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Modeling of freeboard fluidized bed coal gasifier

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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. 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. 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. In this work, modeling of freeboard region has been developed in coal gasifier by taking several assumptions.*

Keywords: Modeling, Freeboard, fluidized bed and coal gasifier

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INTRODUCTION

Gasification is a thermo-chemical process to convert carbon-based products such as biomass and coal into a gas mixture known as synthetic gas or syngas. Various types of gasification methods exist, and fluidized bed gasification is one of them which is considered more efficient than others as fuel is fluidized in oxygen, steam or air [2]. 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.

FREEBOARD MODEL

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 [3]. The freeboard container is normally cylindrical and usually of the same diameter as the bed but sometimes larger.

Important Points for the Consideration of Freeboard

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 Ejection from Dense Phase into the Freeboard

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 [2]. During solid-gas disengagement process, additional particles may also fall down if they hit the wall. A substantial amount of fine particles fall down along the wall. A descending zone near the wall for fine particles. The thickness of the descending zone near the wall is greatest adjacent to the bed surface but decreases as it moves away from the bed surface.

Effect of O_2/Steam Injection on the Freeboard of a Fluidized Bed Gasifier

The loss of carbon from the gasifier system not only leads to a drop in efficiency, but also Blocks the char outlet, Forms "eyebrows" around air nozzles, Solidifies around thermo couples, Fouls hot gas filter. A possible solution to the problem described above is to inject O_2/steam into the freeboard. This will burn the elutriating carbon fines. Which will increase the temperature of the product gases, also decreases extent of fouling in the process and improve the efficiency of the process.

Freeboard Reactions

Heterogeneous gas-solid reactions:

$C + H_2O \longrightarrow CO + H_2$

$C + CO_2 \longrightarrow 2\ CO$

$C + 2\ H_2 \longrightarrow CH_4$

Homogeneous reactions:

$CO + H_2O \longleftrightarrow CO_2 + H_2$

Reaction due to addition of reactant in the freeboard:

$CO + ½\ O_2 \longrightarrow CO_2$

$H_2 + ½\ O_2 \longrightarrow H_2O$

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.

Model Development

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.

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

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

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

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

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

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

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

Boundary conditions:

At *h = 0* $U_{si} = U_{io}$

h = h_{max} $U_{si} = 0$

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

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.

Calculation to obtain initial solid velocity distribution

The initial solid velocity or solid velocity at the bed surface of a given particle size is represented by a unique distribution function. The distribution function for large particle can be obtained from the maximum height and entrainment rate equations. Three steps to calculate initial solid velocity distribution function: a) calculate the relation between h_{max} and U_{io} for particle size $d_{pi.}$ b) Set up flux profile F_i/F_{io} vs. h c)Combine (a) & (b) by plotting the relation of U_{io} vs. F_i/F_{io} gives the cumulative distribution of the ejected particle velocities.

Solid hold-up

In order to simulate solid-gas reactions in the freeboard. It is necessary to estimate the solid holdup or solid concentration in the freeboard. The hold up of particles in the freeboard is calculated by knowing the relation between the solid flux and solid velocity, both upward and downward. The particle holdup is defined as follows

$$dH_{di} = \frac{dF_i}{U_{si}} + \frac{dF_i^{|}}{U_{si}^{|}}$$

Accordingly if the solid velocity is constant at different heights, the solid hold-up can be represented by the following equation

$$H_{di} = \frac{F_i}{U_{si}} + \frac{F_i^{1}}{U_{si}^{|}}$$

If the solid velocity is a distribution function the calculation should be done in the following way

$$H_{di} = H_{di,asc} + H_{di,des}^{|}$$

$$= \int_0^{F_i} \frac{dF_i}{U_{si}} + \int_0^{F_i^{|}} \frac{dF_i^{|}}{U_i^{|}}$$

The downward flow rate of particles $F_i^{|}$ is obtained from material balance of particles in the freeboard as

$$F_i^{|} = \left(F_{io} - F_{i\alpha}\right)\exp\left(-ah\right)$$

Calculation steps for the estimation of solid hold-up:

1. Calculate the velocity distribution profiles, both upward and downward particles at height '*h*' above the bed surface.
2. Estimate the solid hold-up from above equation by integrating area under the curve $\frac{1}{U_{si}}$ vs. F_i and $\frac{1}{U_{si}^{i}}$ vs. F_{si}^{i} to this height.
3. Establish the solid hold-up profile along the freeboard by repeating the steps (1) & (2) for different heights.

The total solid hold-up in the freeboard (H_d) is the summation of the holdup of each particle size (H_{di}) as:

$$H_d = \sum H_{di}$$

Analytical method for calculation of solid hold-up:

The solid entrainment rate calculation:

$$F_{io} = \frac{3.07 * 10^{-9} \rho_g^{3.5} g^{0.5} \left(U_0 - U_{mf}\right)^{2.5} ADBH}{\mu^{0.5}}$$

DBH- bubble diameter of the bed surface *A*- cross sectional area of the bed

The hold-up in the freeboard relates to the entrainment and average holdup't' of the sorbent particles in the freeboard. $H_d = \frac{F_{io}\, At}{\rho_p}$

Reaction model – axial dispersion

In a steady state flow, the material balance equation for any reactant species *i* in a reactor with the length *H* can be derived based on the convection and the axial dispersion as follows

$$E_Z \frac{d^2C_i}{dh^2} - U_g \frac{dC_i}{dh} + R_i = 0$$

R_i - Production rate of species *i*
E_z - Axial dispersion coefficient, which can be estimated from the gas flow Peclet number in the freeboard region.

$$Peclet\, number = \frac{U_g l}{E_z}$$ *l*- characteristic length

Langmuir's "closed-closed vessel" boundary conditions are used for this case. If reaction rate is constant the analytical solution of the concentration profile for the first order reaction is given by Danckwerts. For a homogeneous reaction, the overall reaction rate, R_i is a function of temperature and gas composition. For a heterogeneous reaction, however, R_i is also a function of no. of particles, particle size etc. Axial dispersion model lead to the two limiting cases of ideal flow model i.e. plug flow model when $E_z \longrightarrow 0$ and complete mixing flow model when $E_z \longrightarrow \alpha$.

Freeboard gas-solid phase reaction
The overall reaction rate constant k_{ov} consists of three resistances one due to gas film another due to pores inside the particle and the third due to the chemical reaction.

$$Overall\ reaction\ rate\ cons\tan t = \frac{(1-\varepsilon)}{\left\{\left(\frac{dp}{6h_m}\right) + \left(\frac{(1-\varepsilon_m)}{K_t}\right)\right\}}$$

For a volumetric reaction, the resistance due to gas film is negligible compared to the gas diffusion resistance through the pores. However for a surface reaction on a non porous solid the diffusion through the pores is neglected. The resistance due to the mass transfer of the reactant through the gas film can be represented by the term $\Sigma\, Y_i\, (d_{pi}/6h_{mi})$. Where Y_i is the weight fraction of the particle size d_{pi} in the freeboard, h_{mi} is the mass transfer coefficient across the gas film and can be estimated from the following equation

$$\frac{h_m dp}{D} = 2 + 0.69\left(\frac{\mu}{\rho_g D}\right)^{1/3}\left(\frac{(U_O - U_{ts})dp\,\rho_g^{1/2}}{\mu}\right)$$

$$K_t = K_{to}\exp\left(\frac{-E}{RT}\right)$$

For a volumetric reaction, k_t is independent of particle size; for the surface reaction, however, k_t is a function of a total surface area S. Thus for a first order reaction, R_i can be represented by the following equation

$$R_i = -K_{ov}\, C_i\, (1-\varepsilon)$$

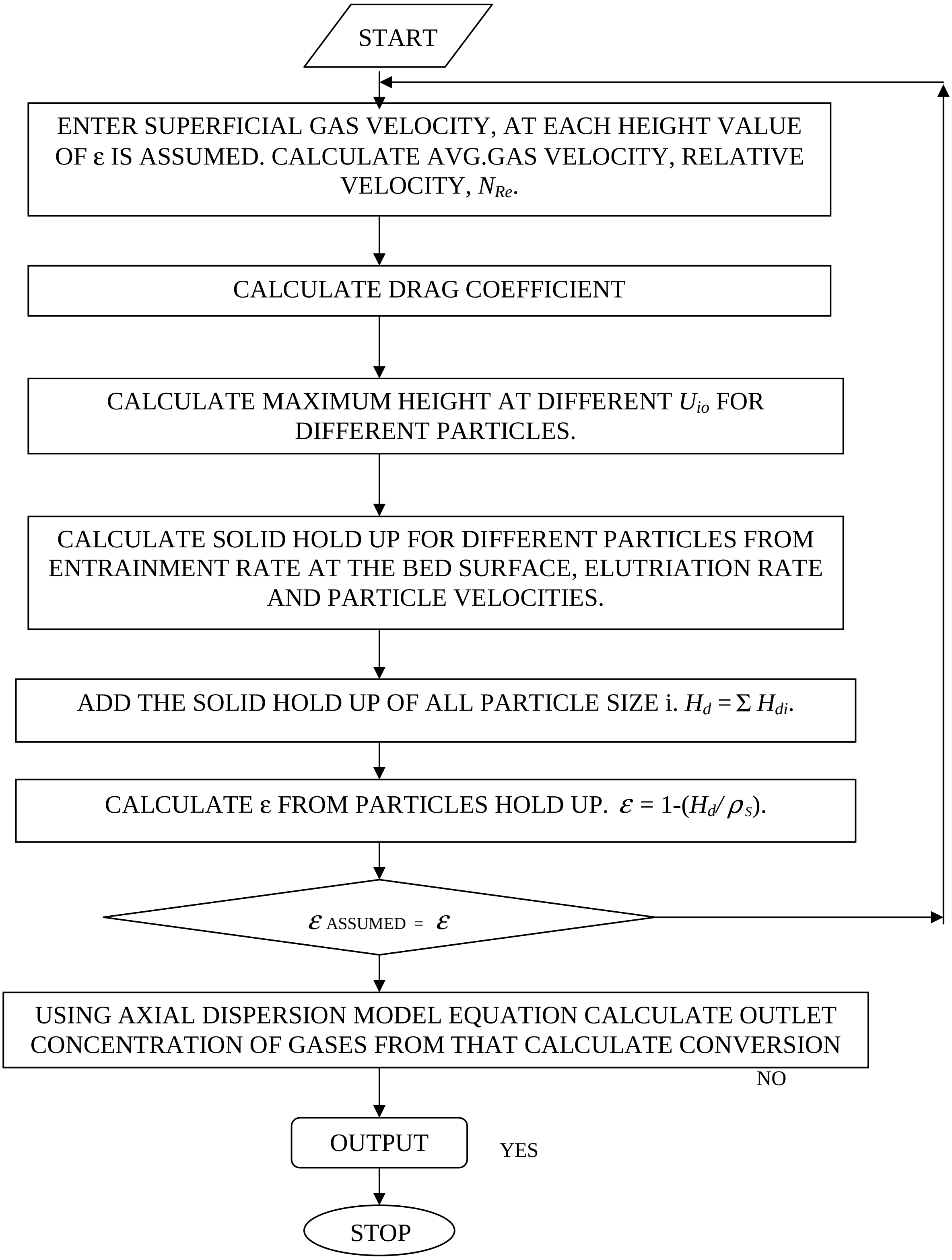
For the surface reaction: $$K_{ov} = \frac{1}{\sum Y_i\left(\frac{dpi}{6h_{mi}}\right) + \frac{(1-\varepsilon)}{K_s S}}$$

For the volumetric reaction: $$K_{ov} = \frac{1}{\sum Y_i\left(\frac{dp}{6D_{eff}}\right)_i + \left(\frac{1}{K_t}\right)}$$

Here D_{eff} is the gas diffusivity through the pores. ε the voidage in the freeboard, can be calculated from the solid hold-up or solid concentration (H_d) as follows

$$\varepsilon = 1 - \left(\frac{H_d}{\rho_s}\right)$$

FREEBOARD MODEL FLOW SHEET



Material balance equations
Gas phase:

$$E_Z \frac{d^2C_i}{dh^2} - U_g \frac{dC_i}{dh} + R_i = 0$$

Solid phase:

$$\frac{dF^u_{i,c}}{dh} - \frac{dF^d_{i,c}}{dh} + \frac{dF^r_{i,c}}{dh} = R_{c,i}$$

Energy balance equation

$$\sum f_{gi,O} H_{gi,O} + \sum f_{si,O} H_{si,O} + Q_{loss} = \sum f_{gi.I} H_{gi,I} + \sum f_{si,I} H_{si,I}$$

Q_{loss}- Heat loss in the freeboard
$f_{si,O}, f_{gi,O}$ – Molar flow rate of solid, gas out
$f_{si,I}, f_{gi,I}$ – Molar flow rate of solid,
H – Enthalpy

RESULTS AND DISCUSSION

When bubble burst at the bed surface particles are ejected into freeboard with different initial velocities. The ejected particles with a terminal velocity greater than average gas velocity will reach a certain height before they fall back into the bed. The ejected particles with a terminal velocity smaller than average gas velocity will be elutriated carried out of the bed. From the maximum height formula h_{max} is a function of initial solid velocity at the bed surface. Initial solid velocity of particle size i at the bed surface is directly proportional to maximum height i.e. initial solid velocity of particle size i at the bed surface increases maximum height also increases, initial solid velocity of particle size i at the bed surface decreases maximum height decreases.

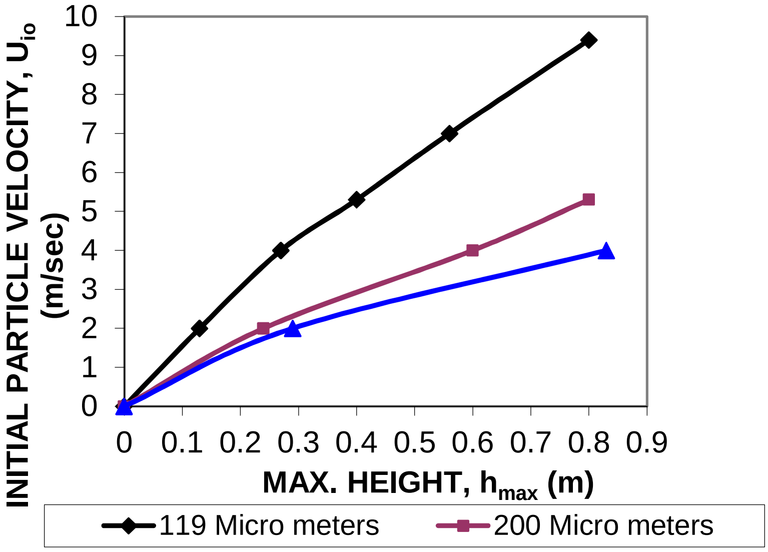


Fig-1. Initial particle velocity Vs Maximum height for different sizes of particles

Cumulative weight fraction is the ratio of entrainment rate of particles size i at any height in the freeboard to the entrainment rate of particles size i at the surface of the bed. As shown in Fig.1, this ratio decreases with freeboard height and at the surface of the bed this ratio is unity.

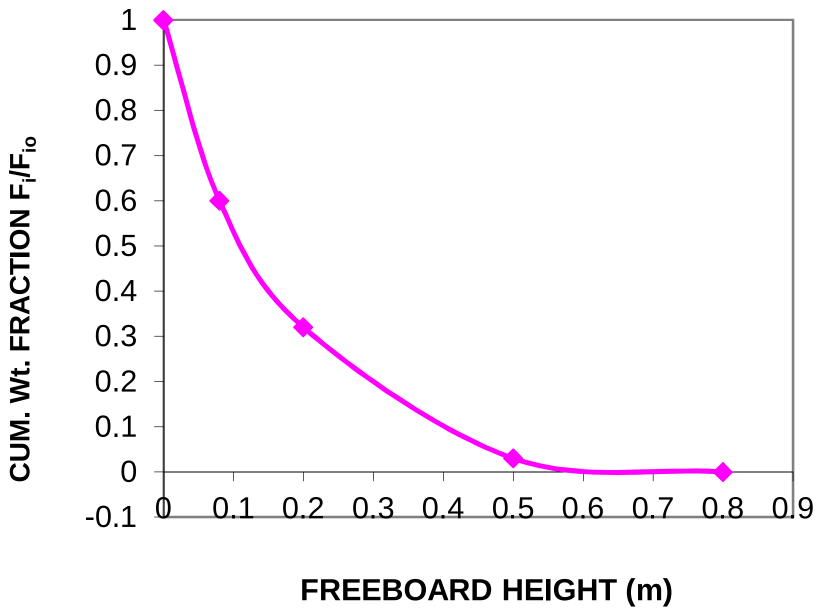


Fig-2. Cumulative weight fraction Vs Freeboard height for the particles size i

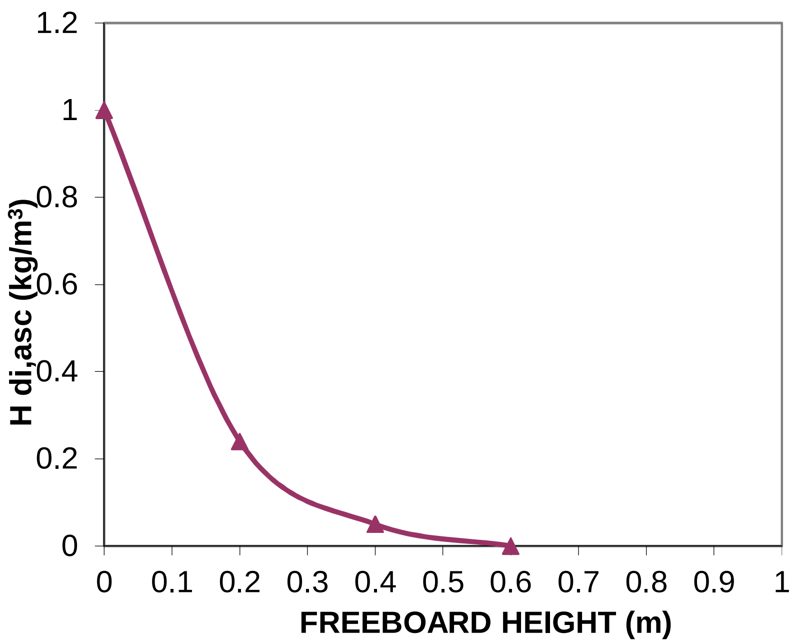


Fig-3. Solid hold-up of ascending particles Vs Freeboard height of particle size i

Initial solid velocity at the surface of the bed is distribution function. Solid velocity decreases with the freeboard height; entrainment rate of ascending particles is also decreases with freeboard height. Solid hold-up of ascending particles is function of entrainment rate of ascending particles and solid velocity. Hence solid hold-up of ascending particles decreases with respect to the freeboard height as shown in Fig.2.

Initial solid velocity at the surface of the bed is distribution function. Solid velocity decreases with the freeboard height; entrainment rate of down ward particles is also decreases with freeboard height. Solid hold-up of descending particles is function of entrainment rate of down ward particles and solid velocity. Hence solid hold-up of down ward particles decreases with respect to the freeboard height.

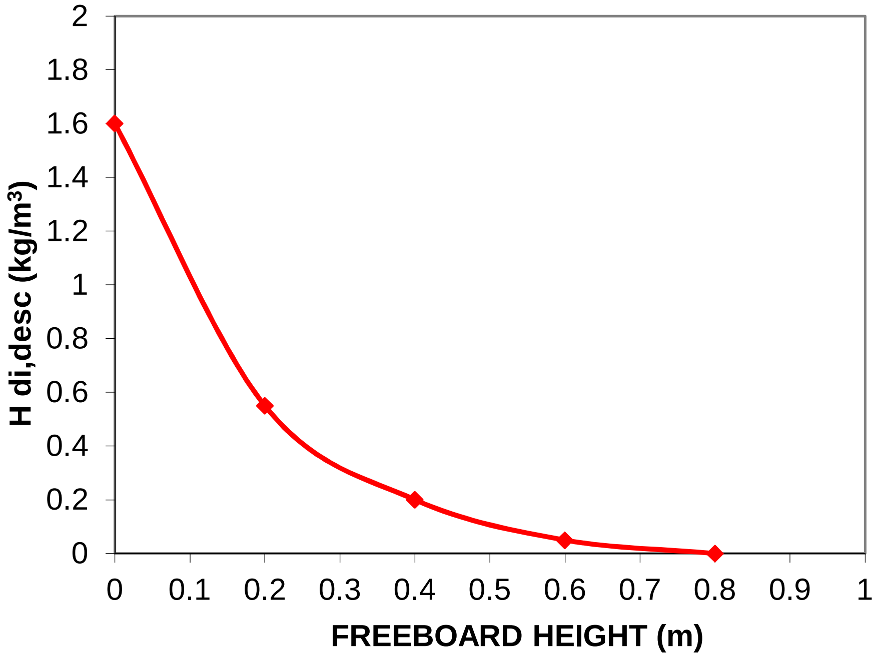


Fig. 4 Solid hold-up of descending particles Vs Freeboard height of particle size i

At the surface of the bed solid hold-up is more voidage is less, as freeboard height increases solid hold-up decreases voidage is increases. From the model also voidage increases with freeboard height.

Initial solid velocity at the surface of the bed is distribution function. Solid velocity decreases with the freeboard height; entrainment rate of particles is also decreases with freeboard height. Solid hold-up of particles is function of entrainment rate of particles and solid velocity. Hence solid hold-up of particles decreases with respect to the freeboard height.

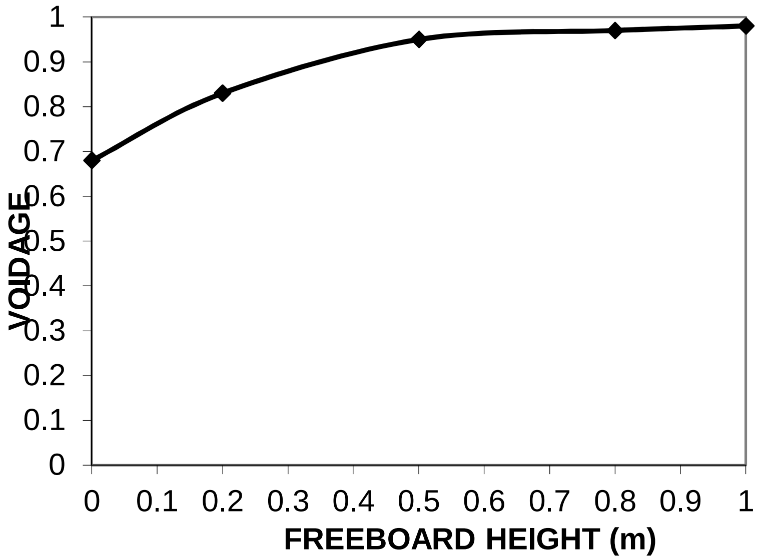


Fig. 5. Voidage Vs Freeboard height

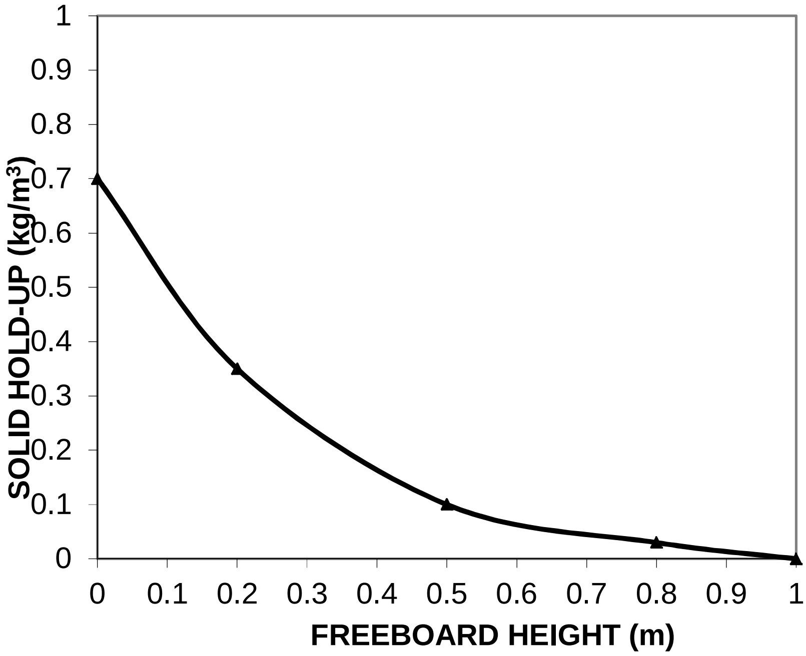


Fig.6 Solid hold-up Vs Freeboard height

In the freeboard solid hold-up decreases as freeboard height increases, voidage increases as freeboard height increases shown in figures 5 & 6.

CONCLUSION

As the reactions are assumed to follow first order reaction kinetics the model predictions are close to experimental data at low pressures (1-10ata). In the freeboard solid hold-up decreases as freeboard height increases, voidage increases as freeboard height increases shown in graphs. Further development can be done by considering higher order reaction kinetics, Methane combustion reaction and Heat loss in freeboard region.

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