Modeling of Freeboard Fluidized Bed Gasifier Integrated to Bubbling Dense Bed

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ABSTRACT

Coal gasification offers one of the most versatile and clean ways to convert coal into electricity, hydrogen, and other energy forms. In this work developed modeling of fluidized bed coal gasifier incorporating fines elutriation and freeboard reactions. Interface the freeboard model with the bed model to predict the performance of gasifier at different simulation parameters. Fluidized bed hydrodynamics play important role. Two phase (Bubble phase and Emulsion phase) hydrodynamics have been considered to represent the physical bed behavior of fluidized bed gasifier. The freeboard region provides additional opportunities for intimate solid-gas contacting the reaction in this regime may be significant in many instances and may not be neglected. Particles carry over from the surface of a fluidized bed into the freeboard depends on the mechanism of bubble eruption. When the bubble burst at the fluidized bed surface, particles are entrained in the freeboard region. The entrained particles with a terminal velocity greater than actual gas velocity $(u_t>u)$ will reach a certain height within the freeboard before they fall back into the bed. However those particles with a terminal velocity smaller than actual gas velocity $(u_t<u)$ will be elutriated and carried out of the bed.
Keywords: Coal gasification, modeling, freeboard and fluidized bed

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INTRODUCTION

Coal gasification offers one of the most versatile and clean ways to convert coal into electricity, hydrogen, and other energy forms. The first coal gasification electric power plants are now operating commercially in the United States and in other nations, and many experts predict that coal gasification will be at the heart of future generations of clean coal technology plants for several decades into the future. Rather than burning the coal directly, gasification breaks down coal-or virtually any carbon-based feed stock – into its basic chemical constituents. In a modern gasifier, coal is typically exposed to hot steam and carefully controlled amounts of air or oxygen under high temperatures and pressures. Under these conditions, carbon molecules in coal break apart, setting off chemical reactions that typically produce a mixture of carbon monoxide, hydrogen and other gaseous compounds. Gasification, in fact, may be one of the best ways to produce clean-burning hydrogen for tomorrow's automobiles and power-generating fuel cells. Hydrogen and other coal gases can also be used to fuel power-generating turbines or as the chemical "building blocks" for a wide range of commercial products.

The main objective of this work is to develop "Mathematical Model of Coal Gasification Process in a Fluidized Bed Reactor" under steady state condition. Fluidized bed hydrodynamics play important role. Two phase (Bubble phase and Emulsion phase) hydrodynamics have been considered to represent the physical bed behavior of fluidized bed gasifier [7]. In the model formulation, fluidized bed is divided in to small strips; the height of each strip corresponds to a small fraction of the total residence time. The model of gas-solid reaction phenomenon in the freeboard is inserted. The freeboard region is important to the physical design and construction of reactor but also to chemical conversion aspects of fluidized bed operations. Knowledge of solid flow patterns at and above the bed surface is necessary to estimate the importance of freeboard region on the overall fluidized bed performance [5]. The freeboard region provides additional opportunities for intimate solid-gas contacting the reaction in this regime may be significant in many instances and may not be neglected.

EXPERIMENTAL SETUP

The required for the validation of the model has been taken from the gasification experiments carried out in 200 mm ID fluidized bed gasifier pilot plant (APFBG test rig). The test rig consists of a single diameter refractory lined fluidized bed made in three sections. The bottom of the gasifier consists of a dismantable plenum which houses the single plate conical distributor made out of SS310 material. Coal is fed into the gasifier through a system of lock hopper consisting of a coal lock and a coal hold up vessel. A rotary feeder mounted below the coal holder vessel transfers the metered quantity of coal flow to the conveying line and is transported into the reactor using a part of the process air. The balance air pass through electrical preheater. Saturated steam is generated in a resistance type electrical boiler at maximum pressure of 7 kg/cm^2 and is super-heated more than 300^0 C in electrical furnace. Preheated air and steam mix just before the plenum. Bottom ash from the gasifier is extracted from a water cooled stand pipe and is collected in ash lock. The raw gas leaving the gasifier

passes through refractory lined cyclone and is cooled with water in a vertical shell and tube synthesis gas cooler. It passes through another cyclone before being vented. The system pressure is controlled by means of a pressure control valve located at the downstream of second cyclone. The system has also a sorbent lock unit and sorbent feeder. However for model validation were of those trials made without sorbent. Then air and steam flows are measured and independently controlled at each stream point. All flow measurements are made with orifice meter with dp transmitter and flow control through automatic control valves. The gasifier has arrangements for temperature measurements and differential pressure measurements at different axial locations. All measurements are automatic and data is logged into PC based data aquition system. Sampling for gas composition is done through a sampling device with filter assembly for fine particulate matter. Gas samples are collected at regular intervals in rubber bladder and analyzed both in gas chromatograph and orsat apparatus. A standard calibration gas mixture is used for the calibration of gas analysis units. This is shown in Fig-1.
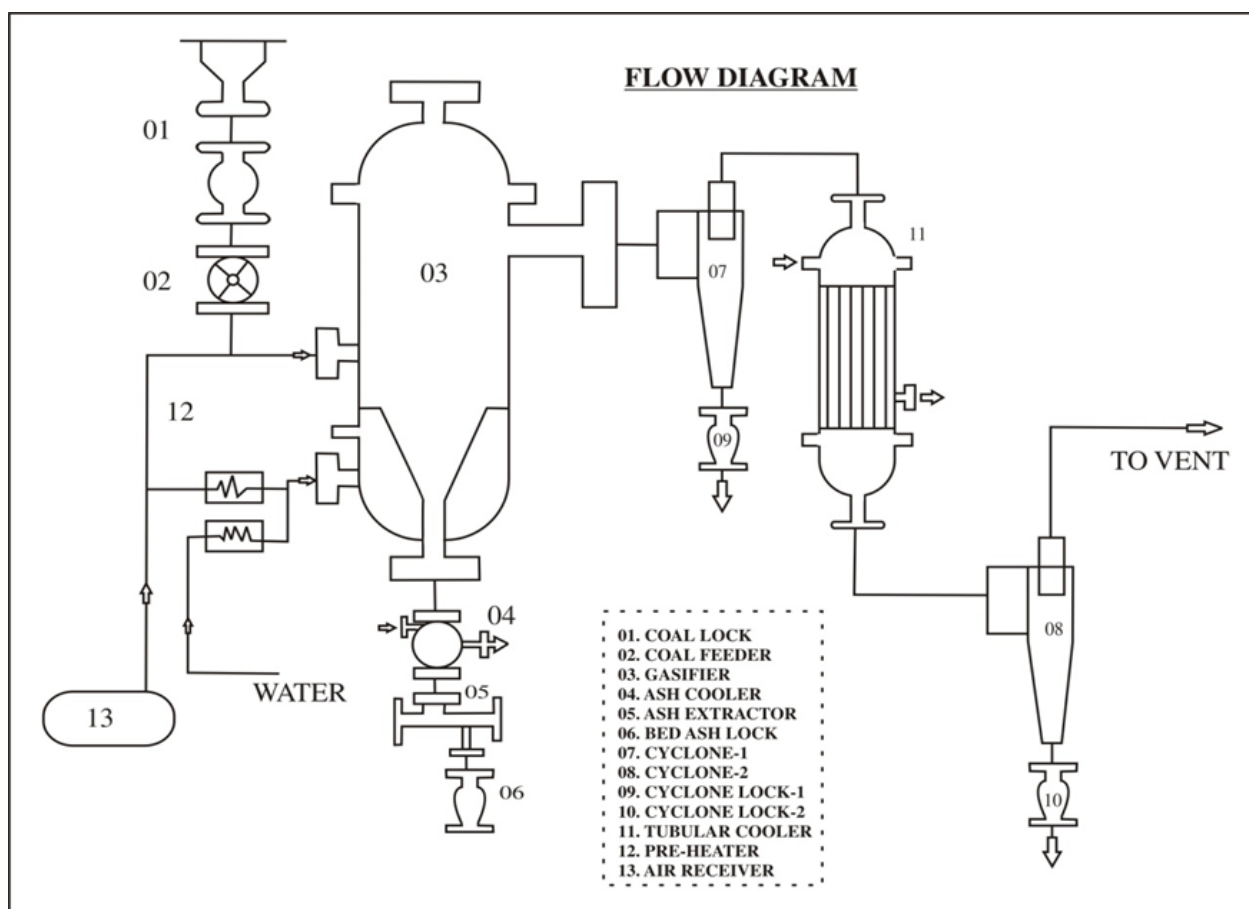

Figure 1: Schematic diagram of Experimental setup.

DESCRIPTION OF THE MODEL

In this model solid flow is considered to be 'mixed flow', gas flow in both emulsion and bubble phases is considered to be 'plug flow'. The solid-gas reactions are assumed to follow a shrinking core model in which there is a continually receding reaction interface surrounded by a porous solid product layer. The main factors in this model are the unchangeability of total particle's shape throughout the reaction though the core radius changes as reaction proceeds and the occurrence of reaction at the surface of particle. Under such conditions, a pseudo steady state assumption can be valid since the rate of recession of the reaction interface is small in comparison to the velocity of diffusion of any gaseous reactant through the product layer. The solid reactant particle is assumed to be spherical. But, in the model combustion reaction is assumed to be instantaneous. Whatever may be the ash that has formed due to the combustion reaction is assumed to be getting peeled off due to high attrition. For remaining reactions shrinking core model (constant volume) is followed. In deriving an overall rate expression to handle the entire reaction zone the following reactions steps were considered. 1. Diffusion of gaseous reactant from bulk gas phase to the ash layer 2. Diffusion through product layer to the reaction interface 3. Reaction at the interface.

MODEL EQUATIONS

Steady State Mass Balance Equation for Each Strip

Bubble phase:

$$U_{bi}\, A_i\, \delta_b\, C_{jbi} = U_{b(i-1)}\, A_{(i-1)}\, \delta_b\, C_{jb(i-1)} + A_i\, \Delta Z\, \delta_b\, K_{be}\left(C_{jei} - C_{jbi}\right) + A_i\, \Delta Z\, \delta_b \sum \beta_{nj}\, R_n$$

Emulsion phase:

$$U_{ei}\, A_i\left(1-\delta_b\right)\varepsilon_{mf}\, C_{jei} = U_{e(i-1)}\, A_{(i-1)}\left(1-\delta_b\right)\varepsilon_{mf}\, C_{je(i-1)} + A_i\, \Delta Z\, \delta_b\, K_{be}\left(C_{jbi} - C_{jei}\right)$$
$$+ A_i \Delta Z\left(1-\delta_b\right)\varepsilon_{mf} \sum \beta_{nj}\, R_n + A_i\, \Delta Z\left(1-\delta_b\right)\left(1-\varepsilon_{mf}\right)\sum \beta_{mj}\, R_m$$

Over All Heat Balance Equations

$$IN\,HEAT = m_{COAL}\, HCV_{COAL} + m_{COAL}\, C_{P\,COAL}\left(T_{COAL} - T_{REF}\right) + m_{AIR}\, C_{P\,AIR}\left(T_{AIR} - T_{REF}\right)$$
$$+ m_{STEAM}\, C_{P\,WATER}\left(T_{BOIL} - T_{REF}\right) + m_{STEAM}\, L_{VAPORISATION} + m_{STEAM}\, C_{P\,STEAM}\left(T_{STEAM} - T_{BOIL}\right)$$

$$OUT\,HEAT = m_{ASH}\, C_{P\,ASH}\left(T_{PROCESS} - T_{REF}\right) + m_{REM\,CARBON}\, CV_{CARBON}$$
$$+ m_{REM\,CARBON}\, C_{P\,CARBON}\left(T_{PROCESS} - T_{REF}\right) + m_{STEAM}\, C_{P\,WATER}\left(T_{BOIL} - T_{REF}\right) + m_{STEAM}\, L_{VAPORIZATION}$$
$$+ m_{STEAM}\, C_{P\,STEAM}\left(T_{PROCESS} - T_{BOIL}\right) + m_{H_2}\, C_{P\,H_2}\left(T_{PROCESS} - T_{REF}\right) + m_{CO_2}\, C_{P\,CO_2}\left(T_{PROCESS} - T_{REF}\right)$$
$$+ m_{CO}\, C_{P\,CO}\left(T_{PROCESS} - T_{REF}\right) + m_{CH_4}\, C_{P\,CH_4}\left(T_{PROCESS} - T_{REF}\right) + m_{N_2}\, C_{P\,N_2}\left(T_{PROCESS} - T_{REF}\right)$$
$$+ m_{H_2S}\, C_{P\,H_2S}\left(T_{PROCESS} - T_{REF}\right) + m_{GAS}\, HCV_{GAS}$$

$$Heatloss = Q_{CONDUCTION} + Q_{CONVECTION} + Q_{RADIATION}$$

$$Q_{CONDUCTION} = \frac{A_{SURFACE}(T_1 - T_4)}{\left[(1/K_1)\ln\left(r_2/r_1\right) + (1/K_2)\ln\left(r_3/r_2\right) + (1/K_3)\ln\left(r_4/r_3\right)\right]}$$

$$Q_{CONVECTION} = h\, A_{SURFACE}(T_4 - T_{AMBIENT})$$

$$Q_{RADIATION} = F_{12}\, \varepsilon\, \delta_{BOLTZ}\, A_{SURFACE}\left(T_4^4 - T_{AMBIENT}^4\right)$$

HYDRODYNAMIC CALCULATIONS

Minimum fluidized velocity: (proposed by Christer et al)

$$R_{eP,mf} = \left[28.7^2 + 0.0494 Ar\right]^{1/2} - 28.7$$

$$Ar = d_P^{\ 3}\, \rho_g\left(\rho_s - \rho_g\right) g\, \mu^{-2}$$

$$R_{eP,mf} = d_P U_{mf}\, \rho_g\, \mu^{-1}$$

Initial bubble diameter:

$$d_{bO} = 1.30 g^{-0.2}\left[\left(U_O - U_{mf}\right) N_{or}^{-1}\right]^{0.4}$$

Maximum bubble diameter   (proposed by Mori and Wen)

$$d_{bm} = 0.65\left[(\pi/4)\, d_t^2\left(U_0 - U_{mf}\right)\right]^{0.4}$$

Bubble diameter at any height:

$$d_b = d_{bm} - \left(d_{bm} - d_{bo}\right)\exp\left(-0.3 z / d_t\right)$$

Single bubble rise velocity: (proposed by Davidson and Harrison)

$$U_{br} = 0.711\left(g\, d_b\right)^{(1/2)}$$

Bubble velocity in the bed:

$$U_b = U_0 - U_{mf} + U_{br}$$

Rise velocity emulsion gas:

$$U_e = \frac{U_{mf}}{\varepsilon_{mf}}$$

Fraction of bed in bubbles:

$$\delta_b = \frac{\left(U_0 - U_{mf}\right)}{\left(U_b - U_{mf}\right)}$$

Fraction of bed in emulsion:

$$\delta_e = 1 - \delta_b$$

Superficial velocity:

$$U_0 = U_b \, \delta_b + U_e \, \delta_e \, \varepsilon_{mf}$$

FREEBOARD MODEL

Definition of freeboard: The freeboard being defined, as the space between surface of the bed and the gas exit at the top of the container and its height is freeboard height. The freeboard above a fluidized bed is the dilute phase region. The freeboard container is normally cylindrical and usually of the same diameter as the bed but sometimes larger. The freeboard region is important to the physical design and construction of reactor but also to chemical conversion aspects of fluidized bed operations. Knowledge of solid flow patterns at and above the bed surface is necessary to estimate the importance of freeboard region on the overall fluidized bed performance. The freeboard region provides additional opportunities for intimate solid-gas contacting the reaction in this regime may be significant in many instances and may not be neglected. Particles carry over from the surface of a fluidized bed into the freeboard depends on the mechanism of bubble eruption. When the bubble burst at the fluidized bed surface, particles are entrained in the freeboard region. The entrained particles with a terminal velocity greater than actual gas velocity ($u_t > u$) will reach a certain height within the freeboard before they fall back into the bed. However those particles with a terminal velocity smaller than actual gas velocity ($u_t < u$) will be elutriated and carried out of the bed.

Model of Solid-Gas Reaction Phenomena in the Fluidized Bed Freeboard

Assumptions:

1. Reaction model- Axial dispersion model (Because of some degree of back mixing of gas in the freeboard region).

2. The water gas shift reaction is kinetically driven (Not in equilibrium)
3. Decrease in solid entrainment rate for large particle due to distribution of initial solid velocity.

Entrainment mechanism

For the solid-gas reaction the solid hold up or concentration in the freeboard will affect the reaction rate. To calculate the solid hold up it is necessary to know the entrainment rates and velocity of solid particles.

The solid entrainment rates calculation: $F_i = F_{i\alpha} + (F_{i0} - F_{i\alpha})\exp(-ah)$

h is height above the dense bed surface.

Solid velocity:

When bubble burst at the bed surface the particles are thrown upwards with different initial velocities. The axial velocity profile in the freeboard for both fine and coarse particles can be obtained from the equation based on the force balance. A balance of drag force, gravitational force, buoyancy force and inertial force for an upward particle is shown as follows

$$\frac{dU_{si}}{dh} = \left\{ \frac{-(3/4)C_D \rho_g U_{sr} |U_{sr}|}{\rho_s d_{pi} U_{si}} \right\} - \left\{ \frac{(\rho_s - \rho_g)g}{\rho_s U_{si}} \right\}$$

Where $U_{sr} = U_{si} - U_g$. U_{sr} is the relative velocity of the particle to the gas stream. C_D is the drag coefficient for multi particle system is represented by the following equation.

$$C_D = C_{DS} \, \varepsilon^{-4.7}$$

ε is voidage in the freeboard. C_{DS} is the drag coefficient for single particle, can be calculated from the following equation.

$$C_{DS} = \left\{ \left(\frac{24}{N_{Re}}\right)\left(1 + 0.15 N_{Re}^{0.687}\right) \right\} + \left\{ \frac{0.42}{\left(1 + 4.25 * 10^4 N_{Re}^{1.16}\right)} \right\}$$

U_g the average gas velocity, is estimated from superficial gas velocity as follows

$$U_g = \frac{U_0}{\varepsilon}$$

$$N_{Re} = \frac{\rho_g d_p |U_{sr}|}{\mu}$$

At each height the value of ε is assumed first to calculate gas, solid velocity and particle hold up. The assumed value ε will then checked with the calculated of value of ε from particle hold up. Large particles projected from the bed surface will reach maximum height where solid velocity changes from upward direction to the downward direction. The maximum projected height of large particle can be calculated from

$$\frac{dU_{si}}{dh} = \left\{ \frac{-(3/4)C_D\,\rho_g\,U_{sr}\,|U_{sr}|}{\rho_s\,d_{pi}\,U_{si}} \right\} - \left\{ \frac{(\rho_s - \rho_g)g}{\rho_s\,U_{si}} \right\}$$

$$K_1 = \frac{-(3/4)C_D\,\rho_g}{\rho_s\,d_{pi}} \qquad\qquad K_2 = \frac{(\rho_s - \rho_g)g}{\rho_s}$$

Boundary conditions:

At $\quad h = 0 \qquad\qquad U_{si} = U_{io}$

$h = h_{max} \qquad\quad U_{si} = 0$

$$h_{\max} = \left\{ \left(\frac{1}{2K_1}\right)\left(1 + \frac{U_g}{\sqrt{\frac{K_2}{K_1}}}\right)\ln\left(\frac{-U_g - \sqrt{\frac{K_2}{K_1}}}{U_{i0} - U_g - \sqrt{\frac{K_2}{K_1}}}\right) \right\} + \left\{ \left(\frac{1}{2K_1}\right)\left(1 - \frac{U_g}{\sqrt{\frac{K_2}{K_1}}}\right)\ln\left(\frac{-U_g + \sqrt{\frac{K_2}{K_1}}}{U_{i0} - U_g + \sqrt{\frac{K_2}{K_1}}}\right) \right\}$$

After reaching the maximum height the particles falls downward at an accelerated velocity. Since the total downward traveling distance is so much greater than the short distance needed for acceleration. The falling velocity of particle can be assumed to be U_{ts}-U_o. For the small particles that fall down along the wall, the freefalling terminal velocity U_{tsi} of the particle is used for the calculation.

RESULTS AND DISCUSSIONS

The experimental total carbon conversion that is calculated based on the solid mass balance is in good agreement with the values obtained using the model. The experimental value of 'net solids out' is also in good agreement with the model result. The deviation between total carbon conversion and net solids out, obtained from the model and the experimental values fall between ± 5%. The molecular weight of the dry gas calculated by model is also closer to experimental value with in ± 2% deviation.

In the case of gas composition for H_2, N_2 model results are deviating with in ± 8% of the experimental values. In the case of CO_2, CO the deviation is found to be within ± 15%. CO_2 volume fraction obtained in the experiment is found to be more than that computed by the model uniformly in all the cases. It appears that the reaction rate assumed for the bouduard

reaction is on the higher side which makes CO volume percentage more through substantial generation from the bouduard reaction. But, in the case of CH_4 the deviation between model and experimental values is more. The percentage value of CH_4 obtained from experiments is far less when compared to the model results. It has been seen through analysis of intermediate steps that CH_4 that formed from methane reaction is less, but that coming due to volatile matter is more. Since in the model CH_4 form volatile matter is computed and given as an input. It appears that more realistic rate process for devolatilisation should be employed in the formula. Further, combustion of that CH_4 has been not taken into account in the model as there is uncertainty about the amount of CH_4 that is undergoing combustion reaction. By the incorporation of CH_4 combustion reaction in the model results will be good in the case of CH_4 composition also. Concentration of gases along the bed height is shown in Fig-2.
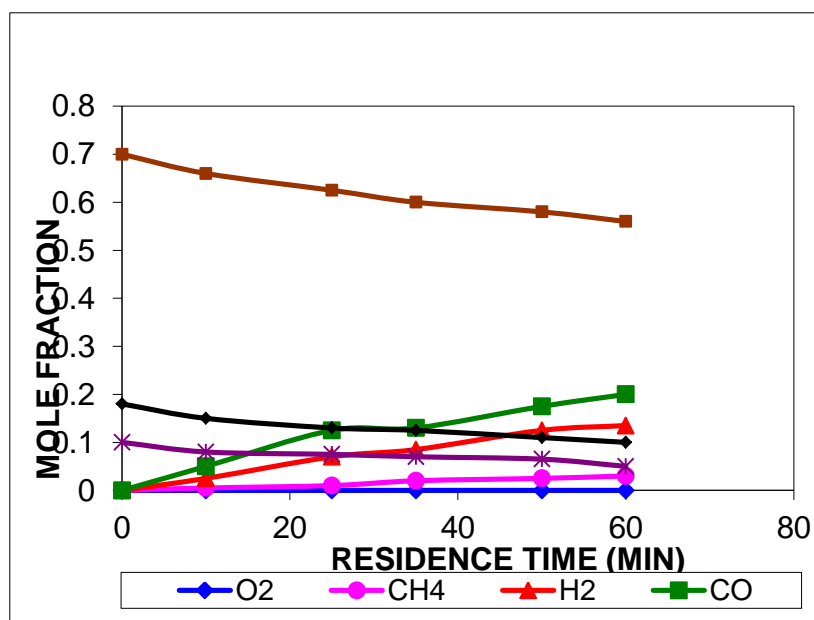

Figure 2:Mole fraction of gases along the height of the bed with residence time.

CONCLUSIONS

Mathematical model for fluidized bed coal gasifier has been developed by considering the assumptions given earlier. The model results are agreeing with experimental values with in ±10% deviation. Only in the case of CH_4, the composition predicted by model is more when compared to experimental data. This is because, in the model only CH_4 formation (From methanation reaction and volatile matter decomposition is considered). But in actual process some amount of methane under goes combustion. This reaction has not been taken into account in the model. The amount of CH_4 that is evolving from volatile matter is also uncertain.

As the reactions are assumed to follow first order reaction kinetics the model predictions are close to experimental data at low pressures (1-10 ata). In the freeboard solid

hold-up decreases as freeboard height increases, voidage increases as freeboard height increases shown in Fig 3 & 4.
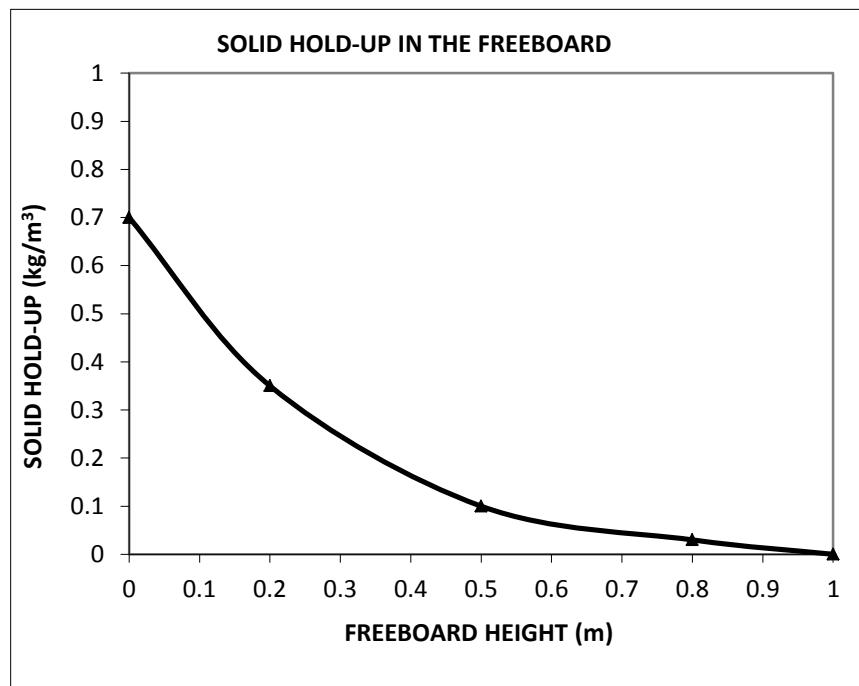

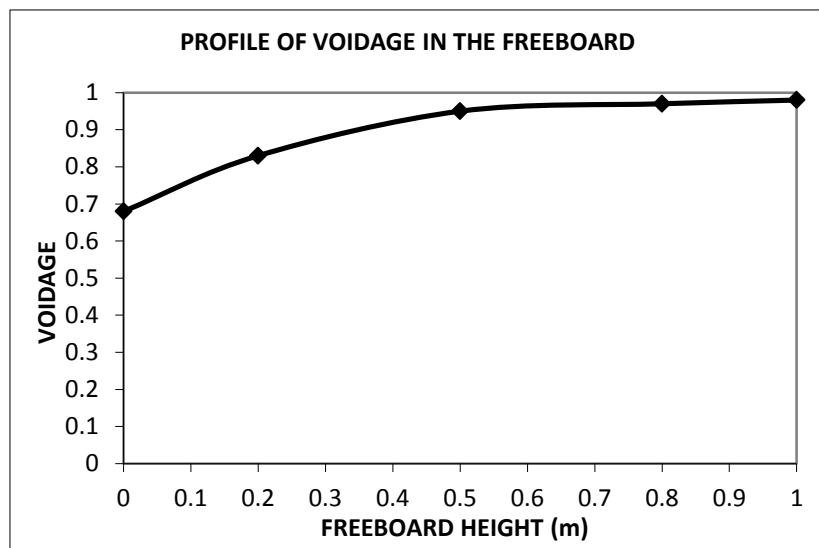**Figure 3: Solid hold-up along the Freeboard height.**

Figure 4: Voidage along Freeboard height.

REFERENCES

[1]   Weimer A.W & David E Clough. Chemical engineering science 1981; 549-567.
[2]   Carl L Yaws. Chemical Engineering science 1976; 22: 153.
[3]   Chen N H & D F Othmer. Journal of Chemical Engineering Data 1962; 7: 37.
[4]   Diazo Kunii, Octave Levenspiel. Fluidization Engineering. Second Edition.
[5]   D C Fee and K M Myles, G Marroquin and Liang-Shih Fan. Chemical Engineering Science 1984; 39(4): 731-737.
[6]   Fabrizio Scala, Piero Salatino. Chemical Engineering Science 2002; 57: 1175-1196.
[7]   F Chejne, J P Hernandez. Fuel journal 2002; 81: 1687-1702.
[8]   Gupta A S and Thodas A. Aiche Journal 1963; 9: 751.
[9]   H M Yan, C Heidenreich and D K Zhang. Fuel Journal 1998; 77: 1067-1079.
[10]   Hugo S Caram and Neal R Amundson. Ind. Eng.chem.process.des.dev 1979; 18(1): 80-102.
[11]   H M Yan, C Heidenreich and D K Zhang. Fuel Journal 1999; 78: 1027-1047.
[12]   H M Yan, C Heidenreich and D K Zhang. Fuel Journal 1998; 77: 1067-1079.
[13]   H M Yan, C Heidenreich and D K Zhang. Fuel Journal 1999; 78: 1027-1047.
[14]   Lowry H R. Chemistry of Coal Utilization. John Willey 1963.
[15]   Michael H Peters and Liang Shih Fan Thomas L Sweeney. Chemical Engineering Science 1983; 38(3): 485-487.
[16]   Perry J H. Chemical Engineer's Hand Book. 5TH Edition.
[17]   Reid R C and T K Sherwood. The Properties of Gases and Liquids. Second Edition.
[18]   R Rusel Rhinehart, Richard M Felder and James K Ferrell. Indian Engineering Chemical Research 1987; 26: 738-745.
[19]   Sherwood T K, Pigford R L and Wilke C R. Mass Transfer. Indian Edition 1975.
[20]   S K Guha, A Kumar and P Sen Gupta. The Canadian Journal of Chemical Engineering 1972; 50: 602-606.
[21]   S T Pemberton and J F Davidson. Chemical Engineering Science 1986; 41: 243-251.
[22]   V S Guru Rajan, P K Agarwal and J B Agnew. Trans I Chem E 1992; 70(A): 211-238.
[23]   Vaclav Baba. Ind Eng chem process des dev 1978; 17(1): 91-98.