

Żogała, A. (2014). Critical analysis of underground coal gasification models. Part I: equilibrium models – literary studies. *Journal of Sustainable Mining*, 13(1), 22–28. doi: 10.7424/jsm140105

## REVIEW PAPER

Received: 10 December 2013 | Revised: 22 May 2014 | Published online: 6 June 2014

# CRITICAL ANALYSIS OF UNDERGROUND COAL GASIFICATION MODELS. PART I: EQUILIBRIUM MODELS – LITERARY STUDIES

Alina Żogała

*Interdisciplinary PhD Studies in Field of Clean Coal Technologies, Central Mining Institute (Katowice, Poland)*  
Corresponding author: e-mail: azogala@autograf.pl, tel.: +48 503 161 360

## ABSTRACT

<b>Purpose</b>	Underground coal gasification is a very difficult process due to changes in the parameters over time and within the space of the reactor and a variety of phenomena that occurs there. Consequently, it is necessary to create appropriate mathematical models, which simplify the optimization and forecast of future results (especially final gas properties). The purpose of this work was the detailed critical analysis of the simplest coal gasification simulations methods, based on thermodynamic calculations of the process. These models, called equilibrium models, can be divided into two groups: stoichiometric and non-stoichiometric. The other aim of this paper was to characterize various engineering methods used in the calculation of equilibrium gasification processes.
<b>Methods</b>	Literary studies, concerned with general aspects of underground coal gasification modeling and the modeling of coal gasification in the manner of equilibrium calculations, were used as a research method applied in presented work.
<b>Results</b>	The critical analysis of equilibrium models of coal gasification and the characterization (including mathematical formulation of process, range of required parameters, rate of convergence of calculations and methodology of searching solutions) of stoichiometric and non-stoichiometric methods were results of numerous considerations presented in this article.
<b>Practical implications</b>	The work presented describes practical issues connected with equilibrium models – their advantages, limitations and possible problems (for example with the determination of required constants) and potential applications (preliminary analysis, point of reference to more complex simulations etc.).
<b>Originality/value</b>	This paper presents state of the art in field of equilibrium coal gasification modeling. This article is also attempt to elaborate on the most important problems connected with thermodynamic models of coal gasification.

## Keywords

*coal gasification, equilibrium, stoichiometric model, non-stoichiometric model*

## 1. INTRODUCTION

Underground coal gasification (UCG), defined as production of gaseous fuels carried directly in coal seam, may be an attractive alternative to surface processes. Firstly, UCG can be used to utilize coal seams which could not be exploit by conventional technologies (too deep or steeply dipping, low rank coals). In comparison to surface gasification, UCG offers lower capital and operating costs, a reduction in underground human labour and environmental benefits (Bhutto, Bazmi, & Zahedi, 2013).

On the other hand underground coal gasification is a complex and technically challenging process. Most of its parameters are changing both during the time of gasification and within the space of the reactor (Kapusta & Stańczyk, 2009). Moreover UCG is determined not only by a complex set of

chemical reactions but also by lots of physicochemical processes, like heat and mass transfer, turbulent mixing, cavity growth and flow through the porous medium. What is more, the same coal is raw material whose properties cannot be strictly characterized, because of their dependence on rank and place of exploitation of the analyzed fuel (Golec & Ilmurzyńska, 2008; Nitao et al., 2011).

The management and running of UCG process will be possible provided that physical and chemical phenomena occurring in gasification and factors effecting them are recognized. Unfortunately, experiments carried out directly in underground reactors are expensive and in some cases impossible to perform. Therefore computer simulations of gasification processes become increasingly significant in science and the industry in general. An appropriate mathematical model will enable not only the theoretical characterization of pro-

cess and its results (which will provide a better understanding of the mechanisms of the process) but also a choice of optimal gasification parameters in order to obtain syngas with suitable properties – chemical composition and heat value (Bialecka, 2008; Wachowicz, Janoszek, & Iwaszenko, 2010).

## 2. MODELING OF UNDERGROUND COAL GASIFICATION – BASIC REMARKS

Underground coal gasification is a process which requires taking many essential decisions, such as: site selection, the geometry of the reactor, the composition and injection rate of the gasifying agent and environmental monitoring. An ideal UCG model should predict each important aspects of the process, e.g.:

- syngas composition and heat value,
- cavity growth,
- water influx to reactor,
- roof collapse and subsidence,
- transport of contaminants out of the reactor (Nitao et al., 2011).

However, due to the complexity of the phenomena occurring during gasification, every model is only an approximation of reality, describing chosen elements of the process. This article presents analysis of UCG models which concentrate on predicting syngas composition.

It is widely known that processes of underground coal gasification should be proceed in a way which provides to obtain syngas with the highest amount of combustible compounds – CO, H<sub>2</sub>, CH<sub>4</sub> and the lowest amount of non-combustible components. It is a very complicated issue, because the final composition of the produced gas depends on many factors, like the properties of the gasifying agent and the analyzed fuel, features of the coal seam and the parameters of the same process (temperature and pressure). Unfortunately, determining their level of importance is extremely difficult. What is more, the aforementioned mentioned factors may positively affect one fraction of the process parameters and negatively on the other part (Żogała, Kabiesz, & Iwaszenko, 2013).

There are a lot of UCG models which vary in level of detail of included phenomena, rate of convergence, mathematical procedures and the required input parameters. These models can be divided into equilibrium models, kinetic models and CFD (*Computational Fluid Dynamics*) models (Golec & Ilmurzyńska, 2008).

This paper presents only the equilibrium approach used in simulations of gasification processes. Kinetic and computational fluid dynamics models were analyzed in a separate part of the article.

## 3. EQUILIBRIUM MODEL

Equilibrium models are based on the thermodynamic analysis of gasification processes. This kind of model assumes that the system reaches a state of equilibrium, which means that the rate of chemical reaction is infinitely fast or the time of reaction is appropriately long (Golec & Ilmurzyńska, 2008).

Equilibrium models of gasification use two general approaches, which vary in the method of formulation of set of equations (describing the state of equilibrium) and scope of input data. The first of them, the stoichiometric model, is based on mass-action law and the equilibrium constants of

chemical reactions. The second model, non-stoichiometric, minimizes the Gibbs free energy of the analyzed system.

The non-stoichiometric method is more general – information about the number and kind of independent reactions and values of equilibrium constants is not necessary. Therefore this model can be used for every case. However it is computationally more complicated because the determination of the minimum of Gibbs free energy is not easy, it requires a long time to calculate, and consequently simulation converges with a lower rate.

The stoichiometric method is computationally simpler and a faster convergent than the non-stoichiometric method. On the other hand it is less general – limited to one set of reactions. Therefore when additional species is included in the process, the whole procedure must be modified (Kozaczka, 1994).

### 3.1. Stoichiometric model

The stoichiometric model of gasification involves defining the following inputs:

- parameters of process (pressure and temperature),
- initial composition of reacting mixture,
- number and kind of independent reactions.

Providing that seven components: C, CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, CH<sub>4</sub>, O<sub>2</sub> take part in gasification, the system is described by chemical matrix **A**:

element \ compound	C	O	H
C	1	0	0
CO	1	1	0
CO <sub>2</sub>	1	2	0
H <sub>2</sub>	0	0	2
H <sub>2</sub> O	0	1	2
CH <sub>4</sub>	1	0	4
O <sub>2</sub>	0	2	0

**A** = (1)

The rank of this matrix is equal to  $R(\mathbf{A}) = 3$ . For the reason that the number of independent chemical reactions is difference between the amount of mixture components and rank of the chemical matrix, the system is determined by four reactions (Tabiś, 2002).

Common calculating methods are generally bases on the following reactions:



The selected chemical model requires the determination of the values of equilibrium constants of the chosen reactions for the defined temperature ( $T$ ) of the process. It may be done by calculating the Gibbs free energy for the analyzed reaction ( $\Delta_R g^\circ$ ). In this way the procedure of computing the equilibrium constant is described by the following algorithm:

1. Collection of thermodynamic data for a particular reactant **i**: specific heat ( $c_{p,i}$ )<sup>1</sup>, enthalpy ( $\Delta_R H_{i,298}^\circ$ ) and entropy ( $\Delta_R S_{i,298}^\circ$ ) in standard temperature ( $T = 298$  K).

<sup>1</sup> Specific heat of reactant **i** is determined in thermodynamic tables by coefficients of polynomial  $c_{p,i} = A_i + B_i T + C_i T^{-2} + D_i T^2$ .

Download English Version:

<https://daneshyari.com/en/article/1758438>

Download Persian Version:

<https://daneshyari.com/article/1758438>

[Daneshyari.com](https://daneshyari.com)