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Mathematical modeling of alternating injection of oxygen and steam in underground coal gasification

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ABSTRACT

Recent successful low-pressure underground coal gasification pilot experiments that use alternating injection of air (oxygen) and steam have shown potential in large scale hydrogen production. This paper extends an existing steady state model to a transient model that can describe an alternating injection of air and steam for deep thin coal layers. The model includes transient heat conduction, where the produced heat during the air injection stage is stored in the coal and surrounding strata. The stored heat is used in the endothermic gasification reactions during the steam injection.

The results show that product composition and temperature oscillation can be predicted with a reasonable accuracy. The stored heat can deliver additional energy that can maintain the gasification during the steam injection period for a limited time. During the steam injection cycle, at low pressure the volumetric flow and the hydrogen content of the product gas are both high, but at higher pressures while the hydrogen composition is still high the coal conversion decreases considerably. The results confirm that the alternating injection of air/steam describes a practical process for UCG at low pressure. However, at high pressure, injecting a mixture of steam and oxygen instead of alternating injection of oxygen/steam results in a higher coal conversion rate, with a final product that contains higher carbon content.

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1. Introduction

The reserves of easily extractable oil and gas are decreasing (Aleklett and Campbell, 2003; Bentley, 2002; Owen et al., 2010). Consequently, there is an increasing interest for coal utilization. Societal concern about global warming makes the use of coal, with an average of only one atom of hydrogen per atom of carbon (CH), be considered less attractive than oil (two hydrogen/carbon, CH_2) or methane (four hydrogen per carbon, CH_4). Therefore it has been suggested to investigate whether it is possible to reduce the carbon footprint of coal if coal is utilized via underground coal gasification (UCG). In European countries like Belgium, The Netherlands, Poland and Great Britain coal is deposited in relatively thin (1–3 m) and deep layers (1000–2000 m) (Białecka, 2008). Moreover issues regarding the carbon footprint are high on the agenda in Europe. Moreover, developed technology can be combined with the ongoing research in the BRICS (Brazil, Russia, India, China, and South Africa) countries (Khadse et al., 2007).

Recent field trials in China and Poland suggested alternating injection of air and steam, where the air injection period serves to heat up the coal and surrounding strata, and the steam injection period serves to produce high quality gas by recuperating the heat from the surrounding strata (Yang et al., 2008). If successful, this alternating injection procedure would allow to separate production periods with high CO_2 and nitrogen content from periods with mainly hydrogen content. If the gas of the first period can be sequestered separately, the hydrogen/carbon ratio can be improved. Stańczyk et al. (Stanczyk et al., 2010; Stańczyk et al., 2011, 2012) gasified the hard coal in a pilot underground gasifier in the Główny Instytut Górnictwa (GIG), Katowice, Poland with alternating injection of oxygen and steam. They successfully produced a fuel gas with more than 50% hydrogen during the steam cycle. In this paper, our focus is on the second pilot experiment, in which, Stanczyk et al. gasified a coal block of $2.4 \times 0.6 \times 0.55$ m^3 (length × height × width) (Stańczyk et al., 2012). We refer to this experiment as the "GIG field trial", and discuss it in more detail in the text.

All the mentioned field trials are carried out in atmospheric pressure. In the gasification of deep coal seams, with the coal connected to an aquifer system, the pressure should be kept high, i.e., slightly higher than the hydrostatic pressure, to avoid underground water flow into the gasification cavity (Camp et al., 1980). This high pressure in the cavity, however, leads to the flow of a variety of hazardous hydrocarbons

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that are formed during the UCG process into the nearby aquifers (Kapusta and Stańczyk, 2011). Therefore, it is advisable to choose a UCG site, where the coal layer is surrounded by low permeable strata. All in all, we include pressure as a parameter in our mathematical model.

A dynamic model is required to study the alternating injection UCG process. The model should be able to predict the composition of gaseous product, the rate of coal consumption, and the heat transfer to the coal layer and the surrounding strata. There is extensive literature on coal gasification models that can predict product gas composition and the rate of cavity growth (Biezen et al., 1995; Britten and Thorsness, 1989; Dinsmoor et al., 1978; Park and Edgar, 1987; Perkins and Sahajwalla, 2005, 2006; Van Batenburg et al., 1994). Some models use only chemical equilibrium on the coal surface to predict the product gas composition (Dufaux et al., 1990). However, this assumption results in an overprediction of the carbon monoxide concentration and an underestimation of the CO_2 content in the product gas.

A model for the chemical reaction of a coal block with air or a mixture of oxygen and steam was developed by Perkins and Sahajwalla (Perkins and Sahajwalla, 2005), which can be applied to underground coal gasification problems for the prediction of the coal consumption rate and the composition of the product gas. The model considers multi-component diffusion, coal drying, pyrolysis, and char/gas chemical reactions. Additionally, Perkins and Sahajwalla (Perkins and Sahajwalla, 2006) studied the effect of various parameters, e.g., pressure, temperature, water influx, and coal properties on the rate of cavity growth and product gas quality. However, to find a numerical solution to their highly nonlinear model, they assume that the bulk gas composition is known.

A cavity growth model developed by Biezen et al. (Biezen et al., 1995) describes cavity development in coal layers. A reasonable agreement with the Pricetown field trial was found, although the model was not developed to predict the product gas composition.

A mathematical model for the cavity growth applicable to UCG in shrinking coal was written by Britten and Thorsness (Britten and Thorsness, 1989). It assumes a fixed low injection point and an axisymmetric cavity around it, well mixed bulk gas, radiation dominated heat transfer, and the spreading of the injected gas through the accumulated rubble on the cavity floor. The model predictions were in agreement with the process data from two UCG field tests (Britten and Thorsness, 1989; Van Batenburg et al., 1994).

A quasi-steady state model developed by Van Batenburg et al. (1994) based on the abovementioned model of Britten and Thorsness, describes the product gas composition in the Pricetown field trial. It is, however, not suitable for alternating injection because it does not consider a time dependent heat conduction module. This study extends the previous quasi steady-state model of Van Batenburg to account for heat accumulation and recuperation from the surrounding strata.

In a conventional underground coal gasification process, oxygen (or air) and steam (or water) are injected simultaneously into a coal layer. The idea behind this process is that oxygen reacts with coal in an exothermic reaction to produce heat, i.e.,

$$CH_aO_b + \left(1-b+\frac{a}{4}\right)O_2 \rightarrow CO_2 + \frac{a}{2}H_2O. \quad (1)$$

Then the injected steam and produced CO_2 react with coal to produce H_2 and CO due to the endothermic Boudouard and shift reactions, i.e.,

$$CH_aO_b(s) + (1-b)CO_2 \rightleftharpoons (2-b)CO + \frac{a}{2}H_2, \quad (2)$$

$$CH_aO_b + (1-b)H_2O \rightleftharpoons CO + \left(1-b+\frac{a}{2}\right)H_2. \quad (3)$$

For simplicity, the methanation reaction is not shown above, but will be considered later in the model. The heat required for the Bouduard and shift reactions is provided by the combustion reaction, i.e., Eq. (1). However in practice injected oxygen reacts instantaneously with the combustible H_2 and CO in the cavity and subsequently the hot gases react with coal. The overall composition of the produced gas (for an air-blown UCG process) is reported in Table 1. It shows that the gas contains 56% N_2 and 18% CO_2, and consequently the fuel gas heating value is low. Downstream separation of N_2 and CO_2, which increases the quality of the product gas, is very energy intensive with the current state of technology and therefore is not practical.

The alternating injection of air and steam is an alternative procedure that separates the combustion and gasification reactions. First air is injected to react with coal and produce heat. It is assumed that the generated heat is stored in the coal and roof layers. The gas produced in this cycle is mainly N_2 and CO_2. Some carbon monoxide and hydrogen can also be produced depending on the composition and water content of the coal. Then air injection is stopped and steam is injected. Steam reacts with the hot coal layer, consumes the heat in the endothermic reactions, and produces a gas with high hydrogen content. Effectiveness of this step highly depends on the pressure. Low pressure is a more favorable condition for this reaction as equilibrium reactions (Eqs. (2) & (3)) shift to the right side to produce more hydrogen and carbon monoxide.

To illustrate these ideas we apply an extended model to low pressure alternating injection underground coal gasification. This model can reproduce the results from the GIG trial, which will also be used as a validation of the model. However, most of the coal layers in Europe appear in deep layers, i.e., over 700 m deep, and therefore the gasification must be done at high pressure. Hence, we investigate the effect of pressure on the product quality of deep UCG. Apart from pressure, the duration of oxygen and steam injection cycles, the time cycle ratio, and the steam/oxygen flow ratio are other important parameters that affect the process and will be studied. Depending on the geometry of the cavity and steam/oxygen flow rates, the produced gas in each stage can be mixed with the product of the previous and/or the next stage. We compare the average composition of the product gas of the alternating injection gasifier with the gasification product of a gasifier, which opposed to alternating injection, uses a continuous injection of a feed stream composed of a mixture of oxygen and steam.

This paper is organized as follows: Section 2 describes the basic assumptions of the model. In Section 2.1 the multi-component mass transfer model and the chemical equilibrium of char/gas are explained. Section 2.2 derives the heat balance equations that include conductive heat loss or gain and radiation between the cavity surfaces. Section 2.3 shows the relation for the calculation of the boundary layer thickness for natural convection dominated flow inside the cavity. Then we give an algorithm to solve the system of nonlinear differential and algebraic equations in Section 3. In Section 4.2, we compare the results of our model with a chemical equilibrium model to show the importance of mass transfer limitations in UCG reactions. We compare our result to the results of the GIG field trial to validate the mathematical model. Then, in Section 4.3 we study the effect of the duration of feed injection and the pressure of the gasifier on the quality of the UCG product.

2. Mathematical model

A schematic representation of the UCG process is shown in the left side of Fig. 1. It includes vertical injection and production wells into a coal layer. The bottom of the wells is interconnected through the coal

Table 1
A typical composition of UCG product gas; average values of the compositions reported in (Khadse et al., 2007).

Component	CO_2	CO	H_2	CH_4	N_2	Other
Mole percent	18.3	7.4	14.9	2.1	55.9	1.4

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