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**Tennessee Valley Authority
Atmospheric Fluidized-Bed
Combustor Simulation Interim
Annual Report**

January 1 Through December 31, 1979

J. W. Wells
R. P. Krishnan

**OPERATED BY
UNION CARBIDE CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY**

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TENNESSEE VALLEY AUTHORITY ATMOSPHERIC FLUIDIZED-BED
COMBUSTOR SIMULATION INTERIM ANNUAL REPORT

January 1 Through December 31, 1979

J. W. Wells
Engineering Division

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Engineering Technology Division

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NOMENCLATURE

- A = heat transfer area, cm^2 (ft^2)
 a_i, b_i = constants for product i , $^{\circ}\text{K}^{-1}$, dimensionless
 A_{xs} = fluidized-bed cross-sectional area, cm^2
 C = molar concentration, g-mol/cm^3
 C_p = specific heat, cal/g-K ($\text{Btu/lb}_m - ^{\circ}\text{R}$)
 D = molecular diffusivity, cm^2/s
 d_B = bubble diameter at some height above the distributor plate, cm
 d_{BM} = maximum attainable bubble diameter due to coalescence, cm
 d_{BO} = initial bubble diameter at the distributor plate, cm
 d_{BS} = maximum stable bubble diameter, cm
 d_p = surface mean diameter of particle, cm
 d_t = diameter of tube, cm (ft)
 D_t = diameter of the fluidized bed, cm
 e = emissivity, dimensionless
 E_j = activation energy of reaction j , kcal/g-mol
 f = frequency of bubble per unit area of the bed, $\text{cm}^{-2} \text{ s}^{-1}$
 F = molar flow of gaseous species, g-mol/s
 F_{ATT} = attrition fines flow rate, g/s
 f_{dp} = fraction of particles in the bed smaller than diameter d_p
 F_f = view factor, dimensionless
 f_w = fraction of particles in the bed smaller than radius R
 F_O = feed rate of solids, g/s
 F_1 = underflow rate of solids, g/s
 F_2 = total rate of elutriated solids, g/s

- g = gravitational acceleration, cm/s^2
 G = cumulative normal Gaussian distribution function
 G_{max} = maximum mass velocity, $\text{G/cm}^2\text{-s}$ ($\text{lb}_m/\text{ft}^2\text{-s}$)
 h_c = convective heat transfer coefficient, $\text{cal/cm}^2\text{-s-K}$ ($\text{Btu/ft}^2\text{-h-}^\circ\text{F}$)
 H_f = heat of formation of component at 298 K reference temperature, cal/g-mol (Btu/lb-mol)
 h_r = radiative heat transfer coefficient, $\text{cal/cm}^2\text{-s-K}$ ($\text{Btu/ft}^2\text{-h-}^\circ\text{F}$)
 k = an adjustable constant in Eq. (3.1), dimensionless
 K = gas exchange coefficient, s^{-1}
 k_{ATT} = attrition rate constant defined by Eq. (4.4), cm^{-1}
 K_{ATT} = attrition rate constant defined by Eq. (4.3), cm^{-1}
 k_{cf} = diffusion rate constant (see Eq. 5.9)
 k_{CR} = chemical reaction rate constant (see Eq. 5.9)
 k_g = gas thermal conductivity, cal/cm-s-K
 k_{j0} = preexponential factor for reaction j , s^{-1}
 k_m = mass transfer coefficient, cm/s
 $K(R)$ = elutriation rate constant of a particle of radius R defined by Eq. (4.5), s^{-1}
 $K^*(R)$ = carryover rate of particle of radius R per unit cross-sectional area of the bed, $\text{g/cm}^2\text{-s}$
 k_1 = reaction rate constant for $\text{C} + 0.5\text{O}_2 \longrightarrow \text{CO}$ (see Table 5.4), $\text{g-mol/cm}^2\text{-s-atm}$
 k_2 = reaction rate constant for $\text{CO} + 0.5\text{O}_2 \longrightarrow \text{CO}_2$ (see Table 5.4), $\text{cm}^3/\text{g-mol-s}$
 k_3 = reaction rate constant for $\text{C} + \text{CO}_2 \longrightarrow 2\text{CO}$ (see Table 5.4), $\text{g-mol/cm}^2\text{-s-atm}$
 L_f = expanded bed height, cm
 L_{mf} = bed height at minimum fluidization, cm

LMTD = log mean temperature difference, K ($^{\circ}$ R)

m = heating rate, K/s

$\dot{m}$ = mass flow rate, g/s (lb_m/s)

M_c = atomic weight of carbon, g-mol

n = number of bubbles at height z above the distributor plate, dimensionless

n_d = number of holes in the distributor plate, dimensionless

N_h = number of incremental volumes ΔV in the bed, dimensionless

$p_A(R)$ = differential attrition fines size distribution, cm^{-1}

$p_B(R)$ = differential particle size distribution in the bed, cm^{-1}

Pr = Prandtl number ($C_p \mu / k_g$), dimensionless

$p_O(R)$ = differential feed size distribution, cm^{-1}

$p_1(R)$ = differential underflow size distribution, cm^{-1}

$p_2(R)$ = differential particle size distribution of elutriated solids, cm^{-1}

Q = heat transfer rate, cal/s (Btu/h)

R = particle radius, cm

Re_t = Reynolds number at terminal velocity $\{[P_g U_t(R) d_p] / \mu_g\}$, dimensionless

R_G = universal gas constant, 1.987 cal/g-mol-K

R_{GG} = universal gas constant, 82.06 atm $\text{cm}^3/\text{g-mol-K}$

$R_{\max}$ = maximum particle radius, cm

$R_{\min}$ = minimum particle radius, cm

$\dot{R}(R)$ = rate of change of particle radius due to attrition for particle radius R , cm/s

$R_T(R)$ = the average rate of total carbon consumption per unit surface area of a particle of radius R , g-mol/ $\text{cm}^2\text{-s}$

- R_1^T = overall rate of $C + 0.5O_2 \longrightarrow CO$ (see Table 5.4),
 $g\text{-mol}/cm^2\text{-s}$
- R_2^T = overall rate of $CO + 0.5O_2 \longrightarrow CO_2$ (see Table 5.4),
 $g\text{-mol}/cm^3\text{-s}$
- R_3^T = overall rate of $CO_2 + C \longrightarrow 2CO$ (see Table 5.4), $g\text{-mol}/cm^2\text{-s}$
- Sh = Sherwood number ($K_m d_p/D$), dimensionless
- T = temperature, K ($^{\circ}R$)
- T_{BED} = average bed temperature, K ($^{\circ}R$)
- TDH = transport disengaging height, cm
- T_p = particle surface temperature, K
- u_B = bubble velocity at height above the distributor plate, cm/s
- U_{mf} = minimum fluidizing velocity, cm/s
- U_{mb} = minimum bubbling velocity, cm/s
- U_o = gas superficial velocity, cm/s (ft/s)
- $\bar{U}_o$ = average freeboard superficial gas velocity, cm/s
- $U_t(R)$ = terminal velocity of particle of radius R , cm/s
- V = volume, cm^3
- V_B = volume of bubble, cm^3
- $\dot{V}_B$ = gas volumetric flow rate through bubble phase, cm^3/s
- $\dot{V}_B'$ = volumetric flux through the bubble phase, $cm^3/cm^2\text{-s}$
- v_i = cumulative yield of product i up to temperature T , wt %
- v_i^* = ultimate yield of product i , wt %
- v_{ij} = cumulative yield of product i by reaction j , wt %
- v_{ij}^* = ultimate yield of product i by reaction j , wt %
- W_B = bed mass, g
- x = weight fraction, dimensionless

X = total amount of reaction component produced or consumed in emulsion phase, g-mol

y = mass fraction passing through screen, dimensionless

z = height above distributor plate, cm

Greek Notation

δ = total void fraction (bubble and emulsion) in control volume ΔV , dimensionless

$\bar{\delta}$ = average total void fraction in the bed, dimensionless

ΔH_R = heat of reaction, cal/g-mol

ϵ_B = bubble voidage at bed height, dimensionless

$\bar{\epsilon}_B$ = average bed bubble voidage, dimensionless

ϵ_{mf} = fractional bed voidage at minimum fluidization, dimensionless

ζ = factor to account for the nonspherical nature of bubble, dimensionless

η = mechanism factor

μ = gas viscosity, g/cm-s ($\text{lb}_m/\text{ft-s}$)

ρ = density, g/cm³ (lb_m/ft^3)

ρ_{char} = density of char, g/cm³

τ = residence time of particles in the bed, s

τ_s = Stefan-Boltzmann constant, cal/cm²-s(K)⁴

ϕ_K = constant defined by Eq. (3.8)

Φ = average amount of component produced or consumed per unit volume of emulsion phase, g-mol/cm³

ψ = constant defined by Eq. (3.7)

Subscripts

BC = bubble to cloud
BE = bubble to emulsion
bund = bundle
CE = cloud to emulsion
CO = carbon monoxide component
CO₂ = carbon dioxide component
F = final
FG = flue gas
g = gas
H₂O = water component
I = initial
O₂ = oxygen component
plug = plug flow
R = reference
W = wall
WW = waterwalls

Superscripts

BUB = bubble phase
EMUL = emulsion phase
I = intrinsic
M = mass transfer
SB = slow bubble

1. SUMMARY

This report contains a detailed description of the work performed during 1979 for the Tennessee Valley Authority (TVA) in support of the TVA Fluidized-Bed Combustor (FBC) Demonstration Plant Program. The work was carried out under task 4, modeling and simulation of atmospheric fluidized-bed combustor (AFBC) systems. The overall objective of this task is to develop a steady-state mathematical model with the capability of predicting trends in bed performance under various feed and operating conditions. As part of this effort, three predictive subprograms (subcodes) were developed during 1979: (1) bubble-growth subcode, (2) sorbent-coal ash elutriation and attrition subcode, and (3) coal combustion subcode. These codes, which are currently being tested with experimental data, are capable of predicting how some of the important operating variables in the AFBC affect its performance (Table 1.1). After testing against field data, these subcodes will be incorporated into an overall AFBC system code, which was developed earlier at ORNL for analysis of the Department of Energy (DOE) Component Test and Integration Unit (CTIU) at Morgantown, West Virginia.

The bubble-growth code developed during this year relates bubble growth to bed expansion. In this procedure, the average bed bubble voidage is predicted by two separate methods. First, applying the two-phase theory, the average bubble voidage is calculated by using the bed expansion expression of Babu, Shah, and Talwalker (1978). Second, using the bubble-growth expression of Mori and Wen (1975), the average bubble voidage is found by calculating the first moment of the specific bubble voidage. These two values of average bed bubble voidage are compared, and the constant in the Mori and Wen correlation is varied until the calculated voidage from both methods agrees. With this constant, the bubble properties as a function of height are estimated.

The sorbent-coal ash elutriation and attrition code completes the material balance about the cell for the sorbent and coal ash solids. This task is done by using the elutriation and attrition expressions of Merrick and Highley (1974) and solving the fluidized-bed performance equations

Table 1.1. Factors affecting atmospheric fluidized-bed combustor performance

Variable	Sorbent utilization	Heat transfer in bed	Combustion efficiency	Bed hydrodynamics
Unit size (bed area)	<i>a</i>		<i>b</i>	<i>b</i>
Bed depth	<i>a</i>		<i>b</i>	<i>b</i>
Tube bank geometry	<i>a</i>	<i>a</i>	<i>a</i>	<i>a</i>
Tube metal temperature		<i>b</i>		
Superficial velocity	<i>a</i>	<i>b</i>	<i>b</i>	<i>b</i>
Coal-limestone feed arrangement	<i>a</i>		<i>a</i>	
Freeboard height	<i>a</i>		<i>a</i>	
Bed temperature	<i>a</i>	<i>b</i>	<i>b</i>	<i>b</i>
Freeboard temperature	<i>a</i>		<i>a</i>	
Excess air	<i>a</i>		<i>b</i>	<i>b</i>
Coal type and size	<i>a</i>		<i>b</i>	
Coal sulfur content	<i>a</i>			
Limestone type and size	<i>a</i>			<i>b</i>
Bed particle size	<i>a</i>	<i>b</i>	<i>b</i>	<i>b</i>
Recycle of elutriated fines	<i>a</i>		<i>a</i>	<i>a</i>

^a Factors known to affect AFBC performance.

^b Factors considered by current codes.

given by Kunii and Levenspiel (1977). As a result, the material balance is closed, and the particle size distribution of the bed and the elutriated solids are found.

The coal combustion code determines the combustion efficiency of the AFBC via a two-phase (emulsion and bubble) bubbling bed model. The bubble characteristics (slow, fast, diameter, fraction, etc.) are predicted via the previous bubble-growth code. Devolatilization of coal is assumed to be uniform throughout the bed, and the yields and composition of volatile products are predicted via the model of Reklaitis et al. (1977) for Illinois No. 6 coal. The subsequent char combustion is assumed to proceed via the following reactions.

For the heterogeneous reactions, Eqs. (1.1) and (1.3), both intrinsic and mass-transfer effects are used to determine the overall rate of the reactions. This information is then used with the elutriation expression of Wen and Hashinger (1960) to close the gas side component balances and the char solids balance. In doing this function, the coal mass balance is closed; concentration profiles for O_2 , CO , and CO_2 are generated; and the char bed weight and size distribution are found.

In addition to these predictive subcodes, the overall system code previously developed for the CTIU is described in this report. The overall system code does not incorporate the above predictive codes. At present, this code closes the material and energy balance for a complete AFBC system. The material balance is closed, based on vendor-supplied data. This balance is then used to predict the heat transfer characteristics of the surfaces (submerged and freeboard) in the AFBC. Existing correlations for heat transfer in AFBC are used in the code along with thermophysical properties of the various streams. These characteristics are used to close the energy balance about the system. The structure of this code allows simulation of many different AFBC configurations.

Typical results from each of the codes are included in this report. Extensive studies with these codes have not been made during this year, due to time limitations. During the upcoming year a sorbent utilization subcode will be developed, and the predictive subcodes will be tested. At this point, these subcodes will be incorporated into the system code. The resulting code will be a flexible predictive code that will be used to simulate the TVA pilot and demonstration plants.

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2. INTRODUCTION

In recent years, the utilization of coal as a primary source of energy has gained increasing importance. A number of new technologies are being developed for the utilization of coal; AFBC is one such technology.

The AFBC concept has many advantages for both utility power and process heat production. Specifically, the AFBC will allow the control of SO_2 and NO_x emissions without the use of external pollution control equipment. Also, the AFBC bed has a fairly uniform temperature throughout and a favorable heat transfer coefficient [$(0.023 \text{ to } 0.028 \text{ W/cm}^2\text{-K})$ ($40 \text{ to } 50 \text{ Btu/h-ft}^2\text{-}^\circ\text{F}$)]. This situation allows lower surface areas for heat transfer compared with pulverized coal-fired boilers. On the other hand, the attrition and elutriation of solids from the AFBC create problems in maintaining a high combustion efficiency and in removing solids from the flue gas. Also, poor solids mixing in the bed and the bypass of gaseous reactants via bubbles may result in localized reducing conditions (corrosion). These conditions may also lead to excessive SO_2 emissions. As with any new technology, these and other difficult problems must be addressed. Many of these questions can be studied by process modeling and simulation together with a carefully planned experimental program. The link between the efforts is, however, very important. The process of comparing the experimental data with the model predictions gives a basic understanding of the various factors affecting AFBC performance. This understanding can then be used to develop a system code that can predict AFBC performance at other operating conditions. The main indicators of performance in the AFBC system are

1. bed hydrodynamics,
2. sorbent utilization,
3. combustion efficiency, and
4. in-bed heat transfer.

These indicators are affected by many design and operating variables, as shown in Table 2.1. The purpose of the modeling effort is to find how each of these variables affects the system performance and to determine

additional variables that are important for design and scale-up. This information can then be used to develop a comprehensive system model for performance prediction. To do this effectively, experimental data must be available in the range of interest. Only recently are data from AFBCs of reasonable size becoming available. The primary sources for data are

1. the Babcock and Wilcox/Electric Power Research Institute (B&W/EPRI) 183- by 183-cm (6- by 6-ft) AFBC at Alliance, Ohio,
2. the Pope, Evans, and Robbins 92- by 92-cm (3- by 3-ft) AFBC at Georgetown, Virginia, and
3. the NASA conical FBC at Cleveland, Ohio.

Table 2.1. Factors affecting atmospheric fluidized-bed combustor performance

Variable	Sorbent utilization	Heat transfer in bed	Combustion efficiency	Bed hydrodynamics
Unit size (bed area)	x		x	x
Bed depth	x		x	x
Tube bank geometry	x	x	x	x
Tube metal temperature		x		
Superficial velocity	x	x	x	x
Coal-limestone feed arrangement	x		x	
Freeboard height	x		x	
Bed temperature	x	x	x	x
Freeboard temperature	x		x	
Excess air	x		x	x
Coal type and size	x		x	x
Coal sulfur content	x			
Limestone type and size	x			x
Bed particle size	x	x	x	x
Recycle of elutriated fines	x		x	x

With this information, the validity of the assumptions made in the modeling process can be confirmed, and an improved AFBC system code will be developed.

This report describes the atmospheric fluidized-bed modeling activities performed for TVA at ORNL during 1979. During this period,

three predictive subcodes were developed: (1) the bubble hydrodynamic routine, (2) the combustion routine, and (3) the sorbent-coal ash elutriation and attrition routine. These three routines can be used to predict the effect of some of the variables listed in Table 2.1 on AFBC performance. In addition, the existing overall AFBC system code originally developed for the Morgantown CTIU facility has been modified to predict the heat transfer coefficients of AFBC heat exchange equipment (submerged surface, freeboard surface, and water wall). This code essentially completes the material and energy balance about the system, based on vendor-supplied data. At present the system code does not incorporate the above predictive subcodes.

Each of the above performance subcodes is described in this report, which includes background material, assumptions, equation derivations, logic diagrams of the codes, limited comparison of computed results to experimental data, and recommendations for further work. The overall system code is also described. Future plans for this calendar year will include the development of a sulfur capture subcode, improvement of the combustion model, incorporation of the predictive subcodes into the existing system code, and simulation of the TVA/B&W pilot plant AFBC.

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3. BUBBLE-GROWTH MODEL

3.1 Background

Simulation of FBCs requires the accurate prediction of bubble size and bubble growth in the bed. The mass transfer of gas between the bubble phase and the emulsion phase is a strong function of bubble size. The prediction of bubble size is necessary for the calculation of combustion efficiencies and sulfur capture in FBCs. The properties of the bubbles in the bed also determine the patterns of solid mixing in the bed and are related to the elutriation of solids from the bed. As a consequence of these effects, the size of the bubble is of primary importance in the scale-up of fluidized beds (Werther 1978 and Bottom 1966). Many bubble-growth correlations have been proposed for small particles and low superficial velocities (Mori and Wen 1975, Cranfield and Geldart 1974, and Werther 1978). Analysis of these correlations shows that they are valid for only a limited range of operating conditions and are inadequate for the large particles and high superficial velocities that are typical of FBC operation.

3.1.1 Bubble growth

Bubble growth in fluidized beds is caused by three mechanisms: (1) the decrease in hydrostatic pressure as the bubble rises, (2) one bubble overtaking another vertically, and (3) one bubble combining with another horizontally. In general, the hydrostatic pressure effect is too small to be significant. For small particles and low superficial velocities, coalescence usually occurs in the vertical direction. Also, it has been reported (Geldart 1977) that the spacing between the bubbles must be within two bubble diameters before vertical coalescence can occur.

For shallow beds of large particles (1000 to 2000 μm), Cranfield and Geldart (1974) observed coalescence to occur primarily by "cross absorption," which corresponds to horizontal bubble growth. Also, for large-particle beds, Cranfield and Geldart (1974) and Cranfield (1978) reported the formation of large lenticular voids a short distance (<2 to 3 cm) above the distributor plate. As this void moves upward, it rapidly breaks up

into small stable bubbles, which has been observed within 5 cm of the distributor plate. In general, for both large- and small-particle beds, the bubbles tend to coalesce toward the center of the bed, leaving a region of descending solids, devoid of bubbles, along the walls of the reactor (Cranfield 1978).

Because of the importance of bubble growth in the prediction of fluidized-bed performance, many correlations for bubble growth have been proposed; these correlations are reviewed in the paper by Mori and Wen (1975). In general, they found that these correlations applied only at the conditions at which the data were taken. It was also noted that the bed diameter affects bubble growth. Following the suggestion of Miwa, Mori, and Muchi (1970), Mori and Wen proposed the following expression:

$$(d_{BM} - d_B)/(d_{BM} - d_{BO}) = \exp(-kz/D_t), \quad (3.1)$$

where d_{BM} is the maximum attainable bubble diameter given by

$$d_{BM} = 0.652[A_{xs}(U_o - U_{mf})]^{2/5}; \quad (3.2)$$

d_{BO} is the initial bubble diameter formed at the distributor plate given by

$$d_{BO} = 0.347[A_{xs}(U_o - U_{mf})/n_d]^{2/5}, \quad (3.3)$$

where z is the height above the distributor plate, D_t is the diameter of the reactor, n_d is the number of holes in the distributor plate, and k is an adjustable constant. By setting the constant k to 0.3, a satisfactory fit of over 400 data points was obtained for a limited range of particle size (60 to 450 μm), superficial velocity (50 to 70 cm/s), and reactor diameter (<130 cm).

More recently Werther (1978) and Cranfield and Geldart (1974) proposed other bubble-growth correlations for fluidized beds. Again, the general applicability of these equations to other systems and conditions is questionable. Cranfield and Geldart's work was specifically for shallow, large-particle beds. Their equation is

$$d_B = 0.0326(U_o - U_{mb})^{1.11} z^{0.81}, \quad (3.4)$$

which tends to overpredict bubble diameters for typical AFBC conditions, as discussed later.

3.1.2 Maximum bubble diameter

Bubble growth can be conceptually limited by two maximum bubble sizes: the size corresponding to complete coalescence of all gas into a single train of bubbles and the stable bubble determined by the bubble hydrodynamics. Mori and Wen (1975) proposed a correlation for the maximum attainable bubble diameter due to complete bubble coalescence d_{BM} , which is the size of a bubble in a train of large, single bubbles rising through a bed such that no vertical coalescence can occur. The value of this bubble diameter was derived by Mori and Wen and is given by Eq.(3.2), which was derived on the basis of the following assumptions. First, the number of bubble diameters that must be maintained between bubbles to prevent vertical coalescence was set at four. Second, the velocity of the bubble was calculated from the work of Davidson and Harrison (1963) as

$$u_B = 0.711 \sqrt{gd_{BM}} \quad (3.5)$$

Third, from two-phase theory, all gas in excess of that required for minimum fluidization passes through the bed as visible bubble flow.

Therefore, the volumetric flux through the bubble phase is

$$\dot{V}_B = \dot{V}_{B/A_{xs}} = (U_o - U_{mf}) \quad (3.6)$$

where $\dot{V}_B$ is the gas volumetric flow rate through the bubble phase, cm^3/s .

Recent observations in fluidized beds have altered these assumptions. First, vertical coalescence appears to be limited by two bubble diameters versus four (Geldart 1977). Next, Werther (1978) found that the velocity of a bubble is a function of the diameter of the reactor and is given by

$$u_B = \psi \sqrt{gd_B} \quad (3.7)$$

where

$$\psi = \begin{cases} 0.64 & D_t \leq 10 \text{ cm} \\ 0.225(D_t)^{0.4} & 10 < D_t < 100 \\ 1.6 & D_t \geq 100 \end{cases}$$

with D_t equal to the diameter of the reactor.

Finally, the volumetric flux through the bubble phase is always smaller than that predicted via two-phase theory and is given by Werther (1978) as

$$\dot{V}_B = \phi_k (U_o - U_{mf}) \quad , \quad (3.8)$$

where $0.67 \leq \phi_k \leq 0.76$. Cranfield and Geldart (1974) proposed the following correlation for predicting the volumetric flux through the bubble phase within $\pm 22\%$:

$$\dot{V}_B = 0.363 (U - U_{mb})^{1.11} z^{0.09} \quad . \quad (3.9)$$

If one repeats the derivation of d_{BM} with these assumptions, the expression for the maximum attainable bubble diameter becomes

$$d_{BM} = 0.431 \left\{ \left[A_{xs} \phi_k (U_o - U_{mf}) \right] / \psi \right\}^{2/5} \quad . \quad (3.10)$$

This value of d_{BM} is the diameter of a train of single bubbles rising along the center of the bed and represents a possible limit to the bubble-growth process.

The second concept of maximum bubble growth is based on bubble hydrodynamics. Experimental observations have shown that bubbles do not grow indefinitely but tend to break up as soon as their diameter exceeds a certain value (Werther 1978 and Matsen 1973). This concept depends on the physical properties of the bed material. A criterion for maximum bubble size based on bubble hydrodynamics is given by Davidson and

Harrison (1963). Here bubble growth is limited by the terminal velocity of the bed material, which is referred to as the maximum stable bubble diameter d_{BS} . By this criterion, the bubble size increases until it reaches the terminal velocity of the surrounding solids. At this point, the internal circulation velocity in the bubble is equal to the terminal velocity of the surrounding solids. If the bubble grows, it becomes unstable and breaks down into smaller bubbles. Specifically, the solids in the wake would be drawn into the bubble, causing the bubble to break up. Hence, the maximum stable diameter would depend on the terminal velocity of the bed material and therefore on the particle size, shape factor, and physical properties of the bed material. Data presented by Rowe and Partridge (1965) and by others (Horio and Wen 1977 and Toei et al. 1974) have raised questions about the validity of this criterion. X-ray profiles of bubbles in three-dimensional beds show the formation of a cusp at the ceiling of the bubble. This cusp grows into a long finger that splits the bubble. Clearly, this is an area that needs further study.

3.1.3 Bed expansion

When the superficial velocity through a fluidized bed is increased above the minimum fluidization velocity, the bed expands. This expansion is due to (1) the formation and coalescence of bubbles or voids of gas and (2) the expansion of the emulsion phase due to an increase in gas flow through this phase, which implies that the bed expansion is related to the bubble diameter and bubble growth. As mentioned previously, the volumetric flux of the gas through the bubble has been observed to be smaller than that predicted by two-phase theory. Therefore, the emulsion phase volumetric flux and expansion should also be greater than predicted by two-phase theory.

A number of correlations to predict bed expansion have been proposed. Recently, Babu, Shah, and Talwalker (1978) reviewed these correlations and found that they do not accurately predict bed expansion at high-pressure and high-density conditions. As a result, a statistical fit of

available data was made, and the following relation was proposed for reactor diameters greater than 6.35 cm:

$$(L_f/L_{mf}) = 1 + \frac{1.9544(U_o - U_{mf})^{0.738} d_p^{1.006} \rho_s^{0.376}}{(U_{mf})^{0.937} \rho_g^{0.126}} \quad (3.11)$$

All terms are expressed in centimeter-gram-second (cgs) units. This correlation is based on data for reactor diameters up to 30.5 cm and was not tested in larger reactors. In this work, bed expansion data from a 183- by 183-cm (6- by 6-ft) AFBC (Modrak et al. 1979) and 61- by 61-cm fluidized beds (Cranfield and Geldart 1974, Staub and Canada 1978, and Canada, McLaughlin, and Staub 1978) have been compared with results from the Institute of Gas Technology (IGT) bed expansion equation [Eq. (3.11)]. This comparison is shown in Sect. 3.4.

The average bubble voidage of the bed can be related to bed expansion by

$$\bar{\epsilon}_B = 1 - (L_{mf}/L_f) \quad (3.12)$$

Equation (3.12) assumes that increased expansion of the emulsion phase due to increased volumetric flux is negligible [i.e., Eq. (3.12) is based on two-phase flow theory].

3.1.4 Effect of horizontal tube bundles

Very little quantitative information is available on the effects of horizontal tubes on bubble growth and bed expansion at high superficial velocities and large particle sizes. For small particles, the effect depends on the relative size of the bubbles and the tubes. Splitting of the bubbles in small-particle beds occurs when bubble diameters are relatively large compared with the tube diameter (Geldart 1977). In current modeling of FBCs, it is usually assumed that bubbles are broken up into a diameter equivalent to the horizontal pitch of the tube bundle (Rengarajan, Krishnan, and Wen 1979). If this assumption were true, it could be shown that the bubble voidage in the bundle would increase and that the observed bed expansion would be higher than that observed with no tube bundles present. Staub and Canada (1978), in their study of large-particle, high-superficial-velocity beds, found that the presence

of tube bundles had no effect on bed expansion. This finding seems to indicate that bubbles are not being broken down into smaller bubbles at the tube bundle. These data were taken with five to ten rows of staggered tubes having a 5.7-cm axial pitch and a 10.2-cm transverse pitch. However, these observations are preliminary and need further experimentation.

3.2 Model Development

From the previous sections, it is qualitatively apparent that average bubble voidage is related to bubble growth. In this section, a quantitative relation between bubble size and average bubble voidage is developed.

3.2.1 Relation between average bubble voidage and bubble growth

First, the number of bubbles per unit volume at some height z above distributor plate is given by

$$n/(A_{xs} \Delta z) = (f/u_B) , \quad (3.13)$$

where f is the frequency per unit area and u_B is the speed of the bubble at height z . Since the volume of a bubble is

$$V_B = (\zeta \pi d_B^3)/6 , \quad (3.14)$$

the bubble volume per unit volume of bed at height z is

$$\epsilon_B = (f/u_B)(\zeta \pi d_B^3)/6 , \quad (3.15)$$

where ζ accounts for the nonspherical nature of the bubble.

Now the volumetric flux through the bubble phase is given by

$$\dot{V}_B' = fV_B = (f\zeta \pi d_B^3)/6 . \quad (3.16)$$

Therefore, the bubble volume per unit volume of bed at some height z can be expressed as

$$\epsilon_B = f/u_B \times \dot{V}_B'/f = \dot{V}_B'/u_B \quad (3.15)$$

From the previous sections, the volumetric flux through the bubble phase is from the work of Werther (1978),

$$\dot{V}_B' = \phi_k (U_o - U_{mf}) ,$$

where $0.67 \leq \phi_k \leq 0.76$, or from Cranfield and Geldart (1974):

$$\dot{V}_B' = 0.363(U - U_{mb})^{1.11} z^{0.09} . \quad (3.9)$$

To obtain the average bed bubble voidage, the first moment of bubble volume per bed volume is found as

$$\bar{\epsilon}_B = \frac{1}{L_f} \int_0^{L_f} (\dot{V}_B' / u_B) dz , \quad (3.18)$$

where L_f is the expanded height of the bed, and, from the work of Werther (1978),

$$u_B = \psi \sqrt{g d_B} ,$$

where ψ is given as a function of reactor diameter by Eq. (3.7). Therefore, bubble diameter (a function of z) can be related to average bed bubble voidage as

$$\bar{\epsilon}_B = \frac{1}{L_f} \int_0^{L_f} (\dot{V}_B' / \psi \sqrt{g d_B}) dz . \quad (3.19)$$

3.2.2 Assumptions

To relate bubble growth to bed expansion quantitatively, certain assumptions are made. First, the volumetric flux through the bubble phase is assumed to be that given by Eq. (3.9). Second, bubble growth is assumed to have the functional form of Eq. (3.1):

$$(d_{BM} - d_B) / (d_{BM} - d_{BO}) = \exp (-kz/D_t) . \quad (3.1)$$

In this expression d_{BM} is given by Eq. (3.10) and d_{BO} is given by Eq. (3.3). Third, the surface mean particle diameter d_p is assumed to be the characteristic particle size in the bed and is calculated as

$$d_p = 1 / [\sum^{all} i (x/d_p)_i] , \quad (3.20)$$

where x is the weight fraction of the i th particle size. Fourth, the increased expansion of the emulsion phase due to the greater volumetric flux through this phase is assumed to be negligible compared with the expansion due to the formation of bubbles. Fifth, the effects of horizontal tube bundle and walls are assumed to be negligible. Of these five assumptions, the fifth is the most questionable. The work of Staub and Canada (1978) seems to indicate no effect of tube bundles on bed expansion. The effects of the walls on d_{BM} and d_{BS} have not been clearly quantized in the literature (Mori and Wen 1975). Utility AFBC applications will dictate large cross-sectional areas, and at present the wall effects are neglected.

3.3 Code Input-Output and Computational Method

Based on the above equations and assumptions, a computer code has been developed for calculation of bubble growth in fluidized beds. The input and the computational scheme of this routine are given and discussed.

The required input parameters and their values are given in Table 3.1. These values are typical of the B&W/EPRI 183- by 183-cm AFBC (B&W 1979a). Figure 3.1 shows the overall computation scheme of the code. First, the average bed bubble voidage is found as

$$\bar{\epsilon}_B = 1 - 1/(L_f/L_{mf}) , \quad (3.12)$$

where L_f/L_{mf} is given by

$$\frac{L_f}{L_{mf}} = 1 + \frac{1.9544(U_o - U_{mf})^{0.738} d_p^{1.006} \rho_s^{0.376}}{(U_{mf})^{0.937} \rho_g^{0.126}} , \quad (3.11)$$

Table 3.1. Input parameters for bubble-growth code

Variable	Value	Definition
D	0.1487	Mean particle diameter in bed, cm
RHOS	2.6	Density of bed material, g/cm ³
RHOG	0.00032	Flue gas density, g/cm ³
MU	0.00044	Gas viscosity, g/(cm-s)
DT	183	Bed diameter, cm
HBED	121.9	Expanded bed height, cm
XND	15,248	Number of orifice openings at distributor plate, dimensionless
UO	243.8	Superficial velocity, cm/s

and the minimum fluidization velocity U_{mf} is calculated by the equation given by Wen and Yu (1966):

$$U_{mf} = \frac{\mu}{d_p \rho_g} \left\{ \left[33.7^2 + \frac{0.0408 d_p^3 \rho_g (\rho_s - \rho_g) g}{\mu^2} \right]^{1/2} - 33.7 \right\}, \quad (3.21)$$

where d_p is the mean particle diameter given by Eq. (3.20).

Next the minimum and maximum diameters are calculated via Eqs. (3.3) and (3.10). At this point the value of the constant k in Eq. (3.1) is assumed and used to determine the average bed bubble voidage from

$$\bar{\epsilon}_B = \frac{1}{L_f} \int_0^{L_f} (\dot{V}_B' / \psi \sqrt{g d_B}) dz, \quad (3.19)$$

where ψ is defined by Eq. (3.7) and $\dot{V}_B'$ is given by Eq. (3.9). The average bubble voidage in Eq. (3.19) is a function of the bubble diameter. Since the bubble diameter in this expression depends on a constant k [see Eq. (3.1)], the value of the bed voidage becomes a function of k . This constant is varied until the value of $\bar{\epsilon}_B$ calculated from Eq. (3.19) agrees with that from Eq. (3.12). The integration of Eq. (3.19) is done

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Fig. 3.1. Flow diagram of computer code.

by Simpson's rule, and the convergence for constant k is obtained by using the Regula-Falsi method (Sokolnikoff and Redheffer 1966). The total fractional bed voidage from the two-phase theory is given by

$$\bar{\delta} = \bar{\epsilon}_B + (1 - \bar{\epsilon}_B) \epsilon_{mf} \quad (3.22)$$

Table 3.2 summarizes typical values generated by the code.

Table 3.2. Output results produced by bubble-growth code

Variable	Value	Definition
HMF	61.7	Height at minimum fluidization, cm
DBO	3.7	Bubble diameter at distributor plate, cm
DBM	157.6	Maximum bubble diameter, cm
DB	See Fig. 3.9	Bubble diameter as a function of bed height, cm
U_B	108.8 - 465.0	Velocity of bubble as function of height, cm/s
EPI	0.49	Average bed bubble voidage, dimensionless
K	0.95 - 1.05	Constant in Eq. (3.1)

3.4 Results and Discussion

Bed expansion results calculated from Eq. (3.11) were compared with experimental data obtained by Modrak et al. (1979), Canada, McLaughlin, and Staub (1978), and Cranfield and Geldart (1974). The comparisons are shown in Figs. 3.2 to 3.6. Figure 3.2 is a comparison of Modrak's experimental data obtained in the B&W/EPRI (183- by 183-cm) bed versus results obtained from Eqs. (3.11) and (3.22). In this calculation, the voidage at minimum fluidization ϵ_{mf} is assumed to be 0.5, based on the work of Hartman and Pata (1978) for limestone solids. As can be seen in Fig. 3.2, only one of the ten data points falls out of the $\pm 10\%$ error zone.

Bed expansion data measured by Canada, McLaughlin, and Staub (1978) are shown in Figs. 3.3 to 3.5. The data were taken in a 61- by 61-cm bed and a 31- by 31-cm bed at 423 K. Figure 3.3 shows a comparison of

Fig. 3.2. Comparison of bed expansion data from Modrak et al. (1979) with that obtained from Eqs. (3.11) and (3.22).

results from bed expansion data obtained with soda lime glass particles ($\rho_s = 2.48 \text{ g/cm}^3$) and Eq. (3.11) for a particle diameter of $650 \mu\text{m}$. A minimum fluidization bed voidage ϵ_{mf} of 0.4 as measured by Canada was used in the calculations. The agreement is reasonable for the majority of points. The results for crown barium glass particles ($\rho_s = 2.92 \text{ g/cm}^3$) of $2600\text{-}\mu\text{m}$ particle diameter are shown in Fig. 3.4, with $\epsilon_{mf} = 0.4$. Again, the agreement is reasonably good except in the lower superficial velocities. Figure 3.5 gives the results for a 50-50 mixture of 650- and $2600\text{-}\mu\text{m}$ particles (Staub and Canada 1978). The voidage was again assumed to be 0.4 as in the other cases, but the agreement is clearly not as good, for which two reasons may exist. First, the value of minimum fluidization

Fig. 3.3. Comparison of bed expansion data from Canada, McLaughlin, and Staub (1978) for 650- μ m particles with results from Eq. (3.11).

voidage was not measured by Staub but was assumed. If this value is increased to 0.5, the agreement becomes better. Second, the different diameter (650 and 2640 μ m) and density (2.48 and 2.92 g/cm³) of the particles cause segregation of the particles, resulting in a nonreproducible bed expansion.

Cranfield and Geldart's bed expansion data, Fig. 3.6, were taken in a 61- by 61-cm bed at 295 K. Alkalized alumina spheres with a mean particle size of 1760 μ m and a density of 1.025 g/cm³ were used as bed material. This figure shows the ratio of the fully expanded bed height to bed height at minimum fluidization versus the superficial velocity. Here the bed expansion equation of Babu, Shah, and Talwalker (1978)

Fig. 3.4. Comparison of bed expansion data from Canada, McLaughlin, and Staub (1978) for 2600- μ m particles with results from Eq. (3.11).

[Eq. (3.11)] does not result in a satisfactory fit. This failure may be attributed to the particle properties, in particular the low density and the rough surface of the alkaliized alumina spheres used in the experiments.

Bubble-growth data for large particles and high superficial velocities are not readily available. Cranfield and Geldart (1974), from data obtained in a 61- by 61-cm bed, have given the following correlation for predicting bubble growth within $\pm 10\%$:

$$d_B = 0.0326(U_0 - U_{mb})^{1.11} z^{0.80} \quad (3.4)$$

Fig. 3.5. Comparison of bed expansion data from Staub and Canada (1978) for a 50-50 mixture of 650- and 2600- μ m particles with results from Eq. (3.11).

Figure 3.7 compares the bubble diameter at the bed surface from this equation with that of the proposed method. Poor agreement at a minimum fluidization height L_{mf} of 30 cm is noted, but, as L_{mf} approaches 10 cm, the agreement between the measured bed expansion and the bed expansion calculated from Eq. (3.11) also became better. This fact establishes the possible premise that, when the bed expansion is predicted correctly, the bubble growth can also be predicted via Eq. (3.1), which has been done in Fig. 3.8 for conditions similar to those used by Modrak et al. (1979) (i.e., an operational AFBC). This figure is a plot of calculated bubble diameter versus expanded bed height for various superficial velocities. By increasing the superficial velocity from 122 to 244 cm/s

Fig. 3.6. Comparison of bed expansion data from Cranfield and Geldart (1974) with results from Eq. (3.11).

(4 to 8 ft/s), the bubble size increases roughly by a factor of 4, which is in accordance with the functional relationship between bubble diameter and bubble velocity.

Finally, Fig. 3.9 compares the bubble growth predicted by the proposed method and those obtained from the Cranfield and Geldart equation [Eq. (3.4)] and Mori and Wen's original equation [Eq. (3.1)] at conditions typical of AFBC operations. Cranfield and Geldart's equation tends to predict very rapid bubble growth, which results in a bubble larger than the bed diameter at a low height above the distributor. The Mori and Wen correlation, which is not applicable to these conditions, predicts a relatively small bubble. The proposed correlation predicts a large bubble (≈ 90 cm) at the surface of the bed. Bubbles of this size have been observed in a 180-cm cold bed using 300- μ m sand (Botton 1966). The

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Fig. 3.7. Comparison of the bubble-growth correlation of Cranfield and Geldart (1974) with the proposed method for bubble growth.

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Fig. 3.8. Calculated bubble diameters at surface versus expanded bed height at typical AFBC condition for 183- by 183-cm bed.

Fig. 3.9. A comparison of bubble-growth relations.

accuracy of the proposed correlations cannot be established, however, without experimental data.

3.5 Recommendations for Future Work

To establish a better understanding of bubble growth in fluidized beds, the following areas should be investigated. First, the relationship between bed expansion and interstitial gas flow does not obey the two-phase theory (Cranfield and Geldart 1974 and Werther 1978), and a predictive method in terms of fluidized-bed properties should be developed. Second, the ratio of the bubble diameter to bed diameter at which the walls of the

reactor affect bubble growth should be determined. This ratio defines minimum reactor size for process testing and scale-up. Third, the effects of horizontal and vertical tube bundles on bubble size, rise velocity, and bed expansion need to be investigated. The bundle configuration should be determined to ensure the appropriate bubble size for maximum combustion rates of chemical reactions and heat transfer in the bundle. Finally, a criterion for the maximum stable hydrodynamic bubble size should be developed based on fluidized-bed properties. Specifically, the effect of fines on hydrodynamic stability of bubbles should be quantified.

3.6 Summary

Simulation of FBCs requires the accurate prediction of the size and growth of bubbles in the bed. The combustion efficiency (coal utilization), the sulfur capture by sorbent in the bed, the elutriation of fines from the bed, and the mass transfer of the gas between the bubble phase and the emulsion phase all depend on bubble size. Empirical correlations available in the literature to predict bubble size are not satisfactory for the large-particle, high-superficial-velocity conditions typical of fluidized-bed combustion.

The bubble-growth subcode developed in this work relates bubble growth to bed expansion. The average bed bubble voidage is calculated from the two-phase theory [Eq. (3.12)] and the bed expansion relation [Eq. (3.11)] proposed by Babu, Shah, and Talwalker (1978). The average bed bubble voidage, which can also be related to bubble size, is found from Eqs. (3.19), (3.9), and (3.1). Equation (3.1) contains an adjustable parameter k , which is varied in the computation to match the values of the average bed bubble voidage calculated from the bed expansion relations [Eqs. (3.11) and (3.12)] and the average bed bubble voidage obtained from bubble size relations [Eqs. (3.1), (3.9), and (3.19)].

The bed expansion and bubble diameters predicted by the code are compared with available experimental data. Experimental data on bubble growth in the range of operating conditions of interest in AFBC are scarce. However, preliminary results indicate that the proposed method for predicting bubble size is reasonable, provided one can estimate bed expansion accurately.

4. LIMESTONE-COAL ASH ELUTRIATION AND ATTRITION MODEL

4.1. Background

The elutriation, or entrainment, of particles is a common problem in all fluidized-bed reactors. This problem stems from the fact that the fluidizing gas velocity usually exceeds the terminal velocities of the finer particles in the bed. These finer particles may come from the bed itself as part of the feed or may be generated in the bed from attrition. Attrition is the reduction of solids particle size by abrasion (grinding) of the particles with the walls, with the internals, and among themselves. In fluidized-bed combustion, the major loss in combustion efficiency is due to elutriation of unburned carbon fines in the flue gas. These solids must be removed from the flue gas to maintain a high combustion efficiency. Also, the amount of the fines and their size distribution should be known in order to properly design the solids removal system. These considerations dictate the need for accurate estimation of the attrition and elutriation rates for the bed material (coal char, coal ash, and limestone sorbent).

It is generally accepted that there is a critical particle size in the bed below which all particles are blown out of the bed. This size would be expected to be the particle size having a terminal velocity equal to or less than the superficial velocity. However, experimental observations (Merrick and Highley 1964 and Geldart 1979) indicate that particles with terminal velocities larger than that of the superficial gas are also carried over, thus further complicating the analysis.

Both attrition and elutriation processes depend on the system and operating variables. Some of the more significant among these are

- physical properties of solids — friability, density, and size distribution;
- feed system configuration — elbows and bends, pipe length, pipe diameter, and solids transport velocity;
- bed hydrodynamics — bubble size and bubble velocity, viscosity of gas, density of gas, bed diameter, bed internals, and mass flow of gas; and

- freeboard conditions — freeboard dimensions, mass flow of gas, and freeboard temperature.

Each of the above affects the amount of solids blown out of the bed. Qualitatively, the effect of these variables can be stated, but quantitative predictions are yet difficult. A limited number of correlations have been proposed for predicting attrition and elutriation rates for limestone and coal ash. However, these rate expressions are system specific and have limited application. There are no correlations available to estimate the attrition and elutriation rates of coal char. The procedure for estimating the rates for coal char is described in Chap. 5 of this report.

In this section, an attrition and elutriation model is developed. The model considers only limestone and coal ash. The experimental correlations developed for limestone and coal ash are discussed next.

4.1.1 Attrition

Solids loading and size distribution due to attrition are generally difficult to estimate. The rate constant is assumed to be related to the particle diameter d_p , the difference in the superficial velocity and minimum fluidization velocity $U_o - U_{mf}$, and the bed mass W_B .

Preliminary estimates from experimental data indicate that roughly 4% of the bed weight is attrited in 1 h (Newby et al. 1978). Results from the Westinghouse fluidized-bed data on limestone have been correlated (Newby et al. 1978) as follows:

$$F_{ATT} = K_{ATT} (U_o - U_{mf}) \tau^{-n}, \quad (4.1)$$

where

F_{ATT} = attrition rate, g/s,

K_{ATT} = attrition rate constant,

n = constant,

τ = residence time of particles in the bed, s,

U_o = superficial gas velocity, cm/s,

U_{mf} = minimum fluidization velocity based on mean bed particle size, cm/s.

The attrition rate constant K_{ATT} is of the order of 3×10^{-4} , and n is given as 0.7. Ciliberti, Ranadive, and Keairns (1979) proposed the following expression for sorbent and coal ash:

$$[d(d_p)/dt]_{\text{sorbent}} = K_{ATT}(d_p - 0.1), \quad (4.2)$$

where K_{ATT} is $1.9 \times 10^{-5} \text{ s}^{-1}$ for coal ash and $5.7 \times 10^{-6} \text{ s}^{-1}$ for sorbent, $d(d_p)/dt$ is rate of change of particle radius with respect to time, cm/s, and d_p is diameter of particle, cm.

Equation (4.2) assumes that attrition does not appreciably affect particles with a diameter of less than 0.1 cm (1000 μm). The equation was developed from case studies (cases A-Z) described in the Stearns and Rogers title report I and is not based on experimental data from operating FBCs.

Merrick and Highley (1974) propose the following expression for coal ash and limestone attrition:

$$F_{ATT} = K_{ATT}(U_o - U_{mf})W_B, \quad (4.3)$$

where F_{ATT} is the rate of solids formed due to attrition, g/s, K_{ATT} is $9.11 \times 10^{-8} \text{ cm}^{-1}$ for coal ash and $2.73 \times 10^{-8} \text{ cm}^{-1}$ for limestone, and W_B is the mass of the bed, g.

The above expression gives the total mass of solids produced in the bed per unit time due to attrition. For each particle size fraction d_{pi} in the bed, the rate of change of diameter with respect to time is estimated from

$$[d(d_{pi})]/dt = k_{ATT} f_{dp}(U_o - U_{mf})d_{pi}, \quad (4.4)$$

where f_{dp} is the fraction of particles in the bed smaller than d_p . The k_{ATT} is defined as the rate constant such that the total rate of abrasion in the bed is equal to that given by Eq. (4.3). Equations (4.3) and (4.4) were derived from experimental observations made in the National Coal Board (NCB) FBC.

4.1.2 Elutriation

Correlations for predicting elutriation rates are based on the definition of the elutriation rate constant, defined as

$$K(R) = [F_2 p_2(R)] / [W_B p_B(R)] , \quad (4.5)$$

where

F_2 = total rate of elutriated solids (see Fig. 4.1), g/s,

$K(R)$ = elutriation constant, s^{-1} ,

$p_B(R)$, $p_2(R)$ = differential particle size of bed and elutriated solids, respectively (see Fig. 4.1), cm^{-1} ,

R = particle radius, cm.

Experimental data on elutriation rates obtained in both batch and continuous fluidized-bed reactors have been correlated by several investigators.

These correlations, presented in Table 4.1, are usually developed in terms of the rate of solids leaving per unit surface area of the bed [$K^*(R)$].

These constants can be converted to the constant in Eq. (4.5) as

$$K(R) = [K^*(R) A_{xs}] / W_B , \quad (4.6)$$

where A_{xs} is total cross-sectional area of the bed, cm^2 . Except for the Highley and Merrick and Wen and Hashinger correlations, all others were developed for solids other than coal char, limestone, and coal ash. Wen and Hashinger obtained the data for coal and glass beads in a batch system in columns of 51 and 10.2 cm diam. The Highley and Merrick (1971) data were obtained in a 30.5- by 30.5-cm fluidized-bed combustion pilot plant with coal ash and sorbent as bed material. A new correlation different in form from the previous correlations was developed.

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Fig. 4.1. The fluidized bed operated at steady state.

In the design of the solids removal system, it is desirable to know a priori the height in the freeboard beyond which the elutriation rate of solids is constant. This height is referred to as the transport disengaging height (TDH). Above the TDH, the entrainment rate of particles is relatively constant and presumably is equal to the maximum saturation, dilute-phase, particle-carrying capacity of the gas stream at its superficial velocity. The TDH is strongly influenced by the gas properties at freeboard conditions, the bubble size at the bed surface, the presence of internals in the freeboard, and the solid properties. The TDH can be calculated by following the procedure outlined by Zenz and Weil (1958). However, the method was developed for fluidized-bed catalytic cracker (FCC) catalyst in the 11- to 168- μm size range in a two-dimensional bed, and its applicability for AFBC is questionable. Amitin et al. (1968) proposed the following correlation for estimating TDH:

$$\text{TDH} = 0.147 \bar{U}_0^{1.2} (22.4 - 1.2 \ln \bar{U}_0) , \quad (4.7)$$

Table 4.1. Some commonly used correlations for entrainment

Yagi and Aochi (1955)

$$\frac{K^* g d_p^2}{\mu (U_o - U_t)^2} = 0.0015 \text{Re}_t^{0.6} + 0.01 \text{Re}_t^{1.2}$$

Wen and Hashinger (1960)

$$\frac{K^*}{\rho_g (U_o - U_t)} = 1.7 \times 10^{-5} \left[\frac{(U_o - U_t)^2}{g d_p} \right]^{0.5} \times \text{Re}_t^{0.725} \left[\frac{\rho_s - \rho_g}{\rho_g} \right]^{1.15} \left[\frac{U_o - U_t}{U_t} \right]^{0.1}$$

Tanaka and Shinohara (1972)

$$\frac{K^*}{\rho_g (U_o - U_t)} = 4.6 \times 10^{-2} \left[\frac{(U_o - U_t)^2}{g d_p} \right]^{0.5} \text{Re}_t^{0.3} \left[\frac{\rho_s - \rho_g}{\rho_g} \right]^{0.15}$$

Merriok and Highley (1974)

$$\frac{K^*}{\rho_g U_o} = A + 130 \exp \left[-10.4 \left(\frac{U_t}{U_o} \right)^{0.5} \left(\frac{U_{mf}}{U_o - U_{mf}} \right)^{0.25} \right]$$

Zenz and Weil (1958)

Calculate $\frac{U_o^2}{g \rho_s^2 d_p}$ then use graph to find $\frac{K^*}{\rho_g U_o}$

where $\bar{U}_o$ is average freeboard superficial gas velocity, cm/s. If this expression is used at AFBC conditions, the TDH is found to be 12.21 m (40 ft), which is quite unlikely. A rule of thumb given by an industrial source suggests allowing 60.9 cm (2 ft) of freeboard height for every (30.48 cm/s (1 ft/s) superficial velocity in the bed to ensure operation above TDH. Based on this rule, the TDH is roughly one-half the TDH calculated from Eq. (4.7). More data from pilot-plant-scale AFBC units are needed to establish a quantitative relationship for the TDH as a function of operating parameters.

4.2 Model Development

Although the above relations for attrition and elutriation tend to be system specific, they can be used to develop a mathematical model for these processes. Results from this model can then be compared with experimental data to establish a better understanding of the factors affecting attrition and entrainment. In this section, the assumptions, equations, and computational method are given and discussed.

4.2.1. Assumptions

To develop the limestone-coal ash elutriation and attrition model, the following assumptions are made. First, the system is assumed to be at steady state (i.e., time invariant). Second, the solids in the fluidized bed are assumed to be well mixed (back-mix flow), which implies that there is no segregation of the limestone particles from coal ash particles. Third, the attrition rate expressions of Merrick and Highley (1974) are assumed for the limestone and coal ash particles:

$$F_{ATT} = K_{ATT} (\bar{U}_o - U_{mf}) W_B, \quad (4.3)$$

$$dR/dt = k_{ATT} f_w (\bar{U}_o - U_{mf}) R, \quad (4.8)$$

where R is the particle radius, cm, k_{ATT} is the attrition constant, cm^{-1} , and f_w is the fraction of particles in the bed smaller than radius R . Fourth, the particle entrainment rate constants for limestone and coal

ash are also assumed to be those given by Merrick and Highley (1974). Specifically,

$$K(R) = [A + 130 \exp\{-10.4[U_t(R)/U_o]^{0.5}[U_{mf}/(U_o - U_{mf})]^{0.25}\}] \times \frac{\rho_g U_o A_{xs}}{W_B}, \quad (4.9)$$

where A is constant, ρ_g is the density of gas, and $U_t(R)$ is the terminal velocity corresponding to the particle radius R (Kunii and Levenspiel 1977). Fifth, the elutriation and attrition of the limestone are assumed to be independent of the coal ash. This assumption implies that the elutriation and attrition constants for the sorbent are not affected by the coal ash and vice versa. Sixth, the fines produced by abrasion are assumed to be less than 125 μ m (0.005 in.) and are immediately entrained. Finally, the bed expansion is predicted by the IGT bed expansion equation (Babu, Shah, and Talwalker 1978).

Of the above, the most important assumptions are the elutriation and attrition rate expressions. In this work the rate expressions of Merrick and Highley (1974) are chosen. These relations were developed from NCB data for a 30.5- by 30.5-cm (1- by 1-ft) AFBC with a 4-m (13-ft) freeboard and superficial velocities of 61 to 244 g/s (2 to 8 ft/s). As stated previously, the rate expressions are system specific and therefore do not account for differences in feed system, freeboard configuration, etc. However, these expressions do have terms in them to account for bed and freeboard hydrodynamics. Specifically, the elutriation constant expression [Eq. (4.9)] has the terms $U_{mf}/(U_o - U_{mf})$ and $U_t(R)/U_o$. The first group represents the ratio of the amount of gas passing through the emulsion phase to the amount passing through the bubble phase. Since the solids are thrown up in the freeboard by the bubble, the first group represents a measure of the amount of solids entering the freeboard. The second group represents the probability that a particle of radius R in the freeboard will fall back into the bed. The attrition rate expression of Merrick and Highley has the term $(U_o - U_{mf})$ in Eq. (4.3), which is a measure of the agitation due to bubbles (energy input) in the bed. At present,

the work of Merrick and Highley represents the best available correlation for the estimation of attrition and elutriation.

The sixth assumption implies that the fines ($<125\text{ }\mu\text{m}$) produced by abrasion are immediately blown out of the system. The fines produced by abrasion are the small particles broken off a control cone particle as it is reduced by the grinding action of other particles, which allows the abrasion products to be treated as a "pseudo" gas. Data from the NCB combustor seem to support the last assumption and also show that, for a given bed material, the size distribution is independent of both the bed size distribution and operating conditions. A typical distribution for fines given by Merrick and Highley is shown in Table 4.2.

Table 4.2. Typical size distribution of attrition fines (Merrick and Highley 1974)

Size range, μm	125-63	63-31	31-16	16-8	8
Percent by weight	20	20	20	20	20

4.2.2 Limestone-coal ash performance equations

The performance of the limestone-coal ash solids in the fluidized bed is determined by the following quantities (see Fig. 4.1):

1. bed mass W_B ,
2. differential bed size distribution p_B ,
3. underflow rate F_1 ,
4. differential underflow size distribution p_1 ,
5. overflow rate F_2 ,
6. differential elutriated solid size distribution p_2 ,
7. attrition fines flow rate F_{ATT} , and
8. differential attrition fines size distribution p_A .

These quantities must be found for each solid component in the fluidized bed (limestone-coal ash). The data required to find these quantities are the physical properties of the solids and gas, the feed rates F_0 and size distribution of the solids in the feed, the superficial gas velocity through the bed, and the dimensions of the bed. The

equations used to determine the above quantities are developed in this section.

The total mass of limestone-coal ash solids in the bed is given by

$$W_B = L_{mf} A_{xs} (1 - \epsilon_{mf}) \rho_s, \quad (4.10)$$

where

L_{mf} = height of bed at minimum fluidization, cm,

A_{xs} = cross-sectional area of bed, cm^2 ,

ϵ_{mf} = voidage at minimum fluidization, unitless,

ρ_s = average density of solids, g/cm^3 .

The bed height at minimum fluidization is determined by the bed expansion relation of Babu, Shah, and Talwalker (1978). The applicability of this relation was discussed earlier in the bubble-growth section of this report. The mass of the coal ash and limestone in the bed is determined by using the composition of the underflow. This composition is determined by solving the general performance equations of a fluidized bed given by Kunii and Levenspiel (1977). These equations consist of an overall material balance and a differential mass balance on particles between the sizes R and $R + dR$. The derivation of these equations is given by Kunii and Levenspiel (1977) and is not repeated here. The overall mass balance equation of a fluidized bed is given by

$$F_1 + F_2 - F_0 - F_{ATT} - \int_{\text{All } R} [3W_B p_B(R) \dot{R}(R) dR] / R, \quad (4.11)$$

and the differential mass balance is given by

$$\begin{aligned} F_0 p_0(R) - F_1 p_1(R) - W_B K(R) p_B(R) - W_B \frac{d[\dot{R}(R) p_B(R)]}{dR} \\ + \frac{3W_B p_B(R) \dot{R}(R)}{R} = 0, \end{aligned} \quad (4.12)$$

where,

F_0 = solids feed rate, g,

F_1 = underflow rate, g/s,

F_2 = total rate of elutriated solids, g/s,

F_{ATT} = attrition fines flow rate g/s,

$p_0(R)$ = differential feed size distribution, cm^{-1} ,

$p_1(R)$ = differential underflow size distribution, cm^{-1} ,

$p_B(R)$ = differential particle size distribution in the bed, cm^{-1} ,

R = particle radius, cm,

$R(R) = (dR)/(dt)$ = rate of change of particle radius due to attrition for particle radius R , cm/s,

$K(R)$ = elutriation constant of a particle of radius R [defined by Eq. (4.9)],

W_B = bed mass, g.

The above notations are explained in Fig. 4.1. From the second assumption listed above,

$$p_B(R) = p_1(R) ,$$

and the differential balance can then be written as

$$dp_B(R)/dR = \frac{F_0 p_0(R)}{W_B \dot{R}(R)} - \left[\frac{F_1}{W_B \dot{R}(R)} + \frac{K(R)}{\dot{R}(R)} + \frac{1}{\dot{R}(R)} \frac{d\dot{R}(R)}{dR} - \frac{3}{R} \right] p_B(R) . \quad (4.13)$$

Finally, by definition of differential particle size distribution,

$$\int_{\text{All } R} p_B(R) dR = 1 . \quad (4.14)$$

The term $\dot{R}(R)$ represents the rate of particle shrinkage due to attrition and is given by Eq. (4.8), and the term $K(R)$ represents the elutriation constant given by Eq. (4.9). Because of the functional form of Eq. (4.8), the attrition rate decreases as the radius of the particle decreases. For some radius R (usually less than 500 μm) the attrition rate becomes negligible. At this point Eq. (4.12) can be simplified to calculate the particle size distribution in the bed as follows:

$$p_B(R) = \frac{F_0 p_0(R)}{F_1 + W_B K(R)} \quad (4.15)$$

Based on the fifth assumption, Eqs. (4.11) to (4.15) apply separately to the coal ash solids and limestone solids in the bed. As a result, F_1 , F_2 , W_B , and F_{ATT} can be obtained for the ash and sorbent separately. The total mass flow rates of product streams shown in Fig. 4.1 is the summation of the ash and sorbent material balance.

4.3 Code Input-Output and Computational Method

Based on the above assumptions and equations, a computer code has been developed to complete the material balance for the limestone sorbent and coal ash. The input and computational scheme of this routine are given and discussed below.

The required input parameters and their values are given in Tables 4.3 to 4.5. These values are typical of the B&W/EPRI 183- by 183-cm (6- by 6-ft) AFBC (B&W 1979a). Tables 4.4 and 4.5 give the size distribution of coal ash and limestone sorbent, respectively, as fed to the bed. These size distributions are used to calculate the differential size distributions of the feed particles $[p_0(R)]$, which are input to Eqs. (4.13) and (4.15). The function $p_0(R)$ is determined by curve-fitting the given feed size distribution and then taking the derivative of the resulting curve at discrete points. The coal ash feed distribution given in Table 4.4 is shown in Fig. 4.2. The size distribution was estimated from the data for a 1/8- by 0-in. coal ash given by Merrick and Highley (1974).

Table 4.3. Computer input parameters for the limestone-coal ash elutriation and attrition code

Variable	Value	Definition
RHOA	3.0	Density of the coal ash (g/cm ³)
RHOSB	2.6	Density of sorbent (g/cm ³)
RHOG	0.00032	Density of gas (g/cm ³)
MU	0.00045	Viscosity of gas (g/cm-s)
EMF	0.4	Voidage at minimum fluidization
AXS	33445.1	Cross-sectional area of bed (cm ²)
UO	243.7	Superficial velocity (cm/s)
HF	121.2	Expanded height of bed (cm)
DM	0.16	Average diameter of particle in bed (cm)
DML	0.16	Average diameter of sorbent in bed (cm)
DMA	0.10	Average diameter of coal ash in bed (cm)
FRSB	0.96	Weight fraction of sorbent in bed
FLSO	94.5	Feed rate of sorbent (g/s)
FAO	16.9	Feed rate of coal ash (g/s)
SFLS	0.83	Shape factor for sorbent
SFAS	0.83	Shape factor for coal ash
AKSB	2.73×10^{-8}	Overall attrition constant for sorbent
AKAS	9.11×10^{-8}	Overall attrition constant for coal ash
NLS	9	Number of values of sorbent feed size distribution
DLS	Table 4.5	Diameters of feed sorbent (μm)
YLS	Table 4.5	Size distribution of feed sorbent
RLSMIN	20	Minimum radius of sorbent in bed (μm)
RLSMAX	3280	Maximum radius of sorbent in feed (μm)
XSBI	20	Interval used in the integration of Eq. (4.13) (μm)
NAS	6	Number of values of coal ash feed size distribution input
DAS	Table 4.4	Diameters of feed coal ash (μm)
YAS	Table 4.4	Size distribution of feed coal ash
RASMIN	20	Minimum radius of coal ash in bed (μm)
RASMAX	2720	Maximum radius of coal ash in feed (μm)
XASI	20	Interval used in integration of Eq. (4.13) (μm)

Table 4.4. Size distribution of coal ash

Particle diameter (μm)	Weight fraction of solids passing through
4000	0.94
2000	0.83
1000	0.68
500	0.54
250	0.4
125	0.27

Table 4.5. Size distribution of feed sorbent

Particle diameter (μm)	Weight fraction of solids passing through
6350	0.982
4750	0.87
2380	0.607
1190	0.421
595	0.272
297	0.173
149	0.110
74	0.077
44	0.059

The size distribution of the ash can be satisfactorily fit by a straight line on semilog paper. The equation has the following form:

$$R = Ae^{By} \quad , \quad (4.16)$$

where y is the mass fraction passing through the screen, A and B are constants, and R is the radius of particle. This form is different from that used to fit the size distribution of the limestone. The limestone size distribution given in Table 4.5 is also shown in Fig. 4.2 and cannot be fitted by a straight line on semilog paper. Figure 4.3 shows the

Fig. 4.2. Log-log plot of size distribution of coal ash and limestone feed to the bed.

limestone and ash size distributions plotted on log-log paper. A straight line can be drawn through the limestone points but not through the ash points. Thus, for the limestone feed particle size distribution, the best fit can be obtained from the following form:

$$y = AR^B \quad (4.17)$$

The curve fitting is done automatically by the code.

Figure 4.4 shows the overall computational scheme of the code. The weight of the sorbent and coal ash in the bed is calculated, based on an assumed bed composition. This composition is then checked by completing the coal ash and sorbent material balance. The coal ash and limestone sorbent material balance is completed by subroutine ZAP1. The logic diagram is shown in Fig. 4.5. Initially, in this routine the total attrition rate is calculated via Eq. (4.2). Next, initial estimates of

Fig. 4.3. Semilog plot of size distribution of coal ash and limestone feed to the bed.

the attrition constant in Eq. (4.8) and the overflow rate F_2 are made. Starting at the maximum particle radius $R_{\max}$ in the feed, the bed differential particle size distribution $p_B(R)$ is determined by solving Eq. (4.13) at specified intervals between $R_{\max}$ and the minimum particle radius $R_{\min}$ in the bed. The initial boundary condition is that the bed differential particle size distribution of the maximum radius particle be zero. Since all particles are undergoing a size reduction, this condition would appear to be a reasonable assumption. The values of $p_B(R)$ are then integrated between the maximum and minimum radii. By the definition, this quantity should have a value of 1; if not, the overflow from the bed F_2 is varied until Eq. (4.14) is satisfied. If the above condition is met, the total attrition rate is calculated via Eq. (4.2) and is compared with the integral of the attrition rates found at each radius R [Eq. (4.11)]. The integral of Eq. (4.11) is evaluated between the maximum and the minimum

Fig. 4.4. Overall computational scheme of the limestone-coal ash elutriation and attrition code.

Fig. 4.5. Computation scheme for routine ZAP1.

radii. If the two rates are not equal, the overflow rate F_2 and the attrition constant in Eq. (4.8) are varied until agreement is obtained. When this agreement occurs for both the coal ash and limestone sorbent components, the following quantities are known:

1. bed mass W_B ,
2. differential bed size distribution p_B ,
3. underflow rate F_1 ,
4. differential underflow size distribution p_1 ,
5. overflow rate F_2 ,
6. differential elutriated solids size distribution p_2 , and
7. attrition fines flow rate F_{ATT} .

The size distribution of the attrition fines is not calculated in this code. At present, the distribution of these fines is assumed to be the same as that given in Table 4.2. Typical values of output obtained from the code are listed in Table 4.6.

Table 4.6. Computer output from the limestone-coal ash elutriation and attrition code

Definition	Variable	Limestone	Coal ash
Underflow	F1	66.3 g/s (526.2 lb _m /h)	5 g/s (39.4 lb _m /h)
Elutriated solids	F2	12.5 g/s (99.2 lb _m /h)	8.7 g/s (69.0 lb _m /h)
Attrited solids	FATT	15.8 g/s (125.4 lb _m /h)	3.3 g/s (26.2 lb _m /h)
Bed mass	WBED	3,218,366 g (7095.2 lb _m)	214,834 g (473.6 lb _m)
Surface mean particle size	DP	1550 μm (0.061 in.)	1062 μm (0.042 in.)

4.4 Results and Discussion

The results from the code are compared with data obtained from the B&W/EPRI 183- by 183-cm AFBC. This comparison is used to analyze the attrition and elutriation phenomena in a large-scale FBC. Only a limited

comparison of model results is given. More extensive comparisons are planned for next year.

The output material balance information obtained from the code is given in Table 4.6. The total solids being "blown out" of the bed consist of two types: solids fed to the bed with a size small enough to be quickly elutriated and particles formed into such size by attrition. In this model the assumption is made that all attrition products are elutriated. A comparison of the model output with B&W's data (B&W 1979a) is given in Table 4.7. The B&W runs were without reinjection of the elutriated fines. Figures 4.6 and 4.7 show the size distribution of the bed as calculated by the code for the limestone solids and the coal ash.

The comparison in Table 4.7 shows that the current code underpredicts the total solids "blown out" of the bed by 23% and overpredicts the total underflow from the bed by 36%. The overall material balance for limestone-coal ash components from the experimental data is also compared with the

Table 4.7. Comparison of attrition-elutriation
code results with B&W data

Quantity	B&W	ORNL	Difference (%)
Total solids "blown out"	52.4 g/s (415.9 lb _m /h)	40.3 g/s (319.8 lb _m /h)	23.1
Feed limestone-ash solids "blown out"	47.0%	36.3%	
Bed mass	3.295×10^6 g (7264.1 lb _m)	3.433×10^6 g (7568.3 lb _m)	4.0
Underflow	52.5 g/s (417 lb _m /h)	71.3 g/s (565.87 lb _m /h)	36.0
Total limestone and coal ash feed	111.4 g/s (884 lb _m /h)	111.4 g/s (884 lb _m /h)	0
Total sorbent and coal ash leaving bed	105.0 g/s (834 lb _m /h)	111.6 g/s (886 lb _m /h)	6.3
Closure on material balance	-5.7%	0.2%

Fig. 4.6. Particle size distribution for limestone solids.

balance obtained from the model. The closure is acceptable ($<10\%$) in both cases. Also, as stated previously, a preliminary estimate for the limestone sorbent indicates that roughly 4% of the bed mass is attrited in 1 h. The calculations based on this estimate yield an attrition rate for the overall bed of 35.6 g/s as compared with 15.8 g/s predicted by the model. These results imply that the correlations of Merrick and Highley (1974) are not predicting the rates of attrition and elutriation accurately.

To resolve these disagreements, the data from the B&W experimental series 5 and 6 (B&W 1979a) were analyzed and correlated. Specifically,

Fig. 4.7. Particle size distribution for coal ash solids.

the total rate of limestone solids elutriated and the rate due to attrition were calculated from the data. This was done by assuming that the bed drain (underflow) is all limestone solids and that all limestone particles below a certain critical size are blown out of the bed. The series 6 data were correlated by

$$F_{ATT} = 6.74 \sqrt{d_p(FD)} U_o \tau^{-1.224}, \quad (4.18)$$

where

F_{ATT} = attrition rate, g/s,

$d_p(FD)$ = arithmetic average particle diameter of limestone feed, cm,

U_o = superficial velocity, cm/s,

τ = weight space time (weight of the bed divided by limestone flow), h.

The data fit and the derived correlation are shown in Fig. 4.8. The correlation does not fit the series 5 data. Between series 5 and 6, the feed system was modified by enlarging some of the solid transport piping from 3.8 to 5.1 cm in diameter, which may account for the difference. The configuration of the feed system will have a significant effect on the attrition of solids fed to the bed. In most cases, pneumatic feed systems cause the size distribution of the limestone and coal entering the bed to be significantly different from that in the storage bunkers. This change is caused by numerous bends, elbows, and splitters in the pneumatic feed system. The solids undergo substantial attrition during transport. Consequently, a higher amount of solids is blown out of the bed.

In analyzing the B&W data another contradiction was noted. Highley and Merrick (1974) and Geldart (1979) reported that there is a critical particle size in a fluid bed below which all particles are blown out of the bed. Only particles larger than the critical size remain in the bed.

Fig. 4.8. Babcock and Wilcox attrition data.

For inert bed material such as ash and limestone, the critical particle is given by Highley and Merrick as 1.6 times the size of the particle having a terminal velocity equal to the superficial velocity. For the B&W/EPRI 183- by 183-cm conditions, this particle size is about 1270 μm . Therefore, the size distribution of the bed material can be expected to start at about this size. Analysis of the B&W data shows that bed size distribution starts at 300 μm and above for all runs reported, which is contrary to the observations of Highley and Merrick and Geldart. This finding could be due to the decrease in the velocity of the gas as it passes through the freeboard convection section. No freeboard cooling was present in Highley and Merrick's bed. For the B&W data, the freeboard cooling lowers the flue gas temperature from approximately 1144 to 644 K (1600 to 700°F), which results in an increase in gas density and a decrease in the flue gas velocity. The flue gas cannot carry the larger particles beyond the freeboard convection bundles. These particles disengage from the gas and fall down along the walls into the bed. The B&W data from series 4, 5, and 6 support this hypothesis. The data show that the size distribution of the cyclone catch is always 300 μm and less and that of the bed is always 300 μm and larger. It appears that particles larger than 300 μm but smaller than 1270 μm may be trapped in the bed freeboard convection sections and attrited down to 300 μm before they are released to the cyclones. Some results to support this hypothesis are shown in Fig. 4.6, in which the calculated bed particle size distribution is compared with the experimental bed particle size distribution (B&W's data). The shape of the particle size distribution curve calculated by the code is similar to that found with the no-fines recycle. However, the B&W experimental particle size distribution on the bed has the shape that is typical of fines recycle (Merrick and Highley 1974). Since no recycle of fines occurs in this series of tests, it is possible that freeboard cooling might have resulted in an indirect recycle of fines back to the bed.

The above analysis of B&W's data shows that attrition and elutriation possibly depend on (1) feed system, (2) bed hydrodynamics, and (3) freeboard cooling. The Highley and Merrick equations for the attrition and elutriation were developed for a different feed system with no freeboard cooling.

At present, no generalized method exists for predicting the effect of the feed system and freeboard cooling on AFBC performance. To quantify these effects, further experimental studies will be required.

4.5 Recommendations for Future Work

As pointed out in the previous discussions, accurate prediction of the elutriation and attrition results are very difficult at the present time. To improve the understanding of these phenomena, certain areas should be investigated. First, it is suggested that solids samples for size analysis be taken just before the solids enter the bed so that correlations can be developed to predict separately the attrition occurring in the feed system and that occurring in the bed. Second, data on characterizing the solids loading in the freeboard should be taken. Specifically, expressions for prediction of the TDH in terms of particle size, particle density, and gas properties should be developed. Also, the solids thrown into the freeboard just above the bed surface should be related to the bubble size, bubble velocity, bubble frequency, fraction of surface area occupied by the erupting bubble, etc. Finally, accurate rate expressions for attrition of coal ash, limestone and char particles, and elutriation should be developed. These expressions should relate attrition and elutriation to in-bed phenomena and particle-gas properties.

4.6 Summary

In fluidized-bed combustion, the major loss in combustion efficiency is due to elutriation of unburned carbon fines in the flue gas. The fine particles may come directly from the feed or be generated in the bed by attrition. The amount of fines and their size distribution should be known in order to properly design the solids removal system. The limestone-coal ash attrition and elutriation subcode allows estimation of the attrition and elutriation rates of the limestone-coal ash solids and the size distributions of the bed particles and elutriated particles.

In the subcode, several assumptions are made with respect to the solids. The solids in the bed are assumed to be completely mixed. The elutriation and attrition of limestone-coal ash are assumed to be inde-

pendent of each other. The fines produced by attrition of a particle in the bed are assumed to be less than 125 μm and are immediately entrained. Based on these assumptions, the differential mass balance equations are written [Eqs. (4.12) through (4.16)] for limestone and coal ash separately. The attrition rates of limestone and coal ash are calculated from the rate expression of Merrick and Highley [Eq. (4.8)]. The elutriation rate constants for the solids are calculated from the Merrick and Highley correlation [Eq. (4.9)]. The particle size distributions as fed to the bed are obtained from a curve fit of the input particle size distribution data.

The computation is started by assuming an initial bed composition. This composition is then checked by completing the coal ash and sorbent material balance [Eqs. (4.12) through (4.16)]. If the assumed bed composition and the calculated bed composition agree within a set tolerance, the computation is stopped. If not, the bed composition is updated and the iteration is continued. The following quantities are determined by the code:

- bed mass,
- differential bed size distribution,
- underflow rate,
- differential underflow size distribution,
- elutriated solids flow rate,
- differential elutriated solids size distribution, and
- attrition fines flow rate.

The total mass flow rates of product streams are the summation of the ash and sorbent.

The comparison of model results with experimental data from the B&W/EPRI 183- by 183-cm AFBC unit shows that the model underpredicts the total solids "blown-out" of the bed by 23% and overpredicts the underflow from the bed by 36%. The material balance closure is acceptable within $\pm 10\%$ for both coal ash and limestone. The particle size distribution in the bed is a strong function of the attrition rate constant, which is higher in the experimental system than is the rate constant calculated in the model. The predicted results also show that the feed system design, recycle of elutriated material, and freeboard cooling could cause a reduction in the bed particle size distribution.

5. COAL COMBUSTION MODEL

5.1 Background

Many parameters (operational and geometric) affect the amount of heat released and the amount of coal consumed in an AFBC. The main purpose of a combustion model is to predict the rate of coal consumption in the AFBC at a given set of conditions. This quantity depends on (1) coal devolatilization, (2) combustion of volatile products, (3) char combustion, (4) bed hydrodynamics, and (5) elutriation-attrition. Development of a combustion model requires that each of the above factors be quantified. In the following text the background information used to quantify these phenomena is given and discussed, which includes discussions of coal devolatilization, volatile product combustion, and char combustion. A summary of recent combustion models is also given. The background discussions for bed hydrodynamics and elutriation-attrition have been presented in Chaps. 3 and 4, respectively, of this report.

5.1.1 Coal devolatilization

As coal is heated, it initially undergoes thermal degradation into gaseous, liquid, and solid products. This process is referred to as devolatilization or pyrolysis, and, as it occurs, both the kind and amount of a particular product formed are functions of the final temperature, heating rate, coal type, time, and gaseous environment.

Roughly speaking, devolatilization can be subdivided into two distinct thermal regimes: slow decomposition and rapid decomposition. The terms *slow* and *rapid* refer to the rate at which the coal is heated. [Nominally, slow decomposition is defined to occur when heating rates range from 1 to 10°C/min, and rapid devolatilization is assumed to occur when heating rates are about 60,000°C/min or greater (Anthony and Howard 1976). At this time no clear-cut definition exists as to where slow decomposition ends and rapid decomposition begins, although Johnson (1974) reported that slow decomposition may persist with heating rates as high as 6000°C/min.]

The fundamental difference between slow decomposition and rapid decomposition is that, when coal is rapidly heated, it generally tends to yield a higher fraction by weight of volatile product than it would if it were heated slowly.

Extensive literature exists on the devolatilization of coal in the slow decomposition regime. Excellent reviews of the available literature are given by Field et al. (1967), Yellow (1975), Gregory and Littlejohn (1965), Jones (1964), Howard (1963), Dryden (1957), and Dutta and Wen (1977). Although a considerable amount of data for slow decomposition has been obtained, a systematic analysis of these data such as to develop a model capable of predicting the yields of individual constituents evolved during devolatilization has not been undertaken. Indeed, this is a formidable task, considering the wide variety of coal types and processing conditions available. About the only work in this area is that of Lowry, Landau, and Naugle (1941), in which a model to predict the volatile yields of gas, light oil, and tar as a function of the ultimate and approximate analysis was obtained. Unfortunately, no additional method has been subsequently developed to predict either the gas composition or the characteristics of the tar and light oil calculated from the correlation of Lowry, Landau, and Naugle (1941).

Unlike slow decomposition, which has a long history and vast literature, rapid decomposition is a relatively recently observed phenomenon and is only now being comprehensively examined. Workers at the British Coal Utilization Research Association (BCURA) cite the work of Shapatina, Kalyuzhani, and Chukharov (1961) as being the earliest in the field. Subsequent research, confirming the general nature of the phenomenon, has been performed by Badzioch (1961), Loison and Chauvin (1964), Howard and Essenhigh (1967), and Kimber and Gray (1967).

Most of the "advanced design" coal gasification and combustion processes involve the injection of coal particles into either a fluidized bed or an entraining gas stream. In these modes of operation, the coal is rapidly heated and consequently undergoes rapid devolatilization. This decomposition tends to produce a greater volatile yield than that obtained by the alternative slow decomposition route, as indicated by the proximate analysis test.

The product yields from rapid devolatilization are strongly influenced by the final temperature, coal type, and gaseous environment. At this time, it is unclear how sensitive these yields are to the heating rate. In fact, the work of Anthony et al. (1976) has indicated that volatile yields from both a subbituminous coal and a lignite appear to be insensitive to changes in the heating rate when it is in the range of 650 to 10,000°C/s. In terms of product distribution, it has been generally observed that rapid heating tends to increase the tar fraction and that higher temperatures decrease the tar to gas ratio (Sass 1974, Peters and Bertung 1965, and Loison and Chauvin 1964).

At least the following three questions must be answered to describe the devolatilization process:

1. Where and how are the volatiles released in the bed?
2. How much of the coal is released as gaseous volatile products?
3. What are the compositions of the gaseous volatile products?

Because of the complex nature of these phenomena, no clear answers currently exist to these questions. But assumptions about the nature of the volatile release process and models for prediction of yields have recently been proposed. Specifically, to answer where and how the volatiles are released, many investigators have assumed the devolatilization to occur instantaneously in the bed, which may be reasonable for small particles ($<100\text{ }\mu\text{m}$). However, as pointed out by Rajan, Krishnan and Wen (1978) and by Beér et al. (1978), this assumption is not justified for large particles in the millimeter-size range. For large particles the devolatilization time can be comparable with the mixing time in the bed (10 to 15 s), which can result in uniform release of volatile products throughout the bed. Furthermore, under fuel-rich operations the assumption of instantaneous devolatilization at the coal feed point is indeed questionable. In the absence of reliable kinetic data and product analysis resulting from devolatilization in FBCs, the devolatilization step cannot be adequately incorporated in FBC models. Determinate approaches (Beér et al. 1978, Rajan, Krishnan, and Wen 1978, Park, Levenspiel, and Fitzgerald 1979, and Wen and Chen 1979) have been taken to model this phenomenon.

In addition, recent attempts have been made to model the yields and composition of the volatile products. Pitt (1962) suggested that rapid devolatilization can be modeled by a series of first-order independent reactions. Anthony et al. (1976) extended this theory by suggesting that rapid decomposition be modeled in terms of an infinite set of parallel reactions in which the activation energy is assumed to follow a Gaussian distribution. Although this model is useful for estimating the total amount of volatile yields, its utility is limited by the fact that it fails to provide information on individual constituent yields. These data are of critical importance, particularly in predicting local reducing-oxidizing conditions in the bed and also in local hot spots. Fortunately, the work of Anthony et al. (1976) has served as a basis for Suuberg, Peters, and Howard (1977) to develop an algorithm for computing the individual product yields occurring from the rapid pyrolysis of Montana lignite. Using the independent parallel reaction concept and the simple decomposition scheme

$$dV_{ij}/dt = k_j (V_{ij}^* - V_{ij}) , \quad (5.1)$$

where

V_{ij}^* = ultimate yield of product i from reaction j at time t, wt %,

V_{ij} = cumulative yield of product i from reaction j at time t, wt %,

k_j = kinetic constant of reaction j, s^{-1} ,

t = time, s.

Appropriate kinetic constants derived for CO, CO₂, CH₄, C₂H₄, hydrocarbons, tar, water, and hydrogen appear in Table 5.1. Meyer et al. (1979) recently simplified Suuberg's model by assuming that the lignite is subject to a constant heating rate and that the kinetic constant is of Arrhenius form:

$$V_{ij} = V_{ij}^* \exp[-(k_{jo} T^2 / mE_j) \exp(-E_j/T)] , \quad (5.2)$$

Table 5.1. Kinetic parameters for lignite pyrolysis^a

Product	Stage	E_i (kcal/mol)	Log (k_{i0}/s^{-1})	V_i^* [wt % of lignite (dry)]
CO ₂	1	36.2	11.33	6.12
	2	64.3	13.71	2.90
	3	42.0	6.74	1.17
CO	1	44.4	12.26	1.90
	2	59.5	12.42	5.74
	3	58.4	9.77	2.42
CH ₄	1	51.6	14.21	0.36
	2	69.4	14.67	0.99
C ₂ H ₄	1	74.8	20.25	0.16
	2	60.4	12.85	0.44
HC ^b		70.1	16.23	1.02
Tar	1	37.4	11.88	2.63
	2	75.3	17.30	3.14
H ₂ O		51.4	13.90	9.7
H ₂		88.8	18.20	0.54
Total				39.2

^aSource: Suuberg et al. (1977).

^bHydrocarbons other than CH₄, C₂H₄, and tar.

where

V_{ij}^* = ultimate yield of product i by reaction j , wt %,

V_{ij} = cumulative yield of product i by reaction j , wt %,

k_{j0} = preexponential factor for reaction j , s^{-1} ,

E_j = activation energy of reaction j , kcal/g-mol,

m = heating rate, K/s,

T = temperature, K.

The computed distribution of the various products versus temperature is shown in Fig. 5.1.

In addition to the Suuberg model, a similar model for the devolatilization of Illinois No. 6 coal has been derived by Reklaitis

Fig. 5.1. Devolatilization products of dry Montana lignite versus temperature.

et al. (1977) at Purdue. Using the available data on the char oil energy development (COED) process and the idea of an infinite set of parallel reactions, the following kinetic parameters have been derived for the model:

$$V_i = V_i^* G(a_i T - b_i) , \quad (5.3)$$

where

V_i^* = ultimate yield of product i , wt %,

V_i = cumulative yield of product i up to temperature T , wt %,

G = cumulative normal Gaussian distribution function,

a_i, b_i = constants for product i , K^{-1} , dimensionless,

T = temperature, K.

These parameters appear in Table 5.2, and the computed distribution of devolatilization versus temperature appears in Fig. 5.2. In the current combustion subcode, it was necessary to characterize the liquid product by the empirical formula $C_1H_{0.800}O_{0.0259}$. This formula was

Table 5.2. Kinetic constants for Illinois No. 6 coal pyrolysis^a

Product	a_i (K^{-1})	$-b_i$	V_i^* (wt % dry coal)
H ₂	0.013293	11.831	1.22
H ₂ O	0.011488	7.898	6.05
CO	0.037222	30.801	4.07
CO ₂	0.054738	43.921	2.22
CH ₄	0.058159	46.236	3.88
C ₂ H ₄	0.023264	17.448	1.54
Oil	0.011632	8.317	18.52
Total			37.50

^aSource: Reklaitis et al. (1977), Reklaitis (1978).

Fig. 5.2. Devolatilization products of dry Illinois No. 6 versus temperature.

derived by Meyer et al. (1979) from the COED project (Jones et al. 1972) data.

It should be emphasized that devolatilization accounts for 25 to 45% of the total weight loss during the combustion process. Although true, it is probably the most poorly understood and inadequately described step in the combustion process.

5.1.2 Combustion of volatile products

At temperatures above 650°C in an oxidizing atmosphere, the rate of burning of volatiles is fast compared with the time required for volatile evolution. However, the combustion of the volatile products (CO, H₂, CH₄, C₂H₆, tar, liquids, etc.) released in the emulsion phase is controlled by the availability of oxygen. Since the oxygen concentration in the emulsion phase is low compared with that in the bubble phase, the volatile products in the emulsion phase first tend to form CO by partial combustion with oxygen, whereas the volatiles exchanged to the bubble phase burn completely to CO₂ because of excess oxygen present in the bubble phase.

Among the combustion reactions of the volatile products, the slowest reaction is the combustion of CO,

The burning time of the volatiles will depend on whether the process is controlled by gas film diffusion (diffusion through the volatile film formed around the particles immediately after pyrolysis) or by the oxidation of CO. Howard and Essenhigh (1967) assumed that burning of volatiles occurs in both the interior of the solid and the laminar layer of gas surrounding the particles. Field et al. (1967), on the other hand, assumed that, because volatiles mix with oxygen at the particle surface and the burning rate is fast, the overall rate is limited by boundary layer diffusion. This subject has been treated extensively by several researchers (Field et al. 1967, Mulcahey and Smith (1969), Sarofim and Beér 1978). An alternative approach, as stated earlier, is

that the volatiles react rapidly to form CO and H₂ and that the rate determining step is the CO oxidation reaction [Eq. (5.4)].

In FBC operation, there is a potential for high emissions of CO, particularly at bed temperatures below 1000 K (Campbell and Davidson 1975, Basu, Broughton, and Elliot 1975, Gibbs, Pereira, and Beér 1975). There is also evidence (Horio et al. 1977) that CO concentration in the emulsion phase is about a factor of 2 larger than the average space concentration. The extent of mixing in the bed will therefore be critical to establish conditions under which local reducing zones and/or local hot spots can prevail in the reactor; it will also influence the extent of freeboard combustion of CO and the char-NO_x reduction reactions. Very little information is currently available on the effect of the feed size distribution and fines content in the feed on CO concentrations in the bed. Until such data become available, the validity of these single-particle combustion models will remain unresolved.

5.1.3 Char combustion

Burning of char, or the char-oxygen reaction, is the fastest among the char gas reactions taking place in the combustor. Although the mechanism of char combustion is better understood than either the pyrolysis reaction or volatile combustion, the mechanisms of char combustion and product gas distributions around the burning char particle are very complex. This complexity is primarily due to the highly exothermic and extremely fast nature of the reaction, which poses difficulties in experimental determination of the particle temperature, which can be 100 to 200°C higher than the bulk gas temperature. Second, the rates of combustion are affected by the coal type, the particle size, and the pore structure, which change during the course of combustion. Consequently, kinetic studies are often limited to oxidation of small carbon or char particles at lower temperatures and pressures. Some of the earlier definitive models related to char combustion in fluidized beds are now discussed briefly.

Avedesian and Davidson (1973) studied the mechanism of combustion of carbon particles (0.23 to 2.61 mm) in a shallow coal ash fluidized bed. Based on their observations, they suggested that O₂ and CO burn rapidly

in a very thin reaction zone surrounding the particle, that carbon monoxide produced at the particle surface diffuses out toward the reaction zone, and that oxygen from the main stream diffuses in and burns in a diffusion flame to produce CO_2 . According to these investigators, no CO appears in the main stream when there is an abundant supply of oxygen. The expression for the burning rate of a single particle was given by

$$\dot{m} = 24\pi \text{Sh} D d_p C_{\text{O}_2} \quad (5.5)$$

where

$\dot{m}$ = burning rate of carbon particle, g/s,

D = molecular diffusion coefficient in the gas phase, cm^2/s ,

d_p = carbon particle diameter, cm,

C_{O_2} = oxygen concentration in the particulate phase, g-mol/ m^3 ,

Sh = Sherwood number, $k_m d_p / D$,

k_m = mass transfer coefficient, cm/s,

$\pi = 3.14$.

Campbell and Davidson (1975) later modified this model and conducted burning rate experiments with char and coke in the size range (1 to 3 mm) in a fluidized bed. Their modified expression is given by

$$\dot{m} = 12b\pi \text{Sh} D d_p C_{\text{O}_2} \quad (5.6)$$

where the constant is defined as $2R/d_p$ and R is the radius of the carbon particle reaction zone.

Basu, Broughton, and Elliot (1975) and Basu (1976) conducted further experiments and concluded that the controlling mechanism may be a combination of diffusion and chemical kinetics. Their expression for the burnup rate is given by

$$\dot{m} = 48\pi D \delta d_p C_{\text{O}_2} (1 + 12C_{\text{O}_2} / \rho_g) \quad (5.7)$$

where $\bar{\delta}$ is the mean fractional void area around a burning carbon particle and ρ_g is the density of fluidizing gas, g/cm³.

Chakraborty and Howard (1978) performed combustion experiments in the temperature range of 1073 to 1173 K with carbon spheres in the range of 0.3 to 12 mm in a shallow fluidized bed (12.5 to 50 mm static bed depth) and computed burning rates from weight loss. They found that, within the range of operating conditions, combustion of particles was mainly kinetically controlled.

These studies clearly show that the mechanism of the char-oxygen reaction is determined by the particle size and temperature. Figure 5.3 illustrates the various rate-controlling regimes in AFBC (Rajan, Krishnan, and Wen 1979). Figure 5.3 shows that the reaction can go to gas-film, diffusion-controlled if the temperature and/or particle size increases. On the other hand, if the temperature and/or particle size decreases substantially, the reaction may proceed toward the chemical reaction

Fig. 5.3. Rate-controlling regimes in AFBC.

control regime and may take place uniformly throughout the internal pore surface of the particle.

The reaction rate expression proposed by Field et al. (1967) for anthracites and brown coal is

$$r_c = \pi d_p^2 k_c C_{O_2}, \quad (5.8)$$

where k_c is the overall rate constant and is given by

$$k_c = [R_{GG} (T_p + T_g)/2Mc] / (1/K_{cR} + 1/K_{cf}) \quad (5.9)$$

where

k_{cR} = chemical reaction rate constant = $8710 \cdot \exp(-35,700/R_G T_p)$,
g/cm²-s-atm,

k_{cf} = diffusion rate constant = $24\eta D/d_p R_{GG} (T_p + T_g)/2$,

d_p = surface volume mean diameter of char, cm,

D = molecular diffusivity, cm²/s,

R_{GG} = universal gas constant, 82.06 atm-cm³/g-mol-K,

T_p = particle surface temperature, K,

T_g = bulk gas temperature, K,

M_c = atomic weight of carbon, g-mol,

C_{O_2} = oxygen concentration in the main stream, g-mol/cm³,

η = mechanism factor.

Of particular importance in the char-oxygen reaction is whether the primary product of the reaction is CO or both CO and CO₂. This question has been addressed by many investigators (Essenhigh 1961, Arthur 1951, Caram and Amundson 1977, Laurendeau 1978, and Field et al. 1967).

The mechanism factor η in Field's rate expression [Eq. (5.8)] takes a value of 2 when CO is the direct product of the char-O₂ reaction,

and a value of 1 when CO₂ is the direct product.

Although several studies have been made to determine the value of η as a function of temperature, particle size, and carbon type, no quantitative conclusions can be drawn.

Other rate expressions for combustion of char have been developed by Smith (1971), Smith and Tyler (1972), Mulcahey and Smith (1969), Hamor, Smith, and Tyler (1973), and Dutta and Wen (1977). All these rate expressions are only approximations to the real combustion process, and the understanding of the phenomenon is far from complete. However, for order-of-magnitude calculations for char combustion, they appear to be reasonable.

5.1.4 Previous combustion models

Models for fluidized-bed combustion are based on an appropriate model for coal combustion that describes the mechanism and rate processes by which a single particle of coal burns. This model is coupled with a model of the fluidized bed that describes the bed hydrodynamics, mass transfer, and heat transfer. Several models of fluidized-bed combustion have appeared in the literature. Table 5.3 represents a partial list of these models, detailed reviews of which can be found in Caretto (1977) and in Wen and Tone (1978). Most of the models developed so far are bubbling bed models based on the two-phase theory of fluidization originally proposed by Toomey and Johnstone (1952) and later modified by Davidson and Harrison (1963). According to the theory, the fluidized bed consists of two phases: (1) a continuous dense particle phase (emulsion phase) and (2) a discontinuous lean gas phase (bubble phase), with exchange of gas between the bubble phase and the emulsion phase. The flow rate of gas through the emulsion phase is assumed to be the incipient fluidization velocity U_{mf} , and the excess gas $U_o - U_{mf}$ flows through the bubble phase. The emulsion phase is considered to have the same void fraction as a bed at minimum fluidization. Extensions of the Davidson and Harrison model visualize, in addition, a thin cloud of surrounding gas and solids around the rising bubble, with a trailing wake of solids at the bottom of the bubble. The cloud wake region is treated separately from the bubble and emulsion phases, and these models fall under the category of three-phase bubbling bed models.

Table 5.3. Classification of models proposed for fluidized-bed combustion

Model description	Investigators	Gas flow pattern		Solids mixing in the bed	Remarks
		Bubble phase	Emulsion phase		
Two-phase bubbling bed model	Avedisian and Davidson (1973)	Plug flow	Plug flow	Complete mixing	Bubble diameter is assumed to be uniform throughout the bed in most cases and is an adjustable parameter; cloud and wake are combined in the emulsion phase; no combustion of carbon in the bubble phase
	Gibbs (1975)	Plug flow	Complete mixing		
	Campbell and Davidson (1975)	Complete mixing	Complete mixing		
	Gordon and Amundson (1976)				
Two-phase compartment in series models	Becker, Beer, and Gibbs (1975)				
	Baron, Hodges, and Sarofin (1977)				
	Horio and Wen (1977)	Complete mixing in each compartment	Complete mixing in each compartment	Complete mixing in each compartment with backflow of solids from one compartment to another	Bubbles grow along the bed height; the backflow solids mixing parameter is adjustable; cloud and wake are combined in the bubble phase; combustion of carbon occurs in both bubble and emulsion phases
Three-phase bubbling bed model	Horio et al. (1977)				
	Rengarajan, Krishnar, and Wen (1979)				
Three-phase bubbling bed model	Chen and Saxena (1977)	Plug flow	Plug flow	Complete mixing	Cloud wake is treated as a separate phase and is in plug flow; solids in the cloud wake are at minimum fluidization; bubbles grow along the bed height; combustion occurs in the cloud wake and emulsion phases; isothermal condition throughout the bed

Source: Wen and Tone (1978).

All bubbling bed models require accurate expressions for prediction of the bubble characteristics, some of which are

1. bubble diameter, d_B ,
2. bed bubble fraction, $\bar{\epsilon}_B$,
3. bubble rise velocity, u_B ,
4. bubble phase volumetric flux, $\dot{V}_B$,
5. gas interchange coefficient from bubble to cloud, K_{BC} , and
6. gas interchange coefficient from cloud to emulsion, K_{CE} .

The relationship among these and other parameters can be found in Kunii and Levenspiel (1977). As can be seen, each of the above quantities is related to the bubble diameter d_B . Bubble size and the interphase gas exchange rate are the major uncertainties in bubbling bed models (Werther 1978 and Yates 1975). At present, no reliable method exists for determining the effective bubble size other than by data fitting (see bubble-growth section), which makes these models unsuitable for scale-up purposes (Werther 1978). Other approaches for estimating bubble size and relating it to characteristic changes in bed hydrodynamics due to changes in reactor geometry, operating pressure, and presence of internals in the bed, etc., are currently being pursued to gain further insight into the scale-up problem.

Recently, the validity of the bubbling bed models for FBC systems, particularly for the designs and operating conditions envisioned for these systems (e.g., TVA's 20-MW AFBC pilot plant), has been questioned.

Park, Levenspiel, and Fitzgerald (1979) recently proposed a radically different model. This model assumed that all coal particles fed to the bed devolatilize instantaneously, which forms a plume of volatile products above the feed point. These products are subsequently combusted at the boundary of the plume. At present, these recent developments have not been significantly reviewed and tested against experimental data, and their validity has not been established.

5.2 Model Development

When coal is fed to an AFBC, the coal devolatilizes and the products (gas and char) are consumed by combustion. In fluidized beds, this process is affected by (1) bed hydrodynamics, (2) solids mixing, (3) solids attrition and elutriation, and (4) kinetics of chemical reactions (devolatilization and combustion). The effects of the above factors on combustion are neither well understood nor quantized for a large-scale AFBC. To develop a combustion model, certain assumptions are required to take into account the above factors. These assumptions can be validated only by comparing the model predictions with experimental results. In the following, the assumptions, derivations of equations, and computational methods are given and discussed.

5.2.1 Assumptions

The following assumptions are made to develop a coal combustion subcode. First, the FBC system is assumed to be at steady state (i.e., the conditions at a point in the bed do not vary with time). Next, two separate phases are considered in the model: the emulsion phase and the bubble phase. The emulsion phase is characterized as the region of the bed devoid of bubbles and containing the solids (limestone, coal ash, and char). The solids present in the emulsion phase are assumed to be well mixed (back-mix). Gas flow through the emulsion phase is in the upward direction and is in plug flow. The voidage of the emulsion phase is assumed to be the voidage corresponding to minimum fluidization in accordance with the two-phase theory. The velocity of the gas flow through the emulsion phase corresponds to the minimum fluidization velocity. The reactions considered in the emulsion phase are

1. $C + 0.5O_2 \rightarrow CO$,
2. $CO + 0.5O_2 \rightarrow CO_2$,
3. $CO_2 \rightarrow C \rightarrow 2CO$, and
4. devolatilization.

The devolatilization reaction is assumed to occur uniformly throughout the emulsion phase in the bed.

For the prediction of the amount of carbon in the volatile gas, the pyrolysis models of Suuberg, Peters, and Howard (1977) and of Reklaitis et al. (1977) developed for Montana lignite and Illinois No. 6 bituminous coal, respectively, are used. The carbon released during devolatilization is assumed to form carbon monoxide instantaneously. The carbon monoxide is then consumed by reaction 2, and the resulting char is consumed by reactions 1 and 3. These reactions are heterogeneous gas-solid reactions. Their overall rates are therefore dependent on both the chemical reaction rate at the solid surface (intrinsic) and the mass transfer rate of gaseous species to the solid surface. Specifically, oxygen and carbon dioxide are transferred to the surface of the particle, where they undergo reactions 1 and 3, respectively. The product carbon monoxide then diffuses back into the interstitial spaces, where it is consumed by reaction 2. The intrinsic rate for reaction 1 was based on the bituminous kinetics of Smith (1971). For the Boudard reaction (reaction 3) the estimate given by Caram and Amundson (1977) was used. The rate expressions for gas species mass transfer to the surface was obtained from Field et al. (1967). The kinetics for the gas phase reaction (reaction 2) was obtained from Horio, Morio, and Muchi (1977). These expressions are summarized in Table 5.4. The expression for reaction 3 (Boudard reaction) has been found to be ten times too high (Horio et al. 1977) and has therefore been reduced by a factor of 10 in the code. For both heterogeneous reactions, the particle surface temperature was calculated via a heat balance between the particle and surrounding gas (Smith 1971):

$$R_1^T(\Delta H_R) = 2k_g(T_p - T_g)/d_p + \epsilon_T S(T_p^4 - T_g^4), \quad (5.11)$$

where

R_1^T = rate of $C + 0.5O_2 \rightarrow CO$, amount of carbon consumed, g-mol/cm²-s,

ΔH_R = heat of reaction, cal/g-mol of carbon,

k_g = gas thermal conductivity, cal/cm-s-K,

T_p = surface temperature of particle, K,

T_g = gas temperature, K,

Table 5.4. Reaction rate expressions

Chemical reaction rate constants (intrinsic)

$$1. \quad C + 0.5O_2 \rightarrow CO: \quad k_1^I = 0.67 \exp(-16,000/R_G T_p) [=] \frac{\text{g-mol carbon consumed}}{\text{cm}^2\text{-s-atm}} \quad (5.12)$$

$$2. \quad CO + 0.5O_2 \rightarrow CO_2: \quad k_2^I = 1.3 \times 10^{14} \exp(-30,000/R_G T_g) [=] \frac{\text{cm}^3 \text{ gas}}{\text{g-mol-s}} \quad (5.13)$$

$$3. \quad CO_2 + C \rightarrow 2CO: \quad k_3^I = \frac{4.2 \times 10^{10}}{R_{GG} T_g} \exp(-59,200/R_G T_g) [=] \frac{\text{g-mol carbon consumed}}{\text{cm}^2\text{-s-atm}} \quad (5.14)$$

Mass transfer reaction rate constants (Field et al. 1967)

$$1. \quad C + 0.5O_2 \rightarrow CO: \quad k_1^M = \frac{4D}{d_p R_{GG} T_g} [=] \frac{\text{g-mol carbon consumed}}{\text{cm}^2\text{-s-atm}} \quad (5.15)$$

$$2. \quad CO + 0.5O_2 \rightarrow CO_2: \quad k_2^M = 0$$

$$3. \quad CO_2 + C \rightarrow 2CO: \quad k_3^M = \frac{4D}{d_p R_{GG} T_g} [=] \frac{\text{g-mol carbon consumed}}{\text{cm}^2\text{-s-atm}} \quad (5.16)$$

Table 5.4 (continued)

Overall reaction rate constants

$$1. \quad C + 0.5O_2 \rightarrow CO: \quad R_1^T = \frac{1}{\left(-1/k_1^I + 1/k_1^M\right)} C_{O_2}^{EMUL} R_{GG}^T \quad [=] \quad \frac{\text{g-mol carbon consumed}}{\text{cm}^2\text{-s}} \quad (5.17)$$

$$2. \quad CO + 0.5O_2 \rightarrow CO_2: \quad R_2^T = k_2^I \left(C_{H_2O}^{EMUL}\right)^{1/2} \left(C_{CO}^{EMUL}\right) \left(C_{O_2}^{EMUL}\right)^{1/2} \quad [=] \quad \frac{\text{g-mol CO consumed}}{\text{cm}^3 \text{ of gas-s}} \quad (5.18)$$

$$3. \quad CO_2 + C \rightarrow 2CO: \quad R_3^T = \frac{1}{\left(1/k_3^I + 1/k_3^M\right)} C_{CO_2}^{EMUL} R_{GG}^T \quad [=] \quad \frac{\text{g-mol carbon consumed}}{\text{cm}^2\text{-s}} \quad (5.19)$$

d_p = diameter of particle, cm,

e = particle emissivity, dimensionless,

τ_S = Stefan-Boltzmann constant, cal/[cm²-s-(K)⁴].

In addition to the emulsion phase, the bubble phase is present throughout the bed. The bubbles are assumed to be devoid of all solids, and the only reaction occurring in the bubble phase is the combustion of carbon monoxide (reaction 2). The rate constant of this reaction is given in Table 5.4. Also, the bubble is assumed to have a very thin cloud. This assumption, which is reasonable for a large-particle, high-superficial-velocity operation, allows the interchange coefficient between the bubble phase and the emulsion phase to be estimated from the Davidson model (Davidson and Harrison 1963):

$$K_{BE} = [4.5(U_{mf}/d_B)] + \left[\left(5.85 D^{1/2} g^{1/4} \right) / \left(d_B^{5/4} \right) \right], \quad (5.20)$$

where

K_{BE} = gas interchange coefficient, 1/s,

U_{mf} = minimum fluidization velocity, cm/s,

d_B = bubble diameter, cm,

D = molecular diffusivity, cm²/s,

g = gravitational acceleration, cm/s².

The bubble size and velocity are estimated from the ORNL bubble-growth model described in this report. Two types of bubbles are assumed to be in the bed: fast and slow. Slow bubbles are voids in the bed, traveling upward at a velocity of less than the interstitial velocity of gases in the emulsion phase. This region is generally found right above the distributor plate. The gases flow through these voids and are not trapped in the voids. At a 10-cm height [calculated via the criteria given by Catipović, Jovanovic, and Fitzgerald (1978)], the bubble velocity increases to a velocity greater than that of the interstitial gas. This

type of bubble is characterized as a "fast" bubble. In addition, it was assumed that the elutriation of char from the bed can be characterized by the elutriation constant of Wen and Hashinger (1960).

Devolatilization of the coal accounts for 25 to 45% of the total coal consumption. For this reason, the devolatilization model and the location where the volatile gas products are released in the bed are very important. In this work, the devolatilization models of Suuberg, Peters, and Howard (1977) and Reklaitis et al. (1977) are chosen. At present these models appear to be reasonable for estimating the total volatile yield and volatile composition. The location of volatile release in the bed depends on the rate of devolatilization and the solids mixing in the bed. In this work, the volatiles are assumed to be released uniformly throughout the bed. Fitzgerald et al. (B&W 1979b) give data showing that the devolatilization time of a coal particle is a function of particle diameter. Specifically, their experimental measurements show that a 200- μm coal particle requires less than 1 s to devolatilize and that a 3000- μm particle requires as much as a 6 to 10 s to devolatilize. This finding implies that fines in the feed are devolatilized rapidly but that large particles require longer. Fitzgerald also gives the mixing time of a fluid bed as about 15 s, which implies that the coal feed particles are uniformly distributed through the bed at the end of 15 s. Highley and Merrick (1971) found that a fluidized bed required 10 to 40 s to become well mixed.

Solids mixing in a fluidized bed is due to the passage of gas bubbles upward through the bed, which induces both lateral and axial mixing. Kunii and Levenspiel (1977) show experimental evidence that vertical mixing is about an order of magnitude greater than is lateral mixing. Data presented by Highley and Merrick (1971) for a 1.5-m-diam (5-ft) coal ash bed show that particles entering the bottom of the bed make their way rapidly (~ 2 s) to the surface of the bed, which implies that coal feed at the bottom of the bed is carried rapidly to the surface of the bed. During this rise, the finer coal particles are completely devolatilized, but the larger particles are only partially devolatilized. Once these particles reach the surface, two things occur: the smaller particles are elutriated, and the larger particles are returned back to the bed.

Although the larger particles (remaining in the bed) have been displaced laterally, the devolatilization process still continues.

As stated previously, the devolatilization time is a function of particle diameter. If large amounts of fines are fed to the bed, a large amount of volatile gas will be rapidly released in the region above the feed point. Therefore, a large amount of oxygen will be consumed, and the possibility exists that reducing conditions will be present in the region above the feed point. At present the nature of the feed coal and solids mixing are assumed to be such that volatiles are released uniformly in the bed. Since very little quantitative information is available on the fluidized-bed devolatilization phenomenon, this assumption is reasonable for the present time. It is hoped that future experimental studies will establish a more realistic approach.

The intrinsic rate expression for the combustion of the char ($C + 0.5O_2 \rightarrow CO$) is important. In this work the bituminous kinetics of Smith (1971) is used. This expression was chosen because the bituminous char structure is different from the structure of lignite and anthracite chars. Bituminous chars contain large and irregularly distributed voids, but lignite and anthracite chars exhibit uniform and narrow pores (Smith 1971). These structural differences affect the intrinsic reaction rate.

Other important assumptions are the bubble-growth correlation and the existence of slow and fast bubbles in the bed. The gas voids in a bed coalesce to form larger voids; from two-phase theory this results in a higher bubble velocity (Cranfield and Geldart 1974). Large bubbles (80 cm) have been observed at the surface of fluidized beds (Botton 1966); from two-phase theory, these should be fast bubbles. The ORNL bubble-growth model predicts large bubbles at the bed's surface. Until more definitive data on bubble growth become available, the current assumptions are reasonable.

Finally, since a major loss of combustion efficiency is due to elutriation, the expression for the elutriation constant is also important. In this work the Wen and Hashinger (1960) expression is used:

$$K(R) = \frac{1.7 \times 10^{-5} \rho_g [U_o - U_t(R)] A_{xs}}{W_B} = \left\{ [U_o - U_t(R)]^2 / 2gR \right\}^{0.5} Re_t^{0.725} \\ \times [(\rho_s - \rho_g) / \rho_g]^{1.15} \left\{ [U_o - U_t(R)] / U_t(R) \right\}^{0.1}, \quad (5.21)$$

where

$K(R)$ = elutriation constant for radius R , s^{-1} ,

ρ_g = gas density, g/cm^3 ,

U_o = superficial velocity, cm/s ,

$U_t(R)$ = terminal velocity for a particle of radius R , cm/s ,

ρ_s = density of particle, g/cm^3 ,

Re_t = Reynolds number based on terminal velocity of particle
 $(Re_t = 2\rho_g R U_t(R) / \mu_g)$, dimensionless,

W_B = mass of char in bed, g ,

R = particle radius, cm .

This expression was chosen because it was developed for coal particles in a fluidized bed. The Merrick and Highley (1971) correlations were not used because they were developed for higher density solids (limestone sorbent and coal ash).

At present, the validity of many of the above assumptions has not been established. For this reason the present combustion subcode has been structured to allow relatively easy modifications as more information becomes available at a later date.

5.2.2 Combustion performance equations

The equations for the solid side (char) and the gas side material balances are developed in this section. These equations are used to

determine the total amount of coal consumed in the bed. The solid side material balance is based on the assumption of well-mixed solids throughout the bed. These equations are similar to those developed in the elutriation-attrition code, except that the balance is performed on char instead of limestone-coal ash solids. The gas side material balance is based on the assumption that the gas flow is characterized by two regions: the slow-bubble region and the fast-bubble region. The criteria for the determination of these regions were given in the assumptions. These regions are shown schematically in Fig. 5.4.

In the slow-bubble region of the bed, the gas flow is treated as plug flow (i.e., all gas moves in a uniform front through the bed). In this

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Fig. 5.4. Schematic of combustion model.

region, the coal devolatilizes to char and volatile gases. The products are consumed in the combustion process (i.e., reactions 1 through 3). In the fast-bubble region two separate phases (the emulsion phase and bubble phase) exist. Each phase is analyzed separately. In the emulsion phase the processes of devolatilization, combustion, and mass transfer of gas species to and from bubbles are assumed to occur. In the bubble phase the combustion of carbon monoxide and mass transfer of gas species to and from the emulsion phase are assumed to occur.

Based on these concepts, the gas side and solid side material balance equations are written as follows.

5.2.2.1 Gas side material balance equation — devolatilization.

Since devolatilization is assumed to occur uniformly through the emulsion phase in both the slow- and fast-bubble regions, the equations developed apply to both regions. The total yields and composition of the volatile gas products are found via the Suuberg, Peters, and Howard (1977) model for lignites or via the Reklaitis et al. (1977) model for bituminous coals. The Reklaitis model is used in the current code. This information is used to determine the average amounts of oxygen consumed and carbon monoxide produced per unit volume of the emulsion phase as follows. First, the volume of the emulsion phase is found as

$$V_{EMUL} = A_{xs} L_f (1 - \bar{\epsilon}_B) , \quad (5.22)$$

where A_{xs} is the total cross-sectional area of the bed, cm^2 , L_f is the expanded bed height, cm , and $\bar{\epsilon}_B$ is the average bed bubble voidage, dimensionless. The average bubble voidage is found from two-phase theory as

$$\bar{\epsilon}_B = 1 - (L_{mf}/L_f) , \quad (5.23)$$

where L_{mf} is the bed height at minimum fluidizing velocity, cm . From the devolatilization code the total amounts of carbon monoxide produced X_{CO} and oxygen consumed X_{O_2} in the bed are found via the volatile yield equations [Eq. (5.2 or 5.3)]. These equations are used to determine the

average amounts of the gases produced and consumed in a unit volume of the emulsion phase as follows:

$$\phi_{O_2} = X_{O_2}/V_{EMUL} , \quad (5.24)$$

$$\phi_{CO} = X_{CO}/V_{EMUL} , \quad (5.25)$$

where ϕ_{O_2} is the average amount of O_2 consumed per unit volume of emulsion phase, g-mol O_2/cm^3 of emulsion, and ϕ_{CO} is the average amount of CO produced per unit volume of emulsion phase, g-mol CO/cm^3 of emulsion. These values are then used in both regions of the bed for the gas side material balance.

5.2.2.2 Gas side component balances. Based on the above devolatilization expressions, a series of differential component material balances are derived. The components considered in these balances are O_2 , CO, and CO_2 . A separate set of differential balances is required for the slow- and fast-bubble regions of the bed; this is due to the difference in bubble characteristics in the slow- and fast-bubble regions in the bed.

The three differential component balances (O_2 , CO, and CO_2) for the slow-bubble region are given in Table 5.5. In this region the gas flowing through the emulsion and bubble is assumed to move in a uniform front (i.e., no axial dispersion). Therefore, the gas composition is only a function of height. The detailed derivation of these expressions is given in Appendix A. The six differential component balances [Eqs. (5.29) through (5.40)] for the fast-bubble region are given in Table 5.6. In this region the gas in the bubble phase is assumed to be "trapped" and is transferred to and from the bubble phase by diffusional mass transfer. This diffusional transfer and the combustion of char in the emulsion phase result in different concentration profiles for the bubble and emulsion phases. Therefore, O_2 , CO, and CO_2 component balances are required for each phase (bubble and emulsion). The detailed derivations of these differential balances are given in Appendix B. The solution to these equations gives profiles of O_2 , CO, and CO_2 through the emulsion and bubble phases in the bed. The solutions are obtained by dividing the bed into small increments N_h of height ΔZ and integrating between the bottom of the bed and the surface of the bed L_f . This procedure is

Table 5.5. Slow-bubble region differential material balances

O₂ balance

$$dC_{O_2}^{SB}/dZ = \frac{A_{xs}}{\dot{V}_T} \left[-\frac{1}{2} \sum_i^{all R} (R_1^T \xi_{plug})_i (1 - \delta) - \frac{1}{2} R_2^T \delta - \phi_{O_2} \frac{1 - \bar{\epsilon}_B}{1 - \bar{\delta}} (1 - \delta) \right] \quad (5.26)$$

CO balance

$$dC_{CO}^{SB}/dZ = \frac{A_{xs}}{\dot{V}_T} \left\{ \left[\sum_i^{all R} (R_1^T \xi_{plug})_i + 2 \sum_i^{all R} (R_3^T \xi_{plug})_i \right] (1 - \delta) - R_2^T \delta + \phi_{CO} \frac{1 - \bar{\epsilon}_B}{1 - \bar{\delta}} (1 - \delta) \right\} \quad (5.27)$$

CO₂ balance

$$dC_{CO_2}^{SB}/dZ = \frac{A_{xs}}{\dot{V}_T} \left[R_2^T \delta - \sum_i^{all R} (R_3^T \xi_{plug})_i (1 - \delta) \right] \quad (5.28)$$

Table 5.6. Fast-bubble region differential material balances

Emulsion phase O₂ balance

$$dC_{O_2}^{EMUL}/dZ = \frac{1}{(1 - \epsilon_B)} \left[(1/U_{mf}) \left(dF_{O_2}^{EMUL}/dV \right) - C_{O_2}^{EMUL} \frac{d(1 - \epsilon_B)}{dZ} \right] \quad (5.29)$$

where

$$dF_{O_2}^{EMUL}/dV = -(1/2) \left[\sum_i^{all} R \left(R_1 T_{\xi_{EMUL}} \right)_i + R_2 T_{\epsilon_{mf}} + 2\phi_{O_2} \right] (1 - \epsilon_B) + K_{BE} \left(C_{O_2}^{BUB} - C_{O_2}^{EMUL} \right) \epsilon_E \quad (5.30)$$

Emulsion phase CO balance

$$dC_{CO}^{EMUL}/dZ = \frac{1}{1 - \epsilon_B} \left\{ (1/U_{mf}) \left(dF_{CO}^{EMUL}/dV \right) - C_{CO}^{EMUL} \left[\frac{d(1 - \epsilon_B)}{dZ} \right] \right\} \quad (5.31)$$

where

$$dF_{CO}^{EMUL}/dV = \left[\sum_i^{all} R \left(R_1 T_{\xi_{EMUL}} \right)_i + 2 \sum_i^{all} R \left(R_3 T_{\xi_{EMUL}} \right)_i - R_2 T_{\epsilon_{mf}} + \phi_{CO} \right] (1 - \epsilon_B) + K_{BE} \left(C_{CO}^{BUB} - C_{CO}^{EMUL} \right) \epsilon_B \quad (5.32)$$

Table 5.6 (continued)

Emulsion phase CO₂ balance

$$dC_{CO_2}^{EMUL}/dZ = \frac{1}{(1 - \epsilon_B)} \left[(1/U_{mf}) \left(dF_{CO_2}^{EMUL}/dV \right) - C_{CO_2}^{EMUL} \frac{d(1 - \epsilon_B)}{dZ} \right] \quad (5.33)$$

where

$$dF_{CO_2}^{EMUL}/dV = \left[R_2^T \epsilon_{mf} - \sum_i^{all} R \left(R_3^T \epsilon_{EMUL} \right)_i \right] (1 - \epsilon_B) + K_{BE} \left(C_{CO_2}^{BUB} - C_{CO_2}^{EMUL} \right) \epsilon_B \quad (5.34)$$

Bubble phase O₂ balance

$$dC_{O_2}^{BUB}/dZ = \left(1/\dot{V}_B \right) \left[\left(dF_{O_2}^{BUB}/dV \right) - C_{O_2}^{BUB} \frac{d\dot{V}_B}{dZ} \right] \quad (5.35)$$

where

$$dF_{O_2}^{BUB}/dV = \left[-(1/2) R_2^T \epsilon_B - K_{BE} \left(C_{O_2}^{BUB} - C_{O_2}^{EMUL} \right) \epsilon_B \right] \quad (5.36)$$

Table 5.6 (continued)

Bubble phase CO balance

$$dC_{CO}^{BUB}/dz = 1/\dot{V}_B \left[\left(dF_{CO}^{BUB}/dV \right) - C_{CO}^{BUB} \left(d\dot{V}_B/dz \right) \right] \quad (5.37)$$

where

$$dF_{CO}^{BUB}/dV = -R_2^T \epsilon_B - K_{BE} \left(C_{CO}^{BUB} - C_{CO}^{EMUL} \right) \epsilon_B \quad (5.38)$$

Bubble phase CO₂ balance

$$dC_{CO_2}^{BUB}/dz = \left(1/\dot{V}_B \right) \left(dF_{CO_2}^{BUB}/dV \right) - C_{CO_2}^{BUB} \left(d\dot{V}_B/dz \right) \quad (5.39)$$

where

$$dF_{CO_2}^{BUB}/dV = R_2^T \epsilon_B - K_{BE} \left(C_{CO_2}^{BUB} - C_{CO_2}^{EMUL} \right) \epsilon_B \quad (5.40)$$

described later. Also, the radius R of the carbon particles existing between the maximum radius $R_{\max}$ and the minimum radius $R_{\min}$ is established by assuming a small increment ΔR , which allows the rate of carbon consumption for each carbon particle of radius R to be found. The average rate of total carbon consumption per unit surface area of a particle of radius R is given by

$$\bar{R}_T(R) = \left\{ \sum_j^{N_h} \left[R_1^T(R) + R_3^T(R) \right] \right\} / N_h, \quad (5.41)$$

where

$R_1^T(R)$ = rate of carbon consumption via reaction 1 (see Table 5.4)
for a particle of radius R , g-mol/s-cm²,

$R_3^T(R)$ = rate of carbon consumption via reaction 3 (see Table 5.4)
for a particle of radius R , g-mol/s-cm²,

N_h = the number of incremental volumes ΔV in the bed, dimensionless.

Also, the rate of change of the char particle radius with respect to time for a particle of radius R can be found as

$$\dot{R}(R) = dR/dt = [\bar{R}_T(R)] / (\rho_{\text{char}}), \quad (5.42)$$

where ρ_{char} is the density of the char in g-mol/cm³.

5.2.2.3 Char particle material balance. By completing the gas component material balance, the rate of change of radius of the char particle can be found via Eq. (5.42). This information is used to solve the general particle side performance equations of a fluidized bed given by Kunii and Levenspiel (1977). These equations consist of an overall material balance and a differential mass balance on particles between R and $R + dR$. The derivation of these equations is given by Kunii and Levenspiel (1977) and is not repeated here. The overall mass balance equation for the char in a fluidized bed is given by

$$F_1 + F_2 - F_0 = \int_{\text{All } R} \frac{3W_B P_B(R) \dot{R}(R)}{R} dR, \quad (5.43)$$

and the differential char mass balance is given by

$$F_0 P_0(R) - F_1 P_1(R) - W_B K(R) P_B(R) - W_B \frac{d[\dot{R}(R) P_B(R)]}{dR} + \frac{3W_B P_B(R) \dot{R}(R)}{R} = 0 \quad (5.44)$$

The above notations are explained in Fig. 5.5. From experimental data obtained from the B&W/EPRI 183- by 183-cm (6- by 6-ft) AFBC (B&W 1979b), the char composition of the underflow F_1 appears to be very small ($\sim 0.1\%$). For this reason, the underflow F_1 is set equal to zero, and the differential balance can then be written as

$$dp_B(R)/dr = \frac{F_0 P_0(R)}{W_B \dot{R}(R)} - \left[\frac{K(R)}{\dot{R}(R)} + \frac{1}{\dot{R}(R)} \frac{d\dot{R}(R)}{dR} - \frac{3}{R} \right] P_B(R) \quad (5.45)$$

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Fig. 5.5. Fluidized bed operated at steady state.

and finally, by definition of differential particle size distribution, as

$$\int_{\text{All } R} p_B(R) dR = 1 . \quad (5.46)$$

In the above equations, $\dot{R}(R)$ represents the rate of particle shrinkage due to combustion as found via the gas component balances [see Eq. (5.42)]. At present, attrition of the char particles is not considered. The term $K(R)$ represents the elutriation constant of Wen and Hashinger (1960) and is given in Eq. (5.21). By solving Eqs. (5.43), (5.45), and (5.46) simultaneously, the char side material is closed. Specifically, the values of F_2 , $p_2(R)$, W_B , and $p_B(R)$ (see Fig. 5.5) are found.

5.3 Code Input-Output and Computational Method

Based on the above assumptions and equations, a computer code has been developed to complete the gas side and char particle side material balance. The input and computational scheme are given and discussed here.

The required inputs and their values are given in Tables 5.7 and 5.8. These values are typical of the B&W/EPRI 183- by 183-cm (6- by 6-ft) AFBC (B&W 1979a). Table 5.8 gives the size distribution of the coal feed. This size distribution is used to calculate the differential size distribution of the feed particle $p_0(R)$, which is an input to Eq. (5.45). The function $p_0(R)$ is determined by curve-fitting the given feed size distribution and then taking the derivative of the resulting curve at discrete points. The coal feed size distribution, shown in Fig. 5.6, was obtained from B&W data (B&W 1979a).

As can be seen, a straight line can be drawn through the data points. Thus, for the coal feed particle size distribution, the best fit can be obtained from

$$Y = AR^B , \quad (5.47)$$

Table 5.7. Input parameters for combustion code

Variable name	Value	Definition
RHOSB	2.6	Sorbent density, g/cm ³
RHOA	3.0	Coal ash density, g/cm ³
RHOC	1.3	Char density, g/cm ³
RHOG	0.00032	Flue gas density, g/cm ³
MU	0.00045	Viscosity of gas, g/(cm-s)
EMF	0.4	Voidage at minimum fluidization, dimensionless
AXS	33445.1	Bed cross-sectional area, cm ²
DT	182.9	Bed diameter, cm
DM	0.1487	Mean particle diameter in bed, cm
FRSB	0.94	Weight fraction sorbent in bed, dimensionless
UO	243.7	Superficial velocity, cm/s
HF	121.9	Expanded bed height, cm
FCOAL	224.8	Coal feed rate, g/s
FCH20	0.95	Weight fraction of dry coal, dimensionless
NCH	8	Number of values of coal feed size distribution input, dimensionless
DCH	α	Feed coal particle diameter, μm
YCH	α	Size distribution of coal feed, dimensionless
RCHMIN	20	Minimum radius of char particle in bed, μm
RCHMAX	2400	Maximum radius of char particle in bed, μm
XCHI	20	Value of ΔR used in the numerical integration of Eq. (5.45), μm
Y(1)	2.3×10^{-6}	Initial value of O ₂ concentration, g-mol/cm ³

^aSee Table 5.8.

Table 5.8. Size distribution of feed coal

Particle diameter (μm)	Weight fraction of solids passing through
4750	0.982
2380	0.633
1190	0.377
595	0.211
297	0.115
149	0.062
74	0.030
44	0.016

Fig. 5.6. Feed coal particle size distribution.

where Y is the mass fraction passing through the screen, A, B are constants, and R is the particle radius. The curve-fitting procedure is done automatically by the code.

Figure 5.7 shows the overall computational scheme of the code. Initial char bed weight and size distribution are assumed. These quantities are used to integrate the differential balances in Tables 5.5 and 5.6 from the distributor plate to the bed surface, which is done by starting with a control volume ($\Delta V = A_{xs} \Delta Z$) at the distributor plate ($Z = 0$). The total rate of carbon consumption due to all char particles in the control volume ($\Delta V = A_{xs} \Delta Z$) is found. The bubble velocity in ΔV is determined and used to establish whether the bubble is fast or slow. Depending on the nature of the bubble, the differential balances in Table 5.5 or 5.6 are solved by using a Runge-Kutta numerical procedure.

Fig. 5.7. Combustion code flow diagram.

The bed height is incremented ($Z_n = Z_n + \Delta Z$), and the calculation is repeated until the surface of the bed is reached. When this occurs, the gas side material balance is considered closed for an assumed char bed mass and particle size distribution. Also, the rate of shrinkage of the char particle due to combustion is known. This rate is then used in routine COMBX to determine a new char bed mass and size distribution.

The logic diagram of routine COMBX is shown in Fig. 5.8. In this routine Eqs. (5.43), (5.45), and (5.46) are solved simultaneously to close the char side material balance. Specifically, starting at the maximum particle radius $R_{\max}$ in the feed, the bed differential particle size distribution $p_B(R)$ is determined by solving Eq. (5.45) at specified intervals between $R_{\max}$ and the minimum particle radius $R_{\min}$ in the bed. The initial boundary condition is that the differential particle size distribution at the maximum radius $R_{\max}$ is zero. Since all particles are undergoing a size reduction, this assumption would appear to be reasonable. The values of $p_B(R)$ are then integrated between the maximum and minimum radii. By definition, this quantity should have a value of 1. If this is not the case, the char bed mass W_B is varied until Eq. (5.46) is satisfied. If the above condition is met, the total overflow rate F_2 is calculated via Eq. (5.43). At this point the char particle side balance is considered closed. The char bed mass determined by routine COMBX is compared with the value used in the gas side balance. If they agree within tolerance, the computation is stopped. At this point both the gas side and particle side balances are considered to be closed, and the following quantities are known:

1. char bed mass, W_{bed} ,
2. differential bed size distribution, $p_B(R)$,
3. char elutriated solids, F_2 ,
4. differential elutriated solids size distribution, $p_2(R)$,
5. for slow-bubble region — gas concentration profiles, $C_{O_2}^{\text{SB}}$, C_{CO}^{SB} , and $C_{CO_2}^{\text{SB}}$, and
6. for fast-bubble region — bubble phase gas concentration profiles, $C_{O_2}^{\text{BUB}}$, C_{CO}^{BUB} , and $C_{CO_2}^{\text{BUB}}$; emulsion phase gas concentration profiles, $C_{O_2}^{\text{EMUL}}$, C_{CO}^{EMUL} , and $C_{CO_2}^{\text{EMUL}}$.

Fig. 5.8. Flow diagram for routine COMBX.

The underflow F_1 is assumed at present to be zero. Table 5.9 and Fig. 5.9 give typical results from this code.

5.4 Results and Discussion

Here the results from the combustion subcode are compared with data obtained from the B&W/EPRI 183- by 183-cm (6- by 6-ft) AFBC. Only a limited comparison of the model results is given. More extensive comparisons are planned during the next year.

The output from the combustion subcode is shown in Table 5.9 and Figs. 5.9 and 5.10. These results were obtained with the input data given in Table 5.7. Table 5.9 gives a preliminary comparison of the model results with B&W experimental results. The char elutriation rate F_2 predicted by the code exceeds the measured value by 31%. Three possible reasons may exist for this discrepancy. First, the current code does not determine the amount of carbon consumed in the freeboard section of the AFBC. Second, the freeboard cooling may cause larger char particles to disengage from the flue gas and fall back into the bed. This increases the residence time of the char particle in the bed and results in improved combustion efficiency. Third, the elutriation constant calculated from Wen-Hashinger's correlation may not be accurate. This correlation was developed for coal beds at conditions different from

Table 5.9. Comparison of combustion subcode results with B&W data

Quantity	Variable name	ORNL	B&W
Char bed mass	WB	22745.3 g (50.11 lb _m)	NA
Char mass, % in bed	PCB	0.7	NA
Char elutriation rate	F2	19.2 g/s (152.4 lb _m /h)	14.6 g/s (116.1 lb _m /h)
Char underflow rate	F1	0.0 g/s	0.06 g/s (0.5 lb _m /h)
Combustion efficiency, %	ETC	91.5	93.0

Fig. 5.9. Calculated gas phase profiles.

typical AFBCs. This table also shows that the assumption of no char underflow is justified due to the very small underflow rate measured by B&W. As can be seen, the predicted and measured values of the combustion efficiencies agree within 1.5%. Figure 5.9 shows the predicted emulsion and bubble phase concentration profiles for O₂, CO, and CO₂ in the bed. The differences in the emulsion and bubble phase concentrations shown in this figure are due to the nature of the fast bubbles. In fast bubbles the gas is essentially trapped and is only transferred to or from the emulsion phase by "pseudo diffusional" mass transfer. In the slow-bubble region (~ 10 cm), since the gas is assumed to move in a uniform front (plug flow), no concentration difference is observed between the bubble and emulsion phases. At present very little experimental data are available for comparison with the computational results. It is hoped that

Fig. 5.10. Predicted bubble diameters as a function of height.

more data will become available in the future. Figure 5.10 shows the calculated average bubble size as a function of height. Again little data are available to prove or disprove results shown in this figure. Large bubbles have indeed been observed by a number of investigators (Cranfield and Geldart 1974, Botton 1966, and Matsen 1973).

5.5 Recommendations for Future Work

The main uncertainties that need to be resolved in the modeling of coal combustion in FBCs are

- the nature and rate of the devolatilization process,
- intrinsic rates of char combustion reactions,
- effects of bubble properties on the mixing and diffusion processes in the bed, and
- carbon loading in the bed and in the freeboard.

These phenomena are not well understood, particularly in large FBCs. Basic experimental and analytical studies are required to formulate better predictive tools. Specifically, experiments should be performed in an entrained tubular reactor to characterize devolatilization and char combustion. This reactor is envisioned as being a hollow tube enclosed in a furnace through which coal particles are blown. Basic kinetic data can be obtained relatively easily from gas concentration profiles and particle residence in the tube. A wide variety of coals can also be studied in these experiments. The information can then be coupled with the bed hydrodynamics.

Another critical area where experimental data are lacking is bubble properties (bubble size, bubble frequency, bubble velocity, gas interchange coefficient, etc.). For application in AFBC modeling, the data should be obtained for large particles and high superficial velocities in a reactor of reasonable dimensions with multiple feed points. Ideally, the data should be obtained in hot beds. However, at present there are no techniques known for such measurements in hot beds. Measurements can be made in cold beds. From the latter, quantitative trends can be established about the nature of bubble growth, gas interchange, solids mixing, and bed expansion in large beds.

5.6 Summary

Many parameters (operational and geometric) affect the heat release and coal utilization in an AFBC. The main purpose of a combustion model is to predict the amount of coal consumed in an AFBC for a given set of conditions.

The combustion subcode calculates the combustion efficiency (coal utilization) of the AFBC and the gas concentration profiles (O_2 , CO , and CO_2) in the bed. A two-phase (bubble and emulsion) bubbling bed model with gas interchange between the bubble phase and the emulsion phase is the basis of the subcode. Bubble properties (speed, diameter, fraction, etc.) in the AFBC are calculated from the bubble-growth subcode. The solids in the emulsion phase are considered to be well mixed, and the voidage of the emulsion phase is the voidage at minimum fluidization. The gas

is assumed to flow through the emulsion phase in plug flow, with its velocity corresponding to the minimum fluidization velocity.

The reactions considered in the emulsion phase are

1. $C + 0.5O_2 \rightarrow CO$,
2. $CO + 0.5O_2 \rightarrow CO_2$,
3. $CO_2 + C \rightarrow 2CO$, and
4. devolatilization of coal.

The devolatilization reaction is assumed to occur uniformly throughout the emulsion phase. For the prediction of the amount of carbon in the volatiles released, the pyrolysis models of Suuberg, Peters, and Howard (1977) and Reklaitis et al. (1977) developed for Montana lignite coal and Illinois No. 6 bituminous coal, respectively, are used. The carbon released during devolatilization is assumed to form carbon monoxide instantaneously. Carbon monoxide is then consumed by reaction 2. The resulting char is consumed by reactions 1 and 3. The reaction rate expressions are given in Table 5.4 [Eqs. (5.12) through (5.19)]. The particle surface temperature is calculated from a heat balance between the particle and the surrounding gas [Eq. (5.11)].

In addition to the emulsion phase, the bubble phase is also considered in the subcode. The bubbles are assumed to have a very thin cloud and are devoid of solids. The only reaction occurring in the bubble phase is the combustion of carbon monoxide (reaction 2). The gas interchange coefficient between the bubble phase and the emulsion phase is estimated from Eq. (5.20). The bubble phase also contains slow and fast bubbles. The elutriation rate constant for char is estimated from Eq. (5.21).

The gas side material balance equations are written for the slow-bubble region [Eqs. (5.26) through (5.28)] and the fast-bubble region [Eqs. (5.29) through (5.40)]. The differential char material balance is given by Eqs. (5.44) through (5.46). Attrition of char is not considered in the subcode. The size distribution of the feed is determined from a curve fit of the given feed size distribution. The computational scheme is shown in Figs. 5.7 and 5.8.

The output from the combustion subcode contains char bed weight and percentage of the total bed weight, char elutriation rate, char underflow

rate, and combustion efficiency. In addition, the output contains the gas profiles (O_2 , CO, and CO_2) in the bubble phase and the emulsion phase. Comparison of the model predictions with experimental data is limited since very little experimental data are available at this time. A preliminary comparison with data from the B&W/EPRI system shows that the predicted combustion efficiency is within 1.6% and that the char elutriation rate exceeds the measured value by 31%. The inaccuracy of the elutriation rate expression and the fact that freeboard reactions are neglected in the subcode could explain the disagreement in the char elutriation rate.

6. ORNL OVERALL SYSTEM CODE

6.1 Background

The purpose of an overall system code is to predict performance trends in AFBC systems for different operating conditions and equipment configurations. This information can be used to formulate the best operating conditions and configuration for a proposed AFBC plant.

Section 6.2 describes the initial effort by ORNL staff to develop a computer code to perform the overall material and energy balance for the coal side of an AFBC.

This code was originally developed to analyze the proposed design of the DOE CTIU at Morgantown, West Virginia. Because the code was written in the English Engineering System (EES) of units, the EES units are used throughout this section. The CTIU design called for multiple heat exchanger equipment arrangements and multiple design operating conditions. To simulate the CTIU, a flexible system code was developed, which was written in sections (subroutines) that simulate equipment configurations commonly used on the coal side of an AFBC. The modular nature of the code permits computation of the coal side energy and material balances for many AFBC configurations. At present this code does not incorporate the bubble-growth code, the elutriation and attrition code, or the combustion code given in Chaps. 3, 4, and 5, respectively. In order to predict the performance of the system, several assumptions are made. These are given and discussed below, along with the input required and a description of the overall code structure. Typical temperature profiles in the system and a system material balance obtained from the code are also presented. During the next year, this code will be extensively modified. Specifically, the material balance (performance) will be calculated after incorporation of the predictive codes developed during this year. In addition, a sulfur capture model will also be developed and included in the code.

6.2 Model Development

The existing ORNL AFBC system code completes the material and energy balance for the coal side of an AFBC and calculates the compositions, mass flow rates, and temperatures of all unknown process streams. This information is then used to establish the tube bundle and waterwall heat duties and the flue gas temperature profile. Since predictive kinetic expressions were not used in this code, many necessary assumptions about performance of the bed are made.

6.2.1 Assumptions

In all regions of the AFBC, (1) the process is assumed to be steady state, (2) the ideal gas law is assumed to apply (no enthalpy correction), and the (3) system is assumed to be adiabatic (no heat loss).

In this code the AFBC main cell is divided into the (1) plenum, (2) bed, (3) less-dense phase (LDP), (4) freeboard, and (5) freeboard bundle (see Fig. 6.1). These sections represent operations or phenomena that are known to occur on the coal side of a typical AFBC. The following sections describe these regions.

6.2.1.1 Plenum. The plenum (sometimes called the wind box) is the region before the distributor plate. Its function is to allow the incoming air velocity to become uniform before entering the bottom of the distributor plate, hence giving uniform fluidization throughout the bed. No chemical reactions occur in the plenum, but heat transfer may occur if waterwalls are present. The program can handle plenums with or without waterwalls. If waterwalls are present, the air is assumed to enter at the temperature at which it leaves the air preheater. The working fluid in the waterwall tubes is assumed to be a saturated liquid flowing via natural convection. The plenum is segmented perpendicular to the direction of flow, and the heat transfer characteristics (surface area) are input for each segment. Material and energy balances are performed to determine the final temperature of the air leaving each segment in the plenum. This determination is done by subroutine NOGEN. The final temperature of the air leaving the plenum is the air temperature entering the bed.

Fig. 6.1. Schematic showing breakdown of AFBC cell into input indexes.

6.2.1.2 Bed. The bed is the dense region above the distributor plate and is characterized as having bubbles of gas passing through a gas-solids emulsion phase. The height of the bed is a function of design and operating conditions. The processes occurring here are elutriation of solids, combustion of carbon and carbon monoxide, calcination of limestone, and SO_2 absorption. Because very few data and quantitative expressions exist to predict these phenomena over a range of design and operating conditions in an FBC, this model, at present, does not incorporate the kinetics of combustion and absorption of SO_2 , nor does it include correlations for calculating the amount of elutriated solids from the bed. To complete the material balance, these processes have to be quantified and certain assumptions made. In the main cell bed, the

following reactions are assumed to represent the processes of combustion, limestone calcination, and sulfur dioxide capture.

1. Combustion:

2. Calcination of limestone:

3. Capture of sulfur dioxide:

The extent of these reactions is set by the following assumptions.
For the combustion reaction:

1. The carbon consumed in the total cell is assumed to be 90%. (Note part of this carbon is consumed in the bed and part in the LDP.)
2. The elemental hydrogen, oxygen, sulfur, nitrogen, and chlorine in the coal are depleted at the same rate as the carbon.
3. Eighty-five percent of the heat is assumed to be released in the bed, based on data obtained from Pope, Evans, and Robins (as cited by Fleischman 1978).
4. In addition, a molar ratio of carbon monoxide to carbon dioxide in the gas leaving the bed is set at 0.29. This value was chosen because it results in a molar flue gas composition of carbon monoxide between 2 and 3%. This level has been predicted by various models (Beer 1978) as the molar composition of the flue gas leaving the bed.

5. The NO_x formation in the combustion process is calculated from the correlation developed by EPRI (1976):

$$\text{NO}_x = (0.28 \times 10^6)(1 + 1.7 \times N)K,$$

where

$$K = 2.19038 \times 10^{-27}(T^{7.23}),$$

T = temperature, °F,

N = nitrogen content of flue gas, wt %,

NO_x = NO_x volume, ppm.

6. The calcination of the limestone is assumed to occur very rapidly and to go to completion.
7. The SO_2 absorption is also assumed to occur in the bed, and the extent of this reaction is set as 85% in the program. This assumption is based on results obtained from the Westinghouse sulfur capture model reported by Henschel (1978).

To estimate the solids elutriated from the bed, three assumptions are made: (1) the composition of the elutriated solids is assumed, (2) the weight ratio of elutriated calcium sulfate to the other elutriated limestone solids is set, and (3) the fraction of the coal ash elutriated is assumed. Based on these assumptions, the amount of solids entrained in the flue gas is found. This is assumed to be constant from the surface of the bed to the outlet of the cell. The only additional assumption required is that the operating temperature of the bed be fixed and known. A material balance is then completed about the main cell bed under the above assumptions. The constraint of an energy balance is also imposed simultaneously, and the heat duty of the water-walls and submerged tube bundle in the bed is determined by calling routines MFBC, BEDBAL, and BED, which are described later.

6.2.1.3 Less-dense phase. The LDP region, just above the level of the bed, has a high particulate loading due to solids elutriated from the bed. Also experimental observation shows a significant amount of

heat released, perhaps due to the combustion of carbon monoxide in this region. Again, little information exists on this region and its behavior, and assumptions are made to close the material and energy balances about the LDP. First, the height of the LDP is assumed to be 4 ft above the bed level for both the carbon burnup cell (CBC) and the main cells. Also, the amount of energy released in this region is assumed to be 15% of the total energy released in the cell, and, finally, the flow of solids is assumed to be the same as that leaving the cell except for the component reacting in the LDP.

Based on these assumptions and the specified heat transfer characteristics of the LDP, a material and energy balance for the LDP is closed by calling routine LDP.

6.2.1.4 Freeboard. The freeboard is a section of the cell above the LDP that has no tube bundles but usually has waterwalls. The only assumptions are that no chemical reactions occur (no heat released) in this section and that solids and gas pass straight through (i.e., there is no disentrainment of solids). Based on these assumptions and the specified heat transfer characteristics, the material and energy balances are closed. In the overall code, this region is simulated by subroutine NOGEN.

6.2.1.5 Freeboard bundle. This section of the cell, defined as the space above the freeboard, has both a tube bundle and waterwalls. Again, the assumptions are that no chemical reactions occur (no heat released) and that solids and gas pass straight through (i.e., there is no disentrainment of solids). Based on these assumptions and the specified heat transfer characteristics, the material and energy balances are closed. Here, heat is being absorbed by both the waterwalls and the bundle. The calculations are performed by subroutine BUND, which completes the material and energy balances and calculates the temperature of the flue gas leaving the bundle.

6.3 Code Input-Output and Overall Structure

Based on the above assumptions, a code was developed to perform the system material and energy balance. The input variables used to specify

bed performance are given in Tables 6.1 to 6.4, with typical values. In addition, the geometries of the heat transfer surfaces are read into the program by dividing the AFBC into several horizontal sections (Fig. 6.1) and assigning an index to each section. For each index, the total heat transfer area of each of the walls, and the inside and outside surface area per unit length of the heat transfer tubes are read in. Table 6.5 gives these parameters and typical values.

The overall flow diagram is shown in Fig. 6.2. Appropriate inputs are used to calculate a material balance about the cell based on 100 lb of run-of-the-mine (ROM) coal fed to the cell. Next, the inlet temperature of the air leaving the air preheater and entering the cell is assumed. The intermediate steam temperatures between the superheater bundles are also assumed. Based on the actual coal feed rate, the material balance developed for 100 lb of ROM coal is used to generate streams entering

Table 6.1. Typical input data supplied by user

Variable	Typical value	Definition
TYPE	Pittsburgh No. 8	Name of coal
STONE	TVA limestone	Name of limestone
UCCOAL	Table 6.2	Composition of run-of-the-mine coal
UCLST	Table 6.3	Composition of limestone
RCATS	6.0	Molar ratio of calcium to sulfur
EEXO2	0.18	Excess air (fractional)
FSO2ES	0.09	Fraction of sulfur escaping
RH	60.0	Relative humidity, %
VPW	0.507	Water vapor pressure, psia
PSTAT	15	Static pressure, psia
ESOLC	Table 6.4	Composition of the elutriated solids
FCEL	0.07	Fraction of carbon elutriated
RACASCA	0.555	Ratio of CaSO_4 to other limestone solids
FC1	0.95	Fractional split across main cell cyclone
CINTP	120	Inlet coal temperature, °F
AINTP	120	Inlet air temperature, °F
SINTP	120	Inlet limestone temperature, °F
FGTP	730	Initial guess of fuel gas temperature leaving cell, °F
STKTP	1550	Main cell spent solids temperature, °F
PRESS	15	System pressure, psia
V	28	Percent volatile of the coal
FASH	1.00	Fraction ash elutriated
FLDP	0.15	Fraction heat release in less-dense phase

Table 6.2. Composition of
Pittsburgh No. 8 coal feed^a

Composition	Weight (%)
Carbon	71.2
Hydrogen	5.1
Oxygen	6.3
Sulfur	4.3
Nitrogen	1.3
Chlorine	0
Ash	8.5
Water	3.3

^aRun-of-the-mine coal.Table 6.3. Composition of TVA
limestone feed^a

Composition	Weight (%)
CaCO ₃	76.5
Fe ₂ (CO ₃) ₃	0.0
MgCO ₃	4.1
Al ₂ O ₃	0.0
SiO ₂	0.0
UND	19.4

^aMolar ratio of calcium to
sulfur = 3.0.

and leaving the cell. Starting with the plenum, subroutines are called that generate the flue gas temperature profile and exchanger heat duties.

The physical characteristics of the heat transfer surfaces in each section are associated with an index or a group of indexes in the input. By transferring these indexes to the appropriate subroutine, the heat duty and temperature leaving that section are found. These routines are discussed in detail in the following sections.

Based on the calculated superheater bundle duties, the intermediate steam side temperature between superheater bundles is calculated. This

Table 6.4. Composition of elutriated solids from the cell^a

Composition	Weight basis (%)
Carbon	35.0
Hydrogen	0.9
Sulfur	4.0
All other	60.1
Molar ratio of CaSO ₄ to other limestone solids elutriated from the cell	0.555

^aFraction of carbon elutriated = 7%; fraction of coal ash elutriated = 100%.

Table 6.5. Typical heat transfer geometry inputs^a

AI	1.52 (bundle) 0.796 (waterwall)	Effective inside area per tube in bundle or waterwall per unit height, in.
AO	2.00 (bundle) 1.297 (waterwall)	Effective outside area per tube in bundle per unit height, in.
DC	6.00	Diameter of fluidized bed, ft
DT	1.75	Outside tube diameter in bundle, in.
DTI	1.33	Inside tube diameter in bundle, in.
DWT2	1.52	Inside tube diameter in waterwall, in.
D2	2.00	Outside tube diameter in waterwall, in.
TD	6.00	Spacing between tubes in tube, in.
TDW2	3.00	Spacing between tubes in waterwall, in.

^aThese values must be given for each index shown in Fig. 6.1.

steam temperature profile is compared with the assumed profile. If the two do not agree within the specified tolerance, the profile is updated and control is returned to calculate the flue gas temperature profiles and heat duties. Once the tolerance is satisfied, the material and energy balances for flue gas and steam sides are closed for the assumed inlet air temperature. At this point, the solids-laden flue gas is sent to the cyclone separators, where solids are removed and solids-free flue gas is sent to air preheater. The temperature of the flue gas

Fig. 6.2. ORNL AFBC system code flow diagram.

leaving the air preheater is set by the dew point of sulfuric acid ($\approx 280^{\circ}\text{F}$). Based on this procedure, the outlet temperature of the air from the preheater is found and then compared with the assumed value. If they do not agree within the tolerance, the steam and flue gas side energy balances are again closed. When the air temperature has finally converged, both the material and energy balances are closed and the output routines are called. At this point, the computation is terminated.

Typical outputs generated from this code are shown in Figs. 6.3 and 6.4. Figure 6.3 is a summary of the overall material balance for the system, and Fig. 6.4 is a summary of the energy balance in the sections (plenum, bed, LDP, and freeboard).

6.4 Description of Routines

The major routines used in the overall simulation can be broken down as follows:

- control routines,
- material balance routines,

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Fig. 6.3. Typical overall AFBC material balance results.

**** ENERGY AND TEMPERATURE PROFILES ****

*** FOR MAIN CELL A ***

PLENUM SECTION

INDEX	HEAT TRANSFER COEFFICIENT BTU/HR-DEG F.-FT2	WATERWALL SURFACE AREA FT2	TEMPERATURE PROFILE DEG. FAHR.
*****	*****	*****	*****
1	2.126	15.56C	500.75C
2	2.126	15.56C	500.65C
3	2.126	15.56C	500.55C
4	2.126	15.56C	500.45C
5	2.126	15.56C	500.35C

TOTAL ENERGY ABSORBED BY WATERWALLS (BTU/HR) - 3487.083

CELL BED

TEMPERATURE OF BED IN DEG. FAHR. - 1550.000
 FRACTION OF TOTAL ENERGY RELEASED IN BED - 0.450
 TOTAL WATERWALL AREA IN BED (FT2) - 62.240
 WATERWALL HEAT TRANSFER COEF. (BTU/HR-FT2-DEG F) - 40.689
 TOTAL WATERWALL HEAT DUTY IN BED (BTU/HR) - 2739*26.000
 TUBE BUNDLE HEAT TRANSFER COEF. (BTU/HR-FT2-DEG F) - 49.304
 TOTAL SUBMERGED TUBE BUNDLE HEAT DUTY (BTU/HR) - 12046454.000

LESS DENSE PHASE (LDP) OF CELL

HEIGHT OF LESS DENSE PHASE (FT) - 4.000
 FRACTION OF ENERGY RELEASED IN LDP - 0.150
 TOTAL WATERWALL AREA IN LDP (FT2) - 62.240
 WATERWALL HEAT TRANSFER COEF. (BTU/HR-FT2-DEG F) - 13.500
 TEMPERATURE OF FLUE GAS LEAVING LDP - 1496.373
 TOTAL WATERWALL HEAT DUTY IN LDP - 103782.688

FREESPACE ABOVE LESS DENSE PHASE (LDP)

INDEX	HEAT TRANSFER COEFFICIENT BTU/HR-DEG F.-FT2	WATERWALL SURFACE AREA FT2	TEMPERATURE PROFILE DEG. FAHR.
*****	*****	*****	*****
1	8.423	7.780	1886.048
2	8.370	17.180	1865.072
3	8.227	22.840	1837.440

TOTAL ENERGY ABSORBED BY WATERWALLS (BTU/HR) - 5503*3.750

BUNDLE 2 IN CELL

TYPE OF BUNDLE - BILIER
 INLET FLUE GAS TEMP. (DEG. F) - 1837.460
 OUTLET FLUE GAS TEMP. (DEG. F) - 966.623
 BUNDLE INLET TUBE SIDE TEMP. (DEG. F) - 527.342
 BUNDLE OUTLET TUBE SIDE TEMP. (DEG. F) - 1000.000

TOTAL TUBE BUNDLE AREA (FT2) - 828.100
 BUNDLE HEAT TRANSFER COEF. (BTU/HR-FT2-DEG. F) - 10.374
 BUNDLE HEAT DUTY (BTU/HR) - 7252598.000
 WATERWALL INLET TUBE SIDE TEMP. (DEG. F) - 480.000
 WATERWALL OUTLET TUBE SIDE TEMP. (DEG. F) - 480.000
 TOTAL WATERWALL AREA (FT2) - 91.360
 WATERWALL HEAT TRANSFER COEF. (BTU/HR-FT2-DEG F) - 5.831
 WATERWALL HEAT DUTY (BTU/HR) - 452196.688

FREESPACE SECTION ABOVE BUNDLE 2

INDEX	HEAT TRANSFER COEFFICIENT BTU/HR-DEG F.-FT2	WATERWALL SURFACE AREA FT2	TEMPERATURE PROFILE DEG. FAHR.
*****	*****	*****	*****
8	3.534	34.270	959.578

TOTAL ENERGY ABSORBED BY WATERWALLS (BTU/HR) - 59409.543

BUNDLE 1 IN CELL

TYPE OF BUNDLE - BILIER
 INLET FLUE GAS TEMP. (DEG. F) - 959.578
 OUTLET FLUE GAS TEMP. (DEG. F) - 681.853
 BUNDLE INLET TUBE SIDE TEMP. (DEG. F) - 480.000
 BUNDLE OUTLET TUBE SIDE TEMP. (DEG. F) - 480.000
 TOTAL TUBE BUNDLE AREA (FT2) - 828.100
 BUNDLE HEAT TRANSFER COEF. (BTU/HR-FT2-DEG. F) - 8.295
 BUNDLE HEAT DUTY (BTU/HR) - 2204611.000
 WATERWALL INLET TUBE SIDE TEMP. (DEG. F) - 480.000
 WATERWALL OUTLET TUBE SIDE TEMP. (DEG. F) - 480.000
 TOTAL WATERWALL AREA (FT2) - 91.360
 WATERWALL HEAT TRANSFER COEF. (BTU/HR-FT2-DEG F) - 3.098
 WATERWALL HEAT DUTY (BTU/HR) - 90826.125

FREESPACE ABOVE BUNDLE 1 IN CELL

INDEX	HEAT TRANSFER COEFFICIENT BTU/HR-DEG F.-FT2	WATERWALL SURFACE AREA FT2	TEMPERATURE PROFILE DEG. FAHR.
*****	*****	*****	*****
13	3.263	187.180	667.198
14	3.222	45.180	663.768
15	3.222	45.180	660.410
16	3.112	45.180	657.122
17	3.102	45.180	653.503
18	3.053	45.180	650.750
19	3.023	45.180	647.661
20	3.074	45.180	644.638
21	3.165	45.180	641.677
22	3.156	45.180	638.775
23	3.146	45.180	635.929
24	3.140	45.180	633.141
25	3.131	45.180	630.409
26	3.124	45.180	627.734
27	3.114	45.180	625.111
28	3.110	29.870	623.497
29	3.802	61.650	620.117

TOTAL ENERGY ABSORBED BY WATERWALLS (BTU/HR) - 497615.563

FINAL EXIT TEMPERATURE OF FLUE GAS FROM CELL - 620.117

Fig. 6.4. Energy and temperature profile for cell.

- energy balance routines,
- property routines, and
- output routines.

These routines are briefly discussed here, but the code listing includes extensive documentation with appropriate comment cards to explain the computational procedure and nomenclature.

6.4.1 Control routines

6.4.1.1 Routine MAIN. In this routine the input shown in Tables 6.1 to 6.4 is read in, and the subroutines required to complete the material balance based on 100 lb_m of ROM coal are called. Control is then passed to subroutine CONTL.

6.4.1.2 Subroutine CONTL. The routine extends the material balance to the actual coal feed rate to the cell and, using the index assigned to each section (plenum, bed, LDP, etc.), calls the appropriate routine necessary to complete the material and energy balances for both the steam side and the flue gas side. This routine is user-specified and must be modified for each new AFBC configuration.

6.4.2 Material balance routines

6.4.2.1 Subroutine MFBC. This routine completes the material balance on the main cell (plenum, bed, LDP, freeboard) based on the 100 lb of the ROM coal.

The input to this routine is given in Table 6.1. Based on this input, all streams entering and leaving the cell are determined. The streams considered here are the coal feed, the limestone feed, the inlet air, the spent solids withdrawn from the cell, and the flue gas leaving the cell. For 100 lb_m/h of ROM coal and the preset Ca/S ratio employed in the bed, the routine calculates the limestone feed and the inlet air requirements. The amount of spent solids withdrawn is the difference between solids fed and solids elutriated. The elutriated solids are calculated on the basis of the composition of these solids and the ratio of the calcium sulfate to other limestone-type solids (CaO, SiO₂, Al₂O₃, etc.). The output generated by the routine is as follows:

C — coal input stream per 100 lb_m of coal (vector),*
 A — air input stream per 100 lb_m of coal (vector),*
 SL — limestone input stream per 100 lb_m of coal (vector),*
 SS — spent solids stream per 100 lb_m of coal (vector),*
 GS — flue gas stream per 100 lb_m of coal (vector),*
 UCARI — molar composition of air (vector),*
 AIRMWT — air molecular weight, lb_m/lb-mol.

6.4.2.2 Subroutine BEDBAL. This routine provides the ratio for the overall material balance computed in subroutine MFBC for 100 lb_m of coal to the specified input feed rate and also calculates the composition of a hypothetical stream leaving the bed and entering the LDP. This stream composition is based on the assumed heat release and the molar ratio of CO to CO₂ in the LDP. Specifically, this stream is generated by the code, and then the heat that is released by combusting the stream is determined. If this release is the same as the assumed heat release, the subroutine is terminated; if not, a new composition is established. Input to this routine, which is either user-supplied information (Table 6.1) or information generated by subroutine MFBC, is as follows:

TCOAL — total coal feed rate,
 C — coal input stream per 100 lb_m of coal (vector),*
 A — air input stream per 100 lb_m of coal (vector),*
 SL — limestone input stream per 100 lb_m of coal (vector),*
 GS — flue gas stream per 100 lb_m of coal (vector),*
 FLDP — fraction heat release in LDP (Table 6.1),
 TBED — temperature of bed.

Output information includes the following:

TC — total coal feed stream (vector),*
 TA — total air feed stream (vector),*
 TSL — total limestone feed stream (vector),*
 TSS — total spent solids stream (vector),*
 TGS — total flue gas stream (vector),*

*The components and units of the vector streams are given in Table 6.6.

Table 6.6. Stream vector components

Subscript	Component	Unit
1	Coal elemental carbon	lb _m /h
2	Coal elemental hydrogen	lb _m /h
3	Coal elemental oxygen	lb _m /h
4	Coal elemental sulfur	lb _m /h
5	Coal elemental nitrogen	lb _m /h
6	Coal elemental chlorine	lb _m /h
7	Coal ash	lb _m /h
8	H ₂ O	lb _m /h
9	O ₂	lb _m /h
10	N ₂	lb _m /h
11	CO ₂	lb _m /h
12	SO ₂	lb _m /h
13	CaCO ₃	lb _m /h
14	Fe ₂ (CO ₃) ₃	lb _m /h
15	MgCO ₃	lb _m /h
16	Al ₂ O ₃	lb _m /h
17	SiO ₂	lb _m /h
18	Undetermined	lb _m /h
19	CaSO ₄	lb _m /h
20	CaO	lb _m /h
21	Fe ₂ O ₃	lb _m /h
22	MgO	lb _m /h
23	HCl	lb _m /h
24	NO _x	lb _m /h
25	Temperature	°F
26	Pressure	psia
27	Total pounds	lb _m /h
28	Total moles of gas	lb-mol/h
29	Standard cubic feet	scf/h
30	Actual cubic feet	acf/h
31	Molecular weight	lb _m /lb-mol

TXX — pseudo flue gas stream leaving the bed (vector),*

QRFB — total energy released in LDP.

6.4.3 Energy balance routines

6.4.3.1 Subroutine TCAL. This routine calculates the final temperature of a stream of gases and solids when a certain amount of heat is transferred to or from the stream. The procedure is iterative, and the convergence method used is the Regula-Falsi. Input to this routine is listed below:

Q — heat transfer to or from stream (Btu/h),

TT — initial temperature of stream ($^{\circ}\text{F}$),

AAA — stream being heated or cooled (vector),*

V — volatility of coal (vector),*

The output is the final temperature T_F of the stream and is found from the sensible heat equation:

$$Q = (\dot{m} C_p) (T_F - T_I) , \quad (6.1)$$

where

C_p = specific heat capacity, Btu/ $^{\circ}\text{R}\text{-lb}_m$,

$\dot{m}$ = mass flow rate, lb_m/h ,

Q = heat transfer, Btu/h,

T_F = final temperature, $^{\circ}\text{R}$,

T_I = inlet temperature, $^{\circ}\text{R}$.

6.4.3.2 Subroutine NOGEN. This routine simulates a section of the freeboard with no heat released and no tube bundle. Only waterwall tubes are present. Input is as follows:

NIP — starting index corresponding to a section of the freeboard,

N — final index corresponding to a section of the freeboard,

* See Table 6.6.

A — area of the waterwall heat transfer surface corresponding to each value of the index (vector),

X — stream components (vector),*

U — waterwall heat transfer coefficients corresponding to section NIP through N,

TI — temperature of the stream entering section NIP of the freeboard.

Output information includes the following:

TF — temperature of the stream leaving section N of the freeboard,

TSO — temperature leaving each increment of freeboard (vector),

Q — total heat transferred to the material in section NIP through N.

The process is iterative, and the convergence method is again Regula-Falsi. Specifically, the sensible heat equation and the following heat transfer design equation are solved simultaneously to determine the final temperature and heat duty of the waterwalls:

$$Q_{ww} = U_{ww} A_{ww} (\text{LMTD}) , \quad (6.2)$$

and

$$Q_{FG} = (\sum \dot{m} C_p)_{FG} (T_F - T_{I,FG}) , \quad (6.3)$$

where

A_{ww} = area of waterwall in this section, ft^2 ,

LMTD = log mean temperature difference, $^{\circ}\text{R}$,

Q_{FG} = energy given up by flue gas, Btu/h,

Q_{ww} = energy absorbed by waterwalls, Btu/h,

U_{ww} = overall heat transfer coefficient of waterwalls, $\text{Btu/h-ft}^2\text{-}^{\circ}\text{R}$.

6.4.3.3 Subroutine BED. This routine determines the heat absorbed in the waterwall section of the bed. Input includes NB, number of segments in the bed; AB, area of waterwall associated with each segment (vector);

* See Table 6.6.

and U, heat transfer coefficients in that segment (vector). Output is QBWW, total energy absorbed by the waterwalls, which is found directly from the heat transfer design equation [Eq. (6.2)].

6.4.3.4 Subroutine LDP. This routine simulates the region just above the bed level. In this region additional heat is released due to combustion of carbon and/or carbon monoxide. This program calculates the heat absorbed by the waterwalls and determines the temperature of the components leaving this region.

This routine requires the following input:

- N — number of segments in this section,
- A — area of the waterwall heat transfer surface in each segment (vector),
- X — stream leaving this region (vector),*
- Y — stream entering this region (vector),*
- U — heat transfer coefficient of each segment in this region (vector),
- Q — heat released in this region due to carbon and/or carbon monoxide combustion.

SHCO — the sensible heat of the carbon monoxide component in stream Y.

The output from this routine is TF, final temperature of the stream leaving the region, and QWW, total energy absorbed by the waterwalls in the region.

The energy liberated in this section must go to one of two places: as sensible heat of the flue gas or as energy absorbed by the waterwalls. Since a chemical reaction is occurring, the total energy released is found by assuming an outlet temperature and evaluating

$$Q_{REL} = \sum \dot{m} [C_p (T_F - T_R) + H_f]_{outlet} - \sum \dot{m} [C_p (T_I - T_R) + H_f]_{inlet} \quad (6.4)$$

where H_f is heat of formation of the components at the reference temperature of 520°R, Btu/lb_m, and T_R is reference temperature, °R. The

* See Table 6.6.

energy absorbed by the waterwalls and the gas is then found from Eqs. (6.2) and (6.3). The estimated value of the temperature is then varied until the heat release is equal to that absorbed by the waterwalls and the gas. The convergence method used is Regula-Falsi.

6.4.3.5 Subroutine BUND. This routine simulates a section of freeboard with a waterwall and a tube bundle. Heat is not released in this section.

Input to this routine includes the following:

X — stream entering the section of freeboard (vector),*
 AB — area of the bundle,
 UB — overall heat transfer coefficient of the bundle,
 NI — index assigned to the first segment in this section,
 NF — index assigned to the final segment in the section,
 TI — temperature of the gas entering the section,
 AW — area of each segment in the waterwall in the section (vector),
 UW — overall heat transfer coefficient of each segment of the waterwall in the section (vector),
 TBOUT — temperature of fluid entering or leaving bundle on the tube side.

Output of this routine includes the following:

TF — final temperature of the flue gas leaving the section,
 QB — heat duty of the bundle in the section,
 QW — heat duty of waterwall in the section,
 TF — final temperature of the gas leaving the bundle.

Energy is being absorbed by both the waterwalls and the bundle. To close the energy balance about this section, the outlet temperature is assumed and the following equations are evaluated:

$$Q_{FG} = (\sum \dot{m} C_p)_{FG} (T_F - T_I)_{FG} , \quad (6.3)$$

* See Table 6.6.

$$Q_{\omega\omega} = U_{\omega\omega} A_{\omega\omega} (\text{LMTD}) , \quad (6.2)$$

and

$$Q_{\text{bund}} = U_{\text{bund}} A_{\text{bund}} (\text{LMTD}) , \quad (6.5)$$

where A_{bund} = area of the tube bundle in the section, ft^2 , Q_{bund} = heat transfer to the bundle, Btu/h , and U_{bund} = overall heat transfer coefficient, $\text{Btu/h ft}^2 \cdot ^\circ\text{F}$. Since

$$Q_{\text{FG}} = Q_{\text{bund}} + Q_{\omega\omega} , \quad (6.6)$$

the temperature of the flue gas is varied until the energy balance Eq. (6.6) is satisfied. The convergence method is Regula-Falsi.

6.4.4 Property routines

These routines calculate either a physical or a thermodynamic property of a stream. The routines, which have been extensively documented in the code, are summarized in Table 6.7. The inputs to these routines are the stream vectors and the constants necessary to calculate the desired property. The values of the constants are given in the reference specified in the table. In addition, a property routine that can calculate the overall heat transfer coefficient was developed by M. H. Culver and is described below.

In each section of an AFBC, heat is transferred for the generation of steam. Heat transfer surfaces are located in each section (plenum, bed, LDP, freeboard, and freeboard bundle). Calculation of the surface heat duties requires the calculation of an overall heat transfer coefficient. The expressions used to calculate these quantities depend on the location (submerged or freeboard) and type of heat duty (boiling or superheating).

The overall heat transfer coefficient is evaluated by this routine. Figure 6.5 is a flow diagram of this routine. An index transferred to the code describes the type and geometry of the heat transfer equipment

Table 6.7. Property subroutines

Subroutine	Properties calculated	Reference
GASCAT	Total pounds, total moles, total standard cubic feet and actual cubic feet of gas stream	None
SOLLAT	Total pounds of solid in the stream	None
HCAL	Total energy of the stream above 25°	Smith and Van Ness, Introduction to Chemical Engineering Thermodynamics, McGraw Hill Co.
SENHT	Total sensible energy of the stream above reference temperature	Smith and Van Ness, Introduction to Chemical Engineering Thermodynamics, McGraw Hill Co.
TCON	Thermal conductivity of the gas stream	Office of Coal Research Report No. 22, Interim Report No. 7
VISC	Viscosity of the gas stream	Office of Coal Research Report No. 22, Interim Report No. 7
HCAP	Heat capacity of the gas stream	Smith and Van Ness, Introduction to Chemical Engineering Thermodynamics, McGraw Hill Co.

present. The physical properties are calculated by property routines described previously. Based on this, the appropriate equations in Tables 6.8 and 6.9 are used to calculate overall heat transfer coefficients.

The LDP is the only region of the fluidized bed that requires an assumption of the heat transfer coefficient. Here the particle concentration gradient and combustion of carbon monoxide make predictions of the radiation and convection components of the heat transfer coefficients difficult. No correlations now exist that allow prediction of this heat transfer coefficient from physical properties.

6.4.5 Output routines

The output routines used in this code are (1) BOP (bed energy balance results), (2) POP (plenum energy balance results), (3) LOP (LDP energy

Fig. 6.5. Flow diagram for subroutine HTCO.

Table 6.8. Heat transfer correlation for submerged surfaces

Horizontal tube bundle

Convection:

For particles $\geq 1000 \mu\text{m}$, L. Glicksman and N. Decker equation (Glicksman and Decker 1979)

$$h_c = (k_g/d_p)(1 - \delta) \left[9.42 + 0.042 \left(\frac{\rho_g d_p U_o}{\mu_g} \right) \text{Pr} \right]$$

For particles $< 1000 \mu\text{m}$, modified Vreedenberg equation (Louis and Tung 1977)

$$h_c = (k_g/d_p)(728)(\text{Pr})^{0.3} \left[1 - 3.44 \left(\frac{U_o \mu_g}{d_p^2 \rho_g} \right)^{1/3} \right] \left(\frac{U_o \mu_g}{d_p^2 \rho_g} \right)^{1/3} (d_p/d_t)^{2/3}$$

Radiation:

Stefan-Boltzmann equation (Kern 1950)

$$h_r = 0.173(F_f) \frac{[(T_g/100)^4 - (T_w/100)^4]}{T_g - T_w}$$

Note: All gas properties are evaluated at the film temperature.

Waterwalls

Convection:

Bartholomew and Katz equation (Bartholomew and Katz 1952)

$$h_c = C_p \rho_g U_o \frac{1.560 + \ln [(\rho_g d_p U_o / \mu_g) F_{dm}^{-2/3} - 0.012]}{-0.227 \text{Pr}^{2/3} F_{dm}^{0.42}},$$

$$\text{where } F_{dm} = [d_p^3 g \rho_g (\rho_s - \rho_g)] / \mu_g^2$$

Table 6.8 (continued)

Radiation:

Stefan-Boltzmann equation (Kern 1950)

$$h_r = 0.173(F_f) \frac{(T_g/100)^4 - (T_w/100)^4}{T_g - T_w}$$

Note: All gas properties are evaluated at the film temperature.

Table 6.9. Heat transfer correlations for freeboard surfaces

Tube bundles

Convection: Grimson correlation (McAdams 1954)

$$h_c = (k_g/d_t)(0.542) \left(\frac{d_{tG_{\max}}}{\mu_g} \right)^{0.568} (Pr)^{1/3}$$

Radiation: Stefan-Boltzmann equation (Kern 1950)

$$h_r = 0.173(F_f) \frac{e_g (T_g/100)^4 - e_w (T_w/100)^4}{T_g - T_w}$$

Waterwalls

Convection: Sieder-Tate equation (Brown and Associates 1966)

$$h_c = (k_g/D_t)(0.023) \left(\frac{D_t U_o \rho_g}{\mu_g} \right)^{0.8} (Pr)^{1/3} (\mu_g/\mu_w)^{0.14}$$

Radiation: Same as in tube bundle

Note: Gas properties are evaluated at the film temperature for tube bundles and at the gas bulk temperature for waterwalls.

balance results), and (4) HOP (freeboard convection section energy balance results). When called, these routines print the headings and the calculated values generated by the code. A typical printout from these routines is shown in Fig. 6.4.

6.5 Results

Typical material balance results for a multicell AFBC are shown in Fig. 6.3, where the results generated by the code are shown in boxes. This balance was completed based on the input data given in Table 6.1. Figure 6.4 shows the energy and temperature profile generated by the code for the main cell, specifically, the temperature profile through each segment of the cell (plenum, bed, LDP, freeboard, and convective bundle). Calculated overall heat transfer coefficients and heat duty for the exchange equipment (submerged and freeboard) are also given. At present, this code has not been used to predict any of TVA's proposed AFBCs.

6.6 Recommendation for Future Work

As can be seen, the current code can simulate many different AFBC configurations, but it is not yet a predictive tool. It closes the material balance based on vendor-supplied data (Table 6.1). In the upcoming year the predictive subcodes described earlier in this report will be incorporated into the overall system code. This overall system code will then be used to analyze and improve proposed TVA AFBC designs.

6.7 Summary

The overall AFBC system code is a flexible code that can simulate the performance of the system for multiple heat exchanger equipment arrangements in the bed and various operating conditions. The code contains several computer routines to perform the material and energy balances for the steam and coal sides of the AFBC. The major routines used in the system code are

1. control routines,
2. material balance,

3. energy balance,
4. physical and thermodynamic properties, and
5. output.

The AFBC main cell is divided into the following sections:

1. plenum,
2. bed (dense region)
3. less-dense region,
4. freeboard, and
5. freeboard bundle.

These sections represent operations of phenomena that are known to occur on the coal side of a typical AFBC. Each of these sections is further divided into indexes. For each index or group of indexes, the geometry of the heat transfer surface is read in. Appropriate correlations in Tables 6.8 and 6.9 are used in the code to calculate the overall heat transfer coefficients in each segment. The material balance calculations are based on user-supplied data (Table 6.1). The energy balance and temperature profile through each segment of the cell are calculated in the code.

The system code is not yet a predictive code. It closes the material balance on user-supplied data. The predictive subcodes described in this report will eventually be integrated into the overall system code. At that point the code can be used to analyze and improve proposed AFBC designs.

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Appendix A

DERIVATION OF SLOW-BUBBLE REGION (PLUG FLOW) COMPONENT BALANCE EQUATIONS

O₂ balance

Considering a control volume $\Delta V = A_{xs} \Delta z$ in the slow-bubble region of the bed, the oxygen mass balance can be written as

$$F_{O_2}^{SB}(V) = F_{O_2}^{SB}(V + \Delta V) + D_{O_2}^{COMB} + D_{O_2}^{DEV}, \quad (A.1)$$

where

$F_{O_2}^{SB}(V)$, $F_{O_2}^{SB}(V + \Delta V)$ = molar flow rate in and out of control volume ΔV , respectively, g-mol/s,

$D_{O_2}^{COMB}$ = O₂ molar consumption rate in ΔV due to reactions 1 and 2 (see Table 5.4), g-mol/s,

$D_{O_2}^{DEV}$ = O₂ molar consumption rate due to devolatilization in ΔV , g-mol/s.

The term $D_{O_2}^{COMB}$ can be expressed as

$$D_{O_2}^{COMB} = \frac{1}{2} \sum_i^{All} R \left(R_1^T \xi_{PLUG} \right)_i (1 - \delta) \Delta V + \frac{1}{2} R_2^T \delta \Delta V, \quad (A.2)$$

where

R_1^T = rate of $C + 0.5O_2 \rightarrow CO$ reaction for a carbon particle of radius R , g-mol of carbon consumed/cm²-s,

ξ_{PLUG} = specific surface area of carbon particles with a radius between R and $R + \Delta R$ per unit volume of the bed, cm²/cm³,

δ = total void fraction of ΔV , dimensionless,

R_2^T = rate of $CO + 0.5O_2 \rightarrow CO_2$ reaction per unit volume of gas, g-mol of CO consumed/cm³.

The expressions for R_1^T and R_2^T are given in Table 5.4. The quantity ξ_{PLUG} for char particles of radius R is defined as

$$\xi_{\text{PLUG}} = \frac{3W_B^{\text{CHAR}} p_B(R) \Delta R}{\rho_{\text{CHAR}} A_{xs} L_f R (1 - \bar{\delta})}, \quad (\text{A.3})$$

where

R = radius of char particle, cm,

W_B^{CHAR} = mass of char in bed, g,

$p_B(R)$ = differential particle size distribution of radius R char in the bed, cm^{-1} ,

ρ_{CHAR} = density of char, g/cm^3 ,

$\bar{\delta}$ = average total voidage of the bed, dimensionless.

In the above expressions the terms δ and $\bar{\delta}$ represent the total void (bubble and emulsion) fraction in the control volume ΔV and the average total void fraction in the bed respectively. These quantities can be expressed as

$$\delta = \epsilon_B + (1 - \epsilon_B) \epsilon_{mf} \quad (\text{A.4})$$

and

$$\bar{\delta} = \bar{\epsilon}_B + (1 - \bar{\epsilon}_B) \epsilon_{mf}, \quad (\text{A.5})$$

where

ϵ_{mf} = void fraction at minimum fluidization, dimensionless,

ϵ_B = bubble voidage in control volume ΔV , dimensionless,

$\bar{\epsilon}_B$ = average bubble voidage of bed defined by Eq. (5.23), dimensionless.

The voidage at minimum fluidization ϵ_{mf} is assumed constant in this work. The value of ϵ_B is determined from the ORNL bubble-growth model as

$$\epsilon_B = \frac{\dot{V}_B}{u_B}, \quad (A.6)$$

where $\dot{V}_B$ is volumetric flux through the bubble phase in control volume ΔV , $\text{cm}^3/\text{cm}^2\text{-s}$, and u_B is velocity of the bubble in control volume ΔV , cm/s . The term $D_{O_2}^{\text{DEV}}$ in Eq. (A.1) is expressed as

$$D_{O_2}^{\text{DEV}} = \phi_{O_2} \frac{1 - \bar{\epsilon}_B}{1 - \bar{\delta}} (1 - \delta) \Delta V. \quad (A.7)$$

These quantities are defined by Eqs. (5.23), (5.24), (A.4), and (A.5).

If Eqs. (A.2) and (A.7) are substituted into Eq. (A.1) and the limit taken as ΔV approaches zero, the following equation results:

$$\begin{aligned} \frac{dF_{O_2}^{\text{SB}}}{dV} = & -\frac{1}{2} \sum_i^{All} R \left(R_1^T \xi_{\text{PLUG}} \right)_i (1 - \delta) - \frac{1}{2} R_2^T \delta \\ & - \phi_{O_2} \frac{(1 - \bar{\epsilon}_B)}{(1 - \bar{\delta})} (1 - \delta). \end{aligned} \quad (A.8)$$

By definition,

$$F_{O_2}^{\text{SB}} = \dot{V}_T C_{O_2}^{\text{SB}} \quad (A.9)$$

and

$$dV = A_{xs} dz, \quad (A.10)$$

where $\dot{V}_T$ is volume flow rate of gas, cm^3/s , $C_{O_2}^{\text{SB}}$ is molar concentration of O_2 , $\text{g-mol}/\text{cm}^3$, and dz is differential increment of height, cm . If constant volumetric flow rate is assumed, the differential material balance [Eq. (A.8)] becomes

$$\frac{dC_{O_2}^{SB}}{dz} = \frac{A_{xs}}{\dot{V}_T} \left[-\frac{1}{2} \sum_i^{All} R \left(R_1^T \xi_{PLUG} \right)_i (1 - \delta) - \frac{1}{2} R_2^T \delta - \phi_{O_2} \frac{(1 - \bar{\epsilon}_B)}{(1 - \bar{\delta})} (1 - \delta) \right], \quad (A.11)$$

which is the differential O_2 balance for the slow-bubble region of the bed.

CO balance

Considering a control volume $\Delta V = A_{xs} \Delta z$ in the slow-bubble region of the bed, the carbon monoxide balance can be written as

$$F_{CO}^{SB}(V) + G_{CO}^{COMB} + G_{CO}^{DEV} = F_{CO}^{SB}(V + \Delta V) + D_{CO}^{COMB}, \quad (A.12)$$

where

$F_{CO}^{SB}(V)$, $F_{CO}^{SB}(V + \Delta V)$ = molar CO flow rate in and out of control volume ΔV , g-mol/s,

G_{CO}^{COMB} = CO generation rate in ΔV due to reactions 1 and 3 (see Table 5.4), g-mol/s,

G_{CO}^{DEV} = CO generation rate in ΔV due to devolatilization, g-mol/s,

D_{CO}^{COMB} = CO consumption rate in ΔV due to reaction 2 (see Table 5.4), g-mol/s.

The term G_{CO}^{COMB} can be expressed as

$$G_{CO}^{COMB} = \left[\sum_i^{All} R \left(R_1^T \xi_{PLUG} \right)_i + 2 \sum_i^{All} R \left(R_3^T \xi_{PLUG} \right)_i \right] (1 - \delta) \Delta V, \quad (A.13)$$

where R_1^T and R_3^T are defined in Table 5.4 and ξ_{PLUG} and δ are defined by Eqs. (A.3) and (A.4), respectively. The term G_{CO}^{DEV} can be written as

$$G_{CO}^{DEV} = \phi_{CO} \frac{(1 - \bar{\epsilon}_B)}{(1 - \bar{\delta})} (1 - \delta) \Delta V, \quad (A.14)$$

where ϕ_{CO} is defined by Eq. (5.25), $\bar{\epsilon}_B$ is defined by Eq. (5.23), $\bar{\delta}$ is defined by Eq. (A.5), and δ is defined by Eq. (A.4). The term D_{CO}^{COMB} can be written as

$$D_{CO}^{COMB} = R_2^T \delta \Delta V, \quad (A.15)$$

where R_2^T is given in Table 5.4 and δ is defined by Eq. (A.4).

If Eqs. (A.13), (A.14), and (A.15) are substituted into Eq. (A.12), the resulting equation is divided by ΔV , and the limit taken as ΔV approaches zero, the following equation results:

$$\begin{aligned} \frac{dF_{CO}^{SB}}{dV} = & \left[\sum_i^{All} R \left(R_1^T \xi_{PLUG} \right)_i + 2 \sum_i^{All} R \left(R_3^T \xi_{PLUG} \right)_i \right] (1 - \delta) \\ & - R_2^T \delta + \phi_{CO} \left[\frac{(1 - \bar{\epsilon}_B)}{1 - \bar{\delta}} \right] (1 - \delta). \end{aligned} \quad (A.16)$$

Then by Eqs. (A.9) and (A.10) and the assumption of constant volumetric flow rate, Eq. (A.16) becomes

$$\begin{aligned} \frac{dC_{CO}^{SB}}{dz} = & \frac{A_{xs}}{\dot{V}_T} \left\{ \sum_i^{All} R \left(R_1^T \xi_{PLUG} \right)_i + 2 \sum_i^{All} R \left(R_3^T \xi_{PLUG} \right)_i (1 - \delta) \right. \\ & \left. - R_2^T \delta + \phi_{CO} \left[\frac{(1 - \bar{\epsilon}_B)}{(1 - \bar{\delta})} \right] (1 - \delta) \right\}, \end{aligned} \quad (A.17)$$

which is the differential CO balance for the slow-bubble region of the bed.

CO₂ balance

Considering a control volume ($\Delta V = A_{xs} \Delta z$) in the slow-bubble region of the bed, the following carbon dioxide balance can be written as

$$F_{CO_2}^{SB}(V) + G_{CO_2}^{COMB} = F_{CO_2}^{SB}(V + \Delta V) + D_{CO_2}^{COMB}, \quad (A.18)$$

where

$F_{CO_2}^{SB}(V)$, $F_{CO_2}^{SB}(V + \Delta V)$ = molar CO₂ flow rate in and out of control volume ΔV , g-mol/s,

$G_{CO_2}^{COMB}$ = CO₂ generation rate due to reaction 2 (see Table 5.4), g-mol/s,

$D_{CO_2}^{COMB}$ = CO₂ consumption rate in ΔV due to reaction 3 (see Table 5.4), g-mol/s.

The term $G_{CO_2}^{COMB}$ in Eq. (A.18) can be expressed as

$$G_{CO_2}^{COMB} = R_2^T \delta \Delta V, \quad (A.19)$$

where R_2^T is given in Table 5.4 and δ is given by Eq. (A.4). The term $D_{CO_2}^{COMB}$ can be written as

$$D_{CO_2}^{COMB} = \sum_{i=1}^{All} R_i \left(R_3^T \xi_{PLUG} \right)_i (1 - \delta) \Delta V, \quad (A.20)$$

where ξ_{PLUG} and δ are defined by Eqs. (A.3) and (A.4).

If Eqs. (A.19) and (A.20) are substituted into Eq. (A.18) and the limit evaluated as ΔV approaches zero, the following equation results:

$$\frac{dF_{CO_2}^{SB}}{dV} = R_2^T \delta - \sum_{i=1}^{All} R_i \left(R_3^T \xi_{PLUG} \right)_i (1 - \delta). \quad (A.21)$$

Then, by Eqs. (A.9) and (A.10) and the assumption of constant volumetric flow rate, Eq. (A.21) becomes

$$\frac{dC_{CO_2}^{SB}}{dz} = \frac{A_{xs}}{\dot{V}_T} \left[R_2^T \delta - \sum_i^{All} R \left(R_3^T \xi_{PLUG} \right)_i (1 - \delta) \right], \quad (A.22)$$

which is the differential CO_2 balance for the slow-bubble region of the bed.

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Appendix B

DERIVATION OF FAST-BUBBLE REGION COMPONENT BALANCES

In the fast-bubble region two separate phases, the bubble and emulsion phases as described earlier, are assumed to exist. In each phase, three balances (O_2 , CO , and CO_2) are made as follows.

Emulsion phase O_2 balance

Considering a control volume ($\Delta V = A_{xs} \Delta z$) in the fast-bubble region of the bed, the following oxygen balance for the emulsion phase can be written as

$$F_{O_2}^{EMUL}(V) + M_{O_2} = F_{O_2}^{EMUL}(V + \Delta V) + D_{O_2}^{COMB} + D_{O_2}^{DEV}, \quad (B.1)$$

where

$F_{O_2}^{EMUL}(V)$, $F_{O_2}^{EMUL}(V + \Delta V)$ = molar flow rate of O_2 in and out of emulsion phase in ΔV , g-mol/s,

M_{O_2} = molar flow rate of O_2 to the emulsion phase from bubble phase, g-mol/s,

$D_{O_2}^{COMB}$ = emulsion phase O_2 consumption rate in ΔV due to reactions 1 and 2 (see Table 5.4), g-mol/s,

$D_{O_2}^{DEV}$ = emulsion phase O_2 consumption rate due to devolatilization in ΔV , g-mol/s.

The term M_{O_2} can be expressed as

$$M_{O_2} = K_{BE} \left(C_{O_2}^{BUB} - C_{O_2}^{EMUL} \right) \epsilon_B \Delta V, \quad (B.2)$$

where

K_{BE} = bubble-emulsion phase interchange coefficient from Eq. (5.20), 1/s,

$C_{O_2}^{BUB}, C_{O_2}^{EMUL}$ = molar concentration of O_2 in bubble and emulsion phases of fast-bubble region, g-mol/cm³,

ϵ_B = bubble voidage at Δz defined by Eq. (A.6), dimensionless.

The term $D_{O_2}^{COMB}$ is defined as

$$D_{O_2}^{COMB} = \frac{1}{2} \left[\sum_i^{All} R \left(\frac{R_1^T}{R_1^T} \xi_{EMUL} \right)_i + R_2^T \epsilon_{mf} \right] (1 - \epsilon_B) \Delta V, \quad (B.3)$$

where

R_1^T, R_2^T = rates of $C + 1/2O_2 \rightarrow CO$ and $CO + 1/2O_2 \rightarrow CO_2$ for a char particle of radius R , g-mol/cm²-s,

ξ_{EMUL} = specific surface area of carbon particles with a radius between R and $R + \Delta R$ per unit volume of the emulsion phase,

ϵ_B = bubble voidage at Δz defined by Eq. (A.6), dimensionless,

ϵ_{mf} = voidage at minimum fluidization, dimensionless.

The expressions for R_1^T and R_2^T are given in Table 5.4. The term ξ_{EMUL} for char particles between R and $R + \Delta R$ is

$$\xi_{EMUL} = \frac{3W_B^{CHAR} P_B(R) \Delta R}{\rho_{CHAR}^A L_f R (1 - \bar{\epsilon}_B)}, \quad (B.4)$$

where

R = radius of char particle, cm,

W_B^{CHAR} = bed weight of char, g,

$P_B(R)$ = differential particle distribution of radius R char in the bed, 1/cm,

ρ_{CHAR} = char density, g/cm³,

$\bar{\epsilon}_B$ = average bubble voidage of bed defined by Eq. (5.23),
dimensionless.

The summation term in Eq. (B.3) represents the total amounts of carbon consumed by the carbon particles existing in control volume ΔV , and the term $D_{O_2}^{\text{DEV}}$ in Eq. (B.1) can be expressed as

$$D_{O_2}^{\text{DEV}} = \phi_{O_2} (1 - \epsilon_B) \Delta V . \quad (\text{B.5})$$

These quantities are defined by Eqs. (5.23) and (A.6).

If Eqs. (B.2), (B.3), and (B.5) are substituted into Eq. (B.1) and the limit taken as ΔV approaches zero, the following equation results:

$$\begin{aligned} \frac{dF_{O_2}^{\text{EMUL}}}{dV} = & -\frac{1}{2} \left[\sum_i^{\text{All}} R \left(R_1^T \epsilon_{\text{EMUL}} \right)_i + R_2^T \epsilon_{\text{mf}} \right] (1 - \epsilon_B) \\ & - \phi_{O_2} (1 - \epsilon_B) + K_{\text{BE}} \left(C_{O_2}^{\text{BUB}} - C_{O_2}^{\text{EMUL}} \right) \epsilon_B . \end{aligned} \quad (\text{B.6})$$

Now the term $F_{O_2}^{\text{EMUL}}$ represents the molar flow rate of O_2 in emulsion phase. Then, by definition,

$$F_{O_2}^{\text{EMUL}} = C_{O_2}^{\text{EMUL}} \dot{V}_{\text{EMUL}} , \quad (\text{B.7})$$

where $\dot{V}_{\text{EMUL}}$ is volumetric flow rate of the gas through the emulsion phase and is equal to

$$\dot{V}_{\text{EMUL}} = U_{\text{EMUL}} A_{\text{EMUL}} = U_{\text{mf}} A_{\text{xs}} (1 - \epsilon_B) = U_{\text{mf}} A_{\text{xs}} (1 - \epsilon_B) . \quad (\text{B.8})$$

Here U_{EMUL} is velocity of the gas in the interstitial spaces of the emulsion phase and A_{EMUL} is the area available for flow in the emulsion phase. Since $dV = A_{\text{xs}} dz$,

$$\begin{aligned} \frac{dF_{O_2}^{EMUL}}{dV} &= \frac{dF_{O_2}^{EMUL}}{A_{xs} dz} = U_{mf} A_{xs} \frac{d \left[(1 - \epsilon_B) C_{O_2}^{EMUL} \right]}{A_{xs} dz} \\ &= U_{mf} \left[C_{O_2}^{EMUL} \frac{d(1 - \epsilon_B)}{dz} + (1 - \epsilon_B) \frac{dC_{O_2}^{EMUL}}{dz} \right] \quad (B.9) \end{aligned}$$

Now Eq. (B.9) is solved for $dC_{O_2}^{EMUL}/dz$,

$$\frac{dC_{O_2}^{EMUL}}{dz} = \frac{1}{(1 - \epsilon_B)} \left[\frac{1}{U_{mf}} \left(\frac{dF_{O_2}^{EMUL}}{dV} \right) - C_{O_2}^{EMUL} \left(\frac{d(1 - \epsilon_B)}{dz} \right) \right], \quad (B.10)$$

where $dF_{O_2}^{EMUL}/dV$ is given by Eq. (B.6). This equation represents the differential O_2 material balance for the emulsion phase in the fast-bubble region of the bed.

Emulsion phase CO balance

Considering a control volume $\Delta V = A_{xs} \Delta z$ in the fast-bubble region of the bed, the following carbon monoxide balance for the emulsion phase can be written as

$$F_{CO}^{EMUL}(V) + G_{CO}^{COMB} + G_{CO}^{DEVOL} + M_{CO} = F_{CO}^{EMUL}(V + \Delta V) + D_{CO}^{COMB}, \quad (B.11)$$

where

$F_{CO}^{EMUL}(V)$, $F_{CO}^{EMUL}(V + \Delta V)$ = CO_2 molar flow rate in and out of the emulsion phase in ΔV , g-mol/s,

M_{CO} = molar flow rate of CO to emulsion phase from bubble phase, g-mol/s,

G_{CO}^{COMB} = emulsion phase CO generation rate in ΔV due to reactions 1 and 3 (see Table 5.4), g-mol/s,

G_{CO}^{DEV} = emulsion phase CO generation rate due to devolatilization in ΔV , g-mol/s,

D_{CO}^{COMB} = emulsion phase CO consumption rate due to reaction 2 (see Table 5.4), g-mol/s.

The term M_{CO} in the above equation is expressed as

$$M_{CO} = K_{BE} (C_{CO}^{BUB} - C_{CO}^{EMUL}) \epsilon_B \Delta V, \quad (B.12)$$

where K_{BE} and ϵ_B are defined by Eqs. (5.20) and (A.4), respectively, and C_{CO}^{BUB} and C_{CO}^{EMUL} are the molar concentrations of the CO in the bubble and emulsion phases respectively. The term G_{CO}^{COMB} is designed as

$$G_{CO}^{COMB} = \left[\sum_i^{All} R \left(R_1^T \xi_{EMUL} \right)_i + 2 \sum_i^{All} R \left(R_3^T \xi_{EMUL} \right)_i \right] \times (1 - \epsilon_B) \Delta V, \quad (B.13)$$

where ξ_{EMUL} and ϵ_B are defined by Eqs. (B.4) and (A.6), respectively, and the expressions for R_1^T and R_3^T are given in Table 5.4. The summation terms in Eq. (B.13) represent the total amount of carbon monoxide produced by the carbon particles existing in control volume ΔV . The term G_{CO}^{DEV} in Eq. (B.11) can be expressed as

$$G_{CO}^{DEV} = \phi_{CO} (1 - \epsilon_B) \Delta V, \quad (B.14)$$

where ϕ_{CO} is defined by Eq. (5.25), ϵ_B is defined by Eq. (A.4), and the term D_{CO}^{COMB} in Eq. (A.11) is defined as

$$D_{CO}^{COMB} = R_2^T \epsilon_{mf} (1 - \epsilon_B) \Delta V, \quad (B.15)$$

where R_2^T is defined in Table 5.4, ϵ_{mf} is voidage at minimum fluidization, and ϵ_B is defined by Eq. (A.6).

If Eqs. (B.12), (B.13), (B.14), and (B.15) are substituted into Eq. (B.11) and the limit taken as ΔV approaches zero, the following equation results:

$$\begin{aligned}
\frac{dF_{CO}^{EMUL}}{dV} = & \left[\sum_i^{All} R \left(R_T^1 \xi_{EMUL} \right)_i + 2 \sum_i^{All} R \left(R_T^3 \xi_{EMUL} \right)_i \right] (1 - \epsilon_B) \\
& - R_2^T \epsilon_{mf} (1 - \epsilon_B) + K_{BE} \left(C_{CO}^{BUB} - C_{CO}^{EMUL} \right) \epsilon_B \\
& + \Phi_{CO} (1 - \epsilon_B) ,
\end{aligned} \tag{B.16}$$

where F_{CO}^{EMUL} is defined as

$$F_{CO}^{EMUL} = C_{CO}^{EMUL} \dot{V}_{EMUL} .$$

Therefore, by Eq. (B.8) and $dV = A_{xs} dz$,

$$\begin{aligned}
\frac{dF_{CO}^{EMUL}}{dV} &= \frac{dF_{CO}^{EMUL}}{A_{xs} dz} = \frac{U_{mf} d \left[(1 - \epsilon_B) C_{CO}^{EMUL} \right]}{dz} \\
&= U_{mf} \left[C_{CO}^{EMUL} \frac{d(1 - \epsilon_B)}{dz} + (1 - \epsilon_B) \frac{dC_{CO}^{EMUL}}{dz} \right] .
\end{aligned} \tag{B.17}$$

Now Eq. (B.17) can be solved as

$$\frac{dC_{CO}^{EMUL}}{dz} = \frac{1}{1 - c_B} \left\{ \frac{1}{U_{mf}} \left[\frac{dF_{CO}^{EMUL}}{dV} \right] - C_{CO}^{EMUL} \left[\frac{d(1 - \epsilon_B)}{dz} \right] \right\} , \tag{B.18}$$

where dF_{CO}^{EMUL}/dV is given by Eq. (B.16). This equation represents the CO material balance for the emulsion phase in the fast-bubble region of the bed.

Emulsion phase CO₂ balance

Considering a control volume ($\Delta V = A_{xs} \Delta z$) in fast-bubble region of bed, the carbon dioxide balance for the emulsion phase can be written as

$$F_{CO_2}^{EMUL}(V) + G_{CO_2}^{COMB} + M_{CO_2} = F_{CO_2}^{EMUL}(V + \Delta V) + D_{CO_2}^{COMB}, \quad (B.19)$$

where

$F_{CO_2}^{EMUL}(V)$, $F_{CO_2}^{EMUL}(V + \Delta V)$ = CO_2 molar flow rate in and out of emulsion phase in ΔV , g-mol/s,

M_{CO_2} = CO_2 molar flow rate to the emulsion phase from the bubble phase, g-mol/s,

$G_{CO_2}^{COMB}$ = emulsion phase CO_2 generation rate in ΔV due to reaction 2 (see Table 5.4), g-mol/s,

$D_{CO_2}^{COMB}$ = emulsion phase CO_2 consumption rate in ΔV due to reaction 3 (see Table 5.4), g-mol/s.

The term M_{CO_2} in the above equation is expressed as

$$M_{CO_2} = K_{BE} \left(C_{CO_2}^{BUB} - C_{CO_2}^{EMUL} \right) \epsilon_B \Delta V, \quad (B.20)$$

where K_{BE} and ϵ_B are defined by Eqs. (5.20) and (A.4), respectively, and $C_{CO_2}^{BUB}$ and $C_{CO_2}^{EMUL}$ are the CO_2 molar concentrations in the bubble and emulsion phases respectively. The term $G_{CO_2}^{COMB}$ is defined as

$$G_{CO_2}^{COMB} = R_2^T \epsilon_{mf} (1 - \epsilon_B) \Delta V, \quad (B.21)$$

where R_2^T is defined in Table 5.4 and ϵ_B is given by Eq. (A.4). The term $D_{CO_2}^{COMB}$ in Eq. (B.19) is given as

$$D_{CO_2}^{COMB} = \sum_i^{All} R \left(R_3^T \xi_{EMUL} \right)_i (1 - \epsilon_B) \Delta V, \quad (B.22)$$

where R_3^T is given in Table 5.4, ξ_{EMUL} is defined by Eq. (B.4), and ϵ_B is given by Eq. (A.4). The summation in the above equation represents the total amount of carbon dioxide consumed by the carbon particles existing in control volume ΔV . If Eqs. (B.20), (B.21), and (B.22) are substituted

into Eq. (B.19) and the limit taken as ΔV approaches zero, the following expression results:

$$\begin{aligned} \frac{dF_{CO_2}^{EMUL}}{dV} = & R_2^T \epsilon_{mf}(1 - \epsilon_B) - \sum_i^{All} R \left(R_3^T \xi_{EMUL} \right)_i (1 - \epsilon_B) \\ & + K_{BE} \left(C_{CO_2}^{BUB} - C_{CO_2}^{EMUL} \right) \epsilon_B, \end{aligned} \quad (B.23)$$

where $F_{CO_2}^{EMUL}$ is defined as

$$F_{CO_2}^{EMUL} = C_{CO_2}^{EMUL} \dot{V}_{EMUL}.$$

Therefore, by Eq. (B.8) and $dV = A_{xs} dz$,

$$\begin{aligned} \frac{dF_{CO_2}^{EMUL}}{dV} &= \frac{dF_{CO_2}^{EMUL}}{A_{xs} dz} = U_{mf} A_{xs} \left\{ \frac{d[(1 - \epsilon_B)] C_{CO_2}^{EMUL}}{A_{xc} dz} \right\} \\ &= U_{mf} \left[C_{CO_2}^{EMUL} \frac{d(1 - \epsilon_B)}{dz} + (1 - \epsilon_B) \frac{dC_{CO_2}^{EMUL}}{dz} \right]. \end{aligned} \quad (B.24)$$

Now the above equation can be rearranged to

$$\frac{dC_{CO_2}^{EMUL}}{dz} = \frac{1}{1 - \epsilon_B} \left[\frac{1}{U_{mf}} \left(\frac{dF_{CO_2}^{EMUL}}{dV} \right) - C_{CO_2}^{EMUL} \frac{d(1 - \epsilon_B)}{dz} \right], \quad (B.25)$$

where $dF_{CO_2}^{EMUL}/dV$ is given by Eq. (B.23). This expression represents the differential CO_2 material balance for the emulsion in the fast-bubble region of the bed.

Bubble phase O₂ balance

Considering a control volume ($\Delta V = A_{xs} \Delta z$) in the fast-bubble region of the bed, the oxygen balance for the bubble phase can be written as

$$F_{O_2}^{BUB}(V) = F_{O_2}^{BUB}(V + \Delta V) + D_{O_2}^{COMB} + M_{O_2} \quad , \quad (B.26)$$

where

$F_{O_2}^{BUB}(V)$, $F_{O_2}^{BUB}(V + \Delta V)$ = O₂ molar flow rate in and out of bubble phase in ΔV , g-mol/s,

M_{O_2} = O₂ molar flow rate from the bubble phase to the emulsion phase, g-mol/s,

$D_{O_2}^{COMB}$ = O₂ molar consumption rate due to reaction 2 (see Table 5.4), g-mol/s.

The term M_{O_2} in the above is defined by Eq. (B.2). Recalling the absence of char in the bubble phase, $D_{O_2}^{COMB}$ can be written as

$$D_{O_2}^{COMB} = + \frac{1}{2} R_2^T \epsilon_B \Delta V \quad . \quad (B.27)$$

If Eqs. (B.2) and (B.27) are substituted into Eq. (B.26) and the limit taken as ΔV approaches zero, the following expression results:

$$\frac{dF_{O_2}^{BUB}}{dV} = \left[- \frac{1}{2} R_2^T \epsilon_B - K_{BE} \left(C_{O_2}^{BUB} - C_{O_2}^{EMUL} \right) \epsilon_B \right] \quad . \quad (B.28)$$

The term $F_{O_2}^{BUB}$ represents the molar flow rate of oxygen in the bubble phase. By definition,

$$F_{O_2}^{BUB} = C_{O_2}^{BUB} \dot{V}_{BUB} \quad , \quad (B.29)$$

where $\dot{V}_{BUB}$ is the volumetric flow rate of the gas through the bubble phase and can be expressed as

$$\dot{V}_{BUB} = U_{BUB} A_{BUB} = \frac{\dot{V}_B}{\cancel{A_B}} (\cancel{A_{xs}} \cancel{A_B}) = \dot{V}_B A_{xs} . \quad (B.30)$$

In this expression $\dot{V}_B$ is the volumetric flux through the bubble phase. The expression for $\dot{V}_B$ is given by Eq. (3.9) in the bubble-growth section. Since $dV = A_{xs} dz$,

$$\frac{dF_{O_2}^{BUB}}{dV} = \frac{dF_{O_2}^{BUB}}{A_{xs} dz} = \frac{\cancel{A_{xs}} d \dot{V}_B C_{O_2}^{BUB}}{\cancel{A_{xs}} dz} = \dot{V}_B \frac{dC_{O_2}^{BUB}}{dz} + C_{O_2}^{BUB} \frac{d\dot{V}_B}{dz} . \quad (B.31)$$

Now Eq. (B.31) is solved for $dC_{O_2}^{BUB}/dz$ to yield

$$\frac{dC_{O_2}^{BUB}}{dz} = \frac{1}{\dot{V}_B} \left(\frac{dF_{O_2}^{BUB}}{dV} - C_{O_2}^{BUB} \frac{d\dot{V}_B}{dz} \right) , \quad (B.32)$$

where $dF_{O_2}^{BUB}/dV$ is given by Eq. (B.28). This equation represents the differential O_2 material balance for the bubble phase in the fast-bubble region of the bed.

Bubble phase CO balance

Considering a control volume ($\Delta V = A_{xs} \Delta z$) in the fast-bubble region of the bed, the carbon monoxide balance for the phase can be written as

$$F_{CO}^{BUB}(V) = F_{CO}^{BUB}(V + \Delta V) + D_{CO}^{COMB} + M_{CO} , \quad (B.33)$$

where

$F_{CO}^{BUB}(V)$, $F_{CO}^{BUB}(V + \Delta V)$ = CO molar flow rate in and out of bubble phase in ΔV , g-mol/s,

M_{CO} = CO molar flow rate from the bubble phase to the emulsion phase, g-mol/s,

D_{CO}^{COMB} = CO molar consumption rate due to reaction 2 (see Table 5.4), g-mol/s.

The term M_{CO} in the above is defined by Eq. (B.12); D_{CO}^{COMB} can be expressed as

$$D_{CO}^{COMB} = R_2^T \epsilon_B \Delta V, \quad (B.34)$$

where R_2^T is given in Table 5.4 and ϵ_B is defined by Eq. (A.6).

If Eqs. (B.12) and (B.34) are substituted into Eq. (B.33) and the limit taken as ΔV approaches zero, the following expression results:

$$\frac{dF_{CO}^{BUB}}{dV} = -R_2^T \epsilon_B - K_{BE} \left(C_{CO}^{BUB} - C_{CO}^{EMUL} \right) \epsilon_B. \quad (B.35)$$

Next via Eq. (B.30) and definition of the control volume ($dV = A_{xs} dz$) the following is obtained:

$$\begin{aligned} \frac{dF_{CO}^{BUB}}{dV} &= \frac{dF_{CO}^{BUB}}{A_{xs} dz} = \frac{\cancel{A_{xs}} d\dot{V}_B C_{CO}^{BUB}}{\cancel{A_{xs}} dz} \\ &= \dot{V}_B \frac{dC_{CO}^{BUB}}{dz} + C_{CO}^{BUB} \frac{d\dot{V}_B}{dz}. \end{aligned} \quad (B.36)$$

Now this expression is solved for dC_{CO}^{BUB}/dz to yield

$$\frac{dC_{CO}^{BUB}}{dz} = \frac{1}{\dot{V}_B} \left(\frac{dF_{CO}^{BUB}}{dV} - C_{CO}^{BUB} \frac{d\dot{V}_B}{dz} \right), \quad (B.37)$$

where dF_{CO}^{BUB}/dV is given by Eq. (B.35). This equation represents the differential CO material balance for the bubble phase in the fast-bubble region of the bed.

Bubble phase CO₂ balance

Considering a control volume $\Delta V = A_{xs} \Delta z$ in the fast-bubble region of the bed, the carbon dioxide balance can be written as

$$F_{CO_2}^{BUB}(V) + G_{CO_2}^{COMB} = F_{CO_2}^{BUB}(V + \Delta V) + M_{CO_2}, \quad (B.38)$$

where

$F_{CO_2}^{BUB}(V)$, $F_{CO_2}^{BUB}(V + \Delta V)$ = CO_2 molar flow rate in and out of the bubble phase in ΔV , g-mol/s,

M_{CO_2} = CO_2 molar flow rate from the bubble phase to the emulsion phase, g-mol/s,

$G_{CO_2}^{COMB}$ = CO_2 molar generation rate due to reaction 2 (see Table 5.4), g-mol/s.

In this expression, the term M_{CO_2} is given by Eq. (B.20); $G_{CO_2}^{COMB}$ can be expressed as

$$G_{CO_2}^{COMB} = R_2^T \epsilon_B \Delta V, \quad (B.39)$$

where R_2^T is given by Table 5.4 and ϵ_B is given by Eq. (A.6). If Eqs. (B.20) and (B.39) are substituted into Eq. (B.38) and the limit taken as ΔV approaches zero, the following expression results:

$$\frac{dF_{CO_2}^{BUB}}{dV} = R_2^T \epsilon_B - K_{BE} \left(C_{CO_2}^{BUB} - C_{CO_2}^{EMUL} \right) \epsilon_B. \quad (B.40)$$

Next, via Eq. (B.30) and definition of the control volume ($dV = A_{xs} dz$), the following expression is obtained:

$$\begin{aligned} \frac{dF_{CO_2}^{BUB}}{dV} &= \frac{dF_{CO_2}^{BUB}}{A_{xs} dz} = \frac{\cancel{A_{xs}} d\dot{V}_B C_{CO_2}^{BUB}}{\cancel{A_{xs}} dz} \\ &= \dot{V}_B \frac{dC_{CO_2}^{BUB}}{dz} + C_{CO_2}^{BUB} \frac{d\dot{V}_B}{dz}. \end{aligned} \quad (B.41)$$

Now, solving for $dC_{CO_2}^{BUB}/dz$ yields

$$\frac{dC_{CO_2}^{BUB}}{dz} = \frac{1}{\dot{V}_B} \left(\frac{dF_{CO_2}^{BUB}}{dV} - C_{CO_2}^{BUB} \frac{d\dot{V}_B}{dz} \right), \quad (B.42)$$

where $dF_{CO_2}^{BUB}/dV$ is given by Eq. (B.40). This equation represents the differential CO_2 material balance for the bubble phase in the fast-bubble region of the bed.

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