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Modeling Cavity Growth during Underground Coal Gasification

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Abstract: Underground coal gasification (UCG) has received renewed interest due to its potential for utilization of the vast amounts of coals available in deep underground seams and the current drive towards clean coal utilization. The UCG process involves the reaction between steam and coal in deep underground seams to form a combustible gas which is brought to surface via a production well and used as a fuel or chemical feedstock. This paper presents a model for the growth of a gasification cavity, which is crucial for determining the duration and extent of the reaction process for a given injection point. COMSOL MULTIPHYSICS software is used to model the combined effects of fluid flow in porous media, mass transfer of species, heat transfer, and reaction kinetics. The growth of the cavity is tracked using ALE moving boundary coupled to reaction physics. The geometry is based on controlled retraction injection point (CRIP), and the change in the geometry is controlled from a MATLAB script. Cavity shape, growth rate, temperature profile and outlet gas compositions are presented and compared to literature values and recent field trials.

Keywords: coal gasification, cavity growth, syn-gas.

1. Introduction

Underground coal gasification (UCG) is a process in which coal is converted into syngas in-situ. Although the concept of the UCG has its roots in 1868, the process was left out mostly because of low prices of gas and oil [1]. Due to increased energy demands and stringent environmental regulations, UCG has regained its popularity in recent years as an immediate alternative for conventional coal power plants.
Drilling is considered to be one of the major steps in UCG. Over the years, two main geometries have been developed. Linked vertical wells (LVW) and controlled-retraction injection point (CRIP). The former one involves the drilling of two vertical wells as injection and production well and establishing a permeable link between these two wells. Field trials of LVW showed decline in quality of produced syngas which could be related to gas and heat and gas loss to overburden [1]. The CRIP method involves a moveable injection point system as shown in Fig.1. The reaction begins near the production well and as the coal between injection and production well is depleted, the head is moved back in a controlled manner.

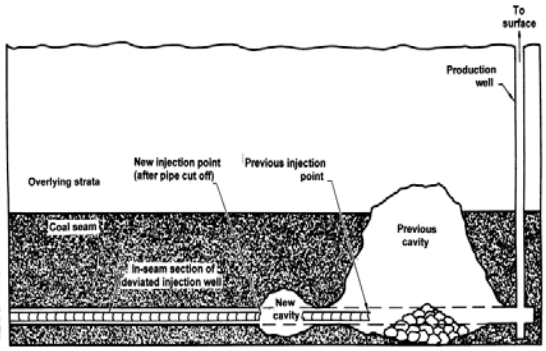


Figure 1. CRIP geometry

1.1 Literature review

UCG is a complex process involving mass and heat transfer in porous media, fluid flow, heterogeneous and homogenous reactions. Three distinct mechanisms are considered as major contributors to cavity growth namely: chemical reaction, thermo-mechanical failure and sidewall and roof collapse.
Several models have been developed over the years to model the UCG process. These models could be categorized in two distinct approaches. Channel models [4-7] treat the cavity as an expanding cylinder in which the chemical reactions occur in the surface of the channel walls. Coal block models [2-3, 8-10] involve gasification in a permeable bed of stationary solids. These studies are either used to simulate laboratory-scale experiments or they have neglected important features of process to compensate for the large-scale computations. In one recent study, a comprehensive model of process has been developed by Nourizadeh [3],

to account for different processes in field-scale trial. However, their final solution is limited to software capabilities to handle complex geometries and depend largely on the mesh grid. This study considers a detailed 2D approximation of UCG process which incorporates flow through varying porous media with the main heterogeneous reactions. These phenomena are coupled with heat and mass transfer equations which yield the temperature and concentration profile along the coal seam at different times.

2. Mathematical Model

Coal is considered as a porous medium with macropores, and micropores. While macropores provides surface area for mass transfer, mircopores provide surface area for chemical reactions. This approach has follows the work of Perkins [3]. Heterogeneous reactions increase the micropores volume, while pyrolysis open up new macropores. Changes in macroporosity could be expressed as follows:

$$\frac{\partial \varphi_m}{\partial t} = \sum (rate_{p_i}) \frac{W_{char}}{W_i} \qquad (1)$$

Variation of microporosity with time is calculated based on the following equation.

$$\frac{\partial}{\partial t}(\varphi_\mu (1-\varphi_m)) = \sum (rate_{gasification_i}) \frac{\rho_{solid}}{W_i} \qquad (2)$$

Chemical reactions during UCG consist of drying, pyrolysis, combustion and gasification. In drying, coal loses its moisture, while in pyrolysis volatile matter is released from coal and a carbon-rich material remains which is called char. The char finally undergoes gasification reactions which yield syngas. These reactions are summarized below:

$$Drying : \quad WetCoal \longrightarrow DryCoal + H_2O \quad \Delta H_{298} = 40 kJ/mol$$

$$Pyrolysis : \quad DryCoal \longrightarrow Char + Volatilematter \quad \Delta H_{298} \sim 0 kJ/mol$$

$$Gasification \begin{cases} C(char) + CO_2 \longrightarrow 2CO & \Delta H_{298} = 172 kJ/mol \\ C(char) + H_2O \longrightarrow CO + H_2 & \Delta H_{298} = 131 kJ/mol \\ C(char) + 2H_2 \longrightarrow CH_4 & \Delta H_{298} = -75 kJ/mol \end{cases}$$

Pyrolysis is taken to be as series of first-order reactions that occur over a range of temperature. This approach is firstly proposed in work of Van Hydek and applied to UCG problem by Tsang. [8]

$$\frac{dm_j}{dt} = rate_{pyrolysis_i} = k^*(m_j^* - m_j) \qquad (5)$$

$$k^* = A\exp(-\frac{E}{RT}) \qquad (6)$$

m_j^* : Potential yield of volatiles(gr)/gr of coal

$$m_j = \frac{\text{gr of specie}}{\text{gr of coal}}$$

Same approach is used to model drying of coal seam. k^* and E are adjusted to yield a sharp peak for rate of evaporation at temperatures around 596 K, which is evaporation temperature of water at 11.5 Mp. Kinetic parameters for pyrolysis are taken from the work of Tsang[8].

In order to describe inhibition effect of H_2 and CO on gasification reactions, Langmuir-Hinshelwood models should be used as kinetics equation, however in this study simple power-law equations are used to describe kinetics of these reactions.

$$rate_i = Sk_{f,i}C_i \qquad (7)$$

where S is specific surface area of coal and C_i is concentration of reactant. Studies have indicated a maximum in rate of gasification reactions vs. conversion. Bhati and Perlmutter[12] have proposed a random pore model to describe variation of surface are with conversion.

$$S = S_0(1-X_c)\sqrt{1-\beta \ln(1-X_c)} \qquad (8)$$

Where β is a structure parameter of the coal and is assumed to have value of 5 according to Perkins [2]. The permeability of coal is a function of its structure and the variation in permability is set to be as a function of changes porosity based on the work of Wang and Bahita[3] who derived the function:

$$\ln\frac{k}{k_0} = \sigma(\varphi - \varphi_0) \qquad (9)$$

$\sigma = 12$, k_0 is the initial coal permeability and

φ_0 the initial porosity. Fluid flow is solved using the Brinkman equation and this varying porosity/permeability. Density of gas is calculated based on Ideal gas law.
Heat transfer equation solved for porous media using:

$$\frac{\partial}{\partial t}(C_{p,eff}T) + \nabla.(\rho_g u_g C_{p,g} T) = \nabla.(k_{eff}\nabla T) + \sum_{i=1}^{n} rate_i \Delta H_i \quad (10)$$

Diffusion of the gas species in the coal seam is calculated using fickian diffusion. Diffusion coefficient for each component of the mixture is calculated from the following relation:

$$D_{im} = \frac{1 - x_i}{\sum \frac{x_k}{D_{ik}}} \quad (11)$$

$$D_{eff_i} = \frac{D_{im}\varphi_g}{\tau}$$

τ : Tortuosity=$\sqrt{2}$

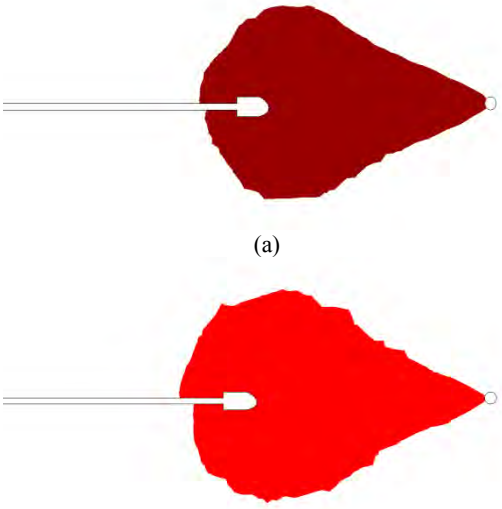
3. Results and discussion

This study focuses on a pilot-scale UCG which is ongoing in Alberta. Coal seam is assumed to be 9m high and the distance between injection header and production well is set to be 4m. Final shape of cavity depends on geological parameters such as permeability. Proximate analysis of coal used in this model is given in table 1.

Fixed Carbon	55
Volatile matter	30
Moisture	5
Ash	10

Table1. Proximate analysis of coal

Homogenous reactions are considered to be very fast compared to heterogeneous reactions that mixture attains equilibrium in each temperature. Figure 2 shows cavity shape after five days. Nourizadeh[3] has calculated unreasonably fast cavity growth in comparison to Perkins [2], Tsang [8] and Abdel-Hadi[11]. In this study average cavity growth rate along cavity center axis is calculated to be 80 cm/day, which is close to data presented elsewhere [2, 8, and 11]. Post-burn experiments have shown the pear-shaped cavity around the injection point. Same trend has been calculated in this model. Proposed model also could be validated based on the backward growth of cavity around injection point, which has shown to be up to 25% of well spacing.



(a)

(b)

Figure 2. Final cavity shape after 5 days. (a) 95071 Degree of freedom (b) 65000 Degree of freedom

Temperature distribution is shown in Figure 3. Mesh dependence of the results have been investigated using three mesh structures. It has been concluded that meshes with meshes generated while parameter has set to be smaller than 50 cm, produces relatively same results for cavity shape.

Figure 4 shows rate of evolution of steam for a point in the coal seam. Two distinct peaks could be identified in this figure. One in lower temperature around 500 K, which is related to evaporation of water, and one wider peak which overlaps with previous peak and has a maximum around 650 K and represents release of steam from pyrolysis.

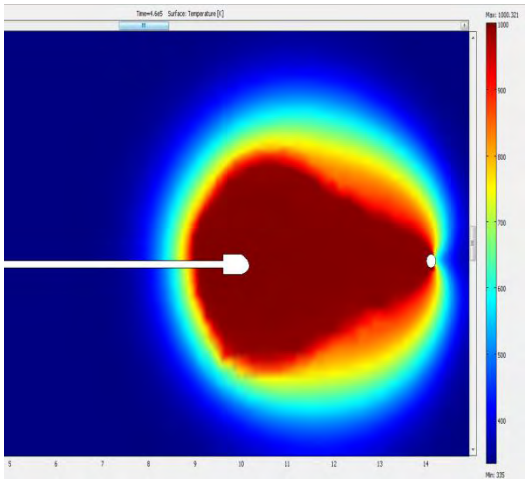


Figure 3. Temperature distribution in cavity after 5 days

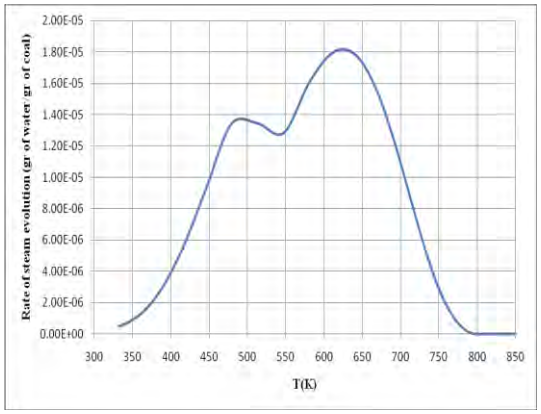
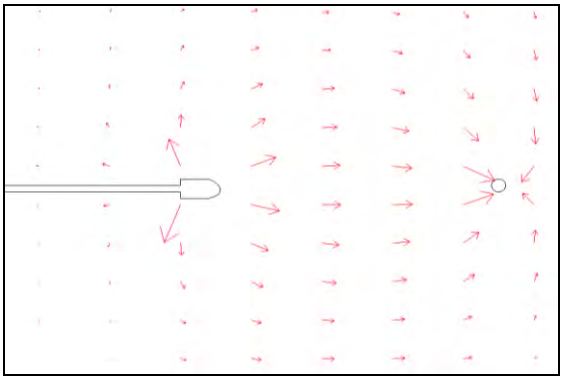


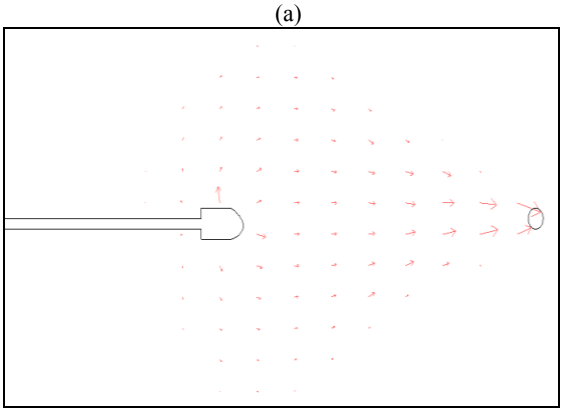
Figure 4. Rate of evolution of steam from evaporation and pyrolysis

The composition of produced gas in production well is presented in Figure 5. Final compositions of produced gases are given in Table 2. (Composition of gases after cavity reaches to production well)

Figure 5 shows velocity vectors at the initial stages of process and after 6 days. As shown in the plots, increase in porosity/permeability due to chemical reaction will lead the flow to restrictively flow in developed cavity with high permeability/porosity rather than almost impermeable virgin coal seam.



(a)



(b)

Figure 5. Velocity vectors (a) Initial stages (b) After 6 days

7. Conclusions

In this paper, a detailed 2D model for cavity growth during UCG process has been developed. Three heterogeneous reactions, pyrolysis and drying have been taken into account. Cavity shape has been shown to be independent of mesh. Final cavity shape and cavity growth rate along the axis of burner head are in good agreement with experimental data from post-burn experiments.

8. References

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