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Mathematical Modelling of Coal Gasification Processes

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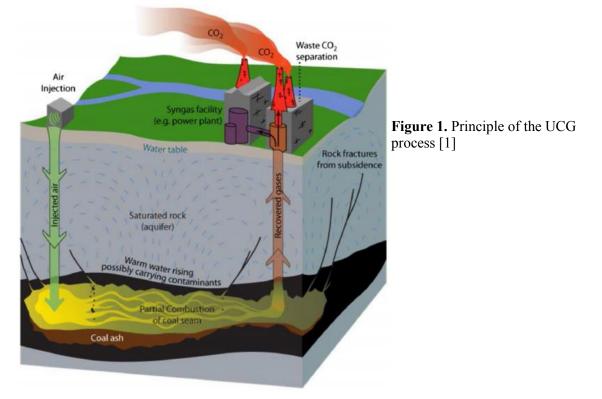* Corresponding Author. Email: tsundar@iitm.ac.in

Abstract. Coal is by far the most commonly employed fuel for electrical power generation around the world. While combustion could be the route for coal utilization for high grade coals, gasification becomes the preferred process for low grade coals having higher composition of volatiles or ash. Indian coals suffer from high ash content- nearly 50% by weight in some cases. Instead of transporting such high ash coals, it is more energy efficient to gasify the coal and transport the product syngas. Integrated Gasification Combined Cycle (IGCC) plants and Underground Gasification of coal have become attractive technologies for the best utilization of high ash coals. Gasification could be achieved in fixed beds, fluidized beds and entrained beds; faster rates of gasification are possible in fluidized beds and entrained flow systems, because of the small particle sizes and higher gas velocities. The media employed for gasification could involve air/oxygen and steam. Use of oxygen will yield relatively higher calorific value syngas because of the absence of nitrogen. Sequestration of the carbon dioxide after the combustion of the syngas is also easier, if oxygen is used for gasification. Addition of steam can increase hydrogen yield in the syngas and thereby increase the calorific value also. Gasification in the presence of suitable catalysts can increase the composition of methane in the product gas. Several competing heterogenous and homogenous reactions occur during coal major heterogenous reaction pathways, while interactions between carbon monoxide, oxygen, hydrogen, water vapour, methane and carbon dioxide result in several simultaneous gas-phase (homogenous) reactions. The overall product composition of the coal gasification process depends on the input reactant composition, particle size and type of gasifier, and pressure and temperature of the gasifier. The use of catalysts can also selectively change the product composition. At IIT Madras, over the last one decade, both experimental and modelling work has been undertaken to investigate the gasification characteristics of high ash Indian coals and compare the yield with those of high grade Australian and Japanese coals. A 20 kW capacity entrained flow gasifier has been constructed and the gasification characteristics have been studied for Indian coals for different particle sizes, system pressures and air flow rates. The theoretical model incorporates the effects of Knudsen diffusion, devolatilization and various heterogenous and homogenous kinetic steps as well as two-phase flow interactions involving the gaseous and particle phases. Output parameters such as carbon conversion, cold gas efficiency and syngas composition have been compared for different grades of coals under a wide range of operating conditions. The model developed for the entrained flow gasifier predicts the gasification characteristics of both Indian and foreign coals well. Apart from the entrained flow gasifier, a bubbling bed gasifier of 100 kW capacity has also been studied. A pilot plant for the gasification of Indian coals has been set up for this capacity and its performance has been investigated experimentally as well as theoretically at different air and steam flow rates. Carbon conversion efficiency of more than 80% has been achieved.

1. Introduction

Coal is by far the major source of energy world-wide and it is likely to remain so, for some more decades to come. India is endowed with large reserves of coal which are expected to last for at least two more centuries, but the coal contains a high percentage (~40% by mass) of ash. The high ash content results in low calorific value and it is also an additional burden when coal is transported to different parts of the country from the mines. Moreover, the presence of fly-ash in the flue gas from coal combustion is a pollution hazard and additional devices such as electrostatic precipitators need to be fitted for the removal of ash particles before the flue gas is exhausted into the atmosphere. Gasification of coal with air/ oxygen/ steam is an attractive option to avoid the ill-effects of fly ash in the combustion products. In fact, underground gasification of coal (UGC) involves the *in situ* conversion of coal into combustible gaseous products containing a mixture of carbon monoxide, carbon dioxide, hydrogen, methane and nitrogen.

During UCG, the coal in the seam reacts at elevated temperatures and pressures to produce gaseous combustible products (Figure 1). The gas composition, as well as the heating value depends on the thermodynamic conditions, grade of coal, and the gasifying agent composition and temperature. The gasification process starts with the ignition of coal seam at the beginning of the gasification channel. After ignition, the gasification agents move the process forward, along the gasification channel towards the production well. The main gasification reactions occur both in the solid and gaseous phases as well on their boundaries. The solid phase undergoes a drying process first to release the water evaporated from the coal; at a slightly higher temperature, pyrolysis processes give rise to some volatile gases. Following the pyrolysis, some homogeneous and heterogeneous reactions occur whose rates primarily depend on temperature (Figure 2). The homogeneous reactions occur completely in the gas phase, while the heterogeneous reactions occur at the solid (coal) surface.
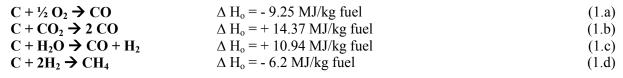

Figure 1. Principle of the UCG process [1]

2. Modelling of coal gasification

2.1. Heterogeneous reactions

Char (solid carbon) is consumed in the following heterogeneous reactions [2-4]:

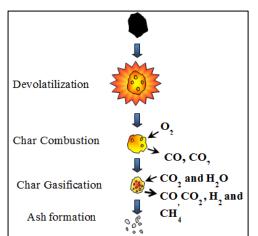|		
C + ½ O$_2$ → CO	Δ H$_o$ = - 9.25 MJ/kg fuel	(1.a)
C + CO$_2$ → 2 CO	Δ H$_o$ = + 14.37 MJ/kg fuel	(1.b)
C + H$_2$O → CO + H$_2$	Δ H$_o$ = + 10.94 MJ/kg fuel	(1.c)
C + 2H$_2$ → CH$_4$	Δ H$_o$ = - 6.2 MJ/kg fuel	(1.d)

Figure 2. Reactions involved in coal gasification

The reactions take place at the surface of char, where a gaseous reactant such as oxygen, CO$_2$ and water vapor reacts with solid carbon and produces gaseous products. In the case of coal, however, after moisture removal and devolatilization, the solid phase consists of char and ash. Thus, after the above-mentioned char reactions, ash is left behind in the form of a porous layer. Although from time to time, the ash layer may break up to form fly ash which is carried away by the product gases, the ash layer forms a barrier for the diffusion of the gaseous reactants towards the char surface. Thus, one needs to consider both chemical kinetics steps for the formation of the product species and also the diffusion aspects of the gaseous reactants through the ash layer. The rate of particle surface species depletion (for species k) in a heterogeneous reaction is given by the expression [2] as:

$$\overline{R}_{k,r} = A_p \eta_r Y_k R_{k,r} \qquad\qquad R_{k,r} = R_{kin,r}\left(p_n - \frac{R_{k,r}}{D_{0,r}}\right)^{N_r}$$

where the kinetic rate is expressed as $R_{kin,r} = A_r T^{n,r} e^{-(E,/RT)}$ and the diffusion coefficient is

given as $D_{0,r} = C_{1,r}\dfrac{[(T_p + T_\infty)/2]^{0.75}}{d_p}$.

Table 1. Composition of Indian coals considered in present study

Coal Types	Proximate Analysis (wt %)				Ultimate Analysis (wt %)					HHV
	Moist	*FC*	*VM*	*Ash*	*C*	*H*	*O*	*S*	*N*	(MJ/kg)
Australian	4.20	56.20	30.90	8.70	76.30	5.31	7.31	0.46	1.54	30
Indian Coal A	4.12	38.05	27.15	30.68	55.66	3.67	8.31	0.40	1.28	19.27
Indian Coal B	6.52	29.86	28.15	35.47	45.15	4.1	13.28	0.91	1.09	16.81
Indian Coal C	4.55	27.6	23.19	44.66	39.7	3.08	15.02	0.59	0.87	14.87

The constants involved in the above kinetic expressions and the diffusion process are taken from the references [2-4]. Apart from the kinetic and diffusion aspects discussed above, additional features that need to be taken into account for high ash Indian coal are the enhanced reactivity due to the mineral matter present in the ash (some of the minerals have catalytic property), decreased reactivity due to low diffusivity, increase in the emissivity of char due to ash and increase in the emissivity of combustor wall due to ash deposition. The net effect of these additional effects will be slower reaction rates for the high ash Indian coals in general, as compared to the low ash foreign coals. The

differences in composition for some Indian coal samples vis-à-vis non-Indian coals are listed in Table 1.

2.2. Heterogeneous reactions
The homogeneous reactions arise from the gas phase processes such as the burning of volatile gases (taken in a general chemical form of CH_xO_y) and the reactions between the gaseous products such as CO, CO_2, H_2O and H_2. Some of the most important homogeneous reactions are listed below:

$CH_xO_y + a\ O_2 \rightarrow CO_2 + b\ H_2O$	(2.a)
$CH_xO_y + c\ O_2 \rightarrow CO + d\ H_2O$	(2.b)
$CO + \frac{1}{2}\ O_2 \longleftrightarrow CO_2$	(2.c)
$H_2 + \frac{1}{2}\ O_2 \longleftrightarrow H_2O$	(2.d)
$CO + H_2O \longleftrightarrow CO_2 + H_2$	(2.e)

Where $a = 1 + x/4 - y/2$, $b = d = x/2$ and $c = (1 - y)/2$, based on stoichiometric balance. The kinetic parameters for the gas-phase reactions have been reported [5-7]. For reversible reactions, equilibrium data (Table 2) is often used to obtain the rates of the backward kinetic steps.

Table 2. Chemical equilibrium constants for carbon reactions [8, 9]

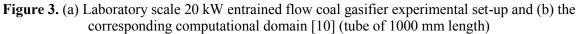| T, K	1/T, K^{-1}	ln K$_p$					
		1.a	C+O$_2$=CO$_2$	1.c	1.b	2.e	1.d
300	0.003333	23.93	68.67	-15.86	-20.81	4.95	8.82
400	0.0025	19.13	51.54	-10.11	-13.28	3.17	5.49
500	0.002	16.26	41.26	-6.63	-8.74	2.11	3.43
600	0.001667	14.34	34.40	-4.29	-5.72	1.43	2.00
700	0.001429	12.96	29.50	-2.62	-3.58	0.96	0.95
800	0.00125	11.93	25.83	-1.36	-1.97	0.61	0.15
900	0.001111	11.13	22.97	-0.37	-0.71	0.34	-0.49
1000	0.001	10.48	20.68	0.42	0.28	0.14	-1.01
1100	0.000909	9.94	18.80	1.06	1.08	-0.02	-1.43
1200	0.000833	9.50	17.24	1.60	1.76	-0.16	-1.79
1300	0.000769	9.12	15.92	2.06	2.32	-0.26	-2.1
1400	0.000714	8.79	14.78	2.44	2.80	-0.36	-2.36

In a typical UCG operation, the heterogeneous reaction of Eq. (1.a) and the homogeneous reactions of (3.a), (3.b), (3.c) and (3.d) may occur at the beginning of the gasification channel, forming what is known as the 'Oxidation Zone'. The endothermic Boudouard's reaction involving CO_2 reduction with char (Eq. 1.b), steam decomposition reaction (Eq. 1.c), the exothermic coal hydration or 'methanation' reaction (Eq. 1.d) may occur towards the later portion of the gasification channel, forming what is known as the 'Reduction Zone'. Over the whole length of the gasification channel, an important gas phase reaction such as the water-gas reaction (Eq. 3.e) can occur. Thus, UGC needs to be considered as a combination of complex flow, heat and mass transfer processes involving several gas phase and solid phase reactions. Often, simplified studies conducted on ground can provide the necessary data for understanding the complex phenomena in UGC.
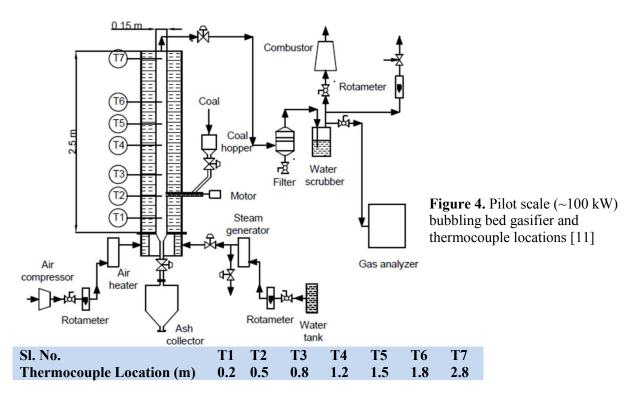
In the Mechanical Engineering Department of IIT Madras, research on surface gasification of coal has been carried out in the last 10 years. A 20 kW laboratory scale entrained flow gasifier and a 100 kW bubbling bed gasifier have been set up, for gasifying high ash Indian coals (see Figures 3 and 4). The characteristics of Indian coal gasification have been compared with those of Australian and Japanese coals of low ash content. CFD simulations have also been performed to analyze the gasification phenomena, using the models presented above and the results have been published as

research papers in archival journals [10-13]. The results obtained in our surface gasification studies of Indian coal are summarized in the next section.

(a)

(b)

Figure 3. (a) Laboratory scale 20 kW entrained flow coal gasifier experimental set-up and (b) the corresponding computational domain [10] (tube of 1000 mm length)

Figure 4. Pilot scale (~100 kW) bubbling bed gasifier and thermocouple locations [11]

Sl. No.	T1	T2	T3	T4	T5	T6	T7
Thermocouple Location (m)	0.2	0.5	0.8	1.2	1.5	1.8	2.8

3. Results and discussion

The laboratory scale entrained gasifier was operated with three grades of Indian coal and its gasification characteristics were compared with those of a typical Australian coal. The compositions of these coals are provided in Table 1. As a first exercise, the predictions of the theoretical model have been compared with available experimental results for an Australian coal and a Japanese coal, in Figure 5 and the associated Table 3. Very good match is observed between the numerical and experimental results in this validation exercise.
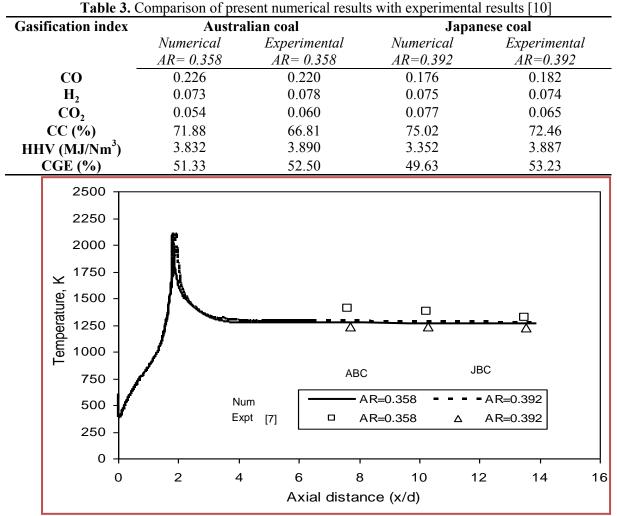
Table 3. Comparison of present numerical results with experimental results [10]

Gasification index	Australian coal		Japanese coal	
	Numerical *AR= 0.358*	*Experimental* *AR= 0.358*	*Numerical* *AR=0.392*	*Experimental* *AR=0.392*
CO	0.226	0.220	0.176	0.182
H$_2$	0.073	0.078	0.075	0.074
CO$_2$	0.054	0.060	0.077	0.065
CC (%)	71.88	66.81	75.02	72.46
HHV (MJ/Nm^3)	3.832	3.890	3.352	3.887
CGE (%)	51.33	52.50	49.63	53.23

Figure 5. Comparison of axial temperature inside the gasifier with experimental results [10]

The effect of pressure on the evolution of gasifier temperature profile is depicted in Figure 6. It is evident that at higher pressure, the oxidation reactions occur at an earlier axial distance, due to the larger concentration of oxygen (per unit volume) in the mixture. The corresponding peak temperatures are also slightly higher. However, the evolution of volatiles is delayed at a higher pressure, as seen in Figure 7. Also, volatile evolution is relatively slower for a larger coal particle than for a relatively smaller particle, evidently due to the diffusion resistance offered by the ash layer. In Figures 8 and 9, it is illustrated that the formation of CO and H$_2$ are also accelerated at higher pressures. Therefore, gasification parameters such as carbon conversion (CC), higher heating value of the gas (HHV) and the cold gas efficiency (CGE) register higher magnitudes at higher system pressures as shown in Table 4. The steam ratio has only a minor effect on all gasification parameters for the high ash Indian coal,

as seen from Table 5. Figure 10 shows that the numerically predicted product gas composition agrees fairly well with the measured gas composition at different air ratios considered.

In Table 6, the conditions studied in the 100 kW pilot scale gasifier are listed. The transient operation of the pilot scale gasifier and the corresponding exhaust temperature variations are shown in Fig. 11. The corresponding gas composition variation with time after an initial transient period of 2 hours is shown in Fig. 12. The average exhaust gas composition for various coal batch sizes is shown in Fig. 13. These studies illustrate that CC is more that 97% in the pilot scale combustor.
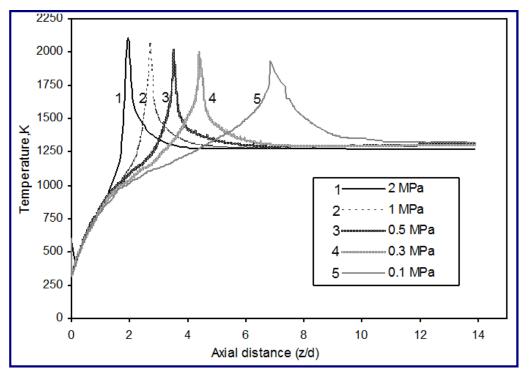

Figure 6. Axial temperature variation inside the gasifier at different operating pressures [10]
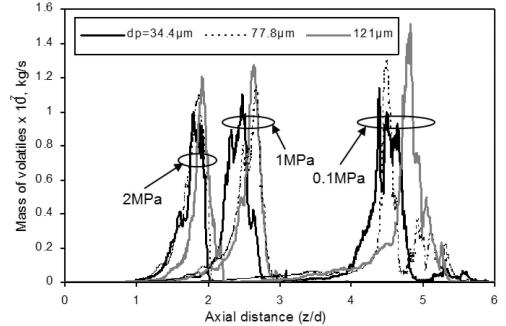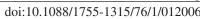

Figure 7. Devolatilization of representative particles at different operating pressures [10]
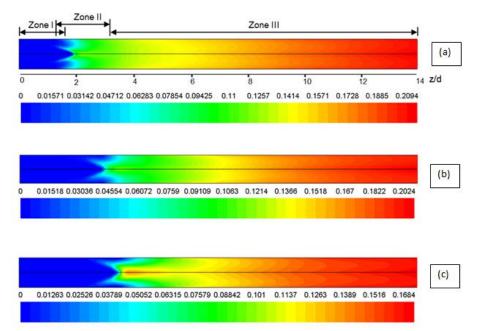
Figure 8. Evolution of CO with axial length in entrained gasifier (a:2 MPa, b:1 MPa, c:0.5 MPa**)** [12]
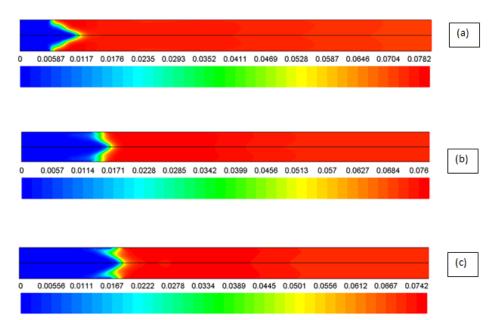

Figure 9. Evolution of H_2 with axial length in entrained gasifier (a:2 MPa, b:1 MPa, c:0.5 MPa) [12]

Table 4. Effect of pressure on gasification parameters for Indian coal- A (SR = steam ratio) [10]

Pressure (MPa)	Carbon conversion CC (%)		HHV (MJ/m^3)		Cold Gas Efficiency (%)	
	SR=0	SR=0.1	SR=0	SR=0.1	SR=0	SR=0.1
2	71.12	69.89	3.543	3.579	47.58	48.03
1	69.32	68.17	3.415	3.373	45.71	46.34
0.5	65.51	64.88	2.912	3.079	41.47	43.04
0.3	62.27	60.86	2.691	2.728	38.55	39.98
0.1	57.85	56.06	2.189	2.235	33.46	34.24

Table 5. Effect of steam ratio on gasification of Austalian and Indian coals, after [10]

Steam Ratio (SR)	CC (%)		HHV (MJ/Nm^3)		CGE (%)	
	ABC	*IC-A*	*ABC*	*IC-A*	*ABC*	*IC-A*
0.0	74.02	71.12	3.641	3.543	52.26	47.58
0.1	73.15	69.89	3.732	3.579	51.02	48.03
0.2	72.62	67.11	3.668	3.552	50.11	47.22
0.3	71.06	66.02	3.602	3.504	49.35	45.41

Figure 10. Comparison of predicted and measured product gas composition [12]

Table 6. Experiments conducted on the pilot scale bubbling bed gasifier [11]

Test run	Power output	Coal feed rate	Air flow rate	ER	Steam flow rate	Steam/coal ratio
	kW	*kg/h*	*kg/h*		*kg/h*	
1	100	20.24	40.6	0.35	-	-
2	80	16.19	32.48	0.35	-	-
3	80	16.19	27.84	0.30	-	-
4	80	16.19	23.20	0.25	2.42	0.15
5	80	16.19	23.20	0.25	3.23	0.25
6	80	16.19	23.20	0.25	4.05	0.30

4. Conclusion

The present experimental and modeling studies illustrate that gasification processes of high ash Indian coals can be modeled fairly accurately. Operation of the gasifier at higher pressure is definitely advantageous to achieve more efficient gasification. As compared to the foreign coals with lower ash content, Indian coals give relatively poorer efficiency during gasification. However, the advantage of not taking the ash out of the mine is greatest for the Indian high ash coals. Although modeling of

surface gasification has been presented in this paper, the methodology outlined here can be combined with the flow, heat transfer and mass transfer processes occurring in UGC, for the development of comprehensive gasification models.
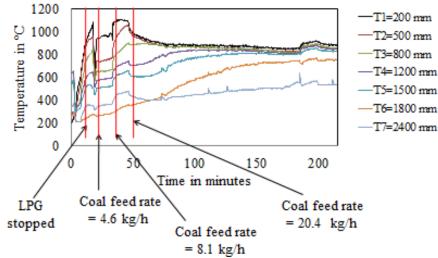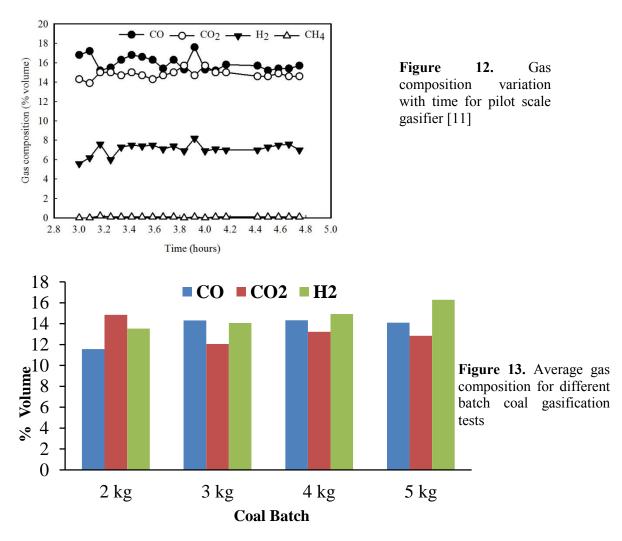

Figure 11. Transient operation of the pilot scale bubbling bed gasifier [11]

Figure 12. Gas composition variation with time for pilot scale gasifier [11]

Figure 13. Average gas composition for different batch coal gasification tests

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