Computational Studies for Underground Coal Gasification (UCG) Process

Dipankar Chatterjee
Advanced Design and Analysis Group, CSIR-Central Mechanical Engineering Research Institute, Durgapur-713209, India
d_chatterjee@cmeri.res.in

Abstract. Underground coal gasification (UCG) is a well proven technology in order to access the coal lying either too deep underground, or is otherwise too costly to be extracted using the conventional mining methods. UCG product gas is commonly used as a chemical feedstock or as fuel for power generation. During the UCG process, a cavity is formed in the coal seam during its conversion to gaseous products. The cavity grows in a three-dimensional fashion as the gasification proceeds. The UCG process is indeed a result of several complex interactions of various geo-thermo-mechanical processes such as the fluid flow, heat and mass transfer, chemical reactions, water influx, thermo-mechanical failure, and other geological aspects. The rate of the growth of this cavity and its shape will have a significant impact on the gas flow patterns, chemical kinetics, temperature distributions, and finally the quality of the product gas. It has been observed that there is insufficient information available in the literature to provide clear insight into these issues. It leaves us with a great opportunity to investigate and explore the UCG process, both from the experimental as well as theoretical perspectives. In the development and exploration of new research, experiment is undoubtedly very important. However, due to the excessive cost involvement with experimentation it is not always recommended for the complicated process like UCG. Recently, with the advent of the high performance computational facilities it is quite possible to make alternative experimentation numerically of many physically involved problems using certain computational tools like CFD (computational fluid dynamics). In order to gain a comprehensive understanding of the underlying physical phenomena, modeling strategies have frequently been utilized for the UCG process. Keeping in view the above, the various modeling strategies commonly deployed for carrying out mathematical modeling of UCG process are described here in a concise manner. The available strategies are categorized in several groups and their salient features are discussed in order to have a good understanding of the underlying physical phenomena. This would likely to be a valuable documentation in order to understand the physical process of UCG and will pave to formulate new and involved modeling and simulation techniques for computationally modeling the UCG process.

1. Introduction
Computational modelling and simulation have become an inexpensive tool for predicting the influence of various physical and operating parameters on the performance of the UCG process, since conducting the UCG trials and data extraction is extremely costly and difficult. A lot of effort is being devoted to model the UCG process along with the field trials. The UCG process as shown in Figure 1 involves several complex mechanisms that happen simultaneously over a range of length and time scales. An
An integrated model involving several submodels is required in order to comprehensively describe the complicated UCG process. These submodels are:

- A coal submodel for investigating evaporation, pyrolysis, self-gasification and combustion of char, the effect of water influx, and heat and mass transport phenomena.
- A cavity submodel to address the cavity growth mechanisms, growth rate, cavity geometry, formation of the rubble pile at the bottom of the cavity, fluid flow, heat and mass transfer within the cavity.
- Gas cleaning and environmental submodels to address the separation of undesired gas species from the product gas, the surface treatment of the syngas for final use, and handling of the produced CO₂, H₂S, etc.

Combining all these sub-models would theoretically give an exact and complete description of the process; however building such a model is an extremely cumbersome task. Therefore all the previous models have mainly focused on studying these aspects in a decoupled manner through several simplifying assumptions.

Current UCG models are mostly based on 1-D study of combustion and gasification of coal using a complex CFD (computational fluid dynamics) approach. These models are used to interpret and predict the performance of laboratory-scale experiments that are generally performed at lower pressures and oxidizing environments as well as a specific portion of field trials operating at pressures up to 5 MPa and shallow depths to 600 m. Some current UCG models assume complicated velocity equations, including the turbulent gas flow inside the cavity, and utilize chemical engineering correlations for a particle size and the porosity of the reactor. In addition, the cavity geometry and growth rate are modelled with an initially pre-assumed shape, either a tiny rectangular cube or a cylinder. Moreover, most of these studies focused on a single cavity and only a few considered interactions with the overburden. These models do not consider interactions between cavities. Due to the enormous complexity and computational cost of these models as the grid numbers increase, they cannot be efficiently used to simulate large-scale field trials. Using the CRIP technology, the coal is gasified in several stages and a sequence of cavities are developed according to the applied retraction strategies. These cavities are known to influence each other thermally. For this reason, the current models are not very appropriate to investigate the performance of different UCG technologies at a large scale.
The UCG models in the literature can be divided into two main categories: global and process models. Global models describe the overall field performance of UCG, while the process models are simple models of specific parts of the process, such as rock and coal spalling and the effect of water influx. The global models incorporate several approaches, such as packed bed, coal block, and channel models. In the following section, a brief overview of some important models will be provided and their approaches will be discussed in brief.

2. Overview of various models

2.1. Packed bed models

In the packed bed model, the process is described as a packed bed reactor. In this concept, the coal seam is considered to be a highly permeable porous media where the bed properties change with reactions. Winslow [2] used this approach to model the process in a 1-D domain with reactions occurring in char particles. Darcy equation was used to describe the fluid flow. Heat and mass transfer was addressed in the gas and solid phases, considering the convection terms only in the governing equations. Experimental correlations were used to describe the heat transfer between the phases. The numerical predictions were in accordance with the experimental results. Thorsness and Kang [3] extended the model by incorporating homogenous reactions, diffusion effects, wall transport, and also by revising the char reaction rates based on the ash segregation (AS) and shell progressive (SP) reaction models (refer to Figure 2).

![Figure 2](image_url)

(a) Shell progressive (SP) model       (b) Ash segregation (AS) model

Figure 2. Different reaction regimes in the packed-bed model [2]

Khadse et al. [4] developed a simple 1-D model to describe the UCG process at char-rubble zone in a cylinder filled with coal particles. They followed a pseudo-steady approach, as there exists a large difference between solid and gas characteristic time-scales. Effect of $O_2$ concentration, Steam/$O_2$ ratio, and the inlet pressure were investigated. They found that increasing both $O_2$ and steam fraction in feed increases the propagation rate of the reaction front. Pressure was found to have insignificant impact. Although packed bed models are able to reproduce the laboratory experiments their extension to field trials is somewhat unfeasible, since other cavity growth mechanisms such as the thermo-mechanical failure cannot be incorporated into the model. Furthermore, this method requires fine grid system in the vicinity of the reaction front that practically limits its applicability.

2.2. Coal slab models

This concept considers the UCG coal seam as a coal slab. The process in these models is described by governing the movement of various defined regions in a coal slab. These regions include: gas film, ash layer, char region, dried coal, and virgin coal. There is an influx of the injection gases towards the cavity wall, while there is a simultaneous counter flux of steam and pyrolysis products from the wall to the cavity. The general framework of these models is depicted in Figure 3.
Tsang [6] first used such approach and developed a 1-D unsteady model. The coal slab was divided into two zones: wet and dry zones. In the wet zone, heat conduction and liquid transfer are solved. It was assumed that all drying occurs in one moving point (Stefan model). This model neglects the effects of steam convection and assumes that the drying process is dominated by the conduction mode of heat transfer. In the dry region, pseudo-steady state assumption was adopted to solve the mass balance, heat transfer and gas-flux. Pyrolysis reactions are modelled as simultaneous independent reactions with kinetic parameters obtained from Campbell [7]. Porosity and permeability change with the extent of the reactions involving the correlations obtained from the oil well acidization. The model was validated with the experimental results of Forrester [8]. The model neglects combustion and provides the heat by putting a high temperature condition at the boundary. Massaquoi and Riggs [9-11] extended Tsang’s model [6] by incorporating the combustion of char and volatiles at the boundary. Three zones outside the coal slab were included: ash zone with a constant thickness, gas film, and the bulk gas. The model was used to describe simultaneous combustion and drying of a wet coal. The results showed that homogenous combustion of coal happen at lower surface temperature than reported for char particles. Furthermore, the burn rate decreases with increase in the concentration of $O_2$, when flame front is located in char face and increases when the flame is located in the gas film. Hong [12] applied previous submodels to develop a cavity model to predict the growth rate and composition of the final product gas. In this approach, the cavity was divided into several compartments representing a TIS model. Each compartment was assumed to include a void and a rubble pile region, representing the two branches of the parallel TIS model. The rubble pile (lower branch) and the void space (upper branch) were modelled using plug flow and continuously stirred tank reactors, respectively. It was assumed that all of the ash particles fall down on the rubble pile. This model was used to simulate the Hoe Creek III field trial. Park and Edgar [13] subsequently developed an unsteady 1-D model with a moving burning front to describe the lateral cavity growth in UCG. They also incorporated the coal shrinkage effect due to drying and pyrolysis, as well as steam and CO$_2$ gasification. Their results were validated with the experimental results of Poon et al. [14]. It was concluded that movement of the cavity wall due to shrinkage is only important in lab-scale process and can be neglected for larger scale process. Their results further indicate that the cavity growth is controlled by the rate of $O_2$ transfer to the cavity wall, when flame is located at the char surface. If flame is in the gas film, CO$_2$ and steam gasification determine the cavity growth rate. Abdel-Hadi and Hsu [15] extended previous coal block models by developing pseudo-2-D geometry with a moving burn front. Perkins and Sahajwalla [16, 17] used the CFD software FLUENT to describe UCG process in a 1-D coal block. This model is an extension of Tsang’s model [6] through the inclusion of multi-component diffusion and random pore model to account for the change of heterogeneous reaction rates with conversion. They have proposed that cavity growth occurs at reducing conditions, therefore only heterogeneous gasification reactions are solved and required heat is provided by defining a constant temperature at the char surface. They assumed that solid and gas phases are in thermal equilibrium and bulk gas has a fixed composition that is representative of the
product gas. Various experiments of pyrolysis and drying of large coal particles are used for model verification and an excellent agreement were reported. However, applicability of the model is limited and cannot be used to predict performance of UCG process because of the unphysical assumptions such as constant temperature at and fixed gas composition at the boundary. Results of their parametric study indicate that temperature of the coal surface, water influx and coal composition have the highest impact on the cavity growth rate. Nourizadeh et al. [18] developed a 3-D model using the reservoir simulation software CMG-STARS based on the finite-difference method. They have introduced an arbitrary clay layer in the seam to investigate effect of inert layers on the process; however thermo-mechanical failure of this layer is not included in the model. Chemical reactions and conduction/convection of heat and species were included in the model. The results reveal a large degree of grid dependence and not validated properly. Further, the model was extended to simulate CRIP with successive ignition points [19]. However, again no validation or comparison with the experimental results was reported.

2.3. Channel models

The UCG process, in this approach, is represented by an expanding channel when two distinct zones of rubble/char and open channel exist. Channel regime could dominate the process at a later stage. Figure 4 shows the basic concept and the underlying physics [17]. Air or O$_2$ flows down the central channel and is transported by turbulent flow to the boundary layer along the channel wall. The O$_2$ diffuses through the boundary layer to the solid surface and reacts. The hot combustion gases diffuse back through the boundary layer to the channel. Magnani [20] developed a 1-D channel model with a fixed diameter, assuming that neither axial nor radial diffusion exists, and there are constant axial convection, two reactions of char oxidation and Boudouard reactions, constant reaction rates, and only axial heat transfer in the solid phase. This model was used to investigate gas composition and temperature profile trends along the channel. Pasha and Farouq-Ali [21] improved the shortcomings of Magnani [20] by including radial and axial diffusion and heat transfer in the solid phase, variable gas velocity and channel diameter.

![Figure 4. Reactions and Transport phenomena in channel model [17]](image)

Dinsmor et al. [22] developed a steady-state 2-D model by assuming that the gasifier is a cylindrical channel with reactions occurring at the walls. Mass transfer correlations were calculated based on the turbulent flow in pipes. It was concluded that the operation of UCG in the channel regime is undesirable and would lead to a decrease in the gas heating value due to the bypass of O$_2$. In this model, larger channels would lead to lower velocity and Reynolds number, which in turn decreases the mass transfer by forced convection. The growth rates obtained from simulation were found lower than
the earlier field trials. However, the model was able to highlight the importance of natural convection in channels, which increases the heat and mass transfer. The effect of natural convection in cavity growth was first considered by Eddy and Shwartz [23] through a 2-D model. They described the evolution of the cavity based on the movement of the cavity wall. All reactions are assumed to occur at the wall under a constant temperature condition. Transport of heat and species inside the cavity is governed by empirical correlations. The results indicated that the natural convection is several orders of magnitude higher than the forced convection. The model was able to reproduce the results of Hanna II and Pricetown field trials qualitatively. Later, Luo et al. [24] extended the model by including the heat transfer and coal wall reactions. Flow inside the cavity is solved following the irrotational fluid flow inside an enclosure (Figure 5). FLUENT was used to predict the cavity shape in different times based on the heterogeneous reaction rates at the cavity wall. The model was validated with Chinchilla and Hanna II results [24]. This model predicts hemispherical cavity geometry, however, its use is limited since heat and mass transfer characteristics are unknown. Also, the coupling of this model with the mechanical failure of coal would be cumbersome as the accumulated rubble changes the transport characteristics inside the cavity.

![Figure 5. UCG cavity defined in the work of Luo et al. [24]](image)

At thin seams, failure of the overburden has a major effect on the process. Such a failure would create open channels; as shown in Figure 6. Various models have so far been developed to describe the process in these channels.

![Figure 6. Channel formation in thin seams [28]](image)

Pirlot and co-workers [25, 26] developed a 1-D steady-state channel model with two distinct zones: high and low permeability rubble. Heat and mass transfer were calculated from empirical equations of packed bed concept. Reaction rates of the gas phase were written for an ideal plug flow. Coal
consumption rate was calculated on the channel wall. The model was further extended to 2-D to simulate the cavity growth and shape. Batenburg et al. [27] developed a steady 2-D model for UCG in open channels. Reaction rates were calculated based on resistances in the system including boundary layer, pore diffusion, surface phenomena and chemical kinetics. Heat transfer was addressed by radiation between walls of channel. The effect of natural convection was also included in their model. Results indicated that natural and forced convection are equally important. Kuyper [28, 29] developed a 2-D model (Figure 7) to describe the UCG process in a cross-section of an open channel. The k-ε turbulence model was used to describe the fluid flow and the heat transfer was governed by radiation and convection. Results showed that O₂ is consumed far from coal wall by combustible gases. Double-diffusive natural convection would cause periodic generation and collapse of CO₂ bubbles. Also, mass transfer is reported to be the controlling mechanism for reduction reactions at coal wall. They also investigated the effect of CO₂ injection into the coal seam and reported that it has similar effect as adding steam; although to a lesser extent.

![Figure 7. Channel geometry in Kuyper’s model [29]](image)

Perkins and Sahajwalla [30] extended Kuyper’s model [28, 29] by including an ash layer at the lower part of the channel. The axi-symmetric model is used to investigate natural convection along with relevant reactions in a partially filled cavity (Figure 8). Flow was assumed to be laminar in the ash zone and turbulent in the void space. They concluded that O₂ should be injected at the bottom of the channel, otherwise, valuable gasification products would be oxidized leading to low heating value of the production gas.

![Figure 8. Channel geometry in Perkins and Sahajwalla [30]](image)

2.4. Other approaches for UCG modelling

2.4.1. Reactor models
In this approach, the UCG process is described as a series of ideal reactors. Such models can be used to predict product gas composition without considering the complex phenomena occurring underground. Chang et al. [31] used this approach to predict the resource recovery during UCG process. In this model, the domain is divided into cylindrical elements, where each element consists of two distinct zones: rubble and void. It is assumed that the rubble zone acts as an ideal Plug Flow Reactor (PFR), while void space is assumed to be perfectly mixed modelled as a CSTR. The spalling
and water influx are calculated based on the empirical correlations. The results revealed the importance of turbulent transport in field trials. Some researchers have used the response of tracer material to characterize various zones in the underground cavity and track the cavity growth. Based on the residence time of tracer elements, cavity is modelled as an arrangement of ideal reactors. Debelle et al. [32] used different chemical engineering reaction models to fit the quasi-exponential decay of tracer response. Different stages of the process such as reverse combustion linking and forward gasification were represented through regression models. For gasification period, it was observed that cavity offers a high level of back-mixing, resembling a well-mixed reactor with a small dead zone. Thorsness [33] performed tracer experiments to explore the extent of water influx and steam injection requirements. Pirard et al. [34] used helium tracer and found that cavity behaves almost like a small number of CSTRs in series with high level of back mixing. Daggupati et al. [35] described the cavity as series of ideal reactors (Figure 9). Residence Time Distribution (RTD) of gases was calculated based on the CFD results. This approach has been validated by laboratory-scale tracer experiments. They summarized that as the cavity size increases, cavity behaviour changes from PFR to CSTR.

Figure 9. Reactor arrangement for cavity in works of Daggupati et al. [35]

2.4.2. Probabilistic simulation
Batenburg and Bruining [36] adopted probabilistic simulation to describe forward gasification in 2-D UCG geometry. The model uses stream function on the grid blocks. The derivative of the stream function along ash-char interface is interpreted as the possibility that interface is moving in a certain block. The applicability of this model is very limited since the temperature of the gases and composition are considered constant in each region. Biezen et al. [37] extended the concept by including movement of several interfaces including ash-void, ash-coal, void-coal, and void-rock (Figure 10). The model consists of two modules: one module solves flow in the entire domain and the other selects a block of coal/rock for gasification or spalling. A single streamline is selected randomly and based on the interface located on the streamline, relevant physical phenomena proceeds. They later extended their model to simulate cavity evolution in a 3-D domain [38]. This model is used to simulate the development of gasifier from early times to a developed stage. Application of this model is limited due to its complex nature and certain unphysical assumptions such as constant temperature at each domain.

2.4.3. Process models
All of these reviewed modelling efforts so far have the deficiency of focusing on some aspect of the UCG process, while neglecting others. During UCG trials in US, LLNL funded many modelling studies for UCG process. Several 1-D models were developed and validated with certain series of data from field trials. These segregated models were later combined together to form the CAVISM process model that represents 15 years of continuous UCG research and development in US [39]. The model is applicable for predicting lateral cavity growth of thick and shrinking coal seams in which O₂ is injected at the bottom of the coal seam. The model is based on some major assumptions such as:
cavity is axisymmetric around injection; thermal radiation is the main heat transfer mechanism in well-mixed void space; cavity growth is dominated by thermo-mechanical failure of wall and a packed bed of char and rubble forms over a thin layer of ash. Various sub-models were added into this model to quantify water influx, flow dispersion through a rubble bed, sidewall growth of cavity due to reactions, and spalling of cavity roof into the domain. This model has reproduced results of some of the field trials in US. Therefore, the model could not be used in other seams, as these parameters are not known \textit{a priori}.

![Figure 10. Probabilistic simulation of UCG process by possibility of movement of following interfaces: 1. Void-Rock; 2. Coal-Rock; 3. Void-Coal; 4. Void-Ash; 5. Ash-Void. [38]](image)

3. UCG studies in India

India has a vast coal reserve which are the fourth-largest in the world, primarily of low grade. UCG may be a very promising technology for such coal reserves in India, to reduce the dependency on the oil and gas imports. UCG is expected to be used to utilize India’s large coal reserves, which are difficult to extract economically using the existing conventional technologies. The Government of India constituted a National Committee on UCG taking experts from the University of Bombay, Ministry of Petroleum, Planning Commission, ONGC, CIL/CMPDI, CIMFR (the then CMRS and CFRI), ABE, EIL and IIT Kharagpur in July 1984. A protocol for UCG development was also signed between the Government of India and the Government of erstwhile USSR in 1981. It was also decided that UCG prospect evaluation for coal seams of less than 300m depth would be handled by ONGC. Gautam and Singh [40] have presented a summary of Indian efforts.

As UCG technology for intermediate depths had already been experimented and commercialized in other countries, therefore, pilot project in India was designed to acquire relevant technology at greater depths. Area chosen was near Mehsana city in North Gujarat province where large coal reserves of about 63 billion tonnes at depths ranging from 700 to 1700 m exist. The study covered an area of about 6.7 sq km having an average thickness of coal seam of 15 m. The recoverable energy from these reserves in the form of gas was estimated to be equivalent to 15,000 BCM of natural gas. ONGC drilled 2 pilot wells UCG-1 and UCG-3 for evaluation of the rock characteristics, sub-surface strata conditions and quality of coal. Coal cores retrieved were analysed for various parameters. Of the 15 coal horizons encountered, 11 coal horizons were of thickness more than 1m occurring between 745-941 m of depth. The cores recovered from a depth of about 852 m were highly fractured. Oil traces were observed along these fractures. The coals were high moisture, high volatile, low rank non-caking lignitious type having carbon content (dry ash free basis) between 72 and 76% but somewhat higher hydrogen content compared to other lignite deposits in India. Appreciable quantities of methane content varying from 1 to 6 m$^3$/t were observed in the coal cores. Keeping in view the geohydrological conditions and roof and floor characteristics, Shobhasan-III seam was identified as the most suitable coal seam for in-situ gasification. However, further studies on the subject have not been made since then. Recently ONGC has signed an MOU with Stochinsky Institute of Mining, Russia for taking up UCG projects in India. ONGC has also signed an MOU with Coal India Limited and another with the Singareni Collieries Company Limited. It is likely that ONGC would very soon enter into an MOU.
with Gujarat State Petroleum Corporation for cooperation in developing and applying the UCG technology. The Ministry of Coal, Government of India, has awarded an S&T study project to the Neyveli Lignite Corporation.

Recently, CFD based studies of complex flow patterns in a developing UCG cavity were conducted by researchers from IIT-Bombay in collaboration with ONGC [41]. The main objective of this work was to understand the velocity distribution and perform residence time distribution (RTD) studies in the UCG cavity. Based on the RTD studies, the actual UCG cavity at different times was modeled as a simplified network of ideal reactors, which might offer a computationally less expensive and easier option to determine UCG process performance as a function of time. In another effort, Chatterjee and co-workers [42] conducted a comprehensive three-dimensional numerical study to understand the hydrodynamics within a given cavity size which would give us a relatively quick but reliable insights into the process. Five different cavity sizes were considered inside which the complete turbulent transport was simulated. Apart from the usual vertical and horizontal injection, the effect of inclined injection on the hydrodynamics was also reported in their study for the first time. The numerical simulation was performed by using a commercial CFD package Ansys Fluent [44].

![Diagram of UCG cavity](image)

**Figure 11.** Geometry of UCG cavity in [42]

4. Summary

Although several numerical models involving varying levels of complexities have been published over the past years, applicability of these models is limited to some specific and isolated cases only and the models could hardly be generalized to predict the performance of the practical UCG trials. Furthermore, most of these models are in the 1-D or 2-D framework. Even the 3D models developed thus far are very simple and did not consider the details of the physical and chemical models. Also, the fluid flow is laminar in early stages of the process while changes to turbulent in a developed channel. Turbulence would arise from natural convection due to thermal and solutal gradients in the cavity. Developed models are meant to simulate one of these stages and could not be used in these two conditions. Hence, the future focus should be dedicated towards developing a model in a 3-D
framework including all the factors affecting the performance of the UCG and can correctly reproduce the practical UCG field trials.

![Diagram of flow dynamics](image)

**Figure 12.** Flow dynamics (pathlines) colored by velocity magnitude (in m/s) at different time steps and different nozzle orientations in [42]

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Acknowledgments
The materials in this review paper are taken from several published works. The author sincerely acknowledges all these contributions. Special acknowledgement to Ahad Sarraf Shirazi (MS Thesis, University of Alberta, 2012) and Mojtaba Seifi (PhD Thesis, University of Calgary, 2014) in this regard. Financial support from CSIR (Govt. of India) through network project (no. ESC0302/05) is gratefully acknowledged.