Chapter 4

Mathematical Modelling of AFBC

4.1 System Model

In the fluidized bed combustor system , there are many different physical and chemical processes occurring,these include dispersion of flowing gasses, gas bubble growth, movement of bubbles, movement of solids, devolatilization of coal, elutriation and overflow of unburned solids out of the bed, gas-solid reaction and gas-gas reaction within the bed. A set of equations describing system behavior, is called a system model. Generally a system model that incorporates all the physical and chemical processes occurring in the system will be extremely complex. In this study a system model will be developed to incorporate all major factors affecting system behavior.

We first examine the physical conditions of a fluidized bed combustor. By identifying the special features of this bed and making reasonable assumptions, we are able to decouple many of the interacting processes and thereby develop a greatly simplified model of atmospheric fluidized bed combustion (AFBC). This model allows predictions of carbon combustion efficiency in the unit.

4.2 Physical Conditions and Certain Specific Features

In developing a model the first step is to understand physical conditions and certain specific features of the fluidized bed combustor. The system used is controlled by 2.54 cm diameter ash discharge pipe located at the center of the bed. There is no immersed heat exchanger tube to control the bed temperature. The freeboard is 1.14 m in height. The heat exchanger tube of 1 cm in diameter and 4.60 m in length is arranged in the freeboard. This tube can prevent some of the particles splashing into the free board by the bursting of bubbles from flowing out of the bed with the flue gas. The distributor is a perforated plate with 103 holes of 1.5 mm. diameter. The mixture of limestone and lignite particles is fed by a screw feeder located above the bed. Hence the particles will disperse and fall into the bed, this helps the particles to be dispersed throughout the bed, there is no particular hotspot at the coal entry port of the bed as in the case with the coal entry port being in the bed.

This particular fluidized bed combustion system has the following specific features:

1. It is used for combusting lignite .

2. The limestone particles typically comprises more than 99 % of the materials in the bed.[35] Hence the physical behaviour of the bed will be governed by limestone particles. This fact allows us to decouple coal combustion from the fluid mechanics of the bed in which limestone is the bed material. The limestone particles used are large particles of type D of Geldart particle classification (see section 3.4)[31]

3. Due to the presence of large particles in the bed, gas velocity is high.

4. The circulation of solids within the bed is fast relative to the carbon-oxidation and sorbent-SO_2 reaction rates as a consequence of which the solids within the bed can be treated as being well mixed.

5. The time for carbon-oxidation is more than two orders of magnitude shorter than that for the sorbent-SO_2 reaction.[35]

6. The excess air is supplied to the bed.

4.3 Assumptions

Subsequent to the above mentioned features of the system the following assumptions are made to simplify the equations describing the behavior of the fluidized bed combustion system.

1. The solids within the bed are well mixed

2. The temperature of the bed is relatively uniform

3. The bed material, limestone, governs the fluid mechanics of the bed.

4. Crowded heat exchanger tube arranged in free-board obstructs the solids splashed by bubble bursting

5. The char density is assumed to be constant. The volatiles are assumed to burn at the same rate as the char.

6. Two phase theory of gas flow is assumed.

7. Char oxidation occurs by a two film mechanism and the diffusion of the oxidant is the limiting step.

8. Large char particles shrink as they burn in the bed, the chance of elutriation increases progressively as particles shrink.

9. Oxygen concentration in the emulsion phase is assumed to be well mixed.

4.4 System Modelling

The system model is constructed with particular attention to the calculation of carbon combustion efficiency. It is composed of many subsystem models. The equations for each subsystem model are reviewed in chapter 3. Now the equations that correspond to the physical conditions and certain specific features with the assumptions given above, are chosen and modified according to system modelling

4.4.1 Mass Balance

The mass balance in the bed may be determined from considerations of a population balance on the carbon particles in the bed. This follows the notation of Kunii and Levenspiel. Equations from mass balance are given. Their derivations can be seen in Chapter 3.

$$F_o - F_1 - F_2 = -\int_{\text{all } R} \frac{3WP_o(R)\,\mathcal{R}(R)\,dR}{R} \qquad \ldots\ldots(3.3.4)$$

$$p_1(R) = \frac{F_o R^3}{W\left|\mathcal{R}(R)\right|} I(R,R_M) \int_{R_i = R}^{R_i=R_M} \frac{P_o(R_i)\,dR_i}{R_i^3\ I(R_i,R_M)} \qquad \ldots\ldots(3.3.17)$$

$$\frac{W}{F_o} = \int_{R_{t\to\infty}}^{R_M} \frac{R^3}{\left|\mathcal{R}(R)\right|} . I(R,R_M)\ dR \int_{R_i=R}^{R_i=R_M} \frac{P_o(R_i)\,dR_i}{R_i^3\ I(R_i,R_M)}$$

$$\ldots\ldots(3.3.18)$$

$$p_2(R) = \frac{\mathcal{K}(R)\ WP_1(R)}{F_2} \qquad \ldots.(3.3.19)$$

$$\text{where} \quad I(R,R^*) = \exp - \int_{R^*}^{R} \frac{R_1 W + \mathcal{K}(R)}{\mathcal{R}(R)}\, dR \qquad \ldots.(3.3.13)$$

4.4.2 Combustion Mechanism

The combustion process is assumed to be diffusion limited with the coal particle behaving as a shrinking core. The two film theory of Avedesian and Davidson is applied. Avedesian and Davidson formulated the rate of combustion as

$$n = 2 \quad R' Sh\ D_A C_{Ap} \qquad \ldots.(3.4.24)$$

where n = The rate of oxygen consumption in combustion of a single carbon particle

R' = radius of reaction sphere

From Eq (3.4.24), The derivation of the shrinking rate of carbon particle can be made.

Let N_s be the number of moles of carbon in a single carbon particle size R

$$N_s = \frac{(4/3)\pi R^3 \rho_s}{12}.$$

$$\frac{dNs}{dt} = \frac{\pi R^2 \rho_s}{3} \frac{dR}{dt}$$

The rate of carbon consumption is equal to the rate of oxygen consumption in a single carbon particle

$$n = \frac{dN_s}{dt}$$

$$\frac{\pi R^2 \rho_s}{3} \frac{dR}{dt} = 2\pi R' ShD_A C_{Ap}$$

$$\frac{dR}{dt} = \frac{6 R' ShD_A C_{Ap}}{R^2 \rho_s}$$

$$\mathcal{R}(R) = \frac{6R' Sh\ D_A\ C_{Ap}}{R^2 \rho_s}$$

where $\mathcal{R}(R) = \frac{dR}{dt}$

= the shrinking rate of carbon particle

Avedesian and Davidson[18] assumed that the radius of reaction sphere was equal to d_p, $R' = d_p$, but Tanaka [36] found that the radius of the reaction zone remains 1.2 times as large as the carbon particle diameter during combustion, $R' = 1.2\ d_p$

Hence, $$\frac{dd_p}{dt} = \frac{57.6 Sh\ D_A\ C_{Ap}}{d_p \rho_s}$$

Let $\frac{dd_p}{dt} = \mathcal{R}(d_p)$

$$\therefore \mathcal{R}(d_p) = \frac{57.6\ Sh\ D_A\ C_{Ap}}{d_p\ \rho_s} \qquad \ldots.(4.4.1)$$

4.4.3 Elutriation Constant

The Merrick and Highley correlation, Eq. 3.4.11,

$$\mathcal{K} = \frac{\rho_g U_o A_t}{W} \quad A+130\ \exp\ -10.4\ \left(\frac{U_t}{U_o}\right)^{0.5} \left(\frac{U_{mf}}{U_o-U_{mf}}\right)^{0.25}$$

$$\ldots.(3.4.11)$$

suitable for this system is developed for limestone and coal char. The exchanger tube arranged in the free-board of this experimental combustor is considered, it obstructs the solid particles splashed into the freeboard by bubble bursting. This performs like a long freeboard. Hence the constant A in Merrick and Highley correlation can be assumed zero.

4.4.4 Sherwood Number

Since the coal typically comprises less than 1 % of the bed material, the carbon particle interaction should be small and the single-particle Sherwood number correlation can be used. The single-particle correlation relates Sherwood number to the Reynolds and Schmidt numbers. It is of the form, Eq. 3.4.25.

$$Sh = 2.0+0.6 \left(\frac{d_p U_o \rho_g}{\mu}\right)^{\frac{1}{2}} \left(\frac{\mu}{\rho_g D_A}\right)^{\frac{1}{3}} \qquad \ldots. (3.4.25)$$

4.4.5 Fluid Mechanics

The fluid mechanic model is based upon the Davidson and Harrison's two-phase theory. From Eq. (3.4.27) the concentration of oxygen in emulsion phase which is assumed to be well mixed depends on the value of X_b. X_b is the number of times that a bubble is flused out-by through-flow and diffusion in passing through the bed. This parameter can represent the fluid mechanic behaviors of the system. It incorporates several fluid mechanic factors.

$$X_b = \frac{(K_{bp})_b H}{U_b} \qquad \ldots. (3.4.28)$$

$$\text{where } U_b = U_o - U_{mf} + 0.711 \, (gd_b)^{\frac{1}{2}} \qquad \ldots. (4.4.2)$$

Both value of $(K_{bb})_b$ from Eq. (3.4.32) and the value of U_b in Eq. (4.4.2) are sensitive to bubble diameter, d_b

For this system, the bubble diameter correlation of Cranfield and Geldart which was developed for the large particles fluidized bed combustion is suitable. This correlation is

$$d_b = 0.0326 \, (U_o - U_{mf})^{1.11} \, h^{0.81} \qquad \ldots. (3.4.35)$$

For predicting minimum fluidizing velocity (U_{mf}) of a bed of limestone, Pata and Hartman [26] found that Ergun equation is suitable. (see Table 3.2)

$$G_a = 150 \frac{(1-\epsilon_{mf})}{\varphi^2 \epsilon_{mf}^3} R_{emf} + 1.75 \frac{R_{emf}^2}{\varphi \epsilon_{mf}^3}$$

4.4.6 Gas Interchange

A number of correlations have been developed to predict gas interchange rates between bubble and dense phases in fluidized beds. Several of these correlations have been evaluated to determine their applicabilities to fluidized bed combustors. The Davidson and Harrison correlation has been chosen for use in this model. The correlation allows for gas interchange by both convection and diffusion mechanism. It is of the form

$$(K_{bp})_b = 4.5 \left(\frac{U_{mf}}{d_b}\right) + 5.85 \left(\frac{D_A^{\frac{1}{2}} \; g^{\frac{1}{4}}}{d_b^{5/4}}\right) \qquad \ldots.(3.4.32)$$

4.4.7 Bed Expansion

Carbon loading is the weight percent of carbon in bed. The total bed weight for calculating carbon loading is assumed to be the total weight of limestone in bed. Equation for calculating bed weight is

$$W_B = L_{mf} A_t (1-\epsilon_{mf}) \rho_s \qquad \ldots.(3.4.50)$$

where ρ_s = density of limestone

At a fixed expanded bed height, the value of L_{mf} can be calculated from the Miller et.al correlation.

Although this correlation was developed particularly for pressurized fluidized bed combustion, the bed pressure range is between 1 atm and 5 atm. Hence this correlation can be used in atmospheric fluidized bed combustion as well. One important condition of this correlation is that the correlation was also developed for large particle fluidized bed combustion. It is of the form

$$L_{mf} = (L_f /(0.583 \, Re_x^{0.12} \cdot d_t^{-0.5}))^{0.667} \qquad \ldots.(3.4.49)$$

4.4.8 Summary of System Model

All equations selected for system modelling are

1) $$\eta_c = \frac{F_o - F_1 - F_2}{F_o} \times 100$$

2) $$\frac{W}{F_o} = \int_{d_p=0}^{d_{pM}} \frac{d_p^3}{|\mathcal{R}(d_p)|} I(d_p, d_{pM}) \, d(d_p).$$

$$\int_{d_{pi} = d_p}^{d_{pM}} \frac{p_o(d_{pi}) \, d(d_p)}{d_{pi}^3 (d_{pi}, d_{pm})}$$

3) $$F_o - F_1 - F_2 = -\int_{\text{all } R} \frac{3W\, p_b(R)\, \mathcal{R}(R)\, dR}{R}$$

4) $$p_1(d_p) = \frac{F_o d_p^3}{W\, \mathcal{R}(d_p)}\, I(d_p, d_{pM}) \cdot \int_{d_{pi}=d_p}^{d_{pi}=d_{pm}} \frac{P_o(d_{pi})\, d(d_p)}{d_{pi}^3\, I(d_{pi}, d_{pM})}$$

5) $$P_2(d_p) = \frac{W}{F_2}\, \mathcal{K}(d_p)\, p_1(d_p)$$

6) $$\mathcal{K}(d_p) = 130 \exp\left[-10.4 \left(\frac{U_t}{U_o}\right)^{0.5} \left(\frac{U_{mf}}{U_o - U_{mf}}\right)^{0.25}\right] \cdot \frac{\rho_g U_o A_t}{W}$$

7) $$\mathcal{R}(d_p) = \frac{d(d_p)}{dt}$$

$$= \frac{57.6\, Sh\, D_A\, C_{Ap}}{d_p \rho_s}$$

8) $$Sh\,(d_p) = 2.0 + 0.6 \left(\frac{U_o \rho_g}{\mu}\right)^{\frac{1}{2}} \cdot \left(\frac{\mu}{\rho_g D_A}\right)^{\frac{1}{3}} \cdot d_p^{\frac{1}{2}}$$

9) $$C_{Ap} = \frac{C_{ab} - C_{Ao} \exp(-x_b)}{1 - \exp(-x_b)}$$

10) $$X_b = \frac{(K_{bp})_b h}{U_b}$$

11) $$K_{bp} = 4.5\left(\frac{U_{mf}}{d_b}\right) + 5.85\left(\frac{D_A^{1/2}\, g^{1/4}}{d_b^{5/4}}\right)$$

12) $$d_b = 0.0326\ (U_o - U_{mf})^{1.11}\ h^{0.81}$$

13) $$U_b = 0.711(gd_b)^{1/2} + U_o - U_{mf}$$

14) $$U_t = \frac{0.153\ d_p^{1.14}\ g^{0.71}\ (\rho_s - \rho_g)^{0.5}\ d_p^{0.5}}{\rho_g^{0.5}} \cdot$$

$$0.843 \log\ \left(\frac{\varphi}{0.065}\right)$$

15) $$Ga = 150\ \frac{1-\epsilon_{mf}}{\varphi^2 \epsilon_{mf}^3}\ Re_{mf} + 1.75 \frac{Re_{mf}^2}{\varphi \epsilon_{mf}^3}$$

$$Ga = g\bar{d}_p^{\,3} \rho_g\ (\rho_s - \rho_g)\ /\ \mu^2$$

$$Re_{mf} = U_{mf}\ \bar{d}_p \rho_g / \mu$$

16) $$\bar{d}_p = \frac{1}{\sum_{all\ i} (x_i / d_{pi})}$$

17) $$\frac{L_f}{L_{mf}} = 0.583\ Re_x^{0.12} \left(\frac{L_{mf}}{d_b}\right)^{0.5} P_B^{-0.2}$$

where $$Re_x = \rho_g (U_o - U_{mf})\, \bar{d}_p / \mu$$

18) $$W_B = L_{mf}(1-\epsilon_{mf})\, \rho_s$$

$\bar{d}_p$, d_{pi} in equation 15, 16, 17 mean diameter of limestone particle, otherwise diameter of coal diameter.