coal Gasification Process in a Flow

Nikolai Nikolaevich Efimov<sup>1</sup>, Alexander Alekseevich Belov<sup>1</sup>, Dmitry Anatolyevich Shaforost<sup>1</sup>, Natalia Vasilyevna Fedorova<sup>1</sup> & Vera Sergeevna Pryatkina

<sup>1</sup> Federal State Budget Educational Institution of Higher Professional Education “Platov South-Russian State Polytechnic University (NPI)”, Rostovskiy region, Novocherkassk city, Russia

Correspondence: Nikolai Nikolaevich Efimov, Federal State Budget Educational Institution of Higher Professional Education “Platov South-Russian State Polytechnic University (NPI)”, Rostovskiy region, Novocherkassk city, Russia

Received: October 16, 2014

Accepted: October 26, 2014

Online Published: January 11, 2015

doi:10.5539/mas.v9n2p223

URL: <http://dx.doi.org/10.5539/mas.v9n2p223>

## Abstract

The work purpose - perfection of gasification technologies of processing low reactive high zole coals. For purpose achievement the method of an intensification of process of gasification of coal in an ascending stream of the oxidizer activated by nanocatalyst, and also a mathematical model of the specified process is offered.

A mathematical model of a process of coal gasification in a one-dimensional steady flow in the form of a system of ordinary differential equations of energy and changes in the concentrations of the reactants is represented in this paper. Model is based on the kinetics of chemical reactions that determine the process. The offered mathematical model will allow to make calculations of parameters of macrokinetics and heat exchange at coal gasification in an ascending stream.

**Keywords:** coal gasification, kinetics, mathematical model, steady-state flow

## 1. Introduction

Coal power industry in Russia is the largest consumer of low-quality Russian steam coal, which is about 90% of the total annual consumption of coal fuel at thermal power plants [1]. According to the Russia energy strategy within the period up to 2030 [1], it is planned to increase the share of coal usage in the energy sector. Thermal power plants are supplied with coal with an ash content of about 30% and low output of volatile materials. Within the flaring of the coal in the furnaces of power boilers, the lighting by gas or fuel oil is required and there appear problems with the ash disposal. The increase of burning low-grade solid fuels puts on the agenda issues of significant improvement in its use as by means of improvement of the traditional way of burning as through the development of new ones.

## 2. Methods

In this regard, the high-promising direction of the use of high-ash low-reactive coals is the use of the gasification technologies.

There are various types of coal gasification technologies [2, 3]: in a fixed bed; in a fluidized bed; in a stream; in melts and plasma gasification.

In this paper, we consider a method of a gasification of solid fuels in an upward jet-vortex flow by the oxidant, activated by nanocatalyst.

A characteristic feature of this method is the gasification of coal dust in a turbulized upstream. In a vertical coil chamber a reaction surface is increased owing to the high turbulence of flow and small particles as well as an intensity of the gasification process, which allows reducing the volume of the reaction chamber and improve a capacity of a gasifier. Coal-derived gas, produced in a gasifier can be further burned in a volume of a burning chamber within rated work or can be transferred to external consumers. This makes it possible, firstly, to conduct processes of gasification at stationary – nominal operating mode, and, secondly, with a decrease in consumption of the electric load to accumulate fuel energy (in this case in the form of coal-derived gas as salable products).

For further intensification of gasification process in the described method it is offered to use an oxidizing agent, activated by nanocatalyst. In this regard, a particular interest is carbon nanostructures of new homologous series – fullerenes and fulleroids [4]. According to experimental studies, such carbon nanomaterials as fullerenes,

astralenes, high-defective multilayered nanotubes, contribute to formation of photophysical reactions of singlet-excited state of contacted molecular air oxygen under electromagnetic radiation. Generated singlet oxygen reacts with the carbon of a fuel with considerably high kinetic efficiency, compared with known active forms of oxygen (atomic oxygen and ozone).

A schematic diagram of a gasifier, which realizes the offered method is shown in Figure 1. Preliminary prepared coal dust is fed into the bottom of the jet-vortex gasifier.

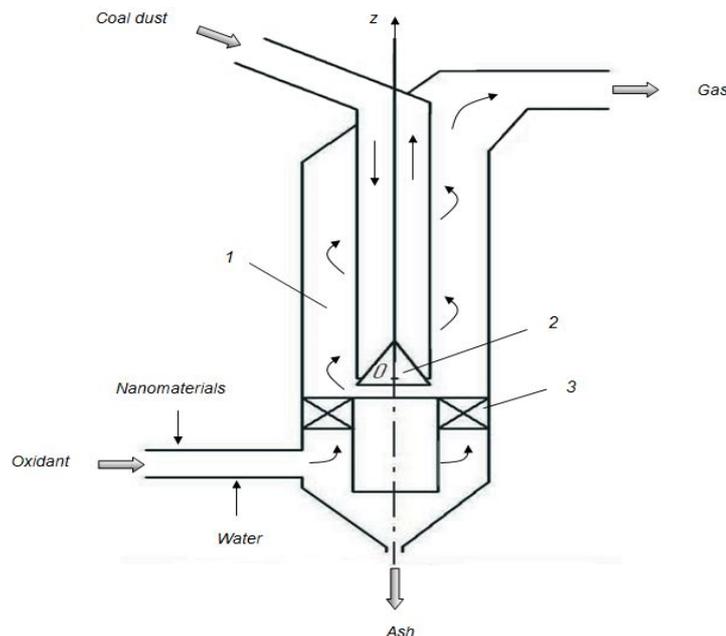


Figure 1. The schematic diagram of a jet-vortex gasification: 1 – gasification chamber; 2 – divider; 3 – swirler

Despite many years of study of burning processes and gasification of coals, in particular [5-20], currently, there are still many unexplored issues. Known models and methods do not allow us to calculate the parameters of macrokinetics and heat exchange in coal gasification in an upward jet-vortex flow. In this regard, it is relevant to develop mathematical models to fill this gap.

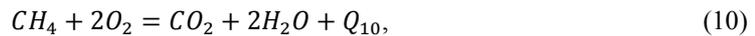
The area of the mathematical modeling is a gasification chamber 1, which is a coil channel with a constant cross-section for gases' pass. The model is one-dimensional with spatial coordinate  $z$ . Coordinate  $z$  axis coincides with the axis of the gasifier and its zero point is at the input section of the coil channel (Figure 1).

During the development of this mathematical model, the following assumptions are accepted:

- 1) The flow and the  $z$ -axis are directed vertically upwards.
- 2) The gasification processes occur in the one-dimensional steady flow.
- 3) Kinetic and potential energy of dispersed flow is small compared to its enthalpy.
- 4) Solid particles and gases have the same temperature.
- 5) To the entrance to the coil channel the particles of coal (coke) come, which passed the stage of drying and devolatilization.
- 6) The gasifier chamber pressure does not depend on  $z$  and is equal to atmospheric one.
- 7) The dispersed flow velocity is equal to the velocity of the gas.
- 8) The hovering velocity is determined for medium-sized solid particles.

During the gasification of low-reactive coal number of chemical reactions takes place, of which the most important are the following:





where  $Q_i$ ,  $i = 1 \dots 10$  – absolute value of heat effects of corresponding reactions kJ/kmole; For reactions (1)-(6) heat effect corresponds to the carbon kmole, for reactions (7)-(8) – to  $CO$  kmole, for (9) – to  $H_2$  kmole, for (10) – to  $CH_4$  kmole.

The developed model is open for other reactions that can make a significant contribution to the results of the gasification process.

The main correlations in the mathematical model are ordinary differential equations, reflecting the law of conservation of energy and mass conservation law for the seven components involved in the reactions (1)-(10). In its turn, the corresponding equations of conservation of mass are based on the kinetics of the processes (1)-(10). The equations of motion in this model are absent because of the small pressure changes by height of the gasification chamber. Aerodynamic resistance of the gasifier can be calculated separately and independently from the energy equation. The system of ordinary differential equations for one-dimensional steady-state flow is as follows:

$$(\rho w)_{mix} \frac{d(cT)}{dz} = f \mu_c \left[ \frac{\mu_{O_2}}{M_{O_2}} (k_1 Q_1 + 2k_2 Q_2) - \frac{\mu_{H_2O}}{M_{H_2O}} (k_3 Q_3 + 0.5k_4 Q_4) - \frac{k_5 \mu_{CO_2}}{M_{CO_2}} Q_5 + \frac{0.5k_6 \mu_{H_2}}{M_{H_2}} Q_6 \right] + \frac{\mu_{CO} \mu_{H_2O}^{0.5}}{M_{CO} M_{H_2O}^{0.5}} \left[ \frac{k_7 \mu_{H_2O}^{0.5}}{M_{H_2O}^{0.5}} Q_7 + \frac{k_8 \mu_{O_2}^{0.25}}{M_{O_2}^{0.25}} Q_8 \right] + \frac{\mu_{O_2}}{M_{O_2}} \left[ \frac{k_9 \mu_{H_2}^{1.5}}{M_{H_2}^{1.5}} Q_9 + \frac{k_{10} \mu_{CH_4}}{M_{CH_4}} Q_{10} \right] - q_0 \frac{P_0}{F} - q_i \frac{P_i}{F} - \frac{dq_r}{dz}, \quad (11)$$

$$\frac{d(w\mu_c^e)}{dz} = -A_c f \mu_c M_c \left[ \frac{\mu_{O_2}}{M_{O_2}} (k_1 + 2k_2) + \frac{\mu_{H_2O}}{M_{H_2O}} (k_3 + 0.5k_4) + \frac{k_5 \mu_{CO_2}}{M_{CO_2}} + \frac{0.5k_6 \mu_{H_2}}{M_{H_2}} \right], \quad (12)$$

$$\frac{d(w\mu_{O_2})}{dz} = -A_{O_2} \left[ f \mu_c \mu_{O_2} (k_1 + k_2) - \frac{0.5k_8 \mu_{CO} \mu_{O_2}^{0.25} \mu_{H_2O}^{0.5} M_{O_2}^{0.75}}{M_{CO} M_{H_2O}^{0.5}} - \frac{0.5k_9 \mu_{H_2}^{1.5} \mu_{O_2}}{M_{H_2}^{1.5}} \right], \quad (13)$$

where  $(\rho w)_{mix}$  – mixture mass rate, kg/(m<sup>2</sup>·s);  $w$  – the flow velocity, m/s;  $c$  – specific heat of gas and solid components' mixture, kJ/(kg·K);  $T$  – the flow temperature, K;  $f$  – specific surface of contact of cokes particles with gases m<sup>2</sup>/kg;  $\mu_c$ ,  $\mu_{O_2}$ ,  $\mu_{H_2O}$ ,  $\mu_{CO_2}$ ,  $\mu_{H_2}$ ,  $\mu_{CO}$ ,  $\mu_{CH_4}$  – correspondingly, carbon, oxygen, water steam, carbon dioxide, hydrogen, carbon and methane oxide, kg/m<sup>3</sup>;  $M_c$ ,  $M_{O_2}$ ,  $M_{H_2O}$ ,  $M_{CO_2}$ ,  $M_{H_2}$ ,  $M_{CO}$ ,  $M_{CH_4}$  – mole mass of the corresponding components, kg/kmole;  $k_1$ - $k_{10}$  – the constants of the velocity of the heterogeneous (1)-(6) and homogenous (7)-(10) chemical reactions;  $q_o$ ,  $q_i$  – the densities of the heat streams on the inner and the outer cylindrical surface of the gasification chamber kJ/(m<sup>2</sup>·s);  $P_o$ ,  $P_i$  – the outer and the inner perimeter of the gasification chamber coil channel, m;  $F$  – the channel cross section, m<sup>2</sup>;  $q_r$  – the density of the resulting radiant heat flux on the coil channel transversal cross section (directed along the  $z$  axis) kJ/(m<sup>2</sup>·s);  $w$  – the gas velocity by  $z$  axis, m/s;  $\mu_c^e$  – expendable carbon concentration, kg/m<sup>3</sup>;  $A_c$ ,  $A_{O_2}$  – empirical coefficients for the carbon and the oxygen concentration change.

For the other homogenous components ( $H_2O$ ,  $CO_2$ ,  $H_2$ ,  $CO$ ,  $CH_4$ ), participating in the reaction (1)-(10), the obtained relations are equal to the equation (13).

The mass velocity  $(\rho w)_{mix}$  in the equation (11) for the considered stationary one-dimension flow does not depend on the  $z$  coordinate:  $(\rho w)_{mix} = G_{mix}/F$ , where  $G_{mix}$  – mass mixture consumption, kg/s.

Let us emphasize that the left side of the equation (12) the expenditure is used, and on the right side the actual concentration of carbon is used. The connection between the expenditure and the true concentration of carbon is obtained in the form of the following equation:

$$\mu_c^e = \frac{\rho_c \mu_c v_c}{\rho_c + \mu(v_c - 1)}$$

where  $\mu_c^e$ ,  $\mu_c$  – expandable and true carbon concentration, kg/m<sup>3</sup>;  $\rho_c$  – the density of the coke particle, kg/m<sup>3</sup>;  $v_c = w_c/w$  – the sliding coefficient for solid particles;  $w_c$ ,  $w$  – the velocity of the solid and gaseous phases, m/s.

The sliding coefficient  $v_c$  is connected with the hovering velocity  $w_{hov}$  by the following way:

$$v_c = 1 - \frac{w_{hov}}{w}$$

Hovering velocity  $w_{hov} = w - w_c$  is calculated for the coke particles of average size.

To solve the system of ordinary differential equations (11)-(13) the following boundary conditions are given:

$$(\mu_c^e)_0 = \frac{C^r/100}{T_0 \alpha V^0 / 273 + d_n / \rho_{H_2O}^0};$$

$$(\mu_{O_2})_0 = \frac{(0.21 \alpha V^0 32 / 22.4 + O^r / 100)}{T_0 \alpha V^0 / 273 + d_n / \rho_{H_2O}^0},$$

$$(\mu_{H_2O})_0 = \frac{W^r / 100 + d_n}{T_0 \alpha V^0 / 273 + d_n / \rho_{H_2O}^0};$$

$$(\mu_{H_2})_0 = \frac{H^r / 100}{T_0 \alpha V^0 / 273 + d_n / \rho_{H_2O}^0};$$

$$(\mu_{CO})_0 = 0; (\mu_{CO_2})_0 = 0; (\mu_{CH_4})_0 = 0.$$

Here  $C^r$ ,  $O^r$ ,  $H^r$ ,  $W^r$  – the carbon, oxygen, hydrogen and moisture content in the work fuel mass %;  $\alpha$  – the air surplus coefficient;  $V^0$  – the air quantity, which is theoretically necessary for the complete burning of 1 kg of the work coil mass, m<sup>3</sup>/kg;  $d_n$  – the weight percent of steam, fed into the gasification chamber, kg/kg,  $T_0$  – the temperature at the gasification chamber outlet, K;  $\rho_{H_2O}^0$  – the density of the water steam at the temperature  $T_0$  and the atmospheric pressure, kg/m<sup>3</sup>.

### 3. Conclusion

Gasification in a stream is perspective way of processing firm petroleum as allows to use coals of any quality and to lower emissions of harmful substances in atmosphere.

Gasification of solid fuel in the upward jet vortex takes place at high turbulence of the medium and small sizes of particles, which increases a reaction surface and the intensity of the gasification process, thus reducing the volume of the reaction chamber at a predetermined capacity of the gasifier.

The offered mathematical model considers the basic features of process of gasification of coal in a stream and represents system of the ordinary differential equations describing cinetic of chemical reactions, proceeding in the gasification chamber.

For further intensification of the gasification process in the described method it is offered to use an oxidizing agent, activated by carbon nanocatalysts of new homologous series – fullerenes and fulleroids. This leads to formation of singlet oxygen which reacts with fuel carbon with considerably high kinetic efficiency.

In model the factors are put, allowing to consider influence of nanoadditives for the speed and depth of course of reactions of gasification of coal.

For mathematical model the assumptions are presented which are not contradicting real features of course of process.

Distribution of the process along the length of the vertical channel provides ample opportunities for control, optimization, and control of gasification parameters.

Mathematical model with distributed parameters will more adequately reflect the low-reactive coal gasification processes than models with lumped parameters. There is the possibility of adapting the model by changing the values of parameters, obtained experimentally.

This work was financially supported by the Ministry of Education and Science of the Russian Federation in the frame of the Federal Target Program "Research and development on priority directions of scientific-technological complex of Russia for 2014-2020" (the agreement #14.574.21.0018 on "Development of a method of intensifying of the low-reactive coal gasification process in an oxidizer upstream jet vortex". Unique identifier of Applied Scientific Research (project) RFMEFI57414X0018).

## References

- Andrew, J. M. (2005). Coal gasification for advanced power generation. *Fuel*, 84, 2222–2235. <http://dx.doi.org/10.1016/j.fuel.2005.08.035>
- Anshakov, A. C. (2013). The generator of plasma of water steam for gasification of firm petroleum. *Thermoenergy*, 12, P.29–32. <http://dx.doi.org/10.1134/S0040363613120023>
- Bautin, S. P., & Obukhov, A. G. (2013). Mathematical modelling of a benthonic part of the ascending twirled stream. *Thermophysics of high temperatures*, 52(2), 567-570. <http://dx.doi.org/10.7868/S0040364413020038>
- Bautin, C. P. (2014) Mathematical modelling of a current in a vertical part of the ascending twirled stream. *Thermophysics of high temperatures*, 52(2), 271-275. <http://dx.doi.org/10.7868/S0040364414020033>
- Bogomolov, A. R. (2013) Modelling of two-phasic gasificator for conversion of coal and шлама in a stream of overwarmed steam. Modern Science Researches, Ideas, Results. *Technologies*, 1(12), 316-321.
- Chang, H., Xiao, F., & Khim, H. C. (2013). Process modeling and thermodynamic analysis of Lurgi fixed-bed coal gasifier in an SNG plant. *Applied Energy*, 111, 742–757.
- Donskiy, I. G. (2013). Calculation of modes of layer gasifications of coal by means of thermodynamic model with macrokinetic restrictions. *Thermoenergy*, 12, 56–61. <http://dx.doi.org/10.1134/S0040363613120060>
- Efimov, N., Oshepkov, A., Rigkov, A., & Shaforost, D. (2011). The method of the oxidizer activity increasing in the processes of the solid fuels combustion and burning. *The news of the high education institutes. North Caucasian region. Technical sciences*, 6, 53-55.
- He, C., Feng, X., Khim, H. C., Li, A. X., & Liu, Y. J. (2014). Industrial-scale Fixed-bed Coal Gasification: Modeling, Simulation and Thermodynamic Analysis. *Chinese Journal of Chemical Engineering*, 22(5) 522–530. [http://dx.doi.org/10.1016/S1004-9541\(14\)60066-5](http://dx.doi.org/10.1016/S1004-9541(14)60066-5)
- Ivanov, P. P. (2013). The thermochemical analysis of efficiency of various technologies of gasification. *Thermoenergy*, 5, 64–70. <http://dx.doi.org/10.1134/S0040363613050056>
- Kalechitsya, I. (1980). *Chemical materials from coal*. Moscow: Chemistry.
- Kantorovich, B. (1958). *The basics of burning and gasification of the solid fuel*. Moscow: Publishing house of USSR Academy of Sciences.
- Koguhovsky, I. (2013). The perspectives of the coal energetics development of Russia. *Power engineer*, 1, 2-8.
- Manenti F., Cieri, S., Restelli, M., Nascimento, L. N. M., & Zuniga, L. L. (2011). Dynamic simulation of lurgi-type reactor for methanol synthesis. *Chemical Engineering Transactions*, 24, 379-384.
- Martin, G., & Bernd, M. (2014). Performance and exergy analysis of the current developments in coal gasification technology. *Fuel*, 116, 910–920.
- Messerle, V. E. (2013). Plasma processing of coals. Ustimenko A.B. *Thermoenergy*, 12, 23–28. <http://dx.doi.org/10.1134/S0040363613120096>
- Predvoditelev, A., Khitrin, L., Tsukhanova, O., Kolodtsev, K. H., & Uhjlzovsky, M. (1949). *The carbon burning*. Moscow-Leningrad.
- Rijkov, A. F. (2013). Working out of low temperature reactors of thermochemical conversion for coal power. *Thermoenergy*, 12, 47–55. <http://dx.doi.org/10.1134/S0040363613120114>
- Ronald, W. B. (2010). Gasification Processes Old and New: A Basic Review of the Major Technologies. *Energies*, 3, 216-240. <http://dx.doi.org/10.3390/en3020216>
- Vilensky, T., & Khzamalyan, D. (1978). *The dynamics of the dust-type fuel burning*. Moscow: Energy.

## Copyrights

Copyright for this article is retained by the author(s), with first publication rights granted to the journal

This is an open-access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/3.0/>).