Process modelling and simulation of underground coal gasification: A Review of work done at IIT Bombay

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Abstract. This paper presents the summary of the work performed over the last decade, at IIT Bombay by the UCG group. The overall objective is to determine the feasibility of a given coal for underground coal gasification and then determine the capacity of a single pair of well through modelling and simulation. It would help one to design a UCG facility for the desired rate of gas production. The simulator developed in this study seeks inputs on four important aspects: Kinetics of all the reactions under the conditions of interest, heat and mass transfer limitations, if any, the flow patterns inside the cavity and lastly the thermo-mechanical failure of the coal. Each of them requires detailed studies in laboratory. Indian Lignite from one of the reserves was chosen as a case study.

1. Introduction

Underground coal gasification is an in-situ process of synthesis gas generation which utilizes deep coal reserves (Figure 1) that are otherwise difficult to mine. India has many such coal reserves and a comprehensive review on the same has been published elsewhere [1]. In UCG process simultaneous combustion and gasification of coal are performed in the presence of gases (oxygen, steam) to generate syngas which finds its application in power generation, nitrogenous fertilizers, petrochemicals, liquid fuels and many such industries. The operation involves drilling of injection and production wells at an appropriate distance. The reagent gases are injected through the injection well into the coal seam. A cavity is formed underground and various gas phase and gas-solid reactions take place. Thus UCG process can be divided into four main steps namely: Drilling, linking, ignition or combustion and gasification.

UCG cavity is a 3-D reactor whose geometry is irregular and is associated with highly non-ideal flow patterns and also the strong interaction between several other chemical and physical processes like chemical reactions, heat and mass transport phenomena and spalling. Water influx further increases the complexity of the process. UCG is a site-specific process and the scope for adjusting the parameters is limited. Thus the development of predictive tools which can determine the behaviour of a UCG reactor under different physical and operating conditions and thus help in control and optimization of the process becomes a need of the day.

This paper summarizes the major contributions and significance of experimental and simulation studies performed at IIT Bombay in collaboration with ONGC over the last decade to develop model which predicts the performance of a UCG process by taking into account the various phenomena which affect the process thus influencing the quality and quantity of product gas [1-11]. Indian Lignite from one of the reserves was chosen as a case study.

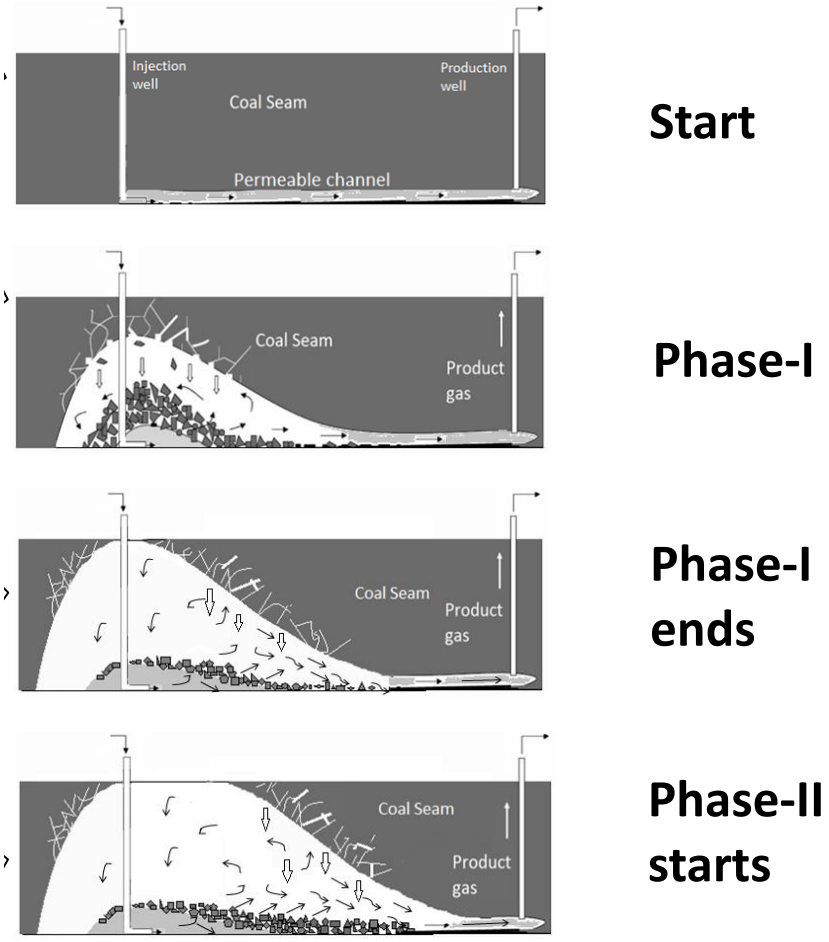

Figure 1. Underground Coal Gasification Process [2]

2. Methodology for model development

The input and output information associated with the simulator developed is shown in figure 2. Model inputs associated with kinetics, heat/mass transfer and spalling have been determined for the coal of interest.

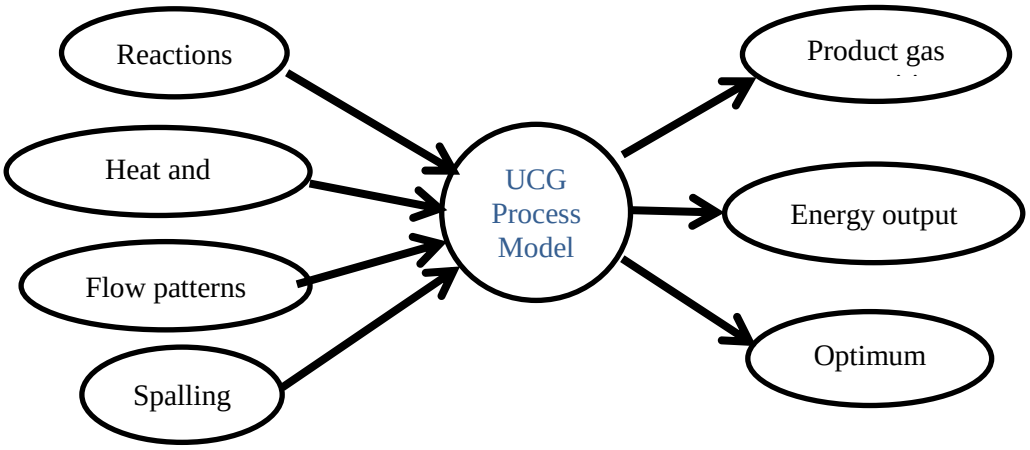

Figure 2. Input and output information for process model [10]

To determine reaction kinetics, laboratory data was generated under UCG-like conditions. Similarly, correlations for heat and mass-transfer coefficients and appropriate spalling (thermo-mechanical failure) parameters were determined for flow and thermal conditions in the UCG geometry [11]. Unlike other parameters, spalling characteristics are expected to be scale-dependent, and therefore these parameters might require tweaking for simulation of field scale experiments. To study the importance of flow fields inside the UCG cavity computational fluid dynamics (CFD) simulations were performed. Based on the detailed study of each one of these inputs the model is developed and the performance is simulated.

2.1 Reaction Kinetics

The steps involved in conversions taking places in UCG cavity are drying, pyrolysis and chemical reactions like combustion, gasification (table 1) and the kinetics of these reactions should be experimentally determined [4, 5].

Table 1. Main Reaction involved in UCG process

Reaction name	Reaction
Drying	$H_2O_{(l)} \overset{heat}{\Longrightarrow} H_2O_{(v)}$
Pyrolysis	$CH_aO_b \overset{k_{f,p}}{\Longrightarrow} a_1C + a_2CH_4 + a_3H_2O + a_4CO + a_5H_2 + a_6CO_2 + a_7C_9H_c$
Char combustion	$\mathrm{C} + \mathrm{O_2} \overset{\mathrm{k_{f,1}}}{\Longrightarrow} \mathrm{CO_2}$
Steam gasification	$\mathrm{C} + \mathrm{H_2O} \overset{\mathrm{k_{f,2}}}{\Longrightarrow} \mathrm{CO} + \mathrm{H_2}$
Boudard reaction	$\mathrm{C} + \mathrm{CO_2} \overset{\mathrm{k_{f,3}}}{\Longrightarrow} 2\mathrm{CO}$
Methanation	$C + 2H_2 \overset{k_{f,4}}{\Longrightarrow} CH_4$
Water-gas-shift	$CO + H_2O \overset{k_{f,5}}{\Longleftrightarrow} CO_2 + H_2$
Gas-phase oxidation	$H_2 + \frac{1}{2}O_2 \overset{k_{f,6}}{\Longrightarrow} H_2O$, $CO + \frac{1}{2}O_2 \overset{k_{f,7}}{\Longrightarrow} CO_2$, $CH_4 + 2O_2 \overset{k_{f,8}}{\Longrightarrow} CO_2 + 2H_2O$
Tar-reforming	$C_9H_c + 9H_2O \rightarrow 9CO + \left(9 + \frac{c}{2}\right)H_2$

Kinetics of char combustion cannot be determined from usual thermo-gravimetric analysis because it is a fast reaction and also the size of coal seam is very large as compared to the size of sample used in TGA. Hence, to overcome this problem a novel reactor setup to determine the fast reaction kinetics was designed which was then used to formulate a kinetic sub-model. Kinetics of other heterogeneous reaction like steam gasification and CO_2 gasification was also studied using specifically designed TGA. To model gas-solid non catalytic reactions a new expression for effectiveness factor in case of random pore model was proposed as given in equation 2.1.4. The rate of reaction by random pore model is given by:

$$\text{rate} = \mathrm{k} * \mathrm{C_{gas,S}} * \mathrm{C_{Char,0}} * (1 - \mathrm{X}) * \sqrt{1 - \psi * \log(1 - \mathrm{X})} \quad (1)$$

Where,

$\boldsymbol{\psi}$ = structural parameter in random pore model

X = local char conversion

The time scales for diffusion and for changes in surface area and effective diffusivity are much different. This constancy of the surface area and that of effective diffusivity are thus considered to get

an expression for Thiele modulus. Later the gas balance equations are solved taking the surface area and effective diffusivity as a functions of solid concentration.

$$M_T = \frac{d}{6} * \sqrt{\frac{k * C_{Char,0}}{D}} \quad (2)$$

$$\eta = \frac{1}{M_T}\left(\frac{1}{\tanh(3M_T)} - \frac{1}{3\,M_T}\right) \quad (3)$$

$$rate = \eta * k * C_{gas,S} * C_{Char,0} * (1 - X) * \sqrt{1 - \psi * \log(1 - X)} \quad (4)$$

This methodology is validated by comparing results with complete diffusion-reaction modeling on a spherical particle [10].

2.2. Flow Patterns

Virtual studies of residence time distribution were performed [2, 6] based on CFD for characterization of non-ideal flow patterns in irregular UCG cavity (figure 3). It may be noted that the basis of the cavity shape comes from the visual observations of cavity formed in several lab scale UCG experiments performed over a small coal block [6].

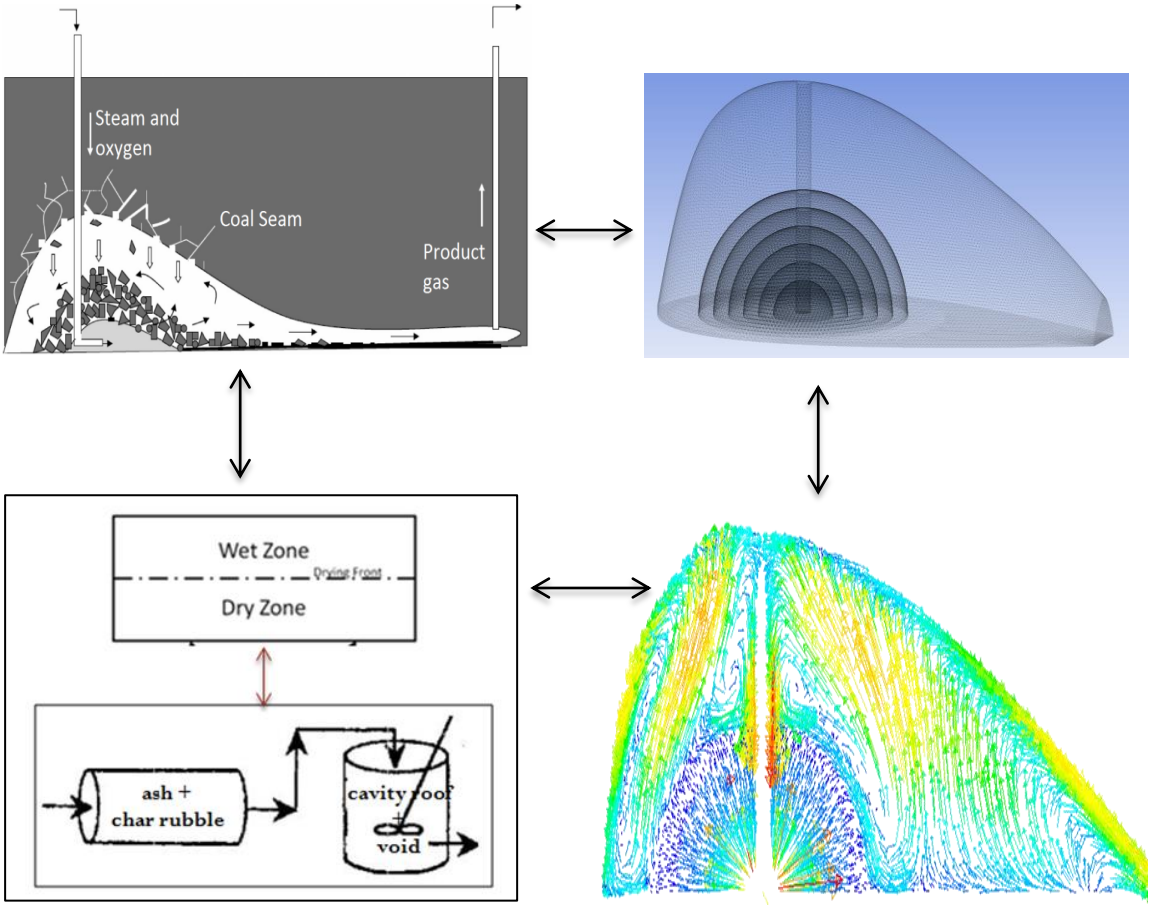

Figure 3. Virtual RTD studies to determine flow patterns and proposed compartment model [10]

The determination of flow patterns in various conditions reveals that one can approximate the cavity as a simplified compartment model that includes Plug flow reactor (corresponding to the rubble fallen on the ground) and the CSTR for the gas flow in the void space of the cavity(Phase-I). Outflow

channel may be assumed as a series of CSTRs (phase-II.). Phase-I concentrates on the vertical growth of cavity till it reaches the overburden after which starts the phase-II where horizontal growth of cavity occurs till it reaches the production well. Compartment modelling simplified the computational intensiveness many fold and made predictions faster. It may be noted that the basis for the shape of cavity comes from several laboratory experiments performed on smaller coal blocks. For details, one can refer the work by Daggupati et al. [6].

2.3. Heat and Mass transfer

The various heat and mass transfer interactions considered during modelling are shown in figure 4. Different modes of heat transfer viz radiation, convection and conduction were considered and appropriate correlations for heat and mass transfer were used in energy and mass balance equations for both gas and solid species in different zones [11].

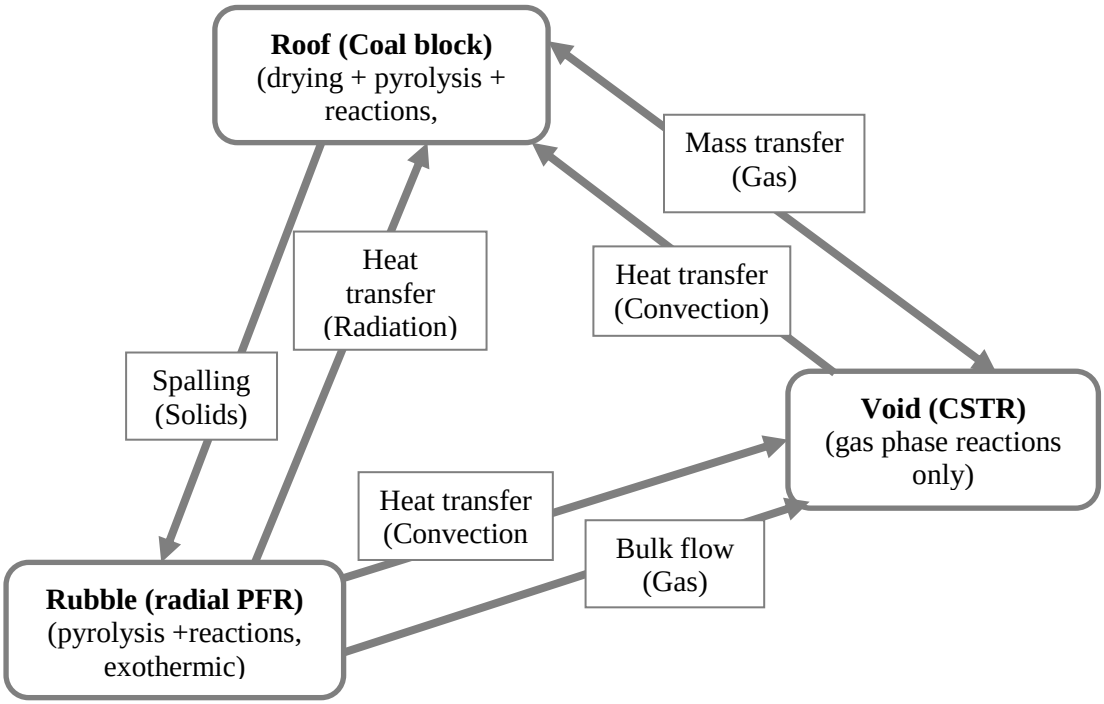

Figure 4. Heat and mass transfer interactions in UCG cavity [2]

2.4. Thermo-mechanical failure (Spalling)

Here, we determined the rate at which the coal/char particles detached from the roof of the cavity and fell on the floor. Rate of spalling is an important parameter because spalling is responsible for creating large external surface for the important gas-solid reactions taking place in the cavity and outflow channel. Thus higher the rate of spalling, higher will be the overall rate.

A special apparatus is designed and fabricated to measure the rate of spalling for the given coal (figure 5). The main part of the apparatus was a furnace in which UCG like conditions were replicated with a plate type heater at the bottom surface of its heating chamber. The heating chamber has inlet and outlet ports for the gas. A coal block holder made up of stainless steel (SS-410) was placed in the chamber, with its bottom face exposed to the hot flowing gas and thermal insulation on all other sides.

This holder was hung from a load cell that was placed outside the furnace, to monitor the weight of the coal block. Figure 6 shows the results obtained from this experiment for the amount of spalled coal with time [8, 9].

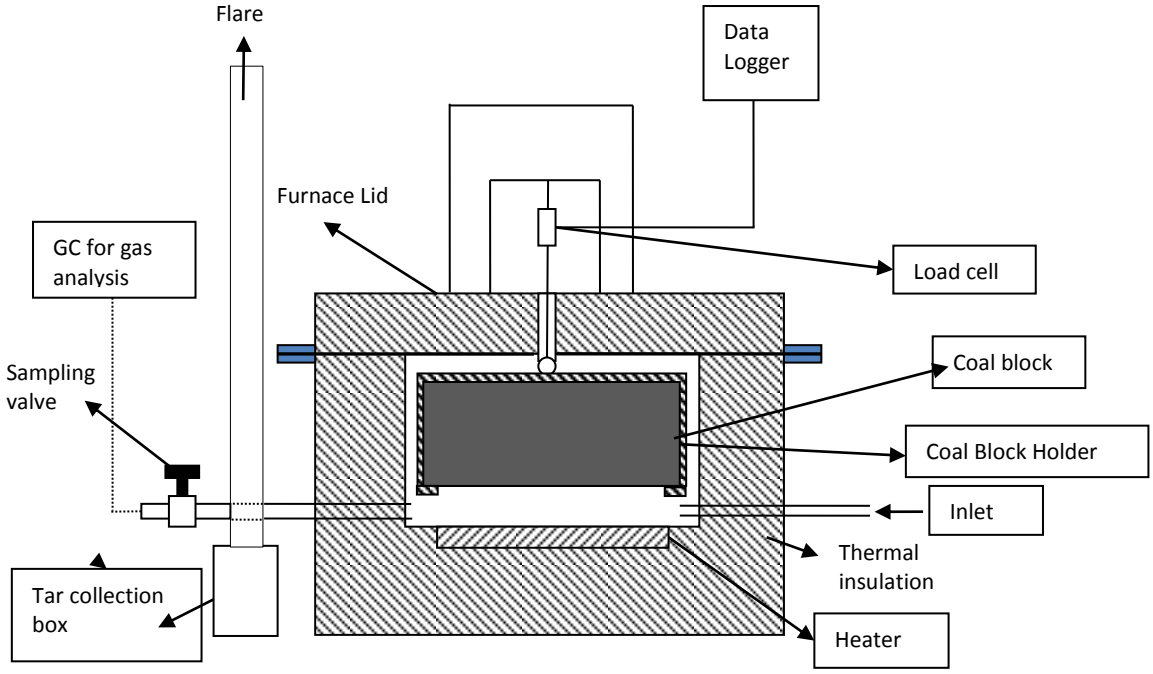

Figure 5. Schematic of the apparatus to measure spalling rate [9]

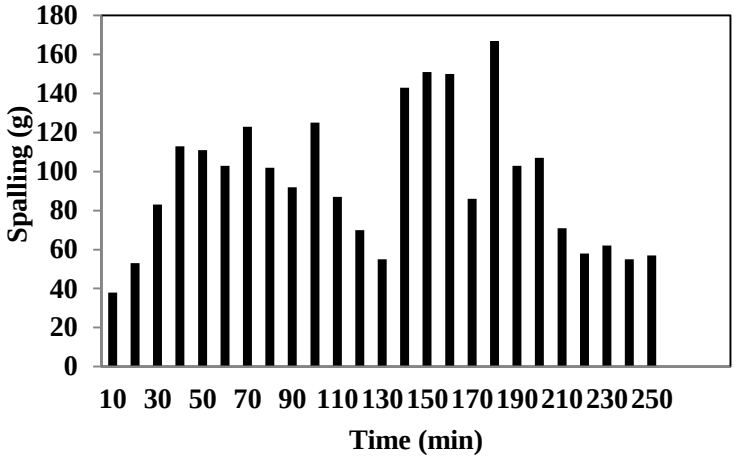

Figure 6. Amount of spalled coal particle with time [9]

It was also observed that the gas calorific value increases with spalling till a critical spalling rate but after that there is no effect. It is due to the reason that after critical spalling the surface available for reaction is large enough and the availability of reacting gas species becomes the limiting factor. The lignite coal of interest gives sufficiently high spalling rates so gas calorific value and exit gas composition were observed to be not so sensitive to a further change in the spalling rate. However, in other cases, where spalling rates are less, a significant impact on the product gas quality can be observed and it may control the performance of the system.

3. Process Model and simulation results

All the above inputs are provided to the process model, which as mentioned above, conceptualizes UCG as a set of multiple zones and compartments linked to each other through heat and mass streams. The model is a set of differential algebraic equations in time and space, and solved using in-house MATLAB program. The dynamic simulation of the model was performed varying the volume of reactor as a function of time based on the amount of coal consumed. With every spalling instance, the volume of rubble zone increases [2, 3].

Figure 7 shows temperature profiles in rubble zone at different times. After every spalling instance temperature in the rubble and roof zone changed due to relatively colder roof. Figure 8 shows plot of char density in the rubble with time.

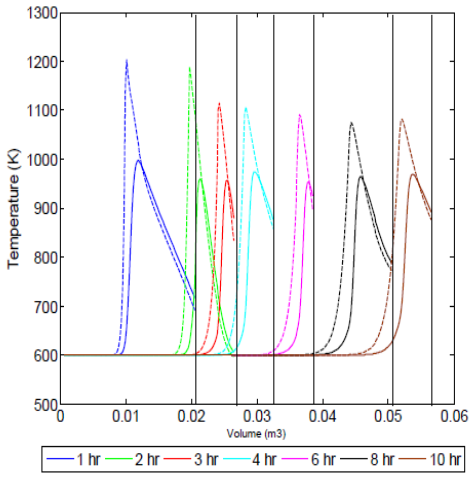

Figure 7. Temperature Profiles at different time [2]

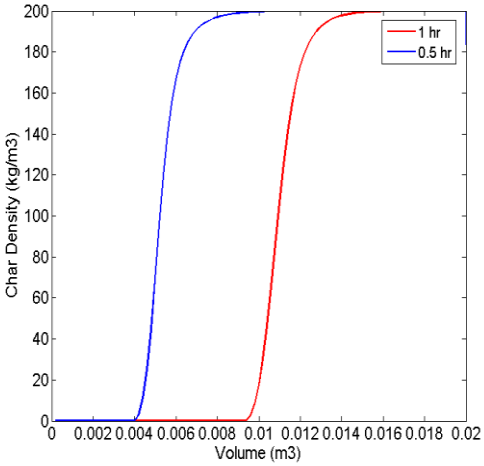

Figure 8. Char density at different times [2]

The change in calorific value with time as observed in the results is shown in figure 9 which shows change in calorific value at every spalling instance. Variation in exit gas mole fraction with time is shown in figure 10 which shows that between two spalling incidents the exit gas fractions remain in a fixed range. The results are validated experimentally with the help of laboratory-scale UCG experiments and the agreement has been satisfactory as shown in figure 11 and table 2. The simulator is computationally intensive and takes long time (20-30 hrs.) to converge to the solution. It is our future task to simplify the model without compromising on the quality of the results.

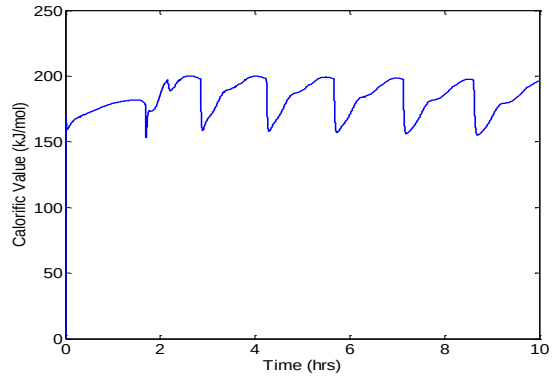

Figure 9. Calorific value of exit gas with time [2]

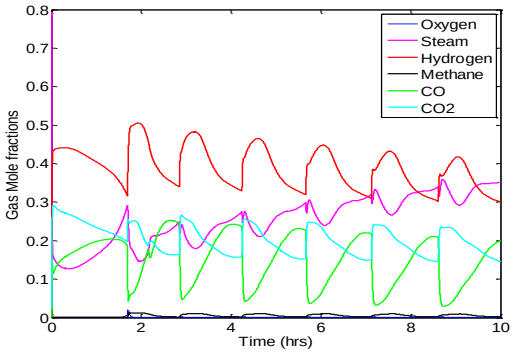

Figure 10. Exit-gas mole fractions with time [2]

Table 2. Comparison of the predicted cavity growth rate and the observed at lab-scale UCG [10]

Parameter	Lab-scale UCG	Process Model
Calorific value (kJ/mol)	~160	157
O_2 Flow Rate (kmole/min)	3.2 x 10^{-5}	3 x 10^{-5}
Total Volume Consumed (cc)	1000	1120

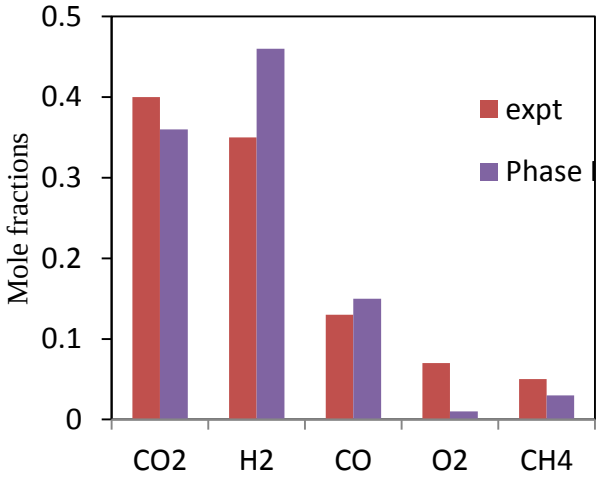

Figure 11. Comparison of experimental and simulation results for UCG results at steady state [10]

4. Conclusion

UCG process model needs inputs on kinetics, flow patterns, spalling and heat and mass transport behaviour of UCG cavity and outflow channel. The kinetic modeling is done for the heterogeneous reactions involved in the UCG process. To determine the kinetics of coal combustion, a novel reactor setup has been designed. Also a simplified procedure for determination of effectiveness factors for RPM kinetics is developed for the first time.

CFD studies were performed to characterize non-ideal flow patterns inside UCG cavity. Based on the flow patterns inside the cavity, compartment modelling approach was devised for different phases of growth of UCG cavity and the resulting model equations were solved for different zones. The attractiveness of this approach is in reducing computational burden and therefore providing faster prediction of the process performance. Spalling is an important phenomena and is responsible for generating large surface area to increase the reaction rates. The data on spalling is generated in laboratory and spalling rate was used as an input parameter. A critical spalling rate is the one beyond which the performance is insensitive to further changes.

The work provides a complete modelling solution for the UCG process. All the important chemical and physical processes have been considered in the model along with the phenomena of spalling and the model agreed well with the CFD and experimental studies performed. Efforts are being made to develop a simplified version of this model in order to reduce the computational time without compromising much on the quality of predictions.

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