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# Simulation study and kinetic parameter estimation of underground coal gasification in Alberta reservoirs

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ABSTRACT

A new method is developed for the estimation of chemical reaction kinetics at high-pressure underground coal gasification from the field produced gas composition. This method combines a developed numerical forward model and field data to investigate uncertain parameters. The forward model is developed on the basis of a unique porous media approach that combines the effects of heat, mass transport, and chemical reactions to simulate the underground coal gasification in three-dimensional basis. The chemical reaction kinetics, that is limited to low pressure, is upscaled based on the available experimental data. A comprehensive sensitivity analysis is carried out to estimate the reaction kinetics and investigate the effect of various parameters, such as pressure, temperature, and reaction environment, on the produced gas composition. The novelty of the developed method is in its applicability as well as its ability to generate the chemical reaction kinetics that corresponds to the field under study. The advantage of the proposed technique is that the sensitivity of the model to different kinetic parameters can be investigated by a graphical method.



*Keywords:* Underground coal gasification; Parameter estimation; Reaction kinetics; Forward model; Porous media approach; Three-dimensional model

## 1. Introduction

Coal is a major fossil fuel and plays a demanding role in the energy sector. Canada is ranked tenth worldwide in coal reserves, and Alberta's 33.6 billion tons of proven mineable coal represents 70% of Canada's reserves. The deep, stranded coal reserves in Canada, which are not part of the coal reserve base, exceed 600 billion tons in Alberta alone (Energy Resources Conservation Board, 2008). Consequently, Alberta's coal resources constitute an enormous source of untapped energy; thus there is a need for the development of novel technologies for the efficient and clean utilization of coal.

Underground coal gasification (UCG) can be considered as a technique that can be applied to convert the abundant coal resources into a synthetic gas. The process involves the injection of steam and air or oxygen into an underground coal seam to ignite and burn coal in situ to produce a combustible gas that can be used either as a fuel or chemical feedstock. UCG has the advantages of high safety, high efficiency, low cost, environmentally friendliness, and a high return rate, compared with surface gasification (Gregg and Edgar, 1978; Burton et al., 2006; Shafirovich and Varma, 2009). In addition, it can be applied to deep and thin coal seams that are not economical for mining.

Accurate production prediction and process optimization are essential to correctly interpret pilot and field data, leading to a better understanding and design of the process in the field. Mathematical models and numerical simulations, as a preliminary study, give better insights to the process. While there have been extensive models for the gasification of coal in one dimension, there are relatively few on the modeling of the process in the three-dimensional space or the field scale. A distinguishing feature of three-dimensional modeling is that the physical and chemical phenomena, such as mass and heat transport, chemical reactions, and geomechanical behavior, become far more complex.

Despite the complexity of the process in the field scale, there are no numerical investigations into the gasification of coal at very high pressure (>10 MPa) and depth (>1000 m). Numerical models developed by Massaquoi and

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**Nomenclature**

| | |
|---|---|
| $A$ | flow area |
| $B$ | reaction components |
| $C$ | solid concentration |
| $D$ | diffusion coefficient |
| $E$ | activation energy |
| $H$ | enthalpy |
| $J$ | sensitivity matrix |
| $k$ | permeability |
| $k_r$ | relative permeability |
| $l$ | distance |
| $M$ | objective function |
| $N$ | number of moles |
| $n$ | number of components |
| $q$ | injection or production rate |
| $R$ | gas constant |
| $r$ | rate of creation and destruction |
| $S$ | fluid saturation |
| $s$ | stoichiometric coefficient |
| $T$ | temperature |
| $t$ | time |
| $U$ | internal energy |
| $V$ | block volume |
| $y$ | mole fraction |
| CMG | computer modeling group |
| exp | experiment |
| GC | gas composition |
| LMA | Levenberg–Marquardt algorithm |
| SAGD | steam assisted gravity drainage |
| UCG | underground coal gasification |
| *Greek letters* | |
| $\chi$ | stopping criteria |
| $\varepsilon$ | reaction rate |
| $\phi$ | porosity |
| $\varphi$ | flow potential |
| $\eta$ | reaction order |
| $\kappa$ | thermal conductivity |
| $\lambda$ | transmissibility |
| $\mu$ | fluid viscosity |
| $\rho$ | density |
| $\sigma$ | adjusting parameter |
| $\omega$ | matrix of gas composition |
| $\xi$ | volatile content of coal |
| $\Omega$ | diagonal matrix |
| *Subscripts* | |
| $f$ | fluid |
| $g$ | gas |
| $s$ | solid |
| $\upsilon$ | iteration number |
| W | water |

Riggs (1983a,b), Park and Edgar (1987), Tsang (1980), and Perkins and Sahajwalla (2005) are for one-dimensional coal gasification up to a pressure of 5 MPa. In some areas, e.g., in Alberta, there are some coal seams in which the coal gasification occurs in situ at a pressure of around 12 MPa, which is substantially higher than the previously cited numerical studies.

One of the major processes in UCG is chemical reaction. The dependence of chemical reactions on the coal block size and the environmental condition in which the chemical reaction occurs can affect the process. The former was studied by Nourozieh et al. (2010) and it was shown that the temperature distribution and chemical process behavior depend on the coal block size. For the latter, experimental study is essential for the modeling of reactions. Most experiments on char reactions have been done at atmospheric conditions and there are only a limited number of studies that measure the kinetics rate of char reaction at high pressure (MacNeil and Basu, 1998; Monson et al., 1995; Roberts and Harris, 2000; Muhlen et al., 1985).

The above-mentioned studies encouraged us to find a parameter estimation method for investigating the chemical reaction kinetics based on field history data. In this method, reaction parameters, which were obtained at low pressures and in laboratory scale, are upscaled and estimated for the field scale. From an engineering point of view, this is an inverse problem.

Generally, two different kinds of problems are considered in engineering – forward and inverse (Schulze-Riegert et al., 2003). For a forward problem, the task is the determination of the model response from the input. In this approach, input data are introduced to the model, which generates the response as output. In an inverse problem, the aim is the determination of model parameter(s) within a certain domain from data, and information may give the boundary of this domain.

Several techniques, such as the Newton method, the steepest descent method, the Levenberg–Marquardt, random search, and genetic algorithms can be used for solving an inverse problem. Some of these methods, such as the random search and genetic algorithms, require many sets of estimated parameters. These methods are not applicable for UCG, where the computational time is too high. Thus it is essential to select a method that has a high convergence rate to estimate parameters with a minimum number of runs. To satisfy the above criteria, the Levenberg–Marquardt method (Levenberg, 1944; Marquardt, 1963) is preferred for parameter estimation.

The objective of the present work is the combination of the developed forward model with field data to investigate uncertain parameters. To this aim, first a three-dimensional model for underground coal gasification in Alberta reservoir is developed. Then, the sensitivity of the model to different kinetic parameters is investigated by a graphical method. Finally, the chemical processes' kinetics based on the literature experimental data are evaluated and estimated for the field under study.

## 2. UCG forward model

In this study, computer modelling group (CMG)'s software STARS is used to build up forward model and study of UCG in deep coal seams. STARS is a semi-compositional porous media based simulator that combines the heat and mass transport equations with chemical reactions to investigate the UCG process. This software as a commercial tool, was developed to simulate the processes such as steam flood, steam cycling, SAGD (steam assisted gravity drainage), dry and wet combustion, along with many types of chemical processes, using a wide range of grid and porosity models in both field and laboratory scale (Computer Modelling Group Ltd., http://www.cmgl.ca/software/stars.htm).