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Effect Of Equivalent Ratio (ER) On the Flow and Combustion Characteristics in A Typical Underground Coal Gasification (UCG) Cavity

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ABSTRACT

Underground Coal Gasification (UCG) is one of the most favourable clean coal technology options from geological-engineering-environmental viewpoint (less polluting and high efficiency) for extracting energy from coal without excavating or burning it on the surface. UCG process requires injecting oxidizing agent (O_2 or air with steam) as raw material, into the buried coal seam, at an effective ratio which regulates the performance of gasification. This study aims to evaluate the influence of equivalent ratio (ER) on the flow and combustion characteristics in a typical half tear-drop shape of UCG cavity which is generally formed during the UCG process. A flow modelling software, Ansys FLUENT is used to construct a 3-D Computational Fluid Dynamics (CFD) model and to solve flow hydrodynamics in the cavity. The boundary conditions are- (i) a mass-flow-inlet passing oxidizer (in this case, air) into the cavity, (ii) a fuel-inlet where the coal volatiles are originated and (iii) a pressure-outlet for flowing the product synthetic gas (syngas) out of the cavity. A steady-state simulation has been run using k-ε turbulence model. The mass flow rate of air varied according to an equivalent ratio (ER) of 0.16, 0.33, 0.49 and 0.82, while the fuel flow rate was fixed. The optimal condition of ER has been identified through observing flow and combustion characteristics, which looked apparently stable at ER 0.33. In general, the flow circulation mainly takes place around the ash-rubble pile. A high temperature zone is found at the air-releasing point of the injection pipe into the ash-rubble pile. This study could practically be useful to identify one of the vital controlling factors of gasification performance (i.e., ER impact on product gas flow characteristics) which might become a cost-effective solution in advance of commencement of any physical operation.

1. Introduction

Underground coal gasification (UCG) is an unconventional industrial method and a thermochemical process of harnessing energy by converting coal in place into combustible product gas. This is known as syngas, a high quality yet a low-cost synthesis gas produced through partial oxidation. UCG is considered favourable for seemingly un-mineable coal (from the point of uneconomical, especially those which are too deep lying at >300 m, low grade, or very thin) with

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minimal surface disturbance [1,2]. Thus the technology becomes lucrative being the more efficient alternative to conventional underground mining.

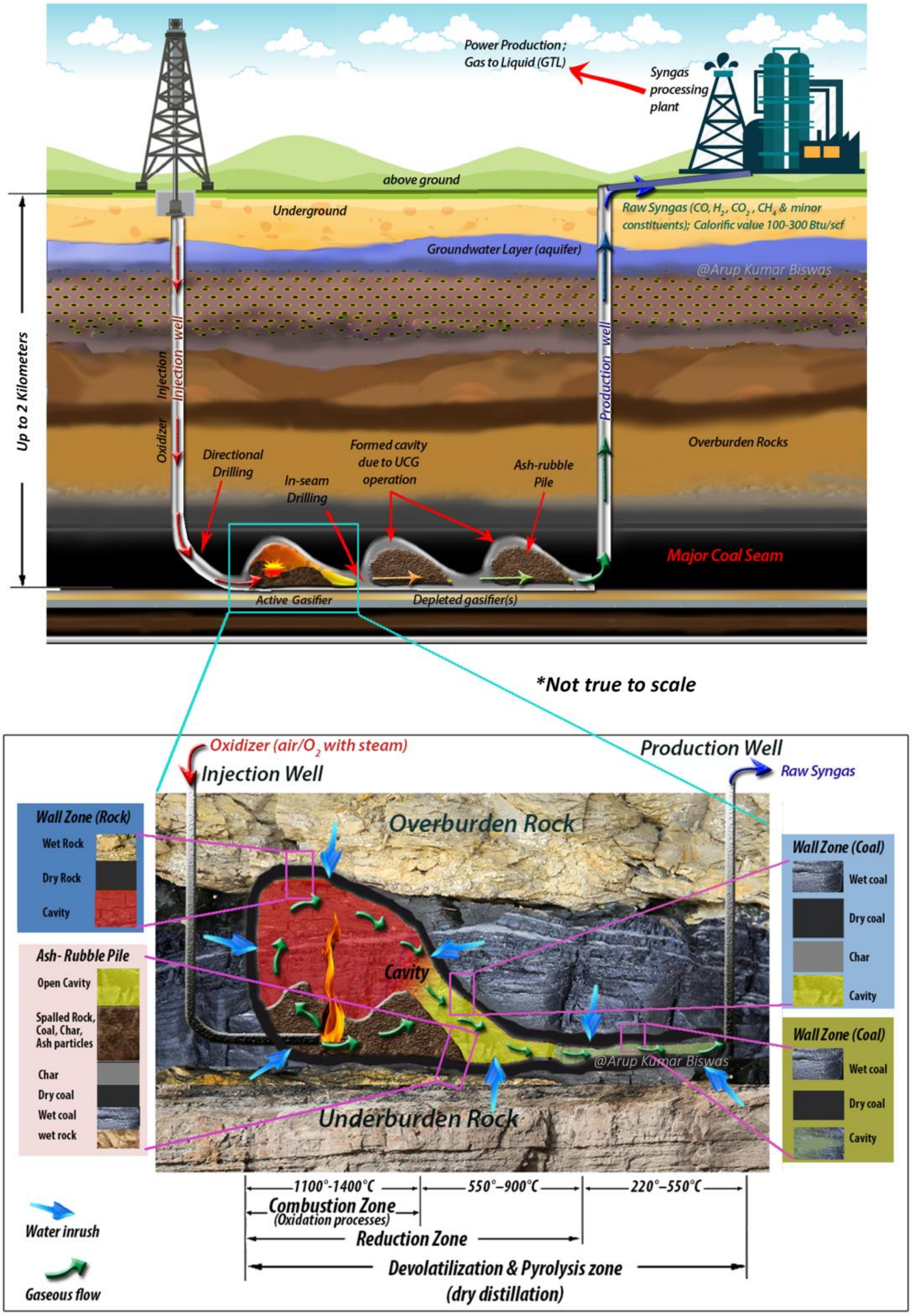


Fig. 1. Schematic of Underground Coal Gasification (UCG) process; *(top)* above ground and underground setup with active and depleted (burnt) gasifiers (formed cavity inside the coal seam); *(bottom)* a typical cavity configuration at a mid-to-late stage of a CRIP (Controlled Retracting Injection Point) module involving distinct physical/chemical-process domain, including ash-rubble zone, in conjunction with the wall zones for both coal and adjacent rock

The process only requires drilling of injection and production wells from surface to the target coal seam. A permeable channel is created between those wells to facilitate a syngas flow-path within the coal seam (Figure 1) [3].

An underground coal gasifier performs complex physico-chemical processes. Chemical processes, occurring in three zones (Figure 1), involve combustion (partial oxidation), reducing reactions leading to gasification and pyrolysis-drying (destructive distillation) simultaneously. Main physical changes taken place, are dewatering, cracking, absorption and contraction of coal with high water content [4–9].

Due to coal combustion fractures develop in surrounding rocks leading to a high temperature cavity formation in the subsurface and grows three dimensionally into the coal seam as the UCG process continues [10,11]. Coal from the surrounding cavity wall is spalled (detached and fallen on the floor into pieces) during gasification process and the cavity gradually appears to be a three-dimensional half teardrop shaped geometry as shown in Figure 2 [12-15]. Thus, the phenomena of thermo-mechanical spalling are responsible for exposing fresh coal to sustain the gasification and increase the reaction rates.

As the feed materials, an oxidant (O_2/air) and steam are only injected for the gasification process to sustain. The gasification performance is predominantly dependent on their effective proportion called equivalence ratio (ER) [16]. Noteworthy, this work focused numerically on the effect of ER in a predefined UCG cavity.

The choice of oxidizer, whether it is O_2 or air, has direct impact on the quality of produced syngas regarding the composition and heat value. Effect of oxidant has been studied by a number of researchers suggesting that using oxygen is preferable over air as oxidant for achieving higher calorific value and higher proportion of potentially useful gases, such as hydrogen, carbon monoxide and methane [17-19]. In this study, however, air has been used as gasification agent for simulating UCG as because the quality of syngas is out of the scope of this research.

The product gas contains high percentage of CO and H_2 (cumulative sum may reach up to 85%) and CO_2 (sometimes may be present up to 40%) with minor CH_4 and higher hydrocarbons, traces of tars and pollutants [20–22]. In UCG process, residual ash is kept sealed within the reservoir. Alina Żogała [22] summarized that temperature raise in UCG reactor increases H_2 and CO concentration as well as higher calorific value in the product gas, while enhancing pressure results in the boosting of CO_2, N_2, H_2O, CH_4. Syngas can be utilized as raw materials for producing chemicals, e.g., fertilizers, ammonia, methanol, hydrogen, SNG (synthetic natural gas), etc. or to generate electricity.

Several studies investigated the effect of ER on gasification performance. Most of those experiments were held in conventional gasifiers operating on surface. Typical surface gasifiers are Fixed-bed, Fluidized bed and Entrained flow gasifier. Liu *et al.,* conducted 3-D CFD simulation of a Circulating Fluidized Bed (CFB) for biomass gasification. The study described steady state model to study effects of turbulence model, radiation model, water-gas shift reaction, and ER to achieve thorough result of feedstock gasification in a CFB reactor [24]. Hassan [24] assessed the effect of ER on syngas composition in a biomass gasifier and the effective operating temperature for achieving optimum heating value of dry gas.

Daggupati *et al.,* [25] conducted compartment modeling for flow characterization of UCG cavity, which grows three dimensionally in a nonlinear fashion as gasification proceeds. They ascertained that the cavity shape is predominantly determined by the flow field, being the function of different parameters (e.g., inlet position and orientation), temperature distribution and coal properties (e.g., thermal conductivity). Debelle *et al.,* [26] modelled the flow at Thulin UCG experiments. The hydrodynamics of the flow profile inside the underground reactor were deduced, where the results exhibited little evolution of the flow conditions inside the underground reactor during the series of reverse combustion tests.

ER study related to gasifying coal in the subsurface (i.e., UCG) is relatively rare. In UCG cavity, the interaction of internal flow of gasification agent and syngas needs to be understood. In this work, ER effect on flow and combustion characteristics in UCG cavity have been simulated using CFD besides assessing the impact on the gas production.

2. Physical Problem and Formulation of Simulation

Development of a complete UCG process model involving the thermal transport and chemical reactions would demonstrate the phenomena occurring underground and predict the product gas quality. However, in the present study a simplified three-dimensional modelling approach facilitates the flow visualization inside a typical UCG cavity. Thus, this simplified hydrodynamic analysis helps to determine the steady state flow patterns, as such presenting valuable insights into the flow physics involved in the process. A conceptual framework of a representative UCG cavity has been developed (Figure 2) for the physical and chemical states that are modelled to attain the solution.

2.1 UCG Cavity Geometry

A 3-D numerical domain has been constructed for simulating UCG cavity (Figure 2). The domain geometry is considered as a half teardrop shape, reported earlier by several researches [26,28–30]. The dimension of the cavity is 85 cm in width, 55 cm in height and 210 cm in length. A 5 cm diameter vertical pipe is located at the center of the domain to inject oxidizer/gasification agent (in this case, air). During gasification process, burnt coal from surrounding the cavity wall/ceiling is detached/spalled on the floor with ash, creating the ash-rubble pile which is accumulated around the injection pipe. This ash-rubble pile is considered as a dome shape of 55 cm diameter residing at the bottom of the domain and behaves as a porous medium with 50% porosity [13].

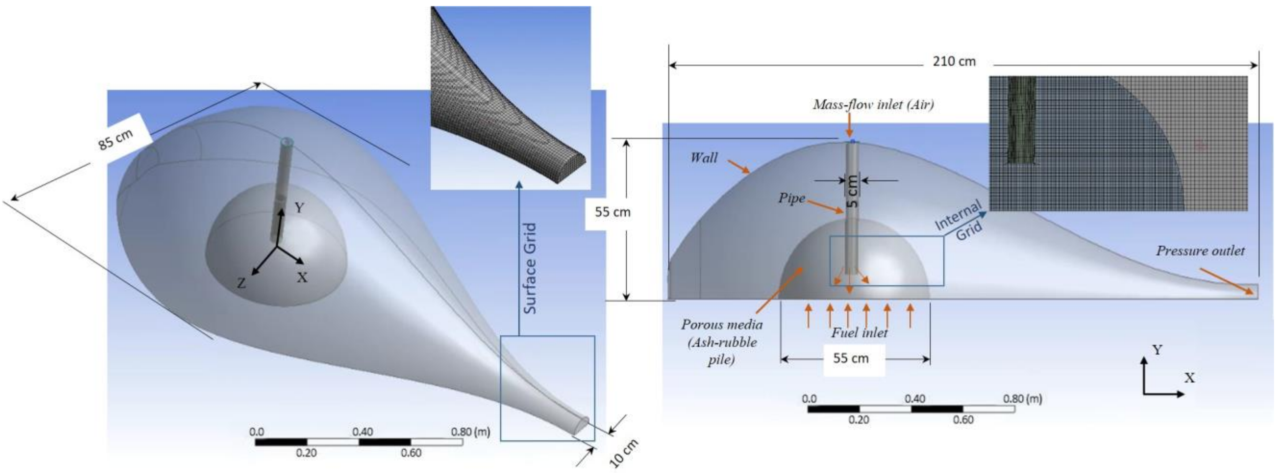


Fig. 2. Geometry, dimension, domain boundaries and constructed grid of the UCG cavity

2.2 Boundary Conditions

An air mass-flow inlet has been assigned at the top of vertical injection pipe. This air is injected into the ash-rubble pile, while the bottom surface of it is set as fuel inlet (Figure 2). Air is inserted at varying rates, 0.0018, 0.0036, 0.0054 and 0.009 kg/s while fuel mass-flow is given at 0.001 kg/s which correspond to equivalent ratio (ER) of ER 0.16, ER 0.33, ER 0.49 and ER 0.82. These values are selected based on the reported optimum ER values for efficient gasification [24,31]. The surface of the cavity is defined as coal wall in this domain. The outlet of syngas is assigned as pressure outlet. The pressure-outlet is located at the narrow end (tail) of the domain (Figure 2). The operating pressure is set to 5 Mpa, as the underground cavity environment is a pressurized zone [13]. Regarding the cell zone conditions, the ash-rubble pile is set to a porous fluid domain assuming that the coal volatiles interact with the incoming oxidizer and the produced gas would come out to flow further.

Table 1
The boundary conditions

Boundary conditions	Value
Mass-flow Inlet (Air)	0.0018 – 0.009 kg/s
Fuel inlet (HV-B type coal)	0.001 kg/s
Outlet	Pressure outlet
Operating pressure	5 MPa
Surfaces of cavity	Adiabatic wall

2.3 Grid Generation and Grid Dependency

Primarily rectangular grid was employed in this numerical modelling (Figure 2). Grids were refined at different points of interest. Assuming the highest velocity gradient at the air inlet, the finest mesh was generated here. Also, grids were finely controlled for the ash-rubble pile, being another higher velocity zone.

A mesh independence analysis has been accomplished to ensure that the result of simulation is independent of the mesh. This analysis can effectively improve the reliability of the simulation and decrease computational time through determining the minimum number of elements for finding optimum result. Varying number of grids in the range of 1.0 – 2.0 million elements were adapted to achieve an accurate solution by taking into account the effects of grid dependency. The temperature profile along X axis was plotted against varying element numbers as shown in Figure 3. It showed that the effect of element number on temperature profile had almost a coinciding trend for both 1.8 and 2.0 million elements. Thus, 1.8 million elements were selected to run the numerical simulation in this study to minimize computational task, also to facilitate the desired result from the modelling.

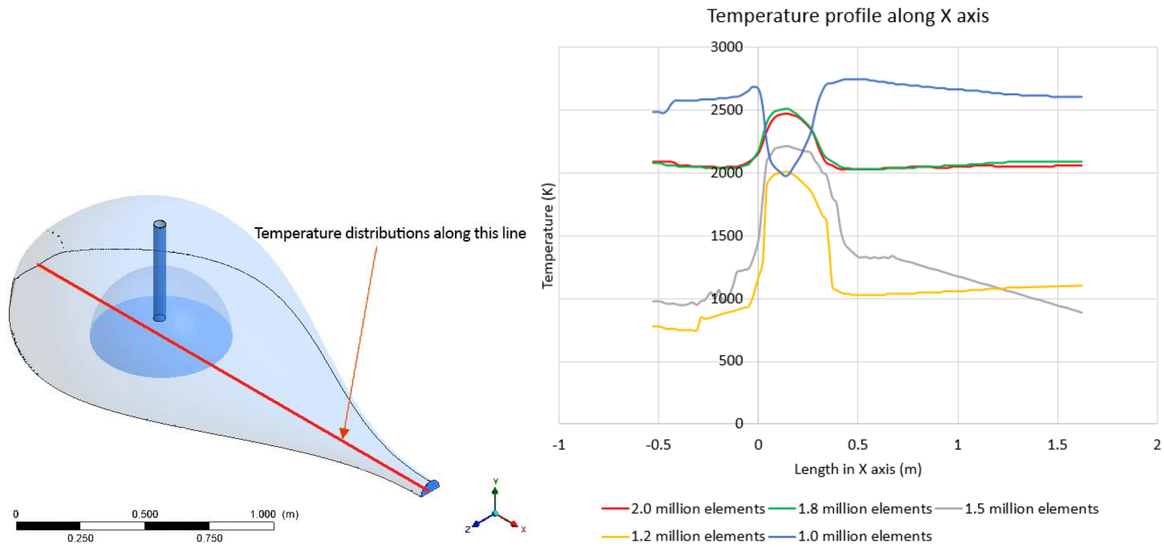


Fig. 3. Grid dependency study by testing different number of mesh elements against temperature profile along the line at the bottom of the mid plane in X axis

2.4 Properties of Fuel (Coal)

The coal samples of interest for this study are collected from Jamalganj coalfield, Bangladesh. This field appears to have the feasibility to conduct UCG, over other 4 discovered coalfields in Bangladesh. UCG in Jamalganj coalfield seems potential in terms of depth of occurrence (~1 Km depth), seam thickness (up to 47 m in places), considerable gap between the coal seam and any significant aquifer, sufficient permeability, coal reserve, areal extent and a manageable overburden [32–34]. Data of proximate and ultimate analysis (Table 2) of these coal samples have been fed into the species transport model.

Table 2
Properties of High-volatile Bituminous (HV-B type) coal from Jamalganj, Bangladesh

Component	Value
Ultimate analysis (dmmf* basis)	
Carbon (as received)	84
Hydrogen (as received)	5
Nitrogen (as received)	1.8
Oxygen (as received)	9
Sulfur (as dried)	0.2
Proximate analysis (% wt)	
Moisture content (as received)	8
Fixed carbon (as received)	45
Volatile matter (as received)	35
Ash (as received)	12

*dmmf = Dry Mineral Matter Free

2.5 Calculation Methodology

Conservation equations for mass, energy and gas species transport are solved to simulate the fluid flow in the cavity. Under prevailing boundary conditions (as mentioned in section 2.2), computations are conducted by solving Reynold's Averaged Navier-Stokes (RANS) equations turbulent flow behavior is considered and accounted for within the hollow region of the cavity. The standard k-ε (2 eqn.) with standard wall functions was used to model the turbulence in the cavity. The transport equations for the turbulent kinetic energy, k and the turbulent dissipation rate, ε (epsilon) have been adopted from Perkins and Sahajwalla [34].

Since heat transport by radiation is deemed important, a radiation model, Discrete Ordinate (DO) is used as the peak temperatures can go high up 2000 K. The species transport model has introduced the properties of Jamalganj High-volatile Bituminous coal.

The discretization scheme for pressure–velocity coupling chosen for the study, is SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm because of its simpler yet robust and effective approach [36]. First order upwind scheme is considered for turbulent kinetic energy, turbulent dissipation rate and DO, while the second order is associated for pressure, momentum, species and energy equations.

In general, a qualitative convergence is obtained when the scaled residuals drop by 3 orders of magnitude. In this study, however, stricter criteria have been followed to achieve convergence being influenced by Shirazi *et al.,* [36]. The convergence of iterative solution is considered to be met when the residuals of all the variables reach at 1×10^{-4} except the energy equation which is set to 1×10^{-6}.

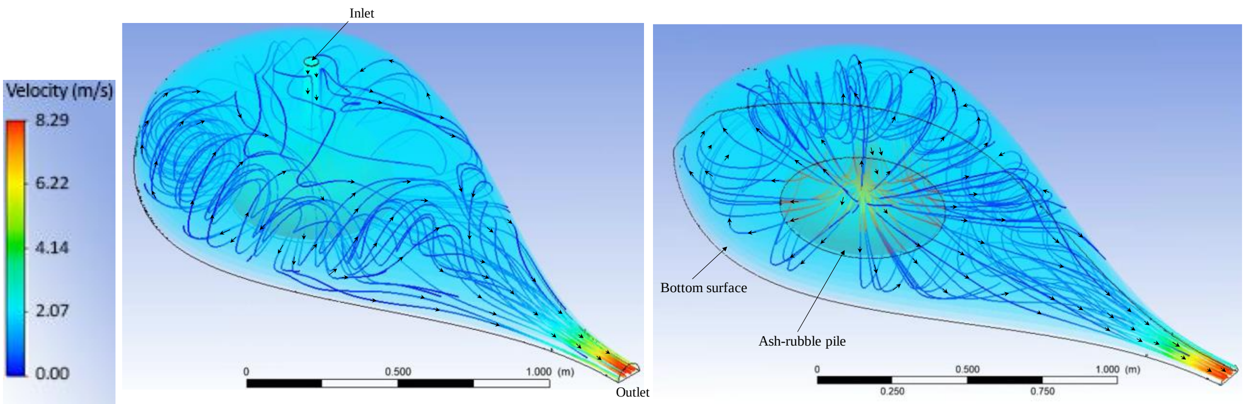
A commercial CFD code is used to perform the modelling, namely ANSYS Fluent which uses a control-volume formulation and the segregated solution method [38].

3. Result and Discussion

3.1 Flow Features

The flow patterns associated with UCG process has been established through the streamlines of flow in UCG cavity (Figure 4). The air, entering at pipe inlet and being discharged into the ash-rubble pile, is interacted with fuel residing at the bottom of the ash-rubble pile, forming exothermic combustion reaction zone. This is identified by higher velocity streamline (at the oxygen release point as in Figure 4(b)) which is caused due to expansion of hot gas. The hot gas flows out from ash-rubble pile forming circulation flow around the pile and subsequently leaving through the cavity outlet.

In this study, it reveals that the circulation flow circles around the ash-rubble pile which is supposed to enhance turbulent flow in the cavity. Presumably, turbulent flow could be attributed to boost up combustion reactions which will be explored in further research work.



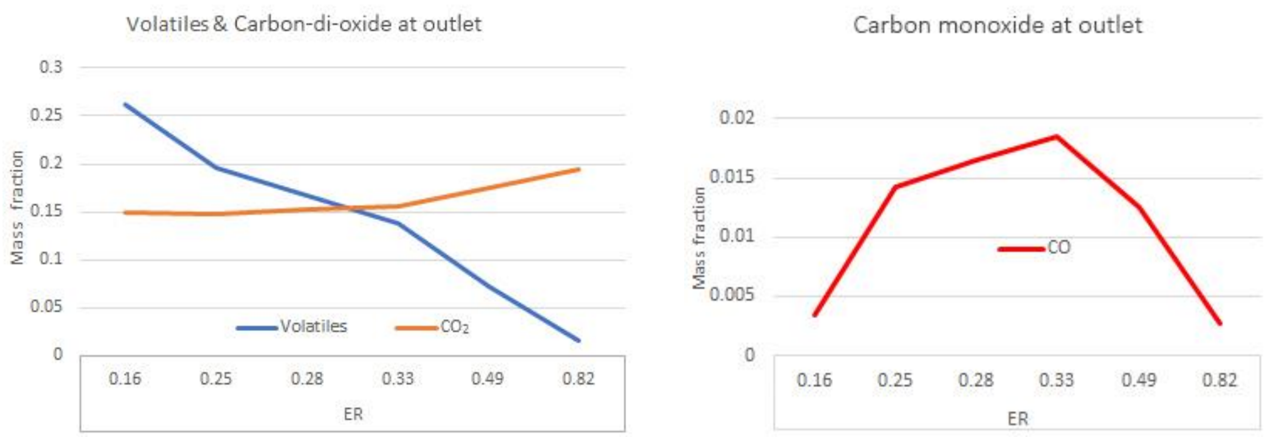
(a) (b)

Fig. 4. Flow Characteristics in UCG cavity (a) Top view (b) Bottom view

3.2 ER Effect on Syngas Composition

The effect of equivalence ratio (ER) in the product gases have been studied numerically. ER has significant impact on the resultant syngas composition. The syngas composition was detected at pressure outlet.

CO_2 concentration rises with increasing equivalence ratio while the concentrations of CO and other volatiles (H_2, CH_4 etc.) decrease in the product gas composition (Figure 5(a)). One of the main constituents of the product syngas, CO is estimated to reach to its maximum level at ER 0.33; but afterwards CO starts falling short in the product syngas and gradually diminishes near ER 1.00 (Figure 5(b)).



(a) (b)

Fig. 5. Product gas composition at different equivalence ratio (a) Mass fraction of Volatiles and CO_2 in syngas (b) Mass fraction of CO in product syngas

3.3 Combustion Characteristics

Temperature contours at cross-section of UCG cavity is shown in Figure 6. As there is no combustion reaction happening within the injection pipe, flow temperature remains very low (around 400 K) in the air pipe. Temperature becomes high (as much as 1900 K, 2200 K and 2600 K at ER 0.16, ER 0.33 and ER 0.49 respectively) in the ash-rubble pile region, especially at the bottom surface, because exothermic combustion reactions take place in this zone. This corresponds to high velocity streamline (see Figure 4(b)) due to expansion of hot gas, affected by combustion reaction. Temperature around the ash-rubble pile becomes moderate (around 1500 K, 1900 K and 2300 K at ER 0.16, ER 0.33 and ER 0.49 respectively) because of the heat loss as hot gas leaves the combustion zone.

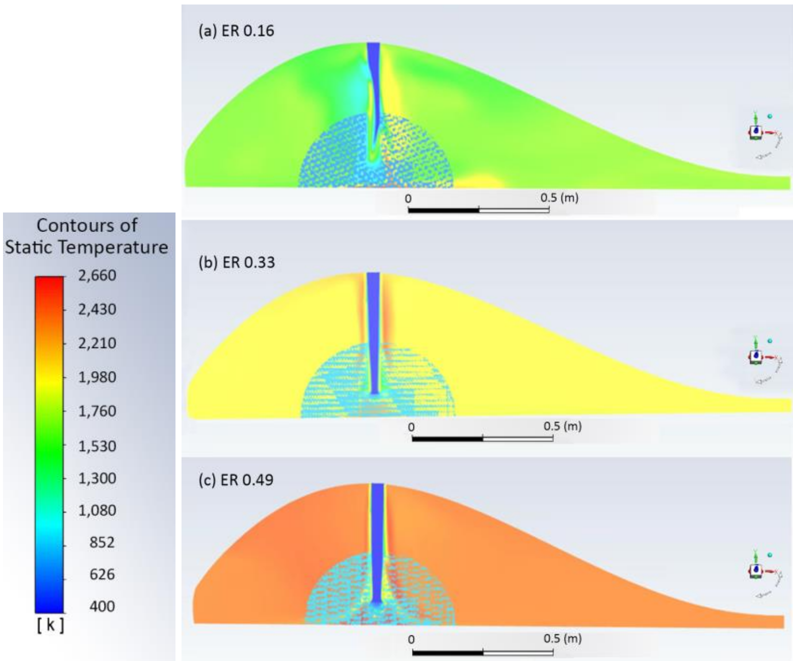


Fig. 6. ER influenced temperature contours at cross-section of UCG cavity (a) low temperature observed at ER 0.16 (b) moderate temperature at ER 0.33 (c) peak temperature at ER 0.49

The simulation results of with varying equivalence ratio from 0.16 to over 0.82 show that, the higher the air ratio, usually the higher the gasifier temperature, as depicted in Figure 6. However, the local temperature peak is observed where the air is released directly from the pipe. For example, at ER 0.33 (Figure 6(b)), region of high temperature (T>2,200 K) lies in the area of the ash-rubble pile. Although the maximum temperature is recorded up to 2550 K, which can be attributed to the fact of no heat loss in simulation method.

Temperature distributions have been found remarkably variable when the ER values are changed (Figure 7). A fluctuating behaviour of temperature is marked along the line at the bottom of the mid plane in X axis (reference line as shown in Figure 3) of UCG cavity. At ER 0.16 and ER 0.82 (the lowest and the highest case considered in this experiment), the resulting temperature rise or fall abruptly as such that the reaction appears to become unstable.

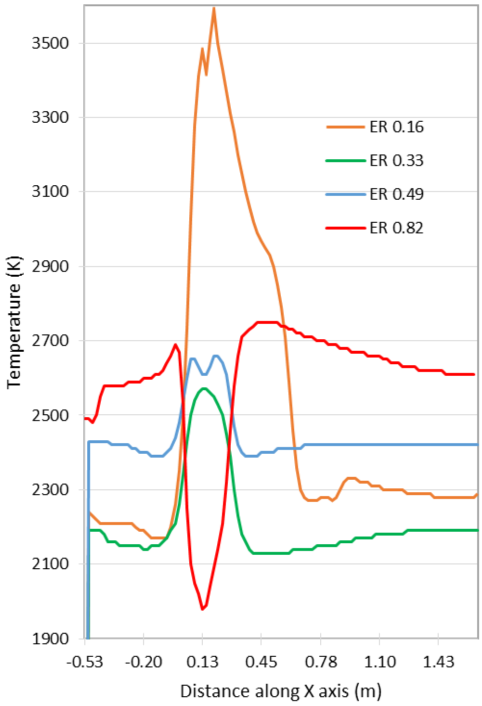


Fig. 7. Temperature fluctuations with varying ER along the line at the bottom of the mid plane in X axis

Thus, the favourable ER for having an efficient underground gasification can be found in between 0.16 to 0.82. In this study, the most effective ER has been determined as 0.33, at which the flow and combustion characteristics are apparently stable and the produced syngas quality appears to be in its best configuration.

4. Conclusion

In this study, a CFD model has been developed which can be used to study the effect of different injection rates. The attempt is to identify the hydrodynamic conditions associated with UCG performance (i.e., composition of the product gas). Thereby the model has simulated the flow and combustion characteristics in a typical UCG cavity. The findings are

i. Syngas composition variation in an Underground Coal Gasification depends on the changing ER as such one of the main constituents of syngas, carbon monoxide (CO) appears best at an equivalent ratio of 0.33.
ii. At an optimal equivalent ratio of 0.33 the flow characteristics are seemingly favourable, while at more or less ER, reactions may become unstable.
iii. It is revealed that the circulation flow, which takes place around the ash-rubble pile, would enhance turbulent flow in the cavity. This turbulent flow is supposedly improved combustion reaction which will be explored in the follow-up work.
iv. The temperature peak is encountered at the air release point directly from the injection pipe. The region of high temperature is lying in the area of the ash-rubble pile.

The study implies the effect of equivalent ratio (ER) on gasification performance along with the flow and combustion characteristics to identify the factors that control UCG performance. Thus, this would become helpful to develop a viable operational strategy in advance of deploying any physical operation which incurs considerable cost.

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