CONTRIBUTION TO CREATING A MATHEMATICAL MODEL OF UNDERGROUND COAL GASIFICATION PROCESS

by

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Original scientific paper
https://doi.org/10.2298/TSCI180316155P

Underground coal gasification, as an auto thermal process, includes processes of degasification, pyrolysis, and the gasification itself. These processes occur as a result of a high temperature and the management of coal combustion during addition of gasification agent. Air, water vapor mixed with air, air or water vapor enriched with oxygen, or pure oxygen, may be used as gasification agents. Resulting gas that is extracted in this process may vary in chemical composition, so it is necessary to adjust it. That is the reason why it is necessary to develop a mathematical model of the underground gasification process prior to any operations in coal deposit, in order to obtain as much accurate prediction of the process as possible. Numerical calculation provides prediction of gas mixture's chemical composition, which enables calculation of gas components' energy contents and total energy content of the gas in predicted underground coal gasification process. It is one of the main criteria in the economic assessment of underground coal gasification process. This paper, based on available data on researches in this area, provides a contribution to creation of mathematical model of underground coal gasification.

Key words: *coal, underground coal gasification, model*

Introduction

In pursuit of alternative energy sources in upcoming years, a gas as an energy source may have a significant role. Deposits of natural gas in Serbia are insignificant, but there are significant possibilities for extraction of a coal gas, as a product of underground coal gasification (UCG), which is the most direct way of in situ conversion of coal seams into gas mixture (synthesis gas). This is especially interesting due to a fact that underground coal mining in Serbia leaves up to 65%, or even 70% of total coal reserves unrecovered [1].

Similar situation is in worldwide coal deposits, too. Considering the presence of massive underground coal deposits, and presence of these deposits in many parts of the world, UCG is defined as one of the main sources for mankind to maintain technological development and keep balance between present and future of the energy [2].

This transition period between present and future, with a constant trend of increase of RES, and decrease of conventional ones, is actually a chance for UCG to step up as the energy

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choice which provides better recovery of remaining coal reserves and improved energetic, economic and environmental parameters.

Gas extracted by UCG (syngas) may be used in thermal power plants, or in gas engines, or as industrial gas in chemical industry. That is why it is very important to adjust its chemical composition depending on its use.

Knowing that, it is very important to create a mathematical model of UCG process prior to in situ operations, in order to define the composition of certain substances and a total energy content of the gas extracted by UCG.

This paper is a contribution to creation of mathematical model of UCG process.

Extraction challenges and technological basis for application of UCG

Mass of combustible coal and moisture in the coal are important influential parameters of UCG process, because they affect the thermal power of coal gas extracted by UCG. Partial or insufficient gasification is mainly performed at the surface facilities, while complete gasification may be applied both on the surface and in underground operations [3] and the latter will be considered in this paper.

Reaction of carbon with oxygen releases the heat (exothermic reaction) by a following process:

$$C + O_2 \rightarrow CO_2 + 4.09 \cdot 104 \text{ [kJkmol}^{-1}\text{]} \tag{1}$$

$$2C + O_2 \rightarrow 2CO + 24.6 \cdot 104 \text{ [kJkmol}^{-1}\text{]} \tag{2}$$

In a presence of extra oxygen, CO can, during combustion, turn into CO_2:

$$2CO + O_2 \rightarrow 2CO_2 + 57.2 \cdot 104 \text{ [kJkmol}^{-1}\text{]} \tag{3}$$

At the same time, in case of high temperature and contact of CO_2 with coal, it will turn into CO:

$$CO_2 + C \rightarrow 2CO - 16.25 \cdot 104 \text{ [kJkmol}^{-1}\text{]} \tag{4}$$

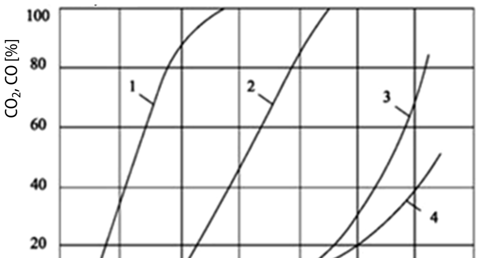

Figure 1. Relation between intensity of turning into CO or CO_2 and temperature [4]; *1 – peat coke, 2 – lignite, 3 – coke, 4 – antracite*

This reaction is evidently endothermic.

Rate of the reaction depends on temperature, as shown on diagram in fig. 1. In the processes of underground coal gasification, the heat, released by reactions shown in eqs. (1)-(3), complies with increase of coal seam temperature and, by that, the endothermic reaction shown in eq. (4).

When water vapor from the overlaying seams comes in contact with carbon from the coal seam, exothermic reaction occurs and combustible gas components are released (CO and CO_2), according to following formulas:

$$C + 2H_2O \rightarrow CO_2 + 2H_2 + 7.54 \cdot 104, \text{ kJ/kmol} \tag{5}$$

$$C + H_2O \rightarrow CO + H_2 + 11.9 \cdot 104, \text{ kJ/kmol} \tag{6}$$

Reactions presented in eqs. (5) and (6) are going on in temperatures above 900 to 1000 °C and rate of the reaction heavily depends on temperature. That way, heat of reaction, presented in eqs. (1)-(3), causes increase of coal temperature, drying of coal, releasing of flying particles which can serve as combustible components (CO, H_2, CH_4, H_2S), and also helps development of reactions (5) and (6).

Rate of chemical reaction between oxygen and carbon on a firm section of a coal seam, basically depends on temperature and specific reaction area. Specific reaction area is defined as area of coal by a unit of its volume where heterogeneous process of chemical reaction between oxygen and carbon are going on [5].

With increase of temperature, rate of reaction increases much faster than the rate of oxygen diffusion in the coal. For instance, if coal temperature rises by 10 °C, rate of heterogeneous reaction of oxygen with coal increases two to three times, while diffusion of air into coal ratio increases only by 20% to 30%. That way, rate of UCG process depends on rate of carbon combustion and rate of diffusion of oxidant into coal. Related to that, we can divide the process of coal combustion in UCG into three phases, or three regimes: diffusion, kinetic, and transition regime [6, 7].

There are four UCG methods: direct heading method, circulation method, frontal method, and flow method. Each UCG method is related to creation of typical zones, each zone is defined by one process, fig. 2: oxidation zone or oxygen zone (OZ), zone of constitution (ZC), zone of thermic decomposition (ZTD), zone of compression (ZCP), zone of drying (ZD) and zone of slag (ZS).

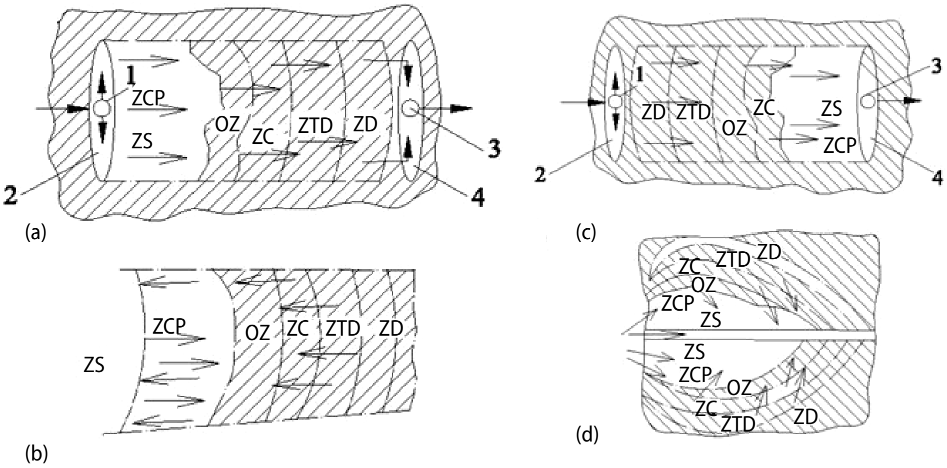

Figure 2. Layout of chemical-technological zones and gasses directions in creation of resulting gas for different UCG methods [3]; (a) direct heating method, (b) circulation method, (c) front method, and (d) flow method ; *1 – injection well, 2 – frontal fire face of gasification, 3 – production well, 4 – rear fire face of gasification*

In direct heading method of UCG, oxygen from the air-flow reacts with coke remnants. Heating of gassy products of gasification creates parts of the seam, or zones, located between combustion and extraction wells. Oxygen from the air-flow is used only for gasification of coke remnants, which could not be gasified in any other way. Also, the heat of the slag is used for heating of air-flow, while the heat of gassy products from the previous zones is used for completion of the process in the end zones. This is possible because, along air-flow direction, zone of thermic decomposition precedes the zone of drying, while zone of stabilization, *i. e.* zone of constitution, precedes the zone of decomposition [8, 9].

Direct heading method of UCG enables highest recovery and it is applicable for coal seams with high initial permeability.

In circulation method of UCG, the oxygen from the air-flow is used not only for coke remnants, but also for gassy combustible components. In comparison of this method with direct heading method, we can see a few disadvantages. For instance, volume of air-flow needed for a unit of heat in created gas is higher, while the heat of combustion is lower. It means that the heat created in the process is not used efficiently. In this method, seam permeability during heating and gasification is constant, while in direct heading method it increases gradually.

In flow method, the oxygen from the air-flow is, similarly to circulation method, distributed both to reaction with coke remnants and combustible gaseous products. However, higher share of oxygen is used for complete reaction with coke remnants. By parameters of heat and chemical-technological parameters, this method provides significant advantages in comparison with direct heading method and circulation method. Gained gas in direct heading method includes levitating combustible components, created in stadium of coal coking without presence of air in final stages of gasification. In circulation method, these levitating components mostly react with oxygen. In flow method, gained gas includes levitating coke gas and gassy products of reaction between oxygen and coke.

Yet another advantage of flow method is possibility of turning of air-flow without changes in technology of gasification process.

Distribution of temperature along the channel of gasification

Temperature regime of the seam along the gasification channel defines the type of gasification. Variation of temperature along the channel is shown in fig. 3. There are eight specific zones [6].

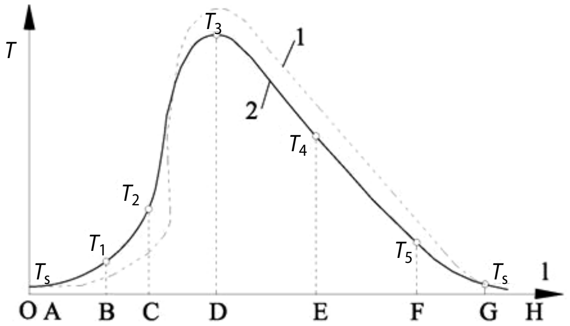

Figure 3. Variation of temperature along gasification channel: *1 – curve for gassy phase, 2 – curve for solid phase (coal surface), OA – air-flow section, AB – part of drying air-flow, BC – part of ignition preparation, CD – exothermic reactions, DE – endothermic reactions, EF – thermal decomposition, FG –drying, GH – gaseous phase*

The O-A is the section where temperature of coal seam and air-flow is almost constant, since at low temperatures the thermal decomposition of coal and its reaction with oxygen is very slow.

Section A-B represents the increase of seam temperature, up to T_1, which is an approximate value of evaporation of moisture from the coal ($T_1 \approx \approx 110$ °C).

Section B-C represents heating of coal from drying temperature (T_1) to ignition temperature ($T_2 \approx 200$ °C for sub-bituminous coal and $T_2 = 300$-350 °C for bituminous coal).

Increase of temperature of coal and air-flow in section O-C actually represents the transfer of heat from areas with higher temperature, located on the right side of the curve from section O-C. Thermal conductivity of the ambience enables this process.

The C-D represents the section with rapid increase of the temperature. This is a section with exothermic reactions, where basic processes are running. Significant amount of heat are lost in surroundings and endothermic reactions. Temperature T_3 is approximately 900-1000 °C.

After this section, the temperature of solid and gaseous phase starts to decrease. Section D-E represents endothermic reactions. In this section, previously emitted heat that was absorbed in the surroundings is now used for endothermic reactions.

Further decrease of temperature from T_4 (580-630 °C) to T_5 in section E-F is the result of heat losses in the surroundings and a process of thermal decomposition of coal.

The F-G represents the section of drying, with decrease of temperature from T_5 (110-130 °C) to seam temperature, T_s. The temperature decreases due to consumption of heat on drying of coal.

Part of the curve to the right of point G is the section with practically constant temperature of both gaseous and solid phase. This temperature is equal to the temperature of the coal seam and this section is called gaseous.

Defining of typical temperatures of specific segments of gasification channel is added up to solving a differential equation of heat conductivity:

$$\frac{\partial T}{\partial \tau} = a\nabla^2 T \tag{7}$$

where a [m^{2}s^{-1}] – is conductivity of temperature, ∇^2 – Laplace's operator, calculated as:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{8}$$

Further elaboration is performed depending on parameters of the coal seam and this could be an interesting topic for further researches.

Numerical calculation of concentration of components during UCG

After the ignition of the coal seam, it turns into a kind of gas generator. Certain amount of created gas starts to flow through pores in a non-stationary manner. When the process of combustion is fully developed, created amount of heat is sufficient to enable more *independent* process of gasification. Zone of gasification is moving and spreading to the depth of the seam, while gasses like CO, CO_2, H_2 and CH_4 are created in the zone of combustion, or the zone of reaction [2, 10-13].

Significant amount of nitrogen can also be found in this gas mixture. Nitrogen originates from the air-flow, but, as an inert gas, it is not interesting for energetic treatment through the final product of gasification [4].

Oxygen, as one of the means of gasification, occurs in final product of gasification bonded usually in CO, or less often in CO_2, but that is not all. It is also possible that small amounts of free O_2 occur as the product of gasification. The amount of O_2 depends on intensity of contact with coal and it should also be included in mathematical model [4].

Considering the water vapor, it could be found in the entry balance, but it diminishes in coal drying process, which is the starting phase of UCG [4].

Carbon from the coal seam is also excluded from the final component balance, because during the process it reacts and turns into slag.

High temperature in gasification zone causes heating, and consequently drying of coal seam, which leads to creation of cracks in the seam. Some of the chemical reactions are exothermic and some of them are endothermic, causing that share of heat is transferred to surrounding rock. Having that in mind, along with a fact that high temperature in reaction zone affects not only porosity and filtration of the seam, but also properties of the seam related to conductivity of mass and heat, it is clear that equations used for defining these processes have to be complex [14-16].

Darcy's equation of continuity, in different forms, is most commonly used for calculations. In this case, it is applied on diffusion of oxygen form the air-flow as agent of gasification.

The equation of oxygen diffusion to coal surface of cylindrical channel can be given in the following form:

$$\frac{\partial C}{\partial \tau}+\left(\vec{\mathrm{v}}\nabla C\right)=D\left[\frac{\partial^2 C}{\partial z^2}+\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial C}{\partial r}\right]+q' \tag{9}$$

where $\vec{\mathrm{v}}$ is the flow velocity ($\vec{\mathrm{v}}=\vec{\mathrm{u}}+\vec{\mathrm{v}}'$), $\vec{\mathrm{u}}$ – the mean air-flow velocity in the channel, $\vec{\mathrm{v}}'$ – the pulsating flow velocity, D – the molar diffusion ratio, z and r – are cylindrical co-ordinates, and q' – the velocity of oxygen diminishing as a result of reactions.

Since the rate of combustion at the wall of cylindrical coal channel is high enough for temperatures above 1000 °C, and main role in the process is oxygen diffusion, its content on the wall is nearing zero:

$$C_{r=R}\approx 0 \tag{10}$$

When the content of the coal is nearing zero, there is no further combustion.

In that case, for stationary turbulent flux, with disregarding of longitudinal diffusion along the channel, the equation transforms into following form:

$$\vec{\mathrm{u}}\frac{\partial C}{\partial z}=\frac{1}{r}\frac{\partial}{\partial r}D_T r\frac{\partial C}{\partial r} \tag{11}$$

where D_T is the ratio of turbulent diffusion.

Differential eq. (11) with Dirichlet's homogenous boundary conditions (10) can be solved using finite difference method. The principle of this method is approximation of all derivatives by finite differences. Prior to that, calculation area is divided into the network in a manner that it enables most accurate approximation of area boundaries and minimal error in area configuration. Rectangular network is most commonly used, or in specific cases square network or polar network.

Substitution of derivatives by corresponding finite differences is performed as follows:

$$\left(\frac{\partial C}{\partial x}\right)_0\approx\frac{C_1-C_2}{2h},\quad\left(\frac{\partial C}{\partial y}\right)_0\approx\frac{C_3-C_4}{2h} \tag{12}$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_0\approx\frac{C_1+C_2-2C_0}{h^2},\quad\left(\frac{\partial^2 C}{\partial y^2}\right)_0\approx\frac{C_3+C_4-2C_0}{h^2} \tag{13}$$

where "0" is a midpoint, where approximation of the operator is performed. The midpoint is surrounded by "1" and "2" on the x-axis, and also "3" and "4" on y-axis, while h is the network pace.

Further procedure is to apply the equations given for point "0" to each point of the entire network. By application of described finite difference method, solution of differential equation (11) is down to solution of a system of algebraic equations.

Numerical solution of that system of equations (by Newton – Raphson method) provides the values of contents in the nodes of the network, *i. e.* variation of oxygen content along the channel, $C = C(z)$, in a form of discrete values. In this case, the discretization is performed using square shaped network, with a pace of h.

Similar differential equations may be formed for other gas components too, such as H_2, CO, CO_2, and CH_4, with their specific parameters and the equations may be solved by the same algorithm applied for O_2.

As a result of calculations, fig. 4 shows the curves of variation of gas components along the channel for an average bituminous coal. The C_0 is the initial concentration of gas components, while $\overline{C}_z$ is the mean concentration of gas components along the channel, on the distance z from the begining of the channel.

The values of concentrations of components gained by numerical calculation are very significant. Based on these values, it is possible to define their energetic values and consequently, total energetic value of the gas produced by UCG. This is very important, because energetic value is one of the main criteria in the economic assessment of UCG processes.

Resulting curves of gas components' concentrations, shown in fig. 4, have a good match with the results gained by experimental tests in actual underground gas generators.

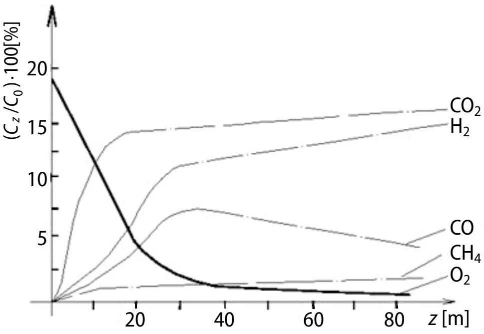

Figure 4. Curves of variation of concentrations of syngas components [3]

Conclusion

Numerical calculations of UCG process parameters provide the possibility to evaluate the eventual application of UCG prior to major investments needed for facilities and field tests of the process. Values of concentrations of gas components and their energetic values can help in economic assessment and so to provide the answer whether it is feasible to extract the coal gas from the deposit after traditional coal mining is ended.

In case of running a case study, it would include actual values of coal seam parameters, as well as parameters of air (p, T). Based on this input parameters, using the numerical approach, it would be possible to gain UCG values for specific coal seam.

Also, this numerical calculation approach can be helpful in adjusting of coal gas component concentration. Depending on gas usage, *i. e.* whether it is going to be used as the energy gas in thermal plants, or as technology gas in chemical industry, it depends on its composition and this is where numerical calculation can provide easier and more accurate setting of UCG process parameters.

Methodology and approach presented in this paper enable more accurate analysis and application of UCG process for any specific case.

References

[1] Petrović, D. *et. al.*, Possibilities of Coal Conversion into Gas Fuel from the Aspect of Greater Valorization of Available Energy Resources in Serbia by Implementing UCG, *RMZ – Materials and Geoenvironment*, *57* (2010), 1, pp. 113-125

[2] Janoszek, T., *et al.,* Modelling Test of Autothermal Gasification Process Using CFD, *Archives of Mining Sciences, 62* (2017), 2, pp. 253-268

[3] Petrović, D., Izučavanje Podzemne Gasifikacije Uglja, Kroz Mogućnosti Primjene Kod Vanbilansnih Rezervi Mrkih Ugljeva (Study of UCG Through Possibility of Application in Out of Balance Coal Reserves – in Serbian), Ph. D thesis, RGF, Tuzla, Yugoslavia, 1988

[4] Krejnin, E. V. *et. al.*, *Podzemnaя gazifikacisя ugolъnыh plastov* (Underground Coal Gasification – in Russian), NEDRA, Moscow, 1982

[5] Andrianopoulos, E. *et. al.*, Chemical Process Modeling of Underground Coal Gasification and Evaluation of Produced Gas Quality for End Use, *Energi Procedia, 76* (2015), Aug., pp. 444-453

[6] Yang, L. H., *et. al.*, Temperature and Gas Pressure Features in the Temperature-control Blasting Underground Coal Gasification, *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*, *32* (2010), 18, pp. 1737-1746

[7] Venugopal, D., *et al.*, Air and Oxygen Gasification Simulation Analysis of Sawdust, *Thermal Science*, *23* (2019), 2B, pp. 1043-1053

[8] Rauk, J., *Wibór Optymalnych Metod Podziemnego Zgazowania Wegla*, (Choice of Optymal Method for Underground Coal Ignition), GIG Katowice, Poland, 1978

[9] Self, S., *et. al.*, Review of Underground Coal Gasification Technologies and Carbon Capture, *Int. J. Energy Environ. Eng.*, *3* (2012), Dec., 16

[10] Sharaf, A., *et. al.*, Modeling Cavity Growth during Underground Coal Gasification, *Proceedings,* Comsol Conference, Boston, Mass., USA, 2011

[11] Perkins, G., Sahajwalla V., A Mathematical Model for the Chemical Reaction of a Semi-infinite Block of Coal in Underground Coal Gasification, *Energy & Fuels*, *19* (2005), 4, pp. 1679-1692

[12] Hatzilyberis, K. S., Androutspoulos, G. P., Lignite Chemical Conversion in an Indirect Heat Rotary Kiln Gasifier, *Thermal Sscience, 10* (2006), 3, pp 181-197

[13] Palarski, J., Gas and Heat transport in the Underground Coal Gasification, *Proceedings,* Symposium Saarbricken, Saarbricken, Germany, 1986

[14] Blinderman, M. S., Friedman, S.J., Underground Coal Gasification with Carbon Capture and Storage: A Pathway to a Low-Cost, Low-Carbon Gas for Power Generation and Chemical Synthesess, NENTL, *Proceedings*, 5th Annual Conference on Carbon Sequestration, Axchange Monitor Publications, Alexandria, Va., USA, 2006

[15] Jovanović, R. D., *et al.*, Novel Fragmentation Model for Pulverized Coal Particles Gasification in Low Temperature Air Thermal Plasma, *Thermal Science, 20* (2016), Suppl. 1, pp. S207-S221

[16] Petrović, D., *et. al.*, Introduction of UCG in Some Parts of Aleksinac Coal Basin (in Serbian), *Proceedings*, Energy 2008, Energy Union Belgrade, Zlatibor, Serbia, 2008

Paper submitted: March 16, 2018
Paper revised: May 8, 2018
Paper accepted: May 10, 2018