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Prediction of cavity growth rate during underground coal gasification using multiple regression analysis

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Abstract During underground coal gasification (UCG), whereby coal is converted to syngas in situ, a cavity is formed in the coal seam. The cavity growth rate (CGR) or the moving rate of the gasification face is affected by controllable (operation pressure, gasification time, geometry of UCG panel) and uncontrollable (coal seam properties) factors. The CGR is usually predicted by mathematical models and laboratory experiments, which are time consuming, cumbersome and expensive. In this paper, a new simple model for CGR is developed using non-linear regression analysis, based on data from 11 UCG field trials. The empirical model compares satisfactorily with Perkins model and can reliably predict CGR.

1 Introduction

Coal is the largest fossil fuel resource in the world, with proven reserves that are adequate to meet the expected demand, without much increase in production costs (Couch 2009). With the depletion in the oil and gas reserves, coal is expected to play a major role in the global energy sector in the near future (BP 2010). Underground coal gasification (UCG) offers the potential for using the energy stored in coal in an economical and environmentally sensitive way, particularly from deposits that are not mineable by conventional methods (Couch 2009). Therefore, UCG is a candidate process for converting the world's coal resources into energy, liquid fuels, and chemicals. If the UCG process is developed commercially, it would increase coal reserves by 60 % (Shirazi 2012). The process of UCG eliminates the costs of mining, lowers water consumption and transportation needs, and generates possible sites for CO_2 sequestration, and gasification installation, which are required for traditional surface gasification process (Gregg and Edgar 1978; Burton et al. 2007). However UCG has some challenges such as process stability, aquifer contamination and ground subsidence.

A schematic diagram of the UCG process is shown in Fig. 1. The procedure for in situ gasification of coal is as follows.

(1) Injection and production wells are drilled from the surface to the coal seam.
(2) Injection and production wells are linked together under ground.
(3) Air or oxygen is sent to the coal seam through the injection well.
(4) The coal is ignited in a controlled manner (Burton et al. 2007; Couch 2009). In the early stages of UCG,

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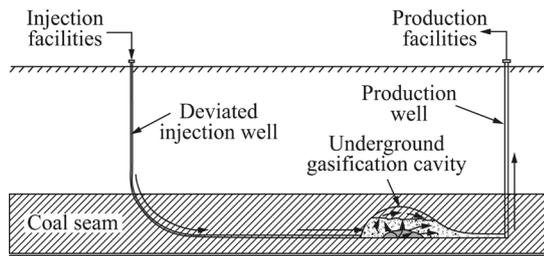[3] Department of Mathematics, Shahrood University, Shahrud, Iran

Fig. 1 Schematic of the components of the UCG process for electricity generation (DTI 2004)

the exothermic coal combustion reaction is required to create a sufficiently large underground cavity, which consists of coal, char, ash, rubble, and void space (Yang et al. 2008). In the cavity the temperature at the roof is in the range of 950–1000 °C, whereas the floor temperature varies between 650 and 700 °C (Bhutto et al. 2012).

(5) Once a stable temperature field is attained, depending on the water present in the coal seam and the surrounding strata, an appropriate amount of steam is injected into the cavity, along with the air or oxygen.

(6) The gas products, such as H_2, CO, CH_4, and CO_2, flow to the surface though the production well

(7) The gas products are sent to the end users after cleaning. The gas products can be used for power generation or to synthesize chemicals, such as methanol, ammonia, and liquid fuels (Khadse et al. 2007; Daggupati et al. 2011)

Prediction of the exact shape and size of the gasification cavity during UCG processes is important for the stability of the upper parts of the geological formation. The size of the cavity directly influences crucial economic and environmental factors. Lateral cavity dimensions influence resource recovery. The hydrological and subsidence responses of the overburden are affected by the spacing between modules, and by the ultimate cavity dimensions. The cavity shape depends on the flow patterns (gas, heat and mass transfer) inside the cavity and its size at any time depends on the rate of coal combustion (Daggupati et al. 2010).

The cavity growth rate (CGR) in different directions is the most important singular phenomenon in UCG. In this research, the definition of CGR is moving rate of the gasification face. There are many parameters that have either a positive or negative effect on the CGR, such as temperature, coal properties (coal volatile matter, fixed carbon, moisture content, ash content, permeability and thermal properties), thermo-mechanical spalling of the coal and roof, water influx, operating pressure and time, distance between wells, and external mass transfer (Perkins

2005; Daggupati et al. 2010, 2011; Prabu and Jayanti 2011).

2 Background

The concept of UCG was first suggested by Sir William Siemens in 1868. At about the same time, in Russia, Dmitry Mendeleyev suggested the idea for drilling injection and production wells (Burton et al. 2007). Since the 1930s, more than 50 pilot UCG plants have been conducted worldwide. These developments have been concentrated in the former USSR, Europe, USA, South Africa, Australia and China.

The UCG process involves complex physical and chemical processes, such as homogeneous and heterogeneous chemical reactions, complex flow patterns of reactant gases, heat and mass transport in porous media, fluid flow and thermo-mechanical failure of the coal seam (Daggupati et al. 2010; Nitao et al. 2010; Sarraf et al. 2011; Shirazi 2012; Najafi et al. 2014). Therefore, the complex interactions among these processes make it challenging to understand UCG. It is difficult to monitor all coal reaction conditions and their effects on the seam and strata (cavity size and shape).

Modeling and laboratory studies have played an important role in UCG studies to predict the effect of various physical and operating parameters on the performance of the process. For modeling of the UCG process, there are two main approaches: the packed bed model and the free channel model. The first approach assumes that the gasification occurs on a stationary coal bed and that the coal seam as a highly permeable porous medium, in which bed properties change with reactions (Magnani and Farouq 1975; Thorsness and Kang 1985; Biezen and Bruining 1995). In the past decade, a number of channel models have been developed to estimate the performance of UCG in thin, deep seams. The channel approach assumes that a permeable channel expands during the UCG process, in which gasification occurs at the roof of the channel (Eddy and Schwartz 1983; Park and Edgar 1987; Kuyper et al. 1994; Perkins and Sahajwalla 2007).

Although several models with varying levels of complexity have been published, the applicability of these models is limited to specific and isolated cases. This has led to a growing interest in laboratory scale experiments, based upon work by Wellborn (1981) and Poon (1985). Experiments at Lawrence Livermore National Laboratory (Shannon et al. 1980; Thorsness and Hill 1981) demonstrated cavity growth in Texas lignite under certain operating conditions in a horizontal channel of a coal block, through which gas flow takes place. Daggupati et al. (2010, 2011) used a systematic series of laboratory scale experiments to study combustion and gasification conditions during cavity evolution. They found empirical correlations

Table 1 Data from UCG field plant studies

UCG site	Fixed carbon (0.01 %)	Volatile matter (0.01 %))	Ash (0.01 %)	Moisture (0.01 %)	Seam thickness (m)	Seam depth (m)	Operating pressure (kPa)	Permeability (Darcy)	Calorific value (kcal/kg)	CGR (m/day)	References
El Tremedal, Spain	0.365	0.275	0.14	0.22	5	580	5000	0.00196	4296	1.2	DTI (2004), Perkins (2005), Couch (2009), Shirazi (2012) Bhutto et al. (2012),
RM1, USA	0.308	0.317	0.289	8.6	7	130	500	0.1	4141	0.65	Lindblom and Smith (1993), Perkins (2005), Dennis (2006), Couch (2009), Shirazi (2012)
Secunda, South Africa	0.501	0.22	0.225	0.504	3	160	140	0.08	4030	0.45	Couch (2009), SSL (2009)
PSC, USA	0.28	0.34	0.21	0.17	6	60	430	0.14	6469	0.82	Perkins (2005), Burton et al. (2007), Couch (2009), Bhutto et al. (2012)
LBK-5, USA	0.355	0.285	0.144	0.216	3	70	150	0.14	6485	0.71	Hill and Thorsness (1982), Perkins (2005), Couch (2009), Bhutto et al. (2012)
Mecsek Hills, Hungary	0.28	0.19	0.473	0.057	7	600	5100	0.15	5346	0.5	Wildhorse Energy Ltd. (2012)
Pricetown, USA	0.495	0.381	0.11	0.014	3	300	2100	0.017	5415	0.48	Perkins (2005), Couch (2009), Bhutto et al. (2012), Shirazi (2012)
Hanna I, USA	0.355	0.285	0.144	0.216	7	80	150	0.13	4143	0.7	Fischer et al. (1977), Lindblom and Smith (1993), Perkins (2005), Burton et al. (2007), Couch (2009), Bhutto et al. (2012), Shirazi (2012)
Hanna II, USA	0.319	0.306	0.289	0.086	9	85	150	0.13	4143	0.5	Fischer et al. (1977), Lindblom and Smith (1993), Burton et al. (2007), Couch (2009), Bhutto et al. (2012), Shirazi (2012)
Chinchilla, Australia	0.276	0.374	0.28	0.07	10	140	1100	0.04	4368	0.5	Blinderman and Jones (2002), Burton et al. (2007), Couch (2009), Luo et al. (2009), Bhutto et al. (2012), Shirazi (2012;)
Bloodwood Creek, Australia	0.285	0.36	0.285	0.07	9	200	1220	0.03	4940.31	0.35	Burton et al. (2007), Couch (2009), Mallett and Burl (2010), Bhutto et al. (2012), Shirazi (2012)

between the cavity volume and the well distance, the gasification time and feed flow rate. They determined that the linear and vertical CGR is 1.1 cm/h using the measured cavity heights at different times, with the other operating conditions being the same. However, experimental tests on UCG are time consuming and expensive. Therefore, there is a need to obtain CGR by a new simple and less expensive method.

The aim of the present paper is to develop a non-linear, multivariable prediction empirical model to predict CGR as a function of coal properties, operation pressure and depth.

3 Data sources

A database was assembled from published sources on coal properties and other parameters from 11 UCG pilot tests in the USA, Europe, Australia and South Africa (Table 1).

4 Simple regression and input data selection

In the first stage of the data analysis, a series of simple regressions were run between the dependent variable (CGR) and 9 independent variables (Table 2) using the data shown in Table 1. Regression analysis was carried out using SPSS (2012), with alpha set at 0.05. The simple regression analyses provide a means of summarizing the relationship between two variables.

As can be seen from Table 2, the relationship between the CGR and some independent variables such as fixed carbon, volatile matter and calorific value are statistically insignificant (based on the r^2 value). The results reveal that no single independent variable explains more than 60 % of the variation in CGR. Therefore, prediction of

Table 2 r^2 values from simple regression between CGR and nine independent variables

Independent variable	Regression model			
	Linear	Power	Logarithmic	Exponential
Moisture	0.586	0.399	0.363	0.557
Ash	0.203	0.224	0.226	0.197
Operating pressure	0.144	0.066	0.043	0.095
Seam thickness	0.114	0.503	0.079	0.151
Seam depth	0.102	0.024	0.007	0.061
Calorific value	0.021	0.016	0.040	0.049
Permeability	0.018	0.241	0.130	0.002
Volatile matter	0.017	0.006	0.008	0.017
Fixed carbon	0.009	0.003	0.001	0.005

CGR based on nine variables is a non-linear multivariable problem.

5 Non-linear multiple regression analysis

Non-linear regression is a method for building a non-linear model of the relationship between the dependent variable and a set of independent variables. Unlike traditional linear regression, non-linear regression can estimate a model with arbitrary relationships between dependent and independent variables (SPSS 2012). In this paper, two non-linear regression equations were developed using SPSS (2012) and the data shown in Table 1. Equation (1) indicates that CGR can be predicted from the coal calorific value, ash content, volatile matter content, moisture content, permeability, and operating pressure. It should be noted that based on Eq. (1), the CGR is not related to fixed carbon, calorific value, seam depth and volatile matter ($R^2 < 0.1$ and $P > 0.05$) and therefore these variables were excluded from the model.

$$\begin{aligned} CGR = {} & 0.076 - 0.32 \log(CA) + 2.181 CM \\ & - 215.102 h^{-28.076} + 0.0000825(OP) \\ & - 399.843 CP^{198.95} \quad R^2 = 0.79 \end{aligned} \quad (1)$$

where CGR is in m/day, OP is the operation pressure (kPa), CP is the coal permeability (Darcy), CM is the coal moisture content (0.01 %), h is the coal seam thickness (m) and CA is the coal ash (0.01 %). It should be noted that the analysis of variances for the significance have been showed this Equation is not valid.

Equation (2) is the basis to develop the second model. In this model the equation representing the model can be written as follows (Choi 1978):

$$Y = \alpha_0 (X_1^{\alpha_1})(X_2^{\alpha_2})\ldots(X_n^{\alpha_n}) \quad (2)$$

where Y is the predicted value corresponding to the dependent variables, α_0 is an arbitrary coefficient, X_1, X_2, …, X_n are the independent variables and α_1, α_2,… α_n are the regression coefficients.

Based upon Eq. (2), the best model for estimating CGR is shown in Eq. (3). It should be noted that the Chinchilla and Mecsek Hills sites were randomly selected to be removed from the dataset to be used as validation data for the model.

$$CGR = \frac{0.004 \times \sqrt{\frac{CCV}{D}} \times (OP)^{0.265} \times (CM)^{0.185}}{CVM \times CA^{0.25} \times CP^{0.159}} \quad (3)$$
$$R^2 = 0.85$$

where CCV is the coal calorific value (kCal/kg), D is the depth of coal seam (m) and CVM is the coal volatile matter (0.01 %). Similar to Eq. (1), CGR is not related to fixed

carbon content, but unlike Eq. (1), it is not related to seam thickness. It is clear that the determination coefficient (R^2), obtained for Eq. (3) is improved relative to that of Eq. (1). Moreover Eq. (3) is simple in comparison to Eq. (1). Therefore, Eq. (3) was selected for the further evaluation.

6 Validation of developed model

Validation of the developed model (Eq. (3)) was carried out in three stages. The first stage considers the determination coefficient the F-test and a plot of observed versus predicted CGR. The statistical results of the model for the 95 % confidence level are given in Table 3. The computed F-value is greater than the tabulated F-value, therefore the null hypothesis (there is not a relationship between the dependent and independent variables) is rejected. Therefore, it is concluded that the model is valid and CGR can be predicted by the developed model.

In the second stage, the developed model was validated using data from the Chinchilla and Mecsek Hills sites, which were not used in the model development dataset. In Table 4 and Fig. 2, the predicted CGR values are compared with the observed CGR values for the Chinchilla and Mecsek Hills UCG sites. The relative errors of the estimated values in Table 2 are represented by the distance of each data point from the 1:1 diagonal line in Fig. 2. The average relative error is 15 %.

In the third stage, the developed empirical model was compared with the Perkins model (2005), which is a channel model that can predict CGR rate mechanisms, the coupled phenomena of heat and mass transfer in combination with chemical reaction, and the factors which affect
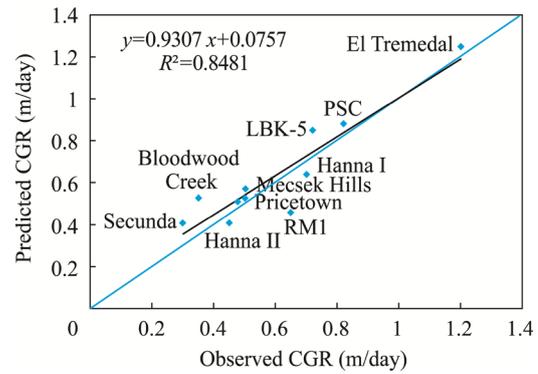
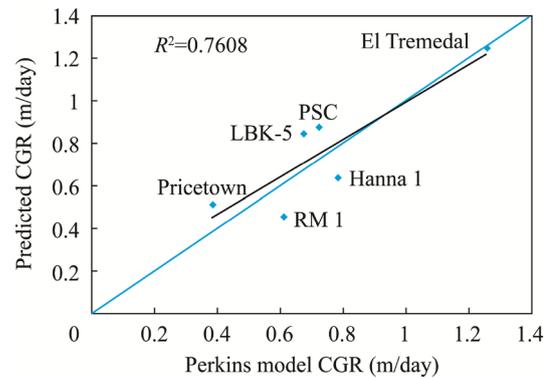**Fig. 2** Predicted CGR versus observed CGR

Fig. 3 Comparison of CGR predicted by the developed empirical model and predicted by the Perkins model

gas production from the gasifier. This model assumption is that the rate of cavity growth is at pseudo-state at all time and that the chemical reactions occur only on the surface of

Table 3 Analysis of variance output for the model in Eq. (3)

	Sum of squares	Degrees of freedom	Mean square	F value	Tabulated F	Significance
Regression	4.594	4	1.025	54	5.19	<0.0001
Residual	0.095	5	0.019			
Total	4.689	11				

Table 4 Predicted and observed CGR values for the development and validation UCG sites

	Model development UCG sites									Model validation UCG sites	
	El Tremedal	RM1	Secunda	PSC	LBK-5	Pricetown	Hanna I	Hanna II	Bloodwood Creek	Chinchilla	Mecsek Hills
Predicted CGR (m/day)	1.25	0.46	0.41	0.88	0.85	0.51	0.64	0.41	0.53	0.53	0.57
Observed CGR (m/day)	1.20	0.65	0.45	0.82	0.72	0.48	0.70	0.30	0.35	0.50	0.50
Relative error (%)	4	28	7	8	18	6	7	17	50	7	15

the coal block (wall). This model is in a one-dimensional spatial domain and validated through comparison with experimental measurements o the pyrolysis of large coal particles and the drying and pyrolysis of cylindrical coal block. It usually predicts a CGR between 0.384 and 1.2 m/day.

The results of this comparison for El Tremedal, RM1, PSC, LBK-5, Pricetown and Hanna1 UCG sites are shown in Fig. 3. It is clear that there is a positive relationship between the empirical model and the Perkins model.

7 Conclusions

The CGR is the most important phenomenon in the UCG process. It directly impacts coal resource recovery and energy efficiency and therefore the economic feasibility of UCG. Prediction of CGR helps to estimate syngas production and cavity shape. In this paper, a new empirical model was developed by non-linear multivariable regression method for predication of the CGR during UCG. During the analysis, nine possible independent variables were evaluated in terms of their ability to predict the CGR. The results of regression analysis excluded two parameters, namely coal seam thickness and fixed carbon content. Hence, the model was created based upon seven independent variables.

The validation exercise demonstrated that Eq. (3) can predict CGR under various conditions. This model provides a quick estimate of CGR at any given set of parameters. The most important application of this model is to predict CGR before the construction of a UCG pilot project. It is evident that the prediction models presented in this paper can be open to further improvements. As an example, if there are sufficient data, other methods such as neural network modeling could be used.

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