NUMERICAL MODELING OF FLUIDIZED-BED COMBUSTOR

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MASTER

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NOMENCLATURE

A	Area as defined
a	Bubble or particle radius
a_m	Limiting bubble radius
b	Tube radius
B	Displacement factor
c_p	Specific heat at constant pressure
c	Specific heat at constant volume
C_D	Drag coefficient
C_{sr}	Interaction coefficient of particles s and r
d	Domain
D	Diffusivity
D_b	Bubble diameter
D_h	Hydraulic diameter
E	Total energy or energy of radiation
f	Field force
$\hat{f}$	Friction factor
F	Inverse relaxation time constant for momentum transfer
$\hat{F}$	Force
g	Gravitational constant
G	Inverse relaxation time constant for energy transfer
$\hat{G}$	Mass Flow
h	Specific enthalpy
$\bar{h}$	Molal enthalpy
$\hat{h}$	Heat transfer coefficient
h, h_b	Bed height
ΔH	Heat of reaction
H	Total enthalpy

NOMENCLATURE

H_{ge}	Local averaged mean curvature
I	Inertial coupling or intensity of radiation
I'	Force due to virtual mass
$\hat{j}$	j-factor for heat transfer
J	Heat flux
k	Rate constant of chemical kinetics
$\hat{k}$	Coalescence coefficient
k^*	Average coalescence coefficient
K	Effectiveness of particle-fluid momentum transfer or equilibrium constant
ℓ	Length or thickness of platelet
$\hat{L}$	Interacting length
L	Length
L	Inertial coupling of energy
L'	Work done due to apparent mass and unsteadiness of flow field
m	Mass per particle of dispersed phase
M	Inverse relaxation time constant for mass transfer or molecular weight
n	Number of terms or number of moles per unit volume or number of intervals in a computer grid
$\hat{n}$	Index of refraction
$\underline{n}$	Unit outward normal vector
N	Number density of particles (or bubbles)
N_{Im}	Impact number
Nu	Nusselt number
p	Force per unit area
P	Pressure
$\hat{P}$	Perimeter
Pr	Prandtl number
Q	Heat transfer coupling

NOMENCLATURE

q	Heat flux at wall
r	Radius
$\underline{r}, \underline{x}$	Space coordinate
r^*	Ratio of the rebound speed to incoming speed
R	Radius of a large bubble
R	Force per unit volume
Re	Reynolds number
$\dot{S}$	Velocity of interface
s	1/2 of tube spacing
$\underline{S}$	Surface of interface
Sc	Schmidt number
Sh	Sherwood number
t	Time
T	Temperature
u	Specific internal energy
U	Velocity
U^*	Characteristic flow velocity
v	Bubble volume
V	Viscous coupling
V'	Force due to unsteadiness of flow field
We	Weber number
$\underline{x}$	Space coordinate
x, y, z	Cartesian coordinates
X	Function as defined
X_0	Characteristic length of a flow passage
s, θ, ϕ	Spherical coordinates
Γ	Mass generation rate per unit volume

NOMENCLATURE

Δ	Shear strain or change in property
α	A constant or stoichiometric number of C atoms in a coal or char molecule or absorptivity
α'_m	Absorption coefficient
α_{lkw}	Accommodation coefficient of impact of lk particles with a wall
β	Number of H atoms in a coal molecule
β_d	Effectiveness of surface porosity of dolomite
γ	Eulers Constant or number of O atoms in a coal molecule
ζ	Bulk viscosity or coordinate as defined
κ	Thermal conductivity
λ	Wavelength
μ	Viscosity
μ^*	Viscosity function as defined
ν	Kinematic viscosity
ρ	Density
$\hat{\rho}$	Density excluding volume occupied by tubes
$\bar{\rho}$	Density of material
σ	Surface tension
σ_r	Stefan-Boltzmann constant of radiation
τ	Viscous stress
ϕ	Volume fraction
ϕ_s	Volume fraction of heat transfer surfaces
ψ	Stream function
Ψ, Φ	Parameters for particle-particle collision
ξ^*	Parameter for length fraction converted
Ω	Solid angle

NOMENCLATURE

Superscript

- (r) Domain (r)
 (—) Material property or molal quantities

Subscript

- a Air
 b Bubble or bulk or black body radiation
 c Char
 d' Half calcined dolomite
 d Sulfated dolomite or reference to tube diameter
 e Dense phase
 E Total energy
 f Free board
 F Fuel or coal
 g Gas
 h Enthalpy
 H Total enthalpy
 i,j Components
 ji Tensorial components
 lk Phase of each species l ($l = c, d, d', b$) and size k
 m Mixture, or limiting value, or maximum value
 mk - of phase k in the mixture
 o Carbon
 rad Radiation
 s Interface or interdomain or pipe surface
 t Tangential direction
 u Overflow pipe

NOMENCLATURE

w Wall

— Vector

x,y,z Components

λ Wavelength

Operator

∇ Gradient

$\nabla \cdot$ Divergence

$$d/dt_k = \partial/\partial t + \underline{U}_k \cdot \frac{\partial}{\partial x}$$

:

 Scalar product of tensors

$()_{,\beta}$ Surface covariant derivative

$\langle \rangle$ Average

1,... Gas components

12 Species 1-2 interaction or coalescence

ABSTRACT

Optimum design of fluidized-bed combustor requires high carbon burn-up, good sulfur retention, minimized sorbent (Ca) utilization, efficient feed distribution and mechanical layout. These parameters are strongly affected by the dynamics of the fluidized bed. The dynamic behavior of fluidized combustor is formulated in terms of multidomain - multiphase mechanics. Fluidization, bubble mechanics, coal combustion, sorbent sulfation, oxidation, solids movement and elutriation, and heat transfer are explicitly taken into account in the proposed numerical model. The model solves conservation equations of mass, momentum and energy coupled with chemical reactions as boundary value problem in space and initial value problem in time. Multi-fluid model and modified implicit multi-field numerical scheme are employed. The objective of this numerical model is for use in engineering design and scaling.

Progress to date shows that all necessary relations can be incorporated within the framework of an overall multidomain - multiphase model for deterministic computation. Provisions are made for subsequent refinements of sub-models of individual mechanism and improvements of the existing numerical model. These refinements and improvements can be achieved as better understanding of physical phenomena and more experimental data become available.

The numerical model outlined in this report is specifically designed for fluidized-bed combustor, however, it can readily be extended to various coal gasification systems.

1.0 Introduction

The basic concepts of multidomain-multiphase mechanics are readily extended to treating a fluidized bed combustion system [1]. The phases will consist of particles of coal, dolomite, gas mixture, ash, and sulfated dolomite of various sizes. The domains include the fluidized bed, the bubbles and the dilute phase in the free board. The basic interactions include momentum, mass and energy transfer and chemical reactions. By correlating and confirming the interacting parameters between the overall data of the experimental system and the results of numerical computations, the numerical model can be used to achieve an optimum design of a fluidized bed combustor.

The following four major concerns in present state-of-art of fluidized bed combustor are briefly discussed and how the proposed numerical model can aid in their resolution is also mentioned.

(a) Combustion Efficiency

To be economically competitive, fluidized bed combustors need to operate with approximately 98% combustion efficiency, measured in forms of the fuel heating value. Experience in small test work to date have shown wide variations in combustion efficiency, ranging from ~50% up to ~100%. Results from pressurized FBC at Exxon indicate that "essentially all of the combustible carbon loss was due to carbon particulates" carried off by elutriation [2]. A similar conclusion was reported from test in England [3]. Thus, it appears that the dynamics of coal/char combustion and elutriation is the determining feature in combustion efficiency. For any given feed of coal, with a spectral mix of particle sizes, sufficient residence time must be obtained to permit essentially complete combustion with less than 1/2% elutriation of coal fines. The competition between combustion reaction and elutriation is affected by solids mixing, gas phase concentration (O_2 , CO , CO_2), and elutriation mechanisms (e.g. bubble-bursts, etc).

The proposed model will permit calculation of the dynamically competing processes (combustion vs. elutriation) for any specific mix of coal feed. Parameter calculations, for varying gas flow rates, tube bundle arrangement, feed point locations, etc. would then establish optimal operating conditions for maximum combustion efficiency.

(b) Feed Distribution

Based on current practice, it has been estimated that an atmosphere pressure fluidized bed combustion plant of 500MW capacity would need some 800 coal and limestone feed points [4]. The necessity for separating and controlling large through-ports of solid granular material to these many distribution points is a problem of major complexity and cost. There is a clear engineering requirement for minimizing the number of feed points, without undue penalty in

combustor performance. The danger in too few and widely scattered feed points is that carbon distribution becomes non-uniform within the bed, resulting in carbon-rich reducing zones which could lead to both poor combustion efficiency and exaggerated corrosion problems.

Clearly, a model which can follow the diffusion of solid feed material as combustion and elutriation progress would be extremely useful in evaluating alternate feed-distribution designs.

(c) Sorbent Utilization

A prime reason for use of fluidized bed combustors is to capture sulfur within the bed. This eliminates the need for stack-gas scrubbing and most important of all, meets current EPA emission standards for SO_2 . If coal of 6-1/2% sulfur content is used as fuel, sulfur retention within the bed must be 90 percent or better. Experimental tests with limestones and dolomite as sorbent indicate wide variations in the ratio of Ca to S required to obtain the desired level of SO_2 . For example, some results [5] indicate better than 95% sulfur retention with a Ca/S molar ratio of 2, while other results [6] indicate that with as high a Ca/S molar ratio as 4, only 70% sulfur retention is obtained. It has been noted [4] that a molar of 4 requires such a high limestones usage rate that the combined problems of waste enthalpy on the "spent" sorbent and the large volume of sorbent to be handled possess "intolerable burdens" for an operating utility.

Recent fundamental studies of the sulfation process on calcined limestone indicate that the effectiveness of the limestone is strongly governed by its pore characteristics [7]. As a limestone particle reacts with SO_2 to form CaSO_4 , its surface pores gradually become plugged and lose effectiveness. Clearly then, for any given type of sorbent limestone, an optimum residence time must be found to obtain a compromise between efficiency of SO_2 capture and minimized sorbent usage. The proposed computer model can include a sub-model for the limestone sulfation process which can be adjusted to represent characteristics of specific stones. This sulfation model, together with the overall bed-dynamic model, will permit calculation of sulfur retention as a function of Ca/S feed ratio, bed residence time for the sorbent, gas superficial velocity, bed height, and other operating variables. Such information is necessary for rational management of sorbent utilization in fluidized bed combustor.

(d) Scaling

Because of complexity of the problem and non-linear nature of fluidized bed combustion systems, no simple scaling law can be found for fluidized bed applications. However, scaling is possible if and only if a comprehensive mathematical model such as proposed here representing dynamic behavior of fluidized bed combustor is formulated. This model must be validated with small scale experimental data and subsequently it can be used for scaling.

This progress report identifies the basic elements of the fluidized bed combustion system and the conservation relations. This is done via gathering of available information and research into the basic interaction. Because of the inherent complexity of the system and the meagerness of experimental data, continuing refinement and adjustment will be made as the numerical program is developed. Most important, the feasibility of numerical modeling is adequately demonstrated.

1.1 General Description

In applications of fluidized-bed combustion, the fuel (coal) is burned in a bed of solids, fluidized by combustion gas in which boiler tubes are immersed to take advantage of the high heat-transfer rates in fluidized beds. Additive, either crushed limestone or crushed dolomite, can be continuously fed to a fluidized-bed combustor to react with SO_2 . Depending on their size, the additive particles and the ash will either be elutriated from the fluidized bed while the major portion will remain in the bed [8]. Typical operating parameters may include 400 μm coal particles, 700 μm dolomite particles at 317.8 to 408.6 kg per 1000kg of coal at a bed temperature 816 to 871°C, with preheated air flowing through a porous distributor plate to sustain the fluidizing and combustion.

The bed may operate at atmospheric pressure or be pressurized as shown in Fig. 1 diagrammatically with horizontal or vertical boiler tubes (Fig. 2) [9]. A pressurized system, including a gas turbine set

Pressure: 1 - 25 atm
 Coal Size: pf - 1/4 in.
 Air Flow: 2 - 15 ft³/sec
 Temperature: 1400 - 1900 °F
 Surface: Water Walls, Horizontal,
 and Vertical Tubes
 in Bed
 Sulfur removal: $\text{CaO} + \text{SO}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{CaSO}_4$

Fig. 1. Fluidized Bed Combustion Boiler
 (Reproduced from Ref. 9)

Fig. 2. Fluidized Bed Combustion Boiler with
Vertical Steam Tubes
(Reproduced from Ref. 9)

for pressurizing and energy recovery, is shown in Fig. 3 [10]. Figure 4 shows a practical design of an atmospheric fluidized bed with boiler tubes and coal distribution system [11].

1.2 Elements of Flow System

Most of the formulations in Report ANL-CT-77-3 (March 1977) [1] are readily applicable to the fluidized bed combustor. Formulations relating to the tube bank are also readily extended from a report on multiphase flow over reactor fuel pins in preparation. Commonality is readily observed; the important thing is to recognize the differences between the fluidized bed combustor and a nuclear reactor. In the present case, the fluidized bed combustion and fluid dynamics are accounted for rigorously. This is to be followed by consistent approximations to obtain solutions demanded by the accuracy being sought.

Figure 5 shows the general behavior of a fluidized bed of particles of mixed sizes. The Cartesian coordinates are the axis of symmetry z in the direction against that of gravity with the x, y axes normal to it. Motion is generated by air entering at the bottom through the porous distributor plate. This air flow imposes upward motion of char and dolomite with simultaneous generation of gas bubbles at the plate. Combustion is maintained by reaction of char and volatile matter with air; SO_2 generated by reaction of sulfur with air is absorbed by dolomite. The heat release, change in temperature and gas composition further affect the motion in the bed. The bubbles, floating upward by buoyancy and gas motion, contribute additional agitation to the bed. As the bubbles coalesce, expand and accelerate upward, they burst at a surface at height h_b . The existence of the interface at height h_b is due to the fact that most of the particles are not ejected by the bubble burst. There are large particles recirculated with the limiting stream surface at h_b except when bubbles emerge. There are other particles which are ejected into the space above h_b , but fall back by gravity in small jet pulses; this category of particles can be represented by the limiting stream surface up to the height h for the uppermost reach of these particles. The fine ash particles are elutriated beyond h and constitute a net elutriation or background elutriation into the exhaust stream from the system.

Table 1 is an outline of domains, phases, and components to be accounted for in the computations.

Fig. 3. 140 MW-Gas-Steam Turbine System
(Reproduced from Ref. 10)

Fig. 4. End view of Coal Fired Fluidized-Bed Utility Boiler
(Reproduced from Ref. 11)

- Stream Surface:
- (a) Of Elutriated Dust
 - (b) Limit of Particle (Small) Ejected by Bursting Bubbles but Returned to Bed.
 - (c) Same as (b) For Large Particles
 - (d) Limit of Particles Not Ejected by Bubble Burst,

Fig. 5. Schematic of Fluidized-Bed Combustor Operating Characteristics

Table 1

An Outline of Domains, Phases, And Components
In Fluidized Bed Combustor

<u>Phases</u>	<u>Components</u>	<u>Moles</u>
<u>Domain: Fluidized Bed</u>		
Fresh coal	$C_{\alpha}, H_{\beta}, O_{\gamma}, N_{\delta}, S_{\epsilon}, A$	n'_o
Air	$O_2, 3.76 N_2$	n'_1, n'_8
Fresh dolomite	$CaCO_3, MgO$	n'_d
Devolatilization of coal		
Char k sizes via reaction $\rho_k, \underline{U}_k, T_k$	$C_{\alpha} S_{\epsilon} A = n_o C + n_s S + n'_o A = n_c$	
Volatile matter	$(1/2) \delta N_2, \gamma H_2O, \frac{\nu}{4n} (CH_2)$	
Comb. gas	$(\alpha = \alpha'_i - \frac{\beta}{2} + \gamma, \frac{\nu}{2} = \beta - 2\gamma)$	
Combustion gas	O_2	n_1
$\rho_g(x_j, t), \underline{U}_g(x_j, t)$	CO	n_2
$T_g(x_j, t)$	CO ₂	n_3
Conservation via individual continuity equation		
	O	n_4
	$\frac{1}{n} (CH_2)_n$	n_5
	H ₂ O	n_6
	SO ₂	n_7
	N ₂	n_8
	NO	n_9
Dolomite, half calcined ↓	CaCO ₃ · MgO	n'_d
Spent dolomite l sizes via reaction $\rho_l, \underline{U}_l, T_l$	CaSO ₄ · MgO	n_d
Bubbles m sizes	Air and gas	
growth and coalescence	Dilute phase	
$\rho_b, \underline{U}_b, T_b$		

Table 1 (Contd.)

An Outline of Domains, Phases And Components
In Fluidized Bed Combustor

<u>Phases</u>	<u>Components</u>	<u>Moles</u>
<u>Domain: Large bubbles (slugging)</u>		
Diameter = $0\frac{1}{2}$ bed diameter]		
<u>Domain: Tube bank</u>	Char, gas	
Fixed porosity	Dolomite, bubbles	
(heat sink, anisotropic resistance)		
<u>Domain: Free board</u>	Ash, gas (background)	
(surface wave, splashing, bubble burst)	Jet pulses of gas and particles due to bubble burst	
<u>Domain: True free board</u>		
(background elutriation of fines)	Fine ash, gas	

1.3 Basic Flow Configurations

Some understanding of the nature of the flow system may assist efficient programming for the numerical computation. This might be achieved by presenting some of the results of later analysis at this point.

The simplest fluidized system will consist of a pure fluid phase, a monodispersed solid phase, without elutriation, without solid removal, and without bubble formation (Appendices A and B). The stream surfaces of the phases for an axial symmetrical bed are as shown in Fig. 6(a). ψ^* is the dimensionless stream function of stream surfaces of air or fluid (dashed lines); $\psi^* = 0$ along axis of symmetry, $\psi^* = 1$ at the wall. The stream surfaces, ψ_p^* of the particles are denoted by closed solid lines since no particle is elutriated. $(\partial z / \partial x) \psi_p^* = 0$ at the top surface is a rigorous relation as shown in Appendix C. This type of recirculating flow pattern was observed by Leva [12] using salt crystals as tracer in a fluidized bed of sand with or without the presence of bubbles in the bed. Physically, the gas velocity at the wall has to be zero. This condition gives, within a distance from the wall, a region where the terminal velocity of the particles exceeds the gas velocity, causing the particles to move downward near the wall. These particles move upward away from the wall when the gas velocity exceeds the terminal velocity of the particles. A circulating motion as shown in Fig. 6(a) is thus produced.

Fig. 6(b) shows the stream surfaces with elutriation and make-up feed. The amount of solid particles transported is represented between $\psi_p^* = 0$ and $\psi_p^* = a$ outside of the $\psi_p^* = 1$ within which particles are recirculated and mixing among particles is effected by diffusion.

In real gaseous fluidized beds, bubbles tend to form at the distributor plate, floating upward by buoyancy, at the same time expanding as the hydrostatic pressure decreases (or by temperature increase or both) and increasing in size by coalescence. These bubbles tend to migrate to the center of the bed by the motion of the particles and the air (Fig. 5) [13]. The ejection of particles by bubble burst occurs producing a higher velocity than the background gas flow in the free board and produces similar mean stream surfaces of the particle phases as in Fig. 6(c) including a transition region of large particles ejected by bubble burst and falling back to the bed over the thickness of this region. This is also in addition to background flow and elutriation of fines. The agitation caused by the bubbles is the predominant mechanism for particle mixing in the bed.

Fig. 6: Basic Flow Configurations

Figure 6(d) illustrates the typical flow pattern, including a pipe for skimming the ash and spent dolomite.

Large fluidized beds with lateral dimensions much greater than bed height will display a number of recirculation zones for solids via instability of the primary recirculating pattern illustrated in Fig. 6(e). A tall bed will tend to have recirculating patterns dividing it in the vertical direction as shown in Fig 6(f).

The above idealized flow patterns merely give some physical insights of complicated flow fields in a fluidized combustor under various operating conditions. These flow patterns can be significantly perturbed by the locations of feed ports, overflow pipe and outlet of fluidized bed where elutriation may exist, the feed rates of coal, dolomite and air, operating temperature and pressure -- and etc. Simplified models such as plug flow model [14, 15] and back mixing flow model [15] have been proposed and used as basis in some investigations. It is considered here that mixing in a fluidized bed is not produced by bubble motion and agitation alone. Although this concept may be open to question [16,17], finite diffusivities have been reported for gas-fluidized [12,18] and liquid-fluidized [19] beds where bubbles did not exist. The proposed model as described in this report is based on the first principle of fluid mechanics.

Detailed data of rate mechanisms of carbon-oxygen reactions, hydrogen-oxygen reactions, hydrocarbon combustion, SO_2 , NO formations, and sulfation are incomplete on the one hand and too complicated for the scope of the present study on the other hand [20,21]. It is necessary to choose pertinent reactions and mechanisms for the temperature range of fluidized bed combustion. It is also necessary to choose between chemical kinetics controlled rate and diffusion controlled rate for the size of particles in heterogeneous reactions. Considerations may include the availability of data to facilitate the computer simulation.

2.0 Chemical Reactions

The main difference between this work and the ANL-CT-77-3 is the chemical reactions associated with combustion.

Depending on the geometry of the coal inlet, devolatilization may take different steps. In the interest of generality, we shall treat this step separately for the present. A coal is identifiable by: [22]

$$\text{C}_{\alpha}, \text{H}_{\beta}, \text{O}_{\gamma}, \text{N}_{\delta}, \text{S}_{\epsilon}, \text{A} \quad (2.1)$$

in which A denotes ash. $\bar{\rho}_F$ is the density of the coal (subscript F for fuel) which might be 1300 kg/m³. Devolatilization takes place to give

With this coal carried in as an air suspension, and heat supplied by radiation from the combustion flame, $C_{\alpha}S_{\epsilon}A$, char, ($\bar{\rho}_c = 1440 \text{ kg/m}^3$) is formed.

The last term is a hypothetical hydrocarbon including tar. As a preliminary step, we shall treat the combustion and multiphase interactions from fuel supplied as described on the right hand side of Eq. (2.2) to react with air in the presence of half calcined dolomite ($CaCO_3 \cdot MgO$). [8] Reaction Eq. (2.2) is a modified form of "rapid rate methanation" proposed for gasification [22] with CH_4 formed instead of $(CH_2)_n$. An empirical equilibrium constant was proposed based on a limited number of experiments, in terms of temperature, partial pressure of hydrogen, and coal type.

To limit the number of variables in the computer program, we assume that this devolatilization step occurs in the feed. However, the devolatilization can be incorporated readily into the proposed model when information on both the rate of devolatilization and the mechanisms become available.

2.1 Species and Kinetics

The minimum number of identifiable reactions and species (and heats of reaction ΔH are:

where k_I , k_{II} , to k_{VII} are reaction rate constants.

Other reactions which might be significant, but will have to be left for future treatment are [23]:

For instance, reactions Eqs. (2.10) and (2.11) for N and O include many more steps [24].

The change in composition via combustion with air is postulated to take the form:

Note that in the overall system, the number of moles of species in Eq. (2.13) are related by the primary conservation of atoms and calcined dolomite molecules. Available data of k and ΔH are tabulated in Table 2 with details depending on availability and reality of diffusion rate controlled reactions.

$$\left. \begin{aligned} \text{C: } n_o + n'_d + n_2 + n_3 + n_5 &= n'_o \alpha + n'_o \frac{v}{4} + n'_{do} \\ \text{O: } 2n'_d + 3n_d + 2n_1 + n_2 + 2n_3 + n_4 + n_6 + 2n_7 &= n'_o \gamma + 2n'_1 + 2n'_{do} \\ \text{H: } n_5 + n_6 &= n'_o \gamma + \frac{v}{4} n'_o \\ \text{S: } n_d + n_s + n_7 &= n'_o \epsilon \\ \text{Calcined dolomite (CaO} \cdot \text{MgO): } n_d + n'_d &= n'_{do} \\ \text{N: } n_8 &= \frac{\delta}{2} n'_o + 3.76 n'_1 \end{aligned} \right\} \quad (2.14)$$

The rate constants of reactions given in Eqs. (2.3) to (2.9) are defined by [19,26]:

$$\begin{aligned} \text{Reaction Eq. (2.3): } \quad \frac{dn_2}{dt} = \frac{dn_1}{dt} = - \frac{dn_3}{dt} = - \frac{dn_4}{dt} &= - k_I n_1 n_2 + k_{I'} n_3 n_4 \\ &= - k_I n_2 n_1 \left[1 - \frac{1}{K_I} \frac{n_3 n_4}{n_2 n_1} \right] \end{aligned} \quad (2.15)$$

$$\text{Reaction Eq. (2.4): } \quad \frac{dn_2}{dt} = \frac{dn_4}{dt} = - \frac{dn_3}{dt} = - k_{II} n_2 n_4 + k'_{II} n_3 \quad (2.16)$$

$$\text{Reaction Eq. (2.5): } \quad \sum \frac{dn_{ok}}{dt} = \frac{dn_3}{dt} = - \frac{1}{2} \frac{dn_2}{dt} = - k_{III} \sum_{ck} A_{ck}^* n_3 \quad (2.17)$$

Table 2

Reaction Rate Constants (In SI Units)
And Heats Of Reaction ($R = 1.98587 \times 10^{-3}$, T in $^{\circ}K$)

ΔH 10^6 J/kg mole		Based on kinetics	Based on Diffusion**	Ref.
- 38.39	k_I	$1.45 \times 10^6 \exp [-26.9/RT] \text{ m}^3/\text{s}$		[26]
	k'_I	$k_I/10^{(\frac{1.510 \times 10^4}{T} - 1.042)}$	m^3/s	[27]
-530.9	k_{II}	$10^5 \exp [-3.8/RT]$	m^3/s	[19]
	k'_{II}	$10^{5.3} \exp [-111/RT]$	$1/\text{s}$	[19]
174.1	k_{III}	$3.4 \times 10^6 \exp [-84/RT]$	m/s	[28]
-393.7	k_{IV}	$2.9 \times 10^7 \exp [-58/RT]$	m/s	[28]
-394.9	k_V	$4 \times 10^6 \exp [-5.79/RT]$	m^3/s	
-296.9	k_{VI}	---	$(D_o/a_c) \text{ m/s}$ (see note)	
-312.2	k_{VII}^*	---	$\frac{3(0.075 + 10^3 n_6)}{\left[1 + \frac{n'_{do} - n'_d}{2n'_d}\right] \frac{\rho'_d}{\rho_d}} \text{ m}^{5/2}/\text{s}$	[25]

Note: to obtain N_c

$$N_c \frac{4\pi}{3} a^3 \rho_{\text{char}} = \rho_{\text{char}} = n'_o [\alpha M_o + \epsilon M_s + M_A]$$

Diffusion coefficient is given by $D_o = 1.202 \times 10^{-7} \frac{\sqrt{T}}{n_1} \text{ m}^2/\text{s}$

where M is the molecular weight, subscripts o , s and A denote carbon, sulfur, and ash respectively, and a is the radius of a particle

* k_{VII} in this form actually depends on the stage of conversion or A_{dk}^* relation is given for $750^{\circ}C$ only.

**

$$\begin{array}{l} \text{Reaction} \\ \text{Eq. (2.6):} \end{array} \quad \sum \frac{dn_{ok}}{dt} = \frac{dn_1}{dt} = - \frac{dn_3}{dt} = - k_{IV} \sum A_{ck}^* n_1 \quad (2.18)$$

$$\begin{array}{l} \text{Reaction} \\ \text{Eq. (2.7):} \end{array} \quad \frac{dn_5}{dt} = \frac{dn_1}{dt} = - \frac{dn_2}{dt} = - \frac{dn_6}{dt} = - k_V n_5 n_1 \quad (2.19)$$

$$\begin{array}{l} \text{Reaction} \\ \text{Eq. (2.8):} \end{array} \quad \sum \frac{dn_{sk}}{dt} = \frac{dn_1}{dt} = - \frac{dn_7}{dt} = - k_{VI} \sum A_{sk}^* n_1 \quad (2.20)$$

$$\begin{array}{l} \text{Reaction} \\ \text{Eq. (2.9):} \end{array} \quad 2 \frac{dn_1}{dt} = \frac{dn_7}{dt} = \sum \frac{dn'_{dk}}{dt} = - \sum \frac{dn_{dk}}{dt} = - \frac{dn_3}{dt} = - k_{VII} \sum A_{dk}^* n_7 n_1^{1/2} \quad (2.21)$$

where K_I is the equilibrium constant of reaction Eq. (2.3), others have negligible reverse reaction, A_{ck}^* , A_{sk}^* , and A_{dk}^* are reference surface areas per unit volume of mixture for phase k of each species. For N_{ck} particles of char per unit volume at a given stage of burning to have n_{ok} moles of carbon per unit volume, the mass of carbon per particle (approximated by a sphere with molecular weight of carbon equal to M_o) is given by:

$$m_{ok} = n_{ok} M_o / N_{ck} = \frac{4\pi}{3} \bar{\rho}_o a_{ck}^3 \quad (2.22)$$

where $\bar{\rho}_o$ is the density of carbon. The surface area per unit volume is:

$$A_{ok}^* = N_{ck} 4\pi a_{ok}^2 = (4\pi)^{\frac{1}{3}} \frac{2}{3} \left[\frac{n_{ok} M_o}{\bar{\rho}_o} \right]^{\frac{2}{3}} N_{ck}^{\frac{1}{3}} = (4\pi)^{\frac{1}{3}} \frac{2}{3} \left(\frac{\rho_{ok}}{\rho_c} \right)^{\frac{2}{3}} N_{ck}^{\frac{1}{3}} \quad (2.23)$$

Similarly

$$A_{sk}^* = (4\pi)^{\frac{1}{3}} \frac{2}{3} \left[\frac{n_{sk} M_s}{\bar{\rho}_s} \right]^{\frac{2}{3}} N_{sk}^{\frac{1}{3}} \quad (2.24)$$

The reason for these choices is that as C and S are consumed, the available surface area could be drastically varying, depending on whether the ash (A) forms a fused globule, leaving a small surface, or forms a porous framework, giving large surface areas.

For the dolomite particles, we have

$$m_{dk} = n_{dk} M_d / N_{dk} = \frac{4\pi}{3} \bar{\rho}_d a_{dk}^3 \quad (2.25)$$

and

$$A_{dk}^* = \beta_d N_{dk} 4\pi a_{dk}^2 = \beta_d (4\pi)^{1/3} \left[\frac{n_{dk} M_d}{\bar{\rho}_d} \right]^{2/3} N_{dk}^{1/3} \quad (2.26)$$

which gives the exposed area of unsulfated dolomite. β_d is an effectiveness of surface porosity. While the choice of these characteristic areas might be made otherwise, a consistent choice will be desirable for determining the correct reaction rate from experiments.

For the convenience of derivations, it is necessary to switch between the use of mass per unit volume (density ρ_k) and moles per unit volume (concentration n_k). The conversion is summarized as follows:

$$\begin{aligned} \rho_k &= \text{mass of species or phase } k \text{ per unit volume} \\ n_k &= \text{number of moles of } k \text{ per unit volume} \\ M_k &= \text{molecular weight of } k \\ \rho_k &= n_k M_k \end{aligned} \quad (2.27)$$

For a multiphase system, a particle (or bubble) cloud has the following relations:

$$m_k = \text{mass per particle} = (4\pi/3) a_k^3 \bar{\rho}_k \quad (2.28)$$

$$N_k = \text{number of particles per unit volume}$$

$$a_k = \text{particle radius}$$

$$\bar{\rho}_k = \text{density of material constituting the particle}$$

$$\phi_k = \text{volume fraction of particles}$$

$$\rho_k = N_k m_k = \phi_k \bar{\rho}_k \quad (2.29)$$

2.2 Rates Limited by Diffusion

In the case of large particles, the reaction rate is often limited by the diffusion of components. This includes: (1) diffusion rates of reactants in the gaseous phase, and (2) diffusion rate of reactants inside

the solid framework. These cases are applicable to the burning of char and absorption of SO_2 by dolomite. When the reaction rate is limited by diffusion rate, the chemical reaction tends to reach equilibrium compositions [25,29].

Take the case of burning of char, for instance, and using a spherical particle of radius a as an approximation, at quasi-steady state, the density of O_2 is given by:

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \rho_1}{\partial r} \right) = 0 \quad (2.30)$$

which for radius $r = a$, $\rho_1 = \rho_a$, and $\rho_1 = \rho_\infty$ at $r \gg a$, we get for diffusivity of O_2 through the gaseous mixture D_1 , or

$$D_1 \frac{\partial \rho_1}{\partial r} \Big|_a = \hat{h}_m (\rho_\infty - \rho_a) \quad (2.31)$$

where $\hat{h}_m$ is the mass transfer coefficient. The Sherwood number is thus

$$\text{Sh} = \frac{\hat{h}_m (2a)}{D_1} = 2 + (\text{convection effects}) \quad (2.32)$$

The O_2 supplied per particle is thus:

$$\begin{aligned} \left(\frac{dm}{dt} \right)_{\text{O}_2} &= \hat{h}_m (4\pi a^2) (\rho_\infty - \rho_a) \\ &= D_1 (\text{Sh}) \frac{(\text{surface area})}{(\text{size})} (\rho_\infty - \rho_a) \end{aligned} \quad (2.33)$$

for equilibrium reaction based on:

at the surface of the char particle and according to the equilibrium constant of each.

Significant simplification was made possible by Avedesian and Davidson [27] by assuming $\rho_a = 0$ and taking only the $\text{C} - \text{O}_2$ reaction and assuming

in the gaseous phase, with $Sh = 1.42$.

In this case, $n_2 = n_4 = 0$, the net rate of gas generation is given by:

$$\begin{aligned} \frac{dn_1}{dt} = - \frac{dn_3}{dt} = \frac{dn_o}{dt} &= - D_1 (Sh) \frac{4\pi a^2}{2a} n_1 N_c \\ &\equiv - k_D n_1 A_c^* \end{aligned} \quad (2.37)$$

or

$$k_D = \frac{D_1 (Sh)}{2a} \quad (2.38)$$

This relation is useful for the simplified C - O reaction in Appendix D.

Sulfation of half-calcined dolomite chips is also diffusion controlled [25]:

Studies at ANL [25] neglected convective diffusion of SO_2 , but molecular diffusion was shown to be the rate limiting process.

Other assumptions are the platelet geometry of $CaCO_3$ crystallites and high diffusion rate of reacting gases through $CaSO_4$ layer. Variable diffusion coefficient of SO_2 was used.

The extent of SO_2 absorption is represented by

$$\xi^* = \ell^* / \ell \quad (2.40)$$

where ℓ is the depth of the platelet, and ℓ^* is the depth at time t . $1 - \xi^*$ is the extent of sulfation of dolomite, or the fraction of sulfated dolomite. In terms of number of moles of dolomite, we have

$$\frac{dn_d}{dt} = \frac{d\xi^*}{dt} \frac{\rho'_d}{M'_d} = - \frac{dn'_d}{dt} \quad (2.41)$$

ρ'_d is the original density of half-calcined dolomite. The conversion rate is given by:

$$\frac{dn'_d}{dt} = - \left[\frac{\hat{k}_1 n_1^m}{\ell \bar{n}'_d} n_7 \right] \left[1 + \frac{\ell \hat{k}_1 n_1^m n_d}{D_e^o n'_d} \right]^{-1} \quad (2.42)$$

where $\bar{n}'_d = \bar{\rho}'_d / M'_d$ is the concentration of CaCO_3 in the crystallite, $n'_d + n_d = n'_{do}$ the original charge, $m = 1/2$ from Eq. (2.9) or (2.39). $D_e^o \xi^* = D_e$, the effective diffusion coefficient. The rate constant $\hat{k}_1$ is affected by the water vapor present, or

$$\hat{k}_1 = \hat{k}_i n_6^n \quad (2.43)$$

where n is the order of reaction with respect to concentration of H_2O , $\hat{k}_i$ is called the "true intrinsic rate constant".

Deducing from the ANL [25] data at 750°C , we get, for low value of n_6 ,

$$\frac{dn'_d}{dt} = - \frac{dn_d}{dt} = - \frac{(0.075 + 10^3 n_6) n_1^{1/2} n_7}{\left[1 + \left(\frac{n'_{do} - n'_d}{2 n'_d} \right) \right] a_d} \quad (2.44)$$

Comparison to Eq. (2.21) gives

$$k_{VII} = \frac{3(0.075 + 10^3 n_6)}{\left[1 + \left(\frac{n'_{do} - n'_d}{2 n'_d} \right) \right] \frac{\rho'_d}{\bar{\rho}'_d}} \quad (2.45)$$

in Table 2. k_{VII} in this form actually depends on the stage of conversion of dolomite or A^*_{dk} because of n'_d and ρ'_d in Eq. (2.45). See Appendix E for applications.

2.3 Densities and Rates of Generation

We need to express the above quantities in terms of those in [1] ANL-CT-77-3, using kinetic rates for illustration. For the char, the densities of components are:

$$N_{cO}^m = n_{oO}^M = \rho_o \quad (\text{carbon}) \quad (2.46)$$

$$N_{cS}^m = n_{sS}^M = \rho_s \quad (\text{sulfur}) \quad (2.47)$$

$$N_{cA}^m = n_{AA}^M = \rho_A \quad (\text{ash}) \quad (2.48)$$

A cloud of particles of char has density given by:

$$\begin{aligned} N_c (m_o + m_s + m_A) &= n_o M_o + n_s M_s + n'_o M_A \\ &= \rho_o + \rho_s + \rho_A = \rho_{char} - \rho_c \end{aligned} \quad (2.49)$$

Initial mass of char per unit volume is given by:

$$n'_o [\alpha M_o + \epsilon M_s + M_A] = N_c \frac{4\pi}{3} a_c^3 \quad \bar{\rho}_c = \rho_c \quad (2.50)$$

Before devolatilizing, the coal suspension has: (subscript F for coal)

$$\begin{aligned} n'_o [\alpha' M_c + \beta M_H + \gamma M_o + \delta M_N + \epsilon M_s + M_A] \\ = N_c m_F = N_c \frac{4\pi}{3} a_F^3 \quad \bar{\rho}_F = \rho_F \end{aligned} \quad (2.51)$$

and for all the gaseous components, $v = 1, 2, \dots, 8$, we have

$$\rho_v = n_v M_v \quad (2.52)$$

For the dolomite, initially we have

$$\rho_d = N'_d m'_d = n'_d M'_d \quad (2.53)$$

For phase ℓ after absorbing of SO_2 , we get

$$\rho_{d\ell} = N_{d\ell} m_{d\ell} = (n_{d\ell} M_d + n'_{d\ell} M'_d) \quad (2.54)$$

The net rates of change of number of moles of each chemical species are as follows:

M-(Molecular wt.)

C (12.01)

$$\sum \frac{dn_{ok}}{dt} = -k_{III} \sum A_{ck}^* n_3 - k_{IV} \sum A_{ck}^* n_1 = M_o^{-1} \Gamma_o \quad (2.55)$$

O₂ (32)

$$\frac{dn_1}{dt} = -k_{I1} n_1 n_2 \left(1 - \frac{n_3 n_4}{K_I n_1 n_2} \right) - k_{IV} \sum A_{ck}^* n_1$$

$$-k_{VI} \sum A_{sk}^* n_1 - k_{V5} n_1 - \frac{1}{2} \sum k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} \quad (2.56)$$

CO (28.01)

$$\begin{aligned} \frac{dn_2}{dt} = & -k_{I1} n_1 n_2 \left[1 - \frac{n_3 n_4}{K_{I1} n_1 n_2} \right] - k_{II} n_2 n_4 + k'_{II} n_3 \\ & + 2 k_{III} \sum A_{ck}^* n_3 + k_{V1} n_5 \end{aligned} \quad (2.57)$$

CO₂ (44.01)

$$\begin{aligned} \frac{dn_3}{dt} = & k_{I1} n_1 n_2 \left[1 - \frac{n_3 n_4}{K_{I1} n_1 n_2} \right] + \sum k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} \\ & + k_{II} n_2 n_4 - k'_{II} n_3 - k_{III} \sum A_{ck}^* n_3 + k_{IV} \sum A_{ck}^* n_1 \end{aligned} \quad (2.58)$$

O (16)

$$\frac{dn_4}{dt} = k_{I1} n_1 n_2 \left[1 - \frac{n_3 n_4}{K_{I1} n_1 n_2} \right] - k_{II} n_2 n_4 + k'_{II} n_3 \quad (2.59)$$

$\frac{1}{n}$ (CH₂)_n (14.026)

$$\frac{dn_5}{dt} = -k_{V1} n_1 n_5 \quad (2.60)$$

H₂O (18.016)

$$\frac{dn_6}{dt} = k_{V1} n_1 n_5 \quad (2.61)$$

SO₂ (64.06)

$$\frac{dn_7}{dt} = k_{VI} \sum A_{sk}^* n_1 - \sum k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} \quad (2.62)$$

Dolomite

d' (140.41)

or
d (176.46)

$$\sum \frac{dn'_{dk}}{dt} = - \sum k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} = - \sum \frac{dn_{dk}}{dt} \quad (2.63)$$

S (32.06)

$$\sum \frac{dn_{sk}}{dt} = -k_{VI} \sum A_{sk}^* n_1 \quad (2.64)$$

For species $v = 0, 1, \dots, 8, d, d', s$, the generation rate in mass per unit volume is given by:

$$\Gamma_v = M_v \frac{dn_v}{dt} \quad (2.65)$$

The net rate of change in number of moles per unit volume in the gas is given by:

$$\begin{aligned} \left(\frac{dn}{dt}\right)_{\text{net gas}} &= \sum \frac{dn_v}{dt} \\ &= k_{III} \sum A_{ck}^* n_3 + \frac{1}{2} \sum k_{VIIk} A_{dk}^* n_7 n_1^{1/2} - k_{II} n_2 n_4 + k'_{II} n_3 \end{aligned} \quad (2.66)$$

In the solid phase of char

$$\begin{aligned} \left(\frac{dn}{dt}\right)_{\text{net char}} &= -k_{III} \sum A_{ck}^* n_3 - k_{IV} \sum A_{ck}^* n_1 - k_{VI} \sum A_{sk}^* n_1 \end{aligned} \quad (2.67)$$

and dolomite:

$$\begin{aligned} \left(\frac{dn}{dt}\right)_{\text{net dolomite}} &= 0 \end{aligned} \quad (2.68)$$

The system has a net change in number of moles of

$$\begin{aligned} \left(\frac{dn}{dt}\right) &= -k_{II} n_2 n_4 + k'_{II} n_3 - k_{IV} \sum A_{ck}^* n_1 - k_{VI} \sum A_{sk}^* n_1 \\ &\quad + \frac{1}{2} \sum k_{VIIk} A_{dk}^* n_7 n_1^{1/2} \end{aligned} \quad (2.69)$$

The net rate of mass generation in the gas phase is

$$\begin{aligned} \Gamma_{\text{gas}} &= \sum \Gamma_{v \text{ gas}} \\ &= M_1 \left[-k_{I1} n_1 n_2 \left(1 - \frac{n_3 n_4}{K_{I1} n_1 n_2} \right) - k_{IV} \sum A_{ck}^* n_1 - k_{VI} \sum A_{sk}^* n_1 \right. \\ &\quad \left. - k_V n_5 n_1 - \frac{1}{2} \sum k_{VIIk} A_{dk}^* n_7 n_1^{1/2} \right] \\ &\quad + M_2 \left[-k_{I1} n_1 n_2 \left(1 - \frac{n_3 n_4}{K_{I1} n_1 n_2} \right) - k_{II} n_2 n_4 + k'_{II} n_3 + \right. \end{aligned}$$

$$\begin{aligned}
 & \left[2k_{III} \Sigma A_{ck}^* n_3 + k_{V1} n_5 \right] \\
 & + M_3 \left[k_{I1} n_2 \left(1 - \frac{n_3 n_4}{K_{I1} n_2} \right) + \Sigma k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} + k_{II} n_2 n_4 \right. \\
 & \quad \left. - k'_{II} n_3 - k_{III} \Sigma A_{ck}^* n_3 + k_{IV} \Sigma A_{ck}^* n_1 \right] \\
 & + M_4 \left[k_{I2} n_1 \left(1 - \frac{n_3 n_4}{K_{I1} n_2} \right) - k_{II} n_2 n_4 + k'_{II} n_3 \right] \\
 & + M_5 \left[-k_{V1} n_5 \right] + M_6 \left[k_{V1} n_5 \right] \\
 & + M_7 \left[-\Sigma k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} + k_{VI} \Sigma A_{sk}^* n_s \right]
 \end{aligned}$$

After rearranging, the above equation becomes:

$$\begin{aligned}
 \Gamma_{gas} &= \Sigma \Gamma_{v gas} \\
 &= M_o \left(k_{III} \Sigma A_{ck}^* n_3 + k_{IV} \Sigma A_{ck}^* n_1 \right) + M_s k_{VI} \Sigma A_{sk}^* n_1 \\
 &+ \left(-M_7 + M_3 - \frac{1}{2} M_1 \right) \Sigma k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} \quad (2.70)
 \end{aligned}$$

$$\Gamma_{char} = M_o \left[-k_{III} \Sigma A_{ck}^* n_3 - k_{IV} \Sigma A_{ck}^* n_1 \right] - M_s \left[k_{VI} \Sigma A_{sk}^* n_1 \right] \quad (2.71)$$

$$\begin{aligned}
 \Gamma_{dolomite} &= \left(M_7 - M_3 + \frac{1}{2} M_1 \right) \Sigma k_{VIIk} A_{dk}^* n_7 n_1^{\frac{1}{2}} \\
 &= -\Gamma_{sulfated dolomite} \quad (2.72)
 \end{aligned}$$

Hence

$$\Gamma_{gas} + \Gamma_{char} + \Gamma_{dolomite} = 0$$

over the unit volume.

(2.73)

2.4 Volumetric Source Terms of Phases

The gas phase has a single mass velocity $\underline{U}_g$ and static temperature T_g .

For each molecular species

$$\frac{\partial \rho_v}{\partial t} + \nabla (\rho_v \underline{U}_g) = \Gamma_v ; \quad (2.74)$$

and for the entire gas mixture,

$$\frac{\partial \rho_g}{\partial t} + \nabla (\rho_g \underline{U}_g) = \Gamma_g , \quad (2.75)$$

where subscript g denotes the whole gas mixture.

For the char which starts with the same size, in the course of reducing to ash (A) each size range k needs to be identified.

We note that Eqs. (2.71) and (2.72) account for chemical conversion of char and dolomite but not the transition from one size of particle to another such as from ck to c(k+1) as carbon is reacted. If we consider the decrease in carbon content of char as combustion occurs to take q steps with simultaneous conversion of sulfur to SO₂ until finally only ash (A) remains, we have

$$\left. \begin{aligned} \rho_{c1} &= N_{c1} \frac{4\pi}{3} a_{c1}^3 \quad \bar{\rho}_{c1} = N_{c1} \frac{m_F}{M_F} \left[c M_O + \epsilon_1 M_S + M_A \right] \\ \rho_{c2} &= N_{c2} \frac{4\pi}{3} a_{c2}^3 \quad \bar{\rho}_{c2} = N_{c2} \frac{m_F}{M_F} \left[\alpha \frac{(q-2)}{(q-1)} M_O + \epsilon_2 M_S + M_A \right] \\ \rho_{c3} &= N_{c3} \frac{4\pi}{3} a_{c3}^3 \quad \bar{\rho}_{c3} = N_{c3} \frac{m_F}{M_F} \left[\alpha \frac{(q-3)}{(q-1)} M_O + \epsilon_3 M_S + M_A \right] \\ \rho_{cq} &= N_{cq} \frac{4\pi}{3} a_{cq}^3 \quad \bar{\rho}_{cq} = N_{cq} \frac{m_F}{M_F} \left[\epsilon_q M_S + M_A \right] \end{aligned} \right\} \quad (2.76)$$

where m_F is the mass of original coal particles (of one size), and M_F is its equivalent molecular weight for α , ϵ , etc., defined by Eqs. (2.1) and (2.2). By taking these finite steps, we are approximating the gradual change in size by stepwise change in size but gradual change in population of particles in each size range. Note that in this formulation sulfur converts at its own rate, from ϵ_1 to ϵ_2 , etc. This added dimension in particle characterization increases computer storage requirement. This increase can be avoided by neglecting the effect of sulfur on the particle dynamics. This is believed valid in that the sulfur rarely amounts to more than 5% by mass of coal. The rate of generation (or consumption) of char can be given by

From Eqs. (2.60):

$$\left. \begin{aligned} \Gamma_{c1} &= M_o \left\{ -k_{III} A_{c1}^* \frac{\rho_{g3}}{M_3} - k_{IV} A_{c1}^* \frac{\rho_{g1}}{M_1} \right\} \\ \Gamma_{c2} &= -\Gamma_{c1} \frac{m_{c2}}{m_{c1}} + M_o \left\{ -k_{III} A_{c2}^* \frac{\rho_{g3}}{M_3} - k_{IV} A_{c2}^* \frac{\rho_{g1}}{M_1} \right\} \\ \Gamma_{c3} &= -(\Gamma_{c2} + \Gamma_{c1} \frac{m_{c2}}{m_{c1}}) \frac{m_{c3}}{m_{c2}} + M_o \dots \end{aligned} \right\} \quad (2.77)$$

where m_{c1} , etc. are the mass of particles in each range.

$$\frac{m_{c2}}{m_{c1}} = \frac{\left(\frac{q-2}{q-1} \right) M_o + \frac{M_A}{\alpha}}{M_o + \frac{M_A}{\alpha}} \quad (2.78)$$

Dolomite particles in their conversion to sulfated dolomite can be treated in a similar manner such that for psizes

$$\left. \begin{aligned}
 \rho_{d1} &= N_{d1} \frac{4\pi}{3} a_d^3 \bar{\rho}_{d1} = N_{d1} m_{d1} = N_{d1} \frac{m_{d1}}{M'_d} M_{d1} \\
 \rho_{d2} &= N_{d2} \frac{4\pi}{3} a_d^3 \bar{\rho}_{d2} = N_{d2} m_{d2} = N_{d2} \frac{m_{d2}}{M'_d} \left[\frac{p-2}{p-1} M'_d + \frac{1}{p-1} M_d \right] \\
 \rho_{d(p-1)} &= N_{dp} \frac{4\pi}{3} a_d^3 \bar{\rho}_{dp} = N_{dp} m_{dp} = N_{dp} \frac{m_{dp}}{M'_d} \left[\frac{1}{p-1} M'_d + \frac{p-2}{p-1} M_d \right]
 \end{aligned} \right\} (2.79)$$

for $1/p-1$ of unsulfated dolomite. Similarly, we have

$$\left. \begin{aligned}
 r_{d1} &= M'_d \left\{ -k_{VII(1)} A_{d1}^* \frac{\rho_{g1}}{M_1} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \right\} \\
 r_{d2} &= r_{d1} \frac{m_{d2}}{m_{d1}} + M'_d \left\{ -k_{VII(2)} A_{d2}^* \frac{\rho_{g2}}{M_1} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \right\}
 \end{aligned} \right\} (2.80)$$

3.0 Bubbles in Fluidized Bed and Free Board

The simplest case of a fluidized bed is a quiescent bed with a simple flat (Appendix C) surface of discontinuity at the top where (subscripts f and z denote quantities above the free surface and component of motion respectively).

$$\rho_g U_{gz} = \rho_{gf} U_{gzf} \quad (3.1)$$

that is, the gas phase flows through and

$$U_{\ell kz} = 0 \quad (3.2)$$

meaning that the solid phase remains in the bed (subscript lk denotes solids of species $l = c$ for char, d for dolomite, and k for various sizes of each). Other conditions across this free surface are:

$$T_g = T_{gf} \quad (3.3)$$

$$\bar{\rho}_g = \bar{\rho}_{gf} \quad (3.4)$$

The real case, however, includes elutriation of fines when

$$U_{gzf} > U_{t(ck)} \quad (3.5)$$

where $U_{t(ck)}$ ^{*} denotes the terminal velocity of fines such as ash so that species of sizes smaller than (ck) are elutriated. This occurs simply because of the existence of these fines even when the bed is quiescent and we shall refer to this mass flux $\rho_{(ck)}' U_{(ck)}' z_f$ as the background elutriation, with

$$U_{(ck)}' z_f = U_{gzf} - U_{t(ck)}' \quad (3.6)$$

$$\rho_{(ck)}' z_f = \rho_{(ck)}' \quad (3.7)$$

The fact that large particles such as dolomite are not elutriated is readily represented by

$$U_{dkz} = 0 \quad (3.8)$$

at the free surface. For those particles which are ejected by bubble burst, but eventually return to the bed by gravity, their mean upward velocity is also zero.

More importantly, the real situation has to include the existence of gas bubbles in the fluidized bed. These bubbles will rise to the surface and eject solid particles as they burst. This is caused by a localized high gas velocity in the form of a jet:

*See page 49

$$U_{Jzf} = U_{bz} + \Delta U_{bz} \quad (3.9)$$

where U_{bz} is the bubble rise velocity as it approaches the surface and ΔU_{bz} is the increase due to bubble burst at the pressure difference ΔP between the inside of the bubble and its surroundings. This localized velocity of a slug of the gas ($U_{Jzf} > U_{gzf}$) ejects additional particles into the free board. These include particles of species (ck)" which are larger than the upper limit of (ck)" because U_{Jzf} is greater than the terminal velocity of (ck)" or

$$U_{Jzf} > U_{t(ck)} \quad (3.10)$$

This particle flux depends on the number of bubbles reaching the surface at a given time. Here we have an additional mass flux $\rho_{(ck)} U_{(ck)} U_{Jzf}$ due to bubble burst. These large particles will rise to a certain height above the free surface and fall back as the gas jet velocity reduces to the background value as the jet is dissipated.

We shall now identify the details concerning the dynamics of bubbles which have an important effect on the mixing process in the fluidized bed. Study of solid-gas reactions in a fluidized bed by Ishida and Wen [30] employed the bubble assemblage model alone as the origin of solid mixing and obtained good agreement with some experimental data.

At this stage of formulating the fluidized bed system, we shall limit ourselves to the range where a free surface is identifiable between the bed and the free board and the number of bubbles reaching the surface is numerous enough such that statistical consideration is applicable, leaving the condition of slugging by a single bubble reaching the surface from time to time for a later treatment.

Bubbles are generated at the porous support of the fluidized bed much like the generation of gas bubbles in a liquid. Prior to obtaining further evidence, we shall characterize the bubble generation at random sites in terms of

probable sites per unit area N'_b

bubble departure diameter $2a_{bo}$

bubble departure velocity U_{boz}

generating frequency $\hat{f}$

For bubbles produced at $N_b'f$ per unit time per unit area, the resulting number of bubbles per unit volume (N_b) at departure is $N_{bo} = N_b'f / U_{boz}$ and the local bubble density is thus

$$\rho_b = N_b \frac{4\pi}{3} a_b^3 \bar{\rho}_b \quad (3.10)$$

$\bar{\rho}_b$ is the bubble material density and may consist of the gaseous phase and a dilute phase of suspension. Exchange of air and combustion gas occur through the phase boundary. As coalescence occurs, the spherical bubbles will transcend to bubble caps. While non-sphericity and existence of wake of a bubble in a fluidized bed is well known [31,32], for simplicity bubbles are assumed to be spherical in shape in this study. This postulation is in conformity to the underlying framework of multiphase mechanics. The detailed structure of a bubble is accounted for in terms of transport parameters, at least at this stage of development of our modeling efforts.

3.1 Bubble Motion

A great deal of descriptive material on bubbles in a fluidized bed has been published. Quantitative information is scarce. Hovmand and Davidson [33] gave for a slugging bed

$$U_{bs} = U_o - U_{mf} + 0.35 \sqrt{g D_B} \quad (3.11)$$

where U_o is the superficial gas velocity, D_B is the bed diameter, U_{bs} is the absolute rise velocity of a slug, U_{mf} is the minimum fluidization velocity [34]. The radius of curvature r_s of the slug was given as

$$r_s = 0.35 D_B \quad (3.12)$$

for beds deeper than 2 bed diameters.

Orcutt, Davidson and Pigford (p. 400 [35]) suggested that the bubble velocity be given as:

$$U_b = U_f - U_{mf} + 0.711 \sqrt{gD_e} \quad (3.13)$$

where U_f is the fluidizing velocity and D_e is the expanded bubble diameter, $D_e = (6v/\pi)^{1/3}$, v is the bubble volume.

Murray (p.398[35]) gave an extensive description of the bubbles and approximated the bubbles as spheres in his theoretical work. He stated that the bubbles are virtually empty particles. They represent moving regions of very high permeability which affect the otherwise uniform upward flow of the gas.

Entrainment and elutriation rates of particles in the exit stream from the fluidized bed were reviewed by Lewis, Gilliland, and Lang [36].

3.2 Bubble Generation

While general data are lacking, work of Werther and Molerus [13] gave for quartz sand at 83 μ m fluidized by air at 9 cm/sec in a 10 cm-diameter bed, 0.5 cm bubble length at the departure from the distributor of sintered metal plates of 5 μ m mean pore size. Bubble sizes up to 10.5 cm at 95 cm height above the distributor, and 1 cm bubble at 5 cm height were measured. At the latter condition an average of 2 cm³/cm² sec of local bubble gas flow was seen. At a minimum fluidization velocity of 1.8 cm/sec (U_{mf}), and a bubble velocity U_{boz} of 10 cm/sec, the generation rate $N_b^{\wedge}$ was nearly 0.2 bubbles/cm² sec., $2 a_{bo} \sim 5 \times 10^{-3}$ m we get

$$2 \times 10^4 / m^3 < N_{bo} < 10^5 / m^3$$

The bubble density at departure ρ_{bo} is

$$\rho_{bo} = N_{bo} \frac{4\pi}{3} a_{bo}^3 \bar{\rho}_b \quad (3.14)$$

and

$$\bar{\rho}_b \sim \bar{\rho}_g \quad (3.15)$$

In the absence of further evidence, an analogy to gas bubbles in a liquid will be made [37].

3.3 Bubble Coalescence

For a chosen range of bubble sizes k , we have

$$\rho_{bk} = \phi_{bk} \bar{\rho}_{bk} \quad (3.16)$$

where $k = 1, 2, 3, 4$ (say) denoting a range of bubble radius a_{bk}

$$\rho_g = \bar{\rho}_g \left(1 - \phi_c - \phi_d - \sum_k \phi_{bk} \right) \quad (3.17)$$

Transition from one species of bubble to another occurs via influx, expansion, and coalescence due to relative motion. To account for expansion and compression due to temperature and pressure variations, we shall choose different k 's according to mass of bubbles rather than size a_k . Therefore, reference to a_k is made for a given temperature and pressure combination.

The generation of species $k + 1$ by influx of gas into k is given by:

$$-\Gamma_{k \text{ bulk}} = M_{kg} (\bar{\rho}_g - \bar{\rho}_{bk}) = \Gamma_{(k+1) \text{ bulk}} \quad (3.18)$$

where M_{kg} is the inverse relaxation time constant for gas influx into the bubble.

In this chapter, we shall use the subscript numerals to denote various bubble sizes omitting subscript b for simplicity.

The choice of the ranges of k is seen in the following example: We note that for chosen a_1 , the coalescence sequence may consist of: (subscript "1" means "b1").

a_1 to a_1	giving	$1.26 a_1$	, choose	$a_2 = 1.26 a_1$	approximately $\hat{k}_{11}$
a_1 to $1.26 a_1$		$1.44 a_1$		$a_3 = 1.44 a_1$	$\hat{k}_{12}$
a_1 to $1.44 a_1$		$1.59 a_1$		$a_4 = 1.59 a_1$	$\hat{k}_{13}$
a_1 to $1.59 a_1$		$1.71 a_1$		$a_5 = 1.71 a_1$	$\hat{k}_{14}$
a_1 to $1.71 a_1$		$1.82 a_1$		$a_6 = 1.82 a_1$	$\hat{k}_{15}$
a_1 to $1.82 a_1$		$1.91 a_1$		$a_7 = 1.91 a_1$	$\hat{k}_{16}$

$1.26 a_1$ to $1.26 a_1$		$1.59 a_1$		$a_4 = 1.59 a_1$	$\hat{k}_{22}$
$1.26 a_1$ to $1.44 a_1$		$1.71 a_1$		$a_5 = 1.71 a_1$	$\hat{k}_{23}$
$1.26 a_1$ to $1.59 a_1$		$1.82 a_1$		$a_6 = 1.82 a_1$	$\hat{k}_{24}$
$1.26 a_1$ to $1.71 a_1$		$1.91 a_1$		$a_7 = 1.91 a_1$	$\hat{k}_{25}$

$1.44 a_1$ to $1.44 a_1$		$1.82 a_1$		$a_6 = 1.82 a_1$	$\hat{k}_{33}$
$1.44 a_1$ to $1.59 a_1$		$1.91 a_1$		$a_7 = 1.91 a_1$	$\hat{k}_{34}$
$1.44 a_1$ to $1.71 a_1$		$2.00 a_1$			$\hat{k}_{35}$

where the empirical coalescence coefficient accounts for the deviations from the discrete choices of bubble sizes (masses).

For the range of a_k 's the scale of bubbles in mass are according to:

$k = 1$	a_1	m_1
2	$a_2 = 1.26 a_1$	$m_2 = 2m_1$
3	$a_3 = 1.44 a_1$	$m_3 = 3m_1$
4	$a_4 = 1.59 a_1$	$m_4 = 4m_1$
5	$a_5 = 1.71 a_1$	$m_5 = 5m_1$

The choice is therefore according to mass m_{bk} with a_{bk} calculated according to the bubble density $\bar{\rho}_{bk}$ (until $a_{bk} \gtrsim a_m$ where transition to multidomain range will occur).

The transition mechanism by coalescence and gas influx is approximated by:

1-1	to 2
1-2	to 3
1-3, 2-2	to 4
1-4, 2-3	to 5 ----

The inexactness in resultant sizes is compensated by the empirical nature of the coalescence coefficients. The conservation of mass, momentum, and energy is maintained by formulating according to: (all subscript numerals mean b_1, b_2 , etc.)

$$\Gamma_{b1} = \Gamma_{1s} - \hat{k}_{11} \rho_1^2 - \hat{k}_{12} \frac{\rho_1^2 \rho_2}{\rho_1 + \rho_2} - \hat{k}_{13} \frac{\rho_1^2 \rho_3}{\rho_1 + \rho_3} - \hat{k}_{14} \frac{\rho_1^2 \rho_4}{\rho_1 + \rho_4} - M_{12} \left(\bar{\rho}_g - \bar{\rho}_1 \right) \quad (3.19)$$

$$\begin{aligned} \Gamma_{b2} = & \hat{k}_{11} \rho_1^2 - \hat{k}_{12} \frac{\rho_1 \rho_2^2}{\rho_1 + \rho_2} - \hat{k}_{22} \rho_2^2 - \hat{k}_{23} \frac{\rho_2^2 \rho_3}{\rho_2 + \rho_3} + M_{12} \left(\bar{\rho}_g - \bar{\rho}_1 \right) \\ & - M_{23} \left(\bar{\rho}_g - \bar{\rho}_2 \right) \end{aligned} \quad (3.20)$$

$$\begin{aligned} \Gamma_{b3} = & \hat{k}_{12} \rho_1 \rho_2 - \hat{k}_{13} \frac{\rho_1 \rho_3^2}{\rho_1 + \rho_3} - \hat{k}_{23} \frac{\rho_2 \rho_3^2}{\rho_2 + \rho_3} + M_{23} \left(\bar{\rho}_g - \bar{\rho}_2 \right) \\ & - M_{34} \left(\bar{\rho}_g - \bar{\rho}_3 \right) \end{aligned} \quad (3.21)$$

$$\begin{aligned} \Gamma_{b4} = & \hat{k}_{13} \rho_1 \rho_3 + \hat{k}_{22} \rho_2^2 - \hat{k}_{14} \frac{\rho_1 \rho_4^2}{\rho_1 + \rho_4} + M_{34} \left(\bar{\rho}_g - \bar{\rho}_3 \right) \\ & - M_{45} \left(\bar{\rho}_g - \bar{\rho}_4 \right) \end{aligned} \quad (3.22)$$

$$\Gamma_{b5} = \hat{k}_{14} \rho_1 \rho_4 + \hat{k}_{23} \rho_2 \rho_3 - \hat{k}_{24} \frac{\rho_2 \rho_4^2}{\rho_2 + \rho_4} + M_{45} \left(\bar{\rho}_g - \bar{\rho}_4 \right) - M_{56} \quad (3.23)$$

The physical meaning is seen in that Γ_{b1} is the net generation via assuming binary coalescence:

Generation of $k = 1$ at surface

Removal from 1 by coalescence 1-1 to 2

Removal from 1 by coalescence 1-2 to 3

Removal from 1 by coalescence 1-3 to 4

Removal from 1 by coalescence 1-4 to 5

Removal from 1 by influx to grow to 2

In an analogous manner Γ_{b2} is given by:

Generation of 2 by coalescence of 1-1 to 2

Removal from 2 by coalescence with 1-2 to 3

Removal from 2 by coalescence 2-2 to 4

Removal from 2 by coalescence 2-3 to 5

Generation of 2 by influx into 1

Removal from 2 by influx into 2

The relaxation time constant M_{12} , say, gives the rate of conversion of species 1 to species 2, rather than a gradual variation of all species 1 to species 2. This needs to be clarified because M here does not account for stepwise change from species 1 to 2.

3.4 Coalescence Coefficients

An important parameter for the multiphase transport is the coalescence coefficient, about which not much is known.

Evidence based on a rather meager amount of experimental results suggest that the binary coalescence coefficients, $\hat{k}_{11}$, $\hat{k}_{12}$, for instance, given in the form:

$$\Gamma_{11} = -\hat{k}_{11}\rho_1^2 \quad (3.24)$$

$$\Gamma_{12} = -\hat{k}_{12}\rho_1\rho_2 \quad (3.25)$$

etc., will have the coalescence coefficient $\hat{k}_{11}$ as:

$$\hat{k}_{11} = k_{11}^* \frac{1}{\rho_e} n_1^{1/3} \left(\overline{\Delta U_1^2} \right)^{1/2} \quad (3.26)$$

where k_{11}^* is the probability of coalescence by 1-1 to 2; $n_1^{-1/3}$ is the actual mean interparticle spacing, $n_1 = 3\rho_1/4\pi a_1^3\rho_1$; ρ_e is the density of the dense phase of the bed excluding particles; and $(\overline{\Delta U_1^2})^{1/2}$ is the intensity of random motion of bubbles relative to the dense phase (subscript m) $\left[\overline{U_1^2} \right]^{1/2} = \left[\overline{U_1^2} - \overline{U_e^2} \right]^{1/2}$, where $\overline{U_1^2}$ and $\overline{U_e^2}$ are the intensities of random motion of each phase. Note that random motion of bubbles exists even in a liquid in laminar motion arising from reaction of the wake of a bubble. Extension to $\hat{k}_{12}$ gives:

$$\hat{k}_{12} = k_{12}^* \frac{1}{\rho_p} (n_1 n_2)^{1/6} \left[\overline{\Delta U_1^2} \overline{\Delta U_2^2} \right]^{1/4} \quad (3.27)$$

ρ_p gives the primary resistance to relative motion in a fluid and the probabilities of coalescence k_{11}^* , k_{12}^* depend on the fluid properties and decrease with increasing velocities of approach. There are no data on k^* 's. However, test computations will make possible some determination via fitting experimental results using lumped parameters.

Simple case: Since details of coefficients of coalescence are not known, we shall obtain typical values from experiments of Werther and Molerus [13]. We take the case of

$$\bar{\rho}_b = \bar{\rho}_g = \text{Constant}$$

and

$$\phi_b = N_b (4\pi/3) a_b^3$$

and apply the approximation, for coalescence coefficient k^* :

$$\frac{dN_b}{dt} = -k^* \left(\frac{N_b}{N_{bo}} \right)^{-1/3} N_b^2 = -k^* \left(N_{bo} \right)^{1/3} \left(N_b \right)^{5/3} \quad (3.28)$$

for the simple case of binary coalescence. Integration gives:

$$N_b^{-2/3} - N_{bo}^{-2/3} = \frac{2}{3} k^* N_{bo}^{1/3} t$$

or

$$\left(\frac{N_b}{N_{bo}} \right)^{-2/3} - 1 = \frac{2}{3} k^* N_{bo}^{1/3} t \quad (3.29)$$

Alternately, we have

$$\left(\frac{\phi_b}{\phi_{bo}}\right)^{-2/3} \left(\frac{a_b}{a_{bo}}\right)^2 - 1 = \frac{2}{3} k^* N_{bo} t \quad (3.30)$$

From Werther and Molerus [6], $h=0.95$ m, $2a_b=0.1$ m, $2a_{bo}=0.005$ m, $U_b=0.1$ m/s,

We get:

$$\frac{2}{3} k^* N_{bo} h/U_b \sim 400, \text{ or } k^* N_{bo} \sim 60 \text{ s}^{-1}$$

for

$$2 \times 10^4 < N_{bo} < 10^5 \text{ m}^{-3}$$

We use as an approximation $k^* \sim 10^{-3} \text{ m}^3/\text{s}$ since we cannot expect better than order of magnitude accuracy from the available experimental data. Accurate determination of k^* calls for further experimental efforts. This approximation, however, makes possible treating bubbles according to $N_b(\underline{x}, t)$ and $a_b(\underline{x}, t)$.

3.5 Bubble Burst and Particle Flux

Background elutriation of fines at the free surface applies only to particles whose terminal velocity is less than the gas velocity entering the free board. Ejection of particles by bubble burst is a localized phenomenon and is in some ways analogous to bubble burst at a liquid surface. Some lead to formulating bubble burst from a fluidized bed and its effects is provided by those studies of gas bubbles in a liquid and ejection of droplets by bursting.

Newitt [38] gave volume of particles in a particle cloud ejected per unit volume of bubble: $\hat{k}_D = 10^{-3}$.

Chao and Medrow [39] determined the floating bubble configuration and the resulting droplet charge from bubble burst. Trajectories of ejected

particles were studied [40], but we need to know the particle flux and velocities via modifying the semi-empirical approach in [41].

First we consider the gas motion resulting from the bubble burst. The gas pulse produced by bubble burst at the free surface has momentarily a velocity produced by the bubble velocity in the bed (U_{bz}) as it approaches the surface and an increase in velocity due to bubble burst (ΔU_{bz}) superposed on it. The latter is due to a pressure difference between the inside of the bubble and the pressure outside of it as it reaches the surface. The case of an incompressible bubble near an equilibrium state is illustrated in Fig. 7(a) and (b), as it rises in the bed. Following the notations in Fig. 7 for a bed with bubbles with the density of the dense phase given by $\rho_e = \rho_g + \sum_{c,d} \sum_k \rho_{lk}$, we have, upon ignoring surface tension effect, the following relations for static pressure inside and outside of the bubble at the distance z' below the surface.

$$P_b + \bar{\rho}_g [U_{gz} (1 - \phi) - U_{bz}]^2 / 2 = P_1 + \bar{\rho}_g U_{gz}^2 / 2 \quad (3.31)$$

and at the surface, the pressure is given by:

$$P_o + \bar{\rho}_g [U_{gz} (1 - \phi)]^2 / 2 = P_2 + \bar{\rho}_g U_{gz}^2 / 2 \quad (3.32)$$

with

$$P_1 - P_2 = \rho_p (\Delta z) g \quad (3.33)$$

g is the gravitational acceleration. Combining these relations, we get

$$P_b - P_o - \bar{\rho}_g [2U_{bz} U_{gz} (1 - \phi) - U_{gzf}^2] / 2 = \rho_e z' g \quad (3.34)$$

or

$$P_b - P_o = (\bar{\rho}_g / 2) [2U_{bz} U_{gz} (1 - \phi) - U_{bz}^2] + \rho_e z' g \quad (3.35)$$

where $U_{gzf} = U_{gz} (1 - \phi)$. Note that $\Delta P = P_b - P_o$ at the surface where $z' = 0$, or $z = h$ (Fig. 5). ΔP is the pressure difference across the bubble surface when bursting occurs, and

$$\Delta U_{bz} = \eta_v [\Delta P / \bar{\rho}_g]^{1/2} \quad (3.36)$$

Fig. 7 Motion Of a Bubble in Fluidized Bed and Bubble Burst

(c) Bursting Bubble & Jet of Gas With Ejected Particles

where η_v is a velocity coefficient. Therefore at the bubble burst, the jet of gas has, momentarily, a velocity of:

$$U_{Jzf} = U_{bz} + \eta_v \left[\frac{P}{\rho_g} \right]^{1/2} \quad (3.37)$$

The influence of bubble burst at the free surface is seen by considering the motion of the gas phase in the free board produced by the jet-like motion. As bubbles burst at various locations over the free surface, intermittent jets of gas are produced, superposed on the background gas flow from the other parts of the bed where no bubble emerges. Statistically, a simplified view is that of distributed gas jets above the surface, ejecting particles to various heights in addition to background elutriation.

Quantitatively, bubbles burst at random at the free surface at the rate of $N_b U_{bz}$ bubbles per unit area per unit time. Since this occurs as a bubble nears the surface traversing a depth of the order of $2a_b$, the diameter of the bubble as it nears the surface, and over a time duration of $2a_b/U_{bz}$, we have at any time $N_b(2a_b)$ gas jets per unit area each having a velocity U_{Jzf} at the free surface.

An estimate of the height in the free board that is influenced by the bursting bubble can be made by treating each jet at an average distance of $[N_b(2a_b)]^{-1/2}$ (large compared to $2a_b$) from each other as a free jet of gas of initial radius a_b according to the approximation of Schlichting and Tollmien [35]. The maximum velocity U_{Jo} along the center line of the jet is seen to decrease according to:

$$U_{Jo} = 2 \gamma D \left[z'' + (\sqrt{3/2}) \gamma a_b \right]^{-1} \equiv 2 \gamma^2 D \zeta^{-1}, \quad (3.38)$$

where $\gamma = (\sqrt{3/4}) a_b U_{Jzf} / D$, the diffusivity D is given by $a_b U_{Jzf} / 35$, z'' is measured above the free surface. The influence of the bubble burst is seen to have completely decayed at $z'' = \Delta z$ where U_{Jo} is equal to U_{gzf} of the region not influenced by the bubble burst. Substituting the values of D , and solving Eq. (3.38) gives:

$$\Delta z = a_b \left[\left(U_{Jzf} / U_{gzf} \right) - 1 \right] (105/8) \quad (3.39)$$

Within this height Δz above the bed, particles of various sizes rise to different heights by the jet action of the bursting bubbles. For example, with $U_{Jzf}/U_{gzf} = 5$, $a_b = 0.025$ m, $\Delta z = 1.31$ m, while at $U_{Jzf}/U_{gzf} = 2$, $\Delta z = 0.53$ m. In this layer above the free surface ejected particles of different sizes rise to different heights. Hence, bubble burst will contribute significantly to the carry-over of solid particles, particularly when the free board is not high enough above the bed. This multidomain region has a velocity distribution of:

$$U_J = U_{Jo} \left[1 + \frac{1}{4} \gamma^2 \frac{r^2}{\zeta^2} \right]^{-1} \quad (3.40)$$

where r is the radius measured from the axis of a jet and ζ is defined in Eq. (3.38). Some particles are lifted along the center of the jet and fall back to the bed in the region between the jets due to bubble burst. In summary, we have:

Mass of gas ejected per bubble burst: $(4\pi/3) a_b^3 \bar{\rho}_g$, kg

Flux of gas jets: $(4\pi/3) a_b^3 \bar{\rho}_g N_b U_{bz}$ kg/m²s

Average flow rate per jet: $(2\pi/3) a_b^2 \bar{\rho}_g U_{bz}$ kg/s

The ejected particles are quantified as follows:

By analogy to bubble burst in liquid [24], we introduce:

Mass of particles ejected per bubble: $m_e = (4\pi/3) \hat{k}_D a_b^3 \bar{\rho}_c$, kg

Mass of species ck ejected per bubble: $m_{ek} = [\rho_{ck} / \sum_{(ck)''} \rho_{ck}] m_e$,

for particles below size $(ck)'$ whose terminal velocity is below U_{bzf} (summation is over sizes up to $(ck)''$).

Mass of particles ejected per second: $(2\pi/3) \hat{k}_D a_b^2 \bar{\rho}_c U_{bz}$, kg/s

Mass of species (ck) ejected per second:

$$(2\pi/3) \hat{k}_D a_b^2 \bar{\rho}_c U_{bz} \left[\rho_{ck} / \sum_{(ck)''} \rho_{ck} \right], \text{ kg/s} \quad (3.41)$$

Total mass flux of particles ejected:

$$\sum_{(ck)''} \rho_{ckf} U_{ckzf} = \hat{k}_D \bar{\rho}_c (\bar{\rho}_b / \bar{\rho}_g) U_{bz} \quad (3.42)$$

Average initial particle density:

$$\hat{k}_D \bar{\rho}_c (\rho_b / \bar{\rho}_g) \frac{\rho_{ck}}{\sum (ck)'' \rho_{ck}} \quad (3.43)$$

A preliminary calculation of density distribution in a jet of ejected solid particles is given in Appendix F.

4.0 Transport Parameters and Constitutive Relations

While similarities are often noted among the formulations of various multiphase systems, the latter differ from one another in their transport parameters.

Knowledge of transport parameters of fluidized beds is incomplete because studies on fluidized beds have been largely observational and inductive. Rigorous treatment of fluidized beds is rather recent. In this chapter, we shall identify all the available information and shall attempt to fill gaps of knowledge whenever possible.

First we need to introduce a systematic set of notations for the species and phases:

Gaseous phase	Species gk , $k = 1, 2, 3, \dots$	Cartesian components $j, 1$ Velocity $\underline{U}_{gk}$
Coal, char (to ash)	Species ck $k = 1, 2, 3, \dots$	Velocity $\underline{U}_{ck}$
Dolomite (to spent dolomite)	Species dk $k = 1, 2, 3, \dots$	Velocity $\underline{U}_{dk}$
Bubble (local gas species)	Species bk $k = 1, 2, 3, \dots$	Velocity $\underline{U}_{bk}$

Tube bank	Species s	Fixed
(volume fraction ϕ_s)		
General representation	Species ℓ	
	$\ell = c, d, b$	

4.1 Interactions and Mean Quantities

Because of large collision frequency of molecules in a gas, all components of a gaseous mixture, except those generated from other phases, are at one mean velocity U_g and

$$\rho_g = \sum \rho_{gk} \quad (4.1)$$

For the whole mixture,

$$\rho_m = \rho_g + \sum_{\text{(char)}} \rho_{ck} + \sum_{\text{(dolomite)}} \rho_{dk} + \sum_{\text{(bubble)}} \rho_{bk} \quad (4.2)$$

and $\underline{U}_m$ is defined by

$$\rho_m \underline{U}_m = \rho_g \underline{U}_g + \sum_k \rho_{ck} \underline{U}_{ck} + \sum_k \rho_{dk} \underline{U}_{dk} + \sum_k \rho_{bk} \underline{U}_{bk} \quad (4.3)$$

4.2 Transfer of Momentum

Because of the large concentration of solids, the presence of the particles sharply affect the motion of the gas phase via the viscous coupling term:

$$\begin{aligned} & - \sum_k \rho_{ck} F_{ckg} (\underline{U}_g - \underline{U}_{ck}) - \sum_k \rho_{dk} F_{dkg} (\underline{U}_g - \underline{U}_{dk}) \\ & - \sum_k \rho_{bk} F_{bkg} (\underline{U}_g - \underline{U}_{bk}) \end{aligned} \quad (4.4)$$

for inverse relaxation times F for momentum transfers. The viscous coupling terms concerning the motion of solid phase k of char are:

$$\begin{aligned}
 & \rho_{ck} F_{ckg} (\underline{U}_g - \underline{U}_{ck}) + \sum_{r \neq k} \rho_{ck} F_{ckcr} (\underline{U}_{cr} - \underline{U}_{ck}) + \sum \rho_{ck} F_{ckdk} (\underline{U}_{dk} - \underline{U}_{ck}) \\
 & \quad \text{(gas)} \quad \quad \quad \text{(other char)} \quad \quad \quad \text{(dolomite)} \\
 & + \sum \rho_{ck} F_{ckbk} (\underline{U}_{bk} - \underline{U}_{ck}) \quad \quad \quad (4.5) \\
 & \quad \quad \quad \text{(bubbles)}
 \end{aligned}$$

The viscous coupling terms for the dolomite and sulfated dolomite are:

$$\begin{aligned}
 & \rho_{dk} F_{dkg} (\underline{U}_g - \underline{U}_{dk}) + \sum_k \rho_{ck} F_{ckdk} (\underline{U}_{cr} - \underline{U}_{dk}) + \sum_{s \neq k} \rho_{dk} F_{dkds} \\
 & \quad \text{(gas)} \quad \quad \quad \text{(char)} \\
 & (\underline{U}_{ds} - \underline{U}_{dk}) + \sum_k \rho_{dk} F_{dkbk} (\underline{U}_{bk} - \underline{U}_{dk}) \quad \quad \quad (4.6) \\
 & \quad \quad \quad \text{(other dolomite particles)}
 \end{aligned}$$

The basic relations giving F's are given in Ch. 5 of [35] .

The F's due to interaction of phases are:

Number of Interactions	g	ck	dk	bk
(ck)-1		$\rho_{ck} F_{ck(ck)}$		
(dk)-1			$\rho_{dk} F_{dk(dk)}$	
(bk)-1				$\rho_{bk} F_{bk(bk)}$
(ck)	$\rho_g F_{gck}$	$= \rho_{ck} F_{ckg}$		
(dk)	$\rho_g F_{gdk}$		$= \rho_{dk} F_{dkg}$	
(bk)	$\rho_g F_{gbk}$			$= \rho_{bk} F_{bkg}$
(ck)(dk)		$\rho_{ck} F_{ckdk}$	$= \rho_{dk} F_{dkck}$	
(ck)(bk)		$\rho_{ck} F_{ckbk}$		$= \rho_{bk} F_{bkck}$
(bk)(dk)			$\rho_{dk} F_{dkbk}$	$= \rho_{bk} F_{bkdk}$

$(ck)(dk) + (dk)(bk) + (bk)(ck) + 2[(ck) + (dk) + (bk)] - 3 =$ Total number of F's which is also the total number of G's, where G is the inverse relaxation time for energy transfer.

Example: For $ck=1$, $dk=1$, $bk=3$, $g=1$ (3 components)

$$1 + 3 + 3 + (2 \times 5) - 3 = 14 \quad \text{F's and G's each.}$$

The value of $F_{\ell kg}$ is given by (pp. 186, 192 of [35]):

$$F_{\ell kg} = \frac{9\bar{\mu}_g F^*}{2a_{\ell k} \bar{\rho}_{\ell k}}, \quad (4.8)$$

where for $\Sigma\phi_{\ell k} < 0.08$,

$$F^* = 1 + 0.0975 \text{ Re} - 0.636 \times 10^{-3} \text{ Re}^2,$$

and

$$\text{Re} = \frac{2a_{\ell k} |U_g - U_{\ell k}| \bar{\rho}_g}{\bar{\mu}_g} \approx 100. \quad (4.9)$$

For

$$\phi = \Sigma\phi_{\ell k} > 0.08,$$

$$F_{\ell kg} = \frac{75}{2} \frac{\phi}{(1-\phi)^2} \frac{\bar{\mu}_g}{\bar{\rho}_{\ell k} a_{\ell k}^2} + \frac{1.75}{2(1-\phi)} \frac{\bar{\rho}_g}{\bar{\rho}_{\ell k}} \frac{[U_g - U_{\ell k}]}{a_{\ell k}}. \quad (4.10)$$

Note: $g/F_{\ell kg}$ is the terminal velocity of free fall of particle ℓk in the gas due to gravitational acceleration g .

To determine $F_{\ell k(\ell'k')} \equiv F_{sr}$ (for collision of s by r),

$$\Psi_{sr} = \left[1 + \frac{a_r^3 \bar{\rho}_r}{a_s^3 \bar{\rho}_s} \right]^{-1} \frac{\bar{\rho}_r [U_s - U_r]}{2(a_s + a_r) 18\bar{\mu}_g} (2a_r)^2 \quad (4.11)$$

$$\Phi_{sr} = \left[1 + \frac{a_r^3 \bar{\rho}_r}{a_s^3 \bar{\rho}_s} \right] \frac{9\bar{\rho}_r^2}{\bar{\mu}_g \bar{\rho}_r} \left[\frac{U_s - U_r}{2(a_r + a_s)} \right] \quad (4.12)$$

The heat transfer coupling for the dolomite and spent dolomite are

$$\begin{aligned} & \rho_{dk} c_{dk} G_{dkg} (T_g - T_{dk}) + \sum_k \rho_{dk} c_{dk} G_{dkck} (T_{ck} - T_{dk}) \\ & \quad \text{(gas)} \quad \quad \quad \text{(char)} \\ & + \sum_{s \neq k} \rho_{dk} c_{dk} G_{dkds} (T_{ds} - T_{dk}) \\ & \quad \quad \quad \text{(other dolomite)} \end{aligned} \quad (4.19)$$

The basic relations giving G's are given in Ch. 5 of [35]. These transfers between solid phases include physical contact and heat transfer within that duration. The bubble temperature is nearly equal to the local gas temperature; heat transfer coupling with the surrounding dense phase is not given.

For the gas-particle heat transfer we have (p. 205 of [35]):

$$G_{\ell k}^* = \frac{3G_{\ell k} \kappa_g^*}{c_{pg} \bar{\rho}_{\ell k} a_{\ell k}^2} \quad (4.20)$$

except for the bubbles where $T_{bk} = T_g$ because the bubbles are thoroughly ventilated; further

$$G_{\ell k}^* = \frac{1}{2} (Nu) (Re) \Big|_{\ell k} \rightarrow 1 \quad (4.21)$$

where Nu is the Nusselt number and Re is the Reynolds number of particle motion:

$$Re_{\ell k} = \frac{2a_{\ell k} \rho_g |\underline{U}_g - \underline{U}_{\ell k}|}{\mu_g} \quad (4.22)$$

For the dense phase (p. 189 of [35]) ,

$$G_{\ell kg} = \frac{\hat{3}h}{\bar{\mu}_{\ell k} a_{\ell k} c_{p\ell k}} \quad (4.23)$$

where

$$\hat{h} = \hat{j} c_{pg} \bar{\rho}_g |\underline{U}_g - \underline{U}_{\ell k}|^{(Pr)^{-2/3}} \quad (4.24)$$

and the $\hat{j}$ factor is given by

$$\hat{j} = 1.77 (Re_{\ell k})^{-0.4} \quad (4.25)$$

for $(Re)_{\ell k} > 30$,

and

$$\hat{j} = 5.7 (Re_{\ell k})^{-0.78} \quad (4.26)$$

for $(Re)_{\ell k} < 30$.

Equation (4.26) is usually applicable to the present study. For solid-solid interaction, the inverse relaxation times are given by (p. 210 of [35]):

$$G_{\ell k(\ell'k')} \equiv G_{sr} = C_{sr} \frac{\rho_r}{\alpha_r} \frac{(U_s U_r)^{1/2}}{c_s \rho_s a_r a_s} \quad (4.27)$$

where the interaction coefficient is given by:

$$C_{sr} = (2.94) \frac{45}{(2^{2/5})^{32\pi}} \eta_{sr} \left[\sqrt{\frac{m_s}{m_r}} + \sqrt{\frac{m_r}{m_s}} \right]^{-4/5} \left[\sqrt{\frac{a_r}{a_s}} + \frac{a_s}{a_r} \right]^{7/5} \left[\sqrt{\frac{k_s}{k_r}} + \sqrt{\frac{k_r}{k_s}} \right]^{4/5} (N_{Im})^{4/5}$$

where m is the particle mass [$m_s = (4\pi/3)a_s^3\rho_s$], c is the specific heat of solids; $k = (1 - \nu^2)/E$, where ν is the Poisson ratio of the solid material, and E the modulus of elasticity; κ_s and κ_r are the thermal conductivity of the materials of the solids; and the impact number

$$N_{Im} = 5\pi^2 \left[\frac{U_s}{\rho_s} - \frac{U_r}{\rho_r} \right]^2 \frac{1}{\rho_r} \sqrt{k_s k_r} \left(\frac{1 + r^*}{2} \right) \quad (4.28)$$

where $r^* \sim 1/2$, the ratio of the rebound speed to incoming speed. In general,

$$\rho_{lk} c_{lk} G_{lk}(\ell'k') = \rho(\ell'k') c(\ell'k') G(\ell'k')(\ell k) \quad (4.29)$$

The heat transfer by impact of particles on a surface (r) becomes important for $m_r \gg m_s$, and $a_r > a_s$ such as in the case of the tube bank and solid wall ($r=\infty$). The heat transfer coefficient $\hat{h}_{ckw}$ is given by:

$$\hat{h}_{ckw} = \alpha_{lkw} (2.94) \left[\frac{3}{4} (2)^{2/5} \right] \rho_{lk} \frac{\kappa_{lk}}{\rho_{lk} a_{lk}} \left(\sqrt{\frac{k_{lk}}{k_w}} + \sqrt{\frac{k_w}{k_{lk}}} \right)^{4/5} (N_{Im})_w^{4/5} \quad (4.30)$$

and

$$(N_{Im})_w = 5\pi^2 \left(U_{lk} \right)^2 \frac{1}{\rho_{lk}} \sqrt{k_{lk} k_w} \left(\frac{1 + r^*}{2} \right) \quad (4.31)$$

where α_{lkw} is the accommodation coefficient of impact of lk particles with the wall, $\alpha_{lkw} < 1$.

The nature of unsteady heat transfer of a spherical particle in contact with a plain surface was studied by Botterill et al. using an annular bed heat exchanger [42] and array of tubes [43]. The difference from the present system was in their use of stirrer blades to produce particle motion in one case and flow loop in the other. Their mean heat transfer coefficients including the effects of bubbles are of the same order of magnitude of $\hat{h}$ in the above relations.

4.4 Viscosities and Thermal Conductivities

Viscosities due to interaction of particle phases are given by (p. 202 of [35]), for binary interaction of species s and r

$$\mu_{sr} \propto n_s n_r a_{sr}^2 \bar{\rho}_p \left| \Delta_r \Delta_r \right|^{1/2} \quad (4.32)$$

where n's are the number densities of the phases and Δ_r is the shear tensor of species r; that is, the viscosity due to particle-particle collision is non-Newtonian. Schugel [44] postulated a correlation of experimental data obtained by shear viscous measurements to give for the mixture:

$$\begin{aligned} \mu_m &= \frac{4a_p^2 \rho_p}{2.65 \times 10^{-2}} \left(4.35 + 0.13 \frac{\phi}{\phi_0 - \phi} \right) \text{ kg/m} \cdot \text{s} \\ &= \frac{4a_p^2 \rho_p}{2.65 \times 10^{-2}} \mu_s^* \end{aligned} \quad (4.33)$$

where ϕ is the volume fraction of solid in our notation.

Schugel's data cover only moderate bed expansion $2 < \phi/(\phi_0 - \phi) < 25$. He also recognized that for $\phi/(\phi_0 - \phi) > 100$ non-Newtonian behavior is seen. Blake [22] accounted for the difficulty that μ_m does not reduce the μ_g of the gas phase alone by postulating for $0 < \phi/(\phi_0 - \phi) < 2$

$$\mu_s^* = 0.5 \mu_{s2}^* \frac{\phi}{\phi_0 - \phi}, \quad (4.34)$$

where μ_{s2}^* is the value of μ_s^* at $\phi/(\phi_0 - \phi) = 2$. By postulating in this manner, the dependence of μ_m on $(\phi/(\phi_0 - \phi))^2$ is accounted for, or

$$\mu_s^* = \frac{4.61}{4} \left(\frac{\phi}{\phi_0 - \phi} \right)^2 \quad (4.35)$$

and

$$\mu_m = \mu_g + \frac{4a_2 \rho_p}{2.65 \times 10^{-2}} \mu_s^* = \mu_g + 150 \sum_{\ell k} a_{\ell k}^2 \rho_{\ell k} \mu_s^*, \quad (4.36)$$

where $\ell = c, d$ only. In general a polynomial expression for μ_s^* is useful to account for higher order collisions:

$$\mu_s^* = a_2 \left(\frac{\phi}{\phi_0 - \phi} \right)^2 + a_3 \left(\frac{\phi}{\phi_0 - \phi} \right)^3 + a_4 \left(\frac{\phi}{\phi_0 - \phi} \right)^4. \quad (4.37)$$

Fitting between $2 < \phi/\phi_0 - \phi < 14$ gives, for $\phi = 0.52$, or $\phi = \sum_{\ell} \sum_k \phi_{\ell k}$,

$\ell = c, d$ only,

$$a_2 = 1.650 \quad a_3 = -0.2709 \quad a_4 = 0.01114. \quad (4.38)$$

The non-Newtonian nature of the suspension will be treated in a future report.

Apparent thermal conductivity of particle clouds was treated in [35]; again experimental data on individual interactions are meager. The average thermal conductivity was corrected by Gelperin and Einstein [45] to give, for mean thermal conductivity of solid κ_s and fluid κ_g , the value of κ_m for the mixture:

$$\frac{\kappa_m}{\kappa_g} = 1 + \frac{\phi \left(1 - \frac{\kappa_g}{\kappa_s} \right)}{\frac{\kappa_g}{\kappa_s} + 0.28 (1 - \phi)^{0.63} (\kappa_s / \kappa_g)^{0.18}}, \quad (4.39)$$

where ϕ denotes the volume fraction of solid. This relation is for a fixed bed and therefore is not satisfactory, but is the only one available.

4.5 Effect of Radiation

In a fluidized combustion system, radiation is a significant mode of heat transfer as given in Chaps. 5 of [35]. Formulation of energy equations including radiation interchange is given in Chaps. 6 of [35]. This is the most important omission in Blake et al. [22].

In this dilute phase where literally every particle sees the wall with which it exchanges heat by radiation, a simple radiation heat balance will be adequate.

In the dense phase, closely spaced particles will emit independently, and the intensity of the radiation will depend on the condition of the particle cloud; therefore, appropriate radiation model must be chosen (p. 232-233 of [35]). The absorption coefficient α'_m (m^{-1}) is given by

$$\alpha'_m = \alpha \pi a^2 N_p, \quad (4.40)$$

where α is the absorbtivity of the surface. Since the solid particles in the present system are opaque, the index of refraction $\hat{n}_m$ of the mixture is that of the gas phase alone.

The radiation exchange constitutes a heat source in a given volume

$$\rho_p \frac{4\pi a^2}{m_p} \int_0^\infty \alpha_\lambda [E_{b,\lambda} - \int_{4\pi} I_\lambda d\Omega] d\lambda, \quad (4.41)$$

where λ is the wavelength; $E_{b,\lambda}$ is the black body radiation (b) at wavelength λ , in energy per unit area per unit time; and I_λ is the intensity of radiation given by (for spherical coordinates s, θ, ϕ)

$$\frac{dI(s, \theta, \phi)}{ds} = -\alpha'_m \left\{ I(s, \theta, \phi) - \hat{n}_m^2 I_{bb}(s) \right\}, \quad (4.42)$$

where I_{bb} is the intensity of black body radiation.

Viskanta and Grosh [35] suggested introducing radiation conductivity of the magnitude

$$\kappa_{rad} = \frac{16\hat{n}_m^2 \sigma_r T^3}{3\alpha'_m}, \quad (4.43)$$

where σ_r is the Stefan-Boltzmann constant of radiation.

In our preliminary calculations, κ_{rad} will be added to κ_m of Eq. (4.39) to account for the effect of diffused radiation. For the purpose of distribution, we use:

$$\alpha'_m = \alpha \pi \sum_{k,c,d} \sum_{\ell k} a_{\ell k}^2 N_{\ell k} = \alpha \frac{3}{4} \sum_{k,c,d} \sum_{\ell k} \frac{1}{a_{\ell k}} \frac{\rho_{\ell k}}{\bar{\rho}_{\ell k}} \quad (4.44)$$

and T is the temperature of the phase under consideration.

The heat source due to diffused radiation J_{Elk} therefore takes the form:

$$J_{Elk} = \frac{\partial}{\partial x_j} \left[\kappa_{rad} \frac{\partial}{\partial x_j} \left(\frac{\rho_{\ell k} c_{\ell k} T_{\ell k}}{\rho_m c_m} \right) \right]. \quad (4.45)$$

Another important aspect of energy balance is the distribution of heat generated by the reaction. Because of high thermal conductivity in solids as compared to the gaseous phase, all the heat generated or absorbed by heterogenous reaction goes to (or is removed from) the solid

phase, with subsequent heat transfer to the gaseous phase via heat transfer coupling (including collision with other solids). The resultant temperature of the solid phase is the flame temperature of that reaction. All the heat produced (or absorbed) by homogeneous reaction goes to (or is removed from) the gaseous phase, with subsequent heat transfer via heat transfer coupling.

5.0 Tube Bundle Modeling

In a fluidized bed combustor, tube bundles are installed in the bed (immersed) and in the free board. The basic configuration of the boiler tube system in a fluidized combustor as shown in Fig. 8, permits simplification of the multi-multiphase formulation by treating the tube system as a quasi-continuum. The discrete nature of the tubes is accounted for via treating the momentum and energy interactions based on the fact that these solid elements and the fluids are mutually exclusive by formulating the system as an anisotropic system of flow resistance and heat source.

The general specification and approach include the following:

- a. The tubes are treated as distributed solid material and heat source (sink). Their exclusive nature is recognized in the flow and heat transfer relations. They are treated as a fixed phase, but differ from a bubble at zero velocity because they do not contribute to inertial coupling.
- b. They offer anisotropic flow resistance and heat transfer to the multiphase fluid.

We shall illustrate with the basic geometry consisting of tubes of radius b on equilateral triangular spacing of $2s$ between centers of tubes; for other geometries, similar derivations can be followed. The present geometry defined in Fig. 8 gives the following quantities defining the system: for the coordinates x, y across the tubes, and z along the tubes:

$$\text{Volume fraction of the tube bundle} = (\pi b^2) / 2\sqrt{3} s^2 \equiv \phi_s$$

$$\text{Porosity} = 1 - \phi_s$$

$$\text{Axial free flow area} = \Delta x \Delta y (1 - \phi_s)$$

Fig. 8. Geometry of Tubes and Coordinates

Minimum cross flow area in the x-direction = $\Delta y \Delta z [1 - (b/s)]$

Minimum cross flow area in the y-direction = $\Delta x \Delta z [1 - (b/3^{1/2}s)]$

Mean free flow area in the x-direction* = $\Delta y \Delta z (1 - \phi_s)$

Mean free flow area in the y-direction = $\Delta x \Delta z (1 - \phi_s)$

The hydraulic diameters are calculated according to the following:

In the axial flow direction we have the perimeter given as

$$3 \frac{\pi}{6} 2b = \pi b = \hat{P} \quad (5.1)$$

and the free flow area for the same unit is

$$\frac{1}{2} 2s \sqrt{3} s - 3 \frac{1}{6} \pi b^2 = s^2 (\sqrt{3}) (1 - \phi_s) = A_z \quad (5.2)$$

For hydraulic diameters given by 4 times flow area divided by the perimeter, for the geometry as shown in Fig. 8, we have:

$$D_{hz} = \frac{4 \sqrt{3} s^2 (1 - \phi_s)}{\pi b} \quad (5.3)$$

$$D_{hx} = \frac{4(2s)(\Delta z)(1 - \phi_s)}{2 \Delta z + 2 \Delta y (1 - \phi_s)} \simeq 4s (1 - \phi_s) \quad (5.4)$$

$$D_{hy} = \frac{4 (2 \sqrt{3} s) (\Delta z) (1 - \phi_s)}{2 \Delta z + 2 \Delta x (1 - \phi_s)} \simeq 4 \sqrt{3} s (1 - \phi_s) \quad (5.5)$$

Other quantities of interest are:

$$\text{Number of tubes per unit cross section area normal to } z = \frac{1}{2 \sqrt{3} s^2} \quad (5.6)$$

$$\text{Solid surface area per unit volume} = \frac{\pi b}{2 \sqrt{3} s^2} \quad (5.7)$$

Note that although the mean porosities in all directions are known, most of the flow and heat convection data for flow across tubes are based on minimum flow areas (see 5.2).

The above averaging for mean flow area appears to be applicable mainly to a system of nearly uniform openings in the x and y direction. Obviously

* $\frac{\text{Mean area between 4 tubes}}{\text{Mean height in x direction}} = \frac{2 [(1/2) 2s \sqrt{3}s - 3(1/6)\pi b^2]}{\sqrt{3} s}$

if, in Fig. 8, $S_{TX} = 2b$, flow area in the x-direction would be zero. The basic equation based on uniform (net flow area)/(free flow area) is still valid because such an opening will give infinite flow resistance.

The above choice in place of a tensorial porosity is made for the following reasons:

(a) Based on the mean velocity in the inter-tubular spaces, the dynamic equations remain the same for all geometries of tube bundle or even without the presence of tubes. The flow parameters such as friction factor and Nusselt numbers, etc., correlated empirically based on minimum openings are readily incorporated into the calculations of forces and relaxation times.

(b) Use of tensorial porosity and still having to use empirical correlations is a redundant effort -- complication without gaining anything conceptually.

(c) Interactions among the phases are related to the components of mean velocities rather than to the maximum velocity components. Formulation based on the minimum flow area in each direction will lead to errors. The use of mean velocities away from the boundary of a particle phase including stationary tubes is one of the basic concepts of multiphase mechanics,

5.1 Tube Geometry and Phase-Domain Transition

Bubbles in a fluidized bed were shown to possess very low surface tension [37]. The integrity of bubbles as they pass the tube banks is in question. However, the measurements by Chen [46] demonstrated that their effect on heat transfer is important. We shall, for the present, treat the problem based on substantial integrity of bubbles as they pass the tube banks. We shall refer to the coordinate system in Fig. 9 with vertical tubes immersed in a portion of the bed.

The limiting size of a bubble is one that fills the space between three tubes, and the limiting radius or the radius at transition a_m is given by

$$\pi a_m^2 / 2 = \sqrt{3} s^2 - (\pi/2)b^2 = \sqrt{3} s^2 (1 - \phi_s) \quad (5.8)$$

or

$$a_m = [2(\sqrt{3}/\pi) (1 - \phi_s)]^{1/2} s \quad (5.9)$$

and the corresponding axial length Δz is given by

$$(\Delta z) \pi a_m^2 = (4\pi/3) a_m^3 \quad (5.10)$$

Fig. 9. Bubbles as Phases, Heterogeneous Phases and Domains and Their Transitions

or $\Delta z = (4/3) a_m$. For bubble radius below a_m , bubbles are at the same temperature as the gas in the bed. For bubble radius above a_m , bubbles are in contact with the tube, causing a decrease in heat transfer rate. Radius a_m , therefore, marks the transition from multiphase regime to the heterogeneous phase regime within the framework of the tube bundle. A multi-heterogeneous phase is one in which the bubble phase encloses solid structures, such as a tube, in the present study. When these bubbles coalesce to a size of characteristic dimension to the same order of magnitude of the tube bundle, each of these bubbles will be treated as a discrete domain (Fig. 9).

Within a volume $\Delta x \Delta y \Delta z$, bubble coalescence forms a new phase, which we have defined as heterogeneous phase. The number of bubbles is now given by:

$$\begin{aligned} & \Delta x \Delta y \Delta z / (1/2) 2s (\sqrt{3}) s (2) (4/3) a_m^3 \\ & = \Delta x \Delta y \Delta z / 2 (\sqrt{3}) (4/3) (\sqrt{3}/\pi)^{1/2} s^3 (1 - \phi_s)^{1/2} \\ & = (\Delta x \Delta y \Delta z) N_v \end{aligned} \quad (5.11)$$

where N_v is the number density of particles at that location. The limiting density of bubble species k is given by:

$$\rho_{bk} = \bar{\rho}_{bk} N_v (4\pi/3) a_m^3 = \bar{\rho}_{bk} \phi_{bk} \quad (5.12)$$

as it should be. Hence, $\phi_{bk} = 1 - \phi_s$ for bubbles to begin to merge.

The bubble of radius R covering several tubes, i.e., a heterogeneous phase has a mass of gas given by, for $R > a_m$

$$(4\pi/3) R^3 \bar{\rho}_{bk} [1 - \phi_s] \quad (5.13)$$

The tube area covered is thus, for bubble volume $V > (4\pi/3) a_m^3$

$$V \frac{\pi b}{2\sqrt{3} s^2} \quad (5.14)$$

and the limiting value for $a = a_m$ (multiphase) or $a = a_m / (1 - \phi_s)^{1/3}$ (heterogeneous phase) is

$$\frac{4 \sqrt{2\pi}}{3^{3/4}} (1 - \phi_s)^{1/2} sb \quad (5.15)$$

Hence we have these cases:

$$a < a_m, \phi_k < 1 - \phi_s$$

multiphase regime, bubbles remain at bed temperature

$a = a_m, \phi_k = 1 - \phi_s$ imminent transition, each bubble contacts a surface area of $4[(2\pi/\sqrt{3})(1 - \phi_s)]^{1/2}$ sb

$a > a_m, \phi_{bk} = N_k (4\pi/3) R^3 - \phi_s$ multiheterogeneous-phase regime, bubbles enclose tubes, with surface area of $\frac{4\pi}{3} R^3 \left(\frac{\pi b}{2\sqrt{3} s^2} \right)$ each.

$R \lesssim R_c$ Discrete domain regime, R_c is the characteristic radius of the tube bundle. (Before a large bubble encompasses the whole region of tube bundle to form a discrete domain). (5.16)

5.2 Flow Resistance and Heat Transfer

Before the raw data from the experimental results on fluidized bed heat transfer [46, 47] are correlated in a manner than can be used in our numerical computation, the flow and heat transfer relations in this section must be treated as tentative, illustrative, or as an approach toward correlation of data. Modification of empirical coefficients will be made in our study as more experimental data become available. For the present study, the longitudinal direction of the tubes and the direction of gravity is aligned with the z axis, with the x and the y axes transverse to it. Botterill, et al. [43] measured flow resistance in the transverse direction. The flow resistance of the tubes per unit volume of the fluid is given in terms of the components R_x, R_y , and R_z , and the heat transfer coefficients at the tube surfaces are given as $\hat{h}_x, \hat{h}_y$, and $\hat{h}_z$.

In general, the flow resistance is given by: (for gas phase ρ_g)

$$R_{gj} = -4\hat{f}_j \bar{\rho}_g |U_{gj}| U_{gj} / 2 D_{hj} \quad (5.17)$$

where $\hat{f}_j$ is the friction factor in the j-direction and the heat flow by convection per unit volume of fluid is given by:

$$\begin{aligned} J_j &= \hat{h}_j (T_w - T_g) \text{ (tube surface area per unit volume)} \\ &= \hat{h}_j (T_w - T_g) (\pi b / 2 \sqrt{3} s^2) \end{aligned} \quad (5.18)$$

where $\hat{h}_j$ is the heat transfer coefficient for flow in the j-direction, subscript w denotes tube wall.

For laminar flow, the friction factor is given by

$$\hat{f}_z = 64/Re_z, \quad (5.19)$$

where Re_z is the Reynolds number for flow in the z-direction, given by

$$Re_z = \frac{D_{hz} |U_{gz}| \bar{\rho}_g}{\mu_g} \quad (5.20)$$

μ_g is the viscosity, $\bar{\rho}_g$ is the density of the gas phase g, and U_{gz} is the mean velocity in the passage. The Nusselt number for heat transfer given by [48]

$$Nu_z = \frac{\hat{h}_z D_{hz}}{\kappa_g} = 4.12, \quad (5.21)$$

where κ_g is the thermal conductivity of the gas phase.

For crossflow in the x and the y directions, the resistance force per unit length of a tube of radius b is given by [49]

$$(\text{Force}/\Delta z)_j = \frac{4 \pi \mu_g U_{gjm}}{1/2 - \gamma - \ln \left(\frac{U_{gjm}}{4v} b \right)} = \frac{4 \pi \mu_g U_{gjm}}{\alpha} \quad (5.22)$$

for $j = x, y$, where v is the kinematic viscosity of the gas phase, γ is the Eulers constant (0.5772157), and U_{gjm} is the maximum velocity. When applied to the tube system, the force exerted on a given volume $\Delta x \Delta y \Delta z$ containing the tubes is given by

$$\text{Force}/(\Delta z \Delta x \Delta y) \frac{1}{2\sqrt{3}s^2} = \frac{4\pi\mu_g U_{gjm}}{\alpha} \Delta z (\Delta x \Delta y) \frac{1}{2\sqrt{3}s^2} \quad (5.23)$$

for $j = x$ or y , or

$$R_{x,y} = \frac{-2\pi \mu_g U_{gjm}}{\sqrt{3} \alpha s^2} \quad (5.24)$$

The Nusselt number for heat transfer is given by

$$Nu_{x,y} = 0.43 + K_d (Re_d)^m (Pr)^{0.31} = \hat{h} 2b / \kappa_g, \quad (5.25)$$

where K_d and m are constants, Re_d is based on tube diameter $2b$, and Pr is the Prandtl number.

For the case of turbulent flow,

$$\hat{f}_z = 0.046(\text{Re})^{-0.2}, \quad (5.26)$$

$$\text{Re}_z = |\hat{G}_z| D_{hz} / \mu_g = \bar{\rho}_g |U_{gz}| D_{hz} / \mu_g, \quad (5.27)$$

$$\hat{j}_z = \hat{f}_z / 2, \quad (5.28)$$

and the heat transfer coefficient

$$\frac{\hat{h}_{gz}}{C_{pg} |\hat{G}_z|} = \hat{j}_z (\text{Pr}_g)^{-2/3}, \quad (5.29)$$

where Pr_g is the Prandtl number of the gas.

The crossflow resistance and heat transfer are not well correlated, for the system given in Fig. 8 [48]

$$R_x = \left(\frac{\Delta P}{L} \right)_x = \frac{-0.0146 \hat{f}_x' |\hat{G}_{gx}| \hat{G}_{gx}}{\bar{\rho}_g \sqrt{s}} \left(\frac{\mu_{gw}}{\mu_g} \right)^{0.14} \quad (5.30)$$

and, similarly, for y component for quantities in SI units, and

$$\hat{f}_x' = \left[0.25 + \frac{0.118}{\left(\frac{S_{TX}}{2b} - 1 \right)^{1.08}} \right] \left(\frac{|\hat{G}_{gx}| 2b}{\mu_g} \right)^{-0.16} \quad (5.31)$$

for staggered tubes, and μ_g , μ_{gw} are the viscosities based on the bulk temperature and wall temperature, and correspondingly for the y-direction. $\hat{G}_g$ is the mass flow at the minimum area in $\text{Kg} / \text{m}^2 \text{ sec}$.

The Nusselt number of heat transfer is given by [48],

$$\text{Nu}_{x,y} = 0.33 C_H \left(\frac{|\hat{G}_{\max}| 2b}{\mu} \right)^{0.5} \text{Pr}_g^{0.3} = h_{gx,y} (2b) / \kappa_g \quad (5.32)$$

where C_H is a constant depending on tube geometry.

In a dense particle suspension, the above relations might be used for estimation purposes with mixture quantities in place of gas quantities. However, when specular reflection of particles is important, we have [35] [50] for the flow along the tubes

$$R_{g\ell kz} = -\frac{(2\pi)^{3/2}}{4} (1 + r^*) \hat{f} \rho_{\ell k} \bar{v}_{\ell k}^{-2} \left(\frac{b}{s}\right) \frac{U_{\ell kz}}{|U_{\ell k}|} \quad (5.33)$$

where $\hat{f}$ is the friction factor and $\bar{v}_{\ell k}^2$ is the mean squared velocity of random motion of the particles. For crossflow over tubes, we have

$$R_{g\ell kx,y} = -\frac{1}{2\sqrt{3}} \left(1 + \frac{r^*}{3}\right) \rho_{\ell k} |U_{x,y}| U_{x,y} \left(\frac{b}{s}\right) \quad (5.34)$$

The corresponding heat transfer coefficient for flow along the tubes is:

$$\hat{h}_{wz} = \alpha_{\ell kw} (2.94) \left(\frac{3}{4}\right)^{2/5} \rho_{\ell k} \frac{\kappa_{\ell k}}{\bar{\rho}_{\ell k} a_{\ell k}} \left(\sqrt{\frac{k_{\ell k}}{k_w}} + \sqrt{\frac{k_w}{k_{\ell k}}}\right)^{4/5} (N_{Im})^{4/5}, \quad (5.35)$$

where $\alpha_{\ell kw}$ is the accommodation coefficient of impact of ℓk particles with the wall, $\alpha_{\ell kw} < 1$, and

$$N_{Im} = 5\pi^2 \bar{v}_{\ell k}^{-2} \frac{\rho_w}{\rho_p} \sqrt{k_{\ell k} k_w} \frac{1 + r^*}{2}.$$

For crossflow

$$\hat{h}_{wx,y} = \alpha'_{\ell kw} (2.94) \frac{15}{(14)8\pi(2)^{2/5}} \rho_{\ell k} \frac{\kappa_{\ell k}}{\bar{\rho}_{\ell k} a_{\ell k}} \left(\sqrt{\frac{k_{\ell k}}{k_w}} + \sqrt{\frac{k_w}{k_{\ell k}}}\right)^{4/5} (N_{Im})_{x,y}^{4/5}, \quad (5.36)$$

where $\alpha'_{\ell kw}$ is the accommodation coefficient for crossflow, and

$$N_{Im} = 5\pi U^2 \bar{\rho}_{lk} \sqrt{k_{lk} k_w} \left(\frac{1 + r^*}{2} \right)$$

5.3 Flow Resistance of the Interface - Heterogeneous Phase and Domain

Because of the amount of solid surfaces present in the tube bundle as depicted in Fig. 8, the interface force is mainly contributed by the surface force at the dense phase-bubble-solid interface. Such a force might be significant for $a > a_m$; that is, in the heterogeneous phase and discrete domain ranges.

For the elementary surface with surface tension σ in Fig. 10 (a) and (b), the force per unit area is given by

$$\hat{p}_{sz} = \left(\frac{\text{No. of tubes}}{\text{area}} \right)_z \sigma (2\pi b) = \frac{1}{2\sqrt{3} s^2} \sigma 2\pi b = \sigma \frac{\pi b}{\sqrt{3} s^2}, \quad (5.37)$$

$$\hat{p}_{sx} = \left(\frac{\text{No. of tubes}}{\text{area}} \right)_x \sigma (b + \Delta z) 2 \approx \frac{\sigma}{s}, \quad (5.38)$$

and

$$\hat{p}_{sy} = \left(\frac{\text{No. of tubes}}{\text{area}} \right)_y \sigma (b + \Delta z) 2 \approx \frac{\sigma}{\sqrt{3} s}. \quad (5.39)$$

in the opposite direction of displacement.

The magnitude of σ is of the order of 10^{-3} N/m for a fluidized bed bubble which is much smaller than ordinary liquids, [37] and these forces are expected to be small.

When applied to the system of tubes and a bubble of radius R , the resistance force acting on this bubble in the z -direction is given by

$$\begin{aligned} \hat{F}_{Az} &= 2 \int_0^{\pi/2} \left[\frac{2\pi b \sigma}{\cos \theta} \right] \left[n_{Az} 2\pi R \sin \theta R d\theta \cos \theta \right] \cos \theta \\ &= 8\pi^2 \sigma n_A b R^2 = \frac{4\pi^2 \sigma}{\sqrt{3} s^2} b R^2, \end{aligned} \quad (5.40)$$

where n_{Az} is the number of tubes per unit area normal to z .

In the x or y direction (length $2R \sin \theta$, number of pins = $\frac{1}{2\sqrt{3} s^2} 2\pi R^2 \sin \theta d\theta$),

$$\begin{aligned} \hat{F}_{Rx} &= \hat{F}_{Ry} = 2 \int \frac{\sigma 2\pi b}{\sin \theta} \frac{1}{2\sqrt{3} s^2} 2\pi R^2 \sin^2 \theta d\theta \\ &= \frac{4\pi^2}{\sqrt{3}} \sigma \frac{b R^2}{s^2} \end{aligned} \quad (5.41)$$

Fig. 10. Resistance to Motion at the Bubble-Solid Wall Interface

For bubble density ρ_b , $a > a_m$, the resistance due to surface force is given by

$$\begin{aligned} R_{sz} &= \sqrt{3} \pi \phi_b (\sigma b^2 / R s^2) (-U_{sj} / |U_{sj}|) \\ &= R_{sx} = R_{sy} \end{aligned} \quad (5.42)$$

It is also interesting to note that for a single bubble of $a_b > a_m$, the drag coefficient is given by: (for ρ_e of the dense phase)

$$C_{Ds} = \frac{8\pi^2 \sigma n_A b R^2}{\pi R^2 \frac{1}{2} \rho_e U_z^2} = \frac{8}{(We)_{b,n_A}} \quad (5.43)$$

where the Weber number is given by:

$$(We)_{b,n_A} = \frac{\rho_e U_z^2}{\sigma} \frac{1}{2\pi n_A b} = \frac{\rho_e U_z^2}{\sigma} \left(\frac{\sqrt{3} s^2}{\pi b} \right)$$

Next we consider the resistance force to bubble expansion. The relations of tangential force F_θ and F_z to radial force F_r are shown in Fig. 10(e).

$$d\hat{F}_\theta = \frac{2\pi b \sigma}{\cos \theta} \left[n_{Az} 2\pi R \sin \theta R d\theta \cos \theta \right] + 2\pi r \sigma n_{Az} 2\pi R^2 \sin^2 \theta \cos \theta d\theta, \quad (5.44)$$

where the first term is the force along spherical surface consisting of force per tube times the number of tubes over $d\theta$ at θ ; and the second term is the θ -component of force in the z -direction.

The r -component of force in the z -direction is given by

$$\begin{aligned} d\hat{F}_r &= \frac{2\pi b \sigma}{\cos \theta} \left[n_{Az} 2\pi R^2 \sin \theta \cos \theta \right] \cos \theta \cos \theta d\theta \\ &= 2\pi b \sigma n_{Az} 2\pi R^2 \sin \theta \cos^2 \theta d\theta. \end{aligned} \quad (5.45)$$

The radial force per unit area of sphere resisting expansion is given by

$$\frac{d\hat{F}_r}{2\pi R \sin \theta R d\theta} = 2\pi b \sigma n_A \cos^2 \theta = f_r \quad (5.46)$$

Similarly, the tangential force per unit area is given by

$$\begin{aligned} \frac{dF_\theta}{2\pi R \sin\theta R d\theta} &= 2\pi b \sigma n_A + 2\pi b \sigma n_A \sin\theta \cos\theta \\ &= 2\pi b \sigma n_A \left[1 + \frac{1}{2} \sin^2\theta \right] \end{aligned} \quad (5.47)$$

It is seen that for a bubble over the tubes to be approximated adequately by a sphere, f_r must be smaller than the surface tension effect, or

$$f_r \sim 2\pi b \sigma n_{Az} \ll \frac{2\sigma}{R},$$

or

$$\pi b \sigma \cdot \frac{1}{2\sqrt{3} s^2} \ll \frac{\sigma}{R} \quad (5.48)$$

giving

$$\pi b^2 \frac{1}{2\sqrt{3} s^2} = \pi b^2 \cdot n_A \ll \frac{b}{R} \quad (5.49)$$

The left-hand side has the meaning of solidity. Hence, approximation of a bubble by a sphere has to satisfy the condition:

$$\frac{b}{s} \ll \frac{\left(\frac{2\sqrt{3}}{\pi}\right)^{1/2}}{(1 - \phi_s)^{1/2}}; \quad (5.50)$$

i.e., small tubes at large spacing.

5.4 Transport Parameters Relating to Tube Bundles

For a chosen range of bubble sizes k ,

$$\rho_{bk} = \phi_{bk} \bar{\rho}_g, \quad (5.51)$$

where $k = 1, 2, 3, 4$

$$\rho_g = \bar{\rho}_g (1 - \phi_s - \sum_{k, \ell} \phi_{\ell k}) \quad (5.52)$$

Transition from one species of bubble to another occurs via generation, expansion, and coalescence due to relative motion. To account for expansion

and compression due to temperature and pressure variations, we shall choose different a_{bk} 's according to mass of bubbles rather than size a_{bk} . Therefore, reference to a_{bk} is made for a given temperature and pressure combination.

After $a_{bk} > a_m$ is reached, increase in bubble size occurs by heating and gas influx, rather than by coalescence via relative motion. Beyond a_m , the bubble radius jumps to $a_{bk}/(1 - \phi_s)^{1/3}$ for $a_{bk} > a_m$. We treat $a_{bk} = a_{bk}(x_j, t)$, and $\rho_{bk} = N_{bk} \frac{4\pi}{3} a_{bk}^3 \bar{\rho}_g$, with N_{bk} , a_{bk} , $\bar{\rho}_{bk}$ as variables. Coalescence occurs by merging when $\phi_b = 1 - \phi_s$ at a given location.

At slow relative motion, the inverse relaxation times for momentum, energy and mass transfer between phases are:

$$F_{\ell kg} = 9 \bar{\mu}_g / 2 a_{\ell k}^2 \bar{\rho}_{\ell k} \quad (5.53)$$

$$G_{\ell kg} = 3 \kappa_g / c_{v\ell k} a_{\ell k}^2 \bar{\rho}_{\ell k} \quad (5.54)$$

$$M_{\ell kg} = (\rho_{\ell k} / \bar{\rho}_{\ell k}) 3 D_{\ell kg} / a_{\ell k}^2 \quad (5.55)$$

where $D_{\ell kg}$ is the diffusivity of the gas phase. Modifications to relative motion at high velocity are given empirically in [35].

For the particular system under consideration, the presence of the tubes gives rise to $R_{\ell kj}$ and $J_{\ell k}$, the volumetric resistance force and heat source (or sink). We define volumetric resistance and volumetric heat source according to the inverse relaxation times F_{kw} and G_{kw} , or

$$R_{\ell kj} = - \rho_{\ell k} F_{\ell kwj} U_{\ell kj} \quad (5.56)$$

$$R_{gj} = - \rho_g F_{gwj} U_{gj}$$

and

$$J_{\ell k} = c_{p\ell k} \rho_{\ell k} G_{\ell kw} (T_w - T_{\ell k}) \quad (5.57)$$

$$J_{Eg} = c_{pg} \rho_g G_{gw} (T_w - T_g) .$$

The surface tension at the interface passing the tubes further gives rise to

$$R_{bksj} = - \rho_{bk} F_{bksi} U_{bkj} \quad (5.58)$$

for the resistance to bubbles moving over tubes.

In the interest of conformity to fundamentals, the Reynolds number is a measure of state of motion in terms of the ratio of inertia force to viscous force. We define:

$$Re_{\ell k} = \frac{\bar{\rho}_{\ell k} |U_{\ell k}| 2b}{\mu_{\ell k}} \quad (5.59)$$

$$Re_g = \frac{\bar{\rho}_g |U_g| 2b}{\mu_g} \quad (5.60)$$

and

$$|U| = \left[U_x^2 + U_y^2 + U_z^2 \right]^{1/2} \quad (5.61)$$

is the net speed of motion past the tubes. Re_{fz} in Eq. (5.20) is thus, because

$$G_z = \bar{\rho}_g U_{gz}:$$

$$Re_{gz} = Re_g \frac{D_{hz}}{2b} \left| \frac{U_{gz}}{U_g} \right| \quad (5.62)$$

and Eq. (5.19) becomes:

$$\hat{f}_z = \frac{64}{Re_{gz}} \frac{2b}{D_{hz}} \left| \frac{U_g}{U_{gz}} \right| \quad (5.63)$$

since

$$\left(\hat{G}_{\max} \right)_j = \bar{\rho}_g \cdot \bar{U}_{gj} \left(\frac{A_{\text{mean}}}{A_{\text{min}}} \right)_j \quad (5.64)$$

or

$$\begin{aligned} \frac{\left(\hat{G}_{\max} \right)_j}{\mu_g} &= \bar{\rho}_g \left(\bar{U}_{gj} \right) \frac{A_{\text{mean}}}{A_{\text{min}}} \cdot \frac{2b}{\mu_g} \\ &= Re_{gj} \left| \frac{U_{gj}}{U_g} \right| \end{aligned} \quad (5.65)$$

In this manner, the relaxation times of gas-tube surface interaction can be obtained from the equations in Sec. 5.2.

(a) Laminar motion: (from Eqs. 5.17, 5.2, and 5.18)

$$F_{g wz} = \frac{4(32)}{Re_g} \frac{1}{\phi_g} \frac{2b}{D_{hz}^2} |U_g|, \quad (5.66)$$

$$F_{g wx, y} = \frac{2}{Re_g \sqrt{3} \alpha} \frac{2b}{s} |U_g|, \quad (5.67)$$

$$G_{g wz} = \left(\frac{\kappa_g}{\bar{\rho}_g c_{pg}} \right) (Nu)_z \frac{1}{\phi_g} \frac{\pi b}{D_{hz} 2\sqrt{3} s^2}, \quad (5.68)$$

where $\kappa_g / \bar{\rho}_g c_{pg}$ is the thermal diffusivity of the gas from Eq. (5.68),

and

$$G_{gwx,y} = \frac{\kappa_g}{\rho_g c_{pg}} (Nu)_{x,y} \frac{\pi b}{D_{hx,y} 2\sqrt{3} s^2} \frac{1}{\phi_g} \quad (5.69)$$

(b) Turbulent flow

$$\hat{f}_{gz} = \frac{0.046}{Re_g^{0.2}} \left[\frac{D_{hz}}{2b} \left| \frac{U_{gz}}{U_g} \right| \right]^{-0.2} \quad (5.70)$$

From Eqs. (5.17), (5.26), (5.30) and (5.31)

$$F_{gwz} = \frac{4(0.046)}{\phi_g (Re_g)^{0.2}} \left[\frac{2b}{D_{hz}} \left| \frac{U_g}{U_{gz}} \right| \right]^{0.2} \frac{U_g}{2D_h} \quad (5.71)$$

$$F_{gwx,y} = \frac{4(0.0146) \hat{f}_{x,y}}{\sqrt{3} s} \frac{|\hat{G}_{gx}|}{\rho_g \phi_g} \left(\frac{\mu_{gw}}{\mu_g} \right)^{0.14} \quad (5.72)$$

$$G_{gwz} = \frac{\hat{f}_{gz}}{2} \frac{Pr^{-2/3}}{\phi_g} U_{gz} \frac{\pi b}{2\sqrt{3} s^2} \quad (5.73)$$

$$G_{gwx,y} = \frac{\kappa_g}{\rho_k c_{pk}} (Nu)_{x,y} \frac{\pi b}{\phi_g D_{hx,y} 2\sqrt{3} s^2} \quad (5.74)$$

The inverse relaxation times of momentum and energy transfer between the particles ℓk ($\ell = c, d$) and the tubes are given by [35]

$$F_{\ell kwz} = \frac{(\overline{U_{\ell k}})^{1/2}}{2\sqrt{\pi}} \frac{\pi b}{2\sqrt{3} s^2} \quad (5.75)$$

$$F_{\ell kwx,y} = \frac{2}{\pi} (\overline{U_{\ell k}})_{x,y} \left(1 + \frac{r^*}{3} \right) \frac{\pi b}{2\sqrt{3} s^2} \quad (5.76)$$

$$G_{\ell kwz} = \frac{\hat{h}_{\ell kwz}}{\rho_{\ell k} c_{\ell k}} \frac{\pi b}{2\sqrt{3} s^2} \quad (5.77)$$

$$G_{\ell kwx,y} = \frac{\hat{h}_{\ell kwx,y}}{\rho_{\ell k} c_{\ell k}} \frac{\pi b}{2\sqrt{3} s^2} \quad (5.78)$$

where the $\hat{h}_{\ell kw}$ terms are from Eqs. (5.35) and (5.36).

The resistance due to surface force is given by

$$\begin{aligned}\hat{F}_{k\sigma} &= \frac{\sqrt{3} \pi \sigma b}{\rho_k U_{kj} R s^2} \\ &= \frac{3}{8} \frac{\rho_e}{\rho_k} C_{d\sigma} \frac{|U_{kj}|}{R}\end{aligned}\quad (5.79)$$

where the drag coefficient

$$C_{d\sigma} = 8 \frac{\pi \sigma b}{\sqrt{3} \rho_e |U_{kj}|^2 s} = \frac{8}{We}, \quad (5.80)$$

and

$$We = \frac{\sqrt{3} \rho_e |U_{kj}|^2 s^2}{\pi \sigma b}, \quad (5.81)$$

and

$$\begin{aligned}R_{b\sigma z} &= -\rho_k F_{k\sigma} U_{kj} = \sqrt{3} \pi \phi_k \sigma b / R s^2 \\ &= -\sqrt{3} \pi \phi_k \frac{\sigma b}{R s^2 |U_{kj}|} U_{kj}.\end{aligned}\quad (5.82)$$

Hence, $R_{b\sigma z}$ is independent of the magnitude of the velocity and is opposite to its direction.

6.0 Basic Equations

In order to treat a fluidized-bed combustion system with a large number of components and phases, systematic identification of various species is necessary. We shall use the convention in Section 4.

Most of the equations are from Ref. [1], although special concern will be given to the energy equation to account for the heat of reaction. For direct application to computer programming, we refer to the Cartesian coordinates in Fig. 5.

We note that although there is a large number of chemical species in the gas phase, all are at the same mass velocity and static temperature. Hence, there are three (Cartesian components) momentum equations, and one energy equation of the gas phase, which has as many continuity equations as there are identifiable chemical species. The other phases are identified similarly as in Ref [1], although the continuity equation of the bubble phase is based on the conservation of the number of bubbles per unit volume.

Simplification is available to the fluidized bed system in:

Momentum equations: neglect the effect of virtual mass and Basset force in the dense phase;

Energy equations: neglect the effects of kinetic energy and viscous dissipation.

Special consideration is needed when dealing with a tube bundle submerged in a fluidized bed. In multiphase mechanics, we define the velocity of the fluid phase in a suspension by neglecting the distribution of velocity around each particle; effects of velocity distribution are accounted for via transport parameters such as the relaxation time for momentum transfer. In the same way, a velocity component of fluid passing a bundle of tubes is the mean velocity component based on the mean flow area* and the flow resistance in that direction; detailed distribution inside the passage is again accounted for via transport parameters.

We may define the density of a phase including the volume allocated to the tubes ρ_{lk} and excluding the volume occupied by the tubes, $\hat{\rho}_{lk}$, thus

$$\rho_{lk} = \hat{\rho}_{lk} (1 - \phi_s)$$

One choice of mean passage area further gives:

$$\hat{U}_{lkj} = U_{lkj} (1 - \phi_s)$$

Hence, we have

$$\rho_{lk} U_{lkj} = \hat{\rho}_{lk} \hat{U}_{lkj}$$

Formulations in this chapter will treat flow, heating and phase change in the tube bundle system according to the following ranges:

Multiphase: $a_{bk} < a_m$

$$\begin{aligned} \rho_g &= \bar{\rho}_g \phi_g \\ \rho_{bk} &= \rho_{bk} \phi_{bk} \end{aligned} \tag{6.1}$$

$$\phi_s + \sum_l \sum_k \phi_{lk} + \phi_g = 1 \tag{6.2}$$

where $l = c, d$ and b .

* We also have the option of choosing the minimum flow area in each direction, but this choice will call for significant modification of the dynamic equation because of anisotropy in the minimum flow area.

In case of an impermeable array of tubes, the velocity component normal to that array goes to zero because resistance goes to infinity.

Bubbles are heated and accelerated (except buoyancy) by the dense phase. Bubble growth occurs with gas influx into it.

Heterogeneous Phase: $a_{bk} \geq a_m$ jumpwise transition to $a_{bk} = a_m / (1 - \phi_s)^{1/3}$

$$\rho_{bk} = \bar{\rho}_{bk} \phi_{bk} \quad (6.3)$$

$$\phi_s + \sum_l \sum_k \phi_{lk} + \phi_g = 1 \quad (6.4)$$

as before, only the volume of a bubble includes that of the tubes encompassed within it.

Bubbles are cooled and slowed down by tubes also; bubble size may change via cooling by the tubes and influx of gas, especially at the interface of three phases, i.e., the dense phase, the bubble and the tube wall. Different bubble sizes exist at different locations. Coalescence occurs when $\phi_{bk} = (1 - \phi_s)$ at a given point.

Discrete domain: $a_{bk} < R_c$ as multiheterogeneous phase bubbles merge by growth. Each domain is treated as a distinct fluid body. A domain may occupy a substantial portion of the volume of the system under consideration. Interface relations become significant only when considering a discrete domain, which appears only under a slugging bed condition. R_c is the equivalent radius of the tube bundle.

Since we are only concerned with components of a suspension at low relative velocities, the effectiveness of momentum transfer $K = 1$, [35]. In addition, because of the presence of the tubes, bubble-bubble interaction is insignificant compared to bubble-dense phase interaction. The bubble suspension is "dilute" except for coalescence. The effect of pressure gradient on bubble motion is negligible [51].

To account for the effect of coalescence and growth, a range of discrete bubble sizes (bk) will be taken. This is to replace the gradual change in sizes by a gradual change in population of bk.

Including the specific system of tube bundles, the computations and formulations will proceed along the following routes. The regimes of calculations are:

(a) locally $a_{bk} \geq a_m$ proceed as heterogeneous phase with a bk as a function of position and time. Bubbles grow and merge into discrete domain when

(b) $a \geq R_c$; R_c is the equivalent radius of the bundle.

Only discrete domains call for calculation including interface equations. Discrete domains may consist of a dense phase with or without bubbles and dilute phase with or without solids. This regime will be treated in a future report.

Tube orientation: The formulations in this chapter are directly applicable to immersed boiler tubes which are vertical (along z) with equilateral triangular spacing (terms of R 's and $\hat{h}_w$). When applied to horizontal or inclined tubes, R 's should be realigned with respect to the orientation of the tubes. Because of the flow patterns in the bed, regardless of the orientation of the tubes, both axial and cross flows occur over the tubes.

6.1 Continuity Equations

The continuity equations for chemical species of the gas phase take the form

$$\frac{\partial \rho_{gk}}{\partial t} + \frac{\partial \rho_{gk} U_{gx}}{\partial x} + \frac{\partial \rho_{gk} U_{gy}}{\partial y} + \frac{\partial \rho_{gk} U_{gz}}{\partial z} = \Gamma_{gk} \quad (6.5)$$

where the Γ_{gk} terms are given by Eqs. (2.56) to (2.62)

$$\Gamma_{gk} = M_k \frac{dn_k}{dt}$$

with $k = 1$ to 8 , and $\Gamma_{g8} = 0$ as postulated. U_g is common to all gas species because they have the same mass velocity at a given position and time. There are altogether gk continuity equations.

The char and dolomite are represented by phases ck and dk based on initial sizes and stages of chemical conversion. Denoting by species lk ($l = c, d$) we have

$$\frac{\partial \rho_{lk}}{\partial t} + \frac{\partial \rho_{lk} U_{lkx}}{\partial x} + \frac{\partial \rho_{lk} U_{lky}}{\partial y} + \frac{\partial \rho_{lk} U_{lkz}}{\partial z} = \Gamma_{lk} \quad (6.6)$$

where the Γ_{lk} terms are given by Eqs. (2.77) and (2.80). This gives an additional (ck) and (dk) equation.

For the bubble phase, continuity is based on conservation in number of bubbles and the effect of coalescence. For bk species, we have

$$\frac{\partial N_{bk}}{\partial t} + \frac{\partial N_{bk} U_{bkx}}{\partial x} + \frac{\partial N_{bk} U_{bky}}{\partial y} + \frac{\partial N_{bk} U_{bkz}}{\partial z} = \Gamma_{(N)bk} \quad (6.7)$$

where the $\Gamma_{(N)bk}$ terms are given by Eqs. (3.19) to (3.23), and $\rho_{bk} = N_{bk} \frac{4\pi}{3} a_{bk}^3 \rho_g$. The bubble phase gives us bk equations.

Hence, we have altogether $(gk) + (ck) + (dk) + (bk)$ continuity equations for each discrete domain.

6.2 Momentum Equations

Since the gas mixture has a single mass velocity $\underline{U}_g$, we have the momentum equations of the gas phase [1]:

$$\begin{aligned}
 & \frac{\partial \rho_g}{\partial t} \underline{U}_{gx} + \frac{\partial \rho_g}{\partial x} \underline{U}_{gx}^2 + \frac{\partial \rho_g}{\partial y} \underline{U}_{gx} \underline{U}_{gy} + \frac{\partial \rho_g}{\partial z} \underline{U}_{gx} \underline{U}_{gz} \\
 &= - \frac{\partial \phi_g}{\partial x} P + \frac{\partial}{\partial x} \left(\tau'_{gx} \right)_{xx} + \frac{\partial}{\partial y} \left(\tau'_{gx} \right)_{yx} + \frac{\partial}{\partial z} \left(\tau'_{gx} \right)_{zx} \\
 &+ \frac{\partial}{\partial x} \rho_g (U_{mx} - U_{gx})^2 + \frac{\partial}{\partial y} \rho_g (U_{mx} - U_{gx})(U_{my} - U_{gy}) \\
 &+ \frac{\partial}{\partial z} \rho_g (U_{mx} - U_{gx})(U_{mz} - U_{gz}) + \Gamma_g U_{mx} - \sum_{ck} \rho_{ck} F_{ckg} (U_{gx} - U_{ckx}) \\
 &- \sum_k \rho_{dk} F_{dkg} (U_{gx} - U_{dkx}) - \sum_k \rho_{bk} F_{bkg} (U_{gx} - U_{bkx}) - \rho_g F_{gwx} U_{gx} \\
 &- \sum I'_{\ell kx} - \sum V'_{\ell kx} , \quad (6.8)
 \end{aligned}$$

where $\rho_g = \sum_k \rho_{gk}$, P is the pressure, I' is the inertial force due to virtual mass, V' is the force due to unsteady flow field, and F_{gw} is the inverse relaxation time of interaction with submerged solid surfaces.

In all momentum equations, we have

$$\begin{aligned}
 I'_{ckj} &= V'_{ckj} = I'_{dkj} = V'_{dkj} = 0, \quad V'_{bkj} \approx 0 \\
 I'_{bkj} &= \frac{1}{2} \rho_b \frac{\rho_e}{\rho_b} \frac{d}{dt} (U_{pj} - U_{bj}), \quad (6.9)
 \end{aligned}$$

$$\left. \begin{aligned}
 \bar{\rho}_b &= \bar{\rho}_g \\
 \rho_e &= \sum_{(ck)} \rho_{ck} + \sum_{(dk)} \rho_{dk} + \rho_g \\
 \rho_p U_{pj} &= \sum_{(ck)} \rho_{ck} U_{ckj} + \sum_{(dk)} \rho_{dk} U_{dkj}
 \end{aligned} \right\} \quad (6.10)$$

$$\begin{aligned}
& \frac{\partial \rho_g}{\partial t} \frac{U_{gy}}{g} + \frac{\partial \rho_g}{\partial x} \frac{U_{gy} U_{gx}}{g} + \frac{\partial \rho_g}{\partial y} \frac{U_{gy}^2}{g} + \frac{\partial \rho_g}{\partial z} \frac{U_{gy} U_{gz}}{g} \\
&= - \frac{\partial}{\partial y} \phi_g P + \frac{\partial}{\partial x} \left(\tau_g \right)_{xy} + \frac{\partial}{\partial y} \left(\tau'_g \right)_{yy} + \frac{\partial}{\partial z} \left(\tau_g \right)_{zy} \\
&+ \frac{\partial}{\partial x} \rho_g (U_{my} - U_{gy})(U_{mx} - U_{gx}) \\
&+ \frac{\partial}{\partial y} \rho_g (U_{my} - U_{gy})^2 + \frac{\partial}{\partial z} \rho_g (U_{my} - U_{gy})(U_{mz} - U_{gz}) + \Gamma_g U_{my} \\
&- \sum_k \rho_{ck} F_{ckg} (U_{gy} - U_{cky}) - \sum_k \rho_{dk} F_{dkg} (U_{gy} - U_{dky}) \\
&- \sum_k \rho_{bk} F_{bkg} (U_{gy} - U_{bky}) - \rho_{gw} F_{gwy} U_{gy} + \sum I'_{lky}, \quad (6.11)
\end{aligned}$$

$$\begin{aligned}
& \frac{\partial \rho_g}{\partial t} \frac{U_{gz}}{g} + \frac{\partial \rho_g}{\partial x} \frac{U_{gm} U_{gy} U_{gx}}{g} + \frac{\partial \rho_g}{\partial y} \frac{U_{gm} U_{gz} U_{gy}}{g} + \frac{\partial \rho_g}{\partial z} \frac{U_{gm}^2}{g} \\
&= - \frac{\partial \phi_g P}{\partial z} + \frac{\partial}{\partial x} \left(\tau_g \right)_{xz} + \frac{\partial}{\partial y} \left(\tau_g \right)_{yz} + \frac{\partial}{\partial z} \left(\tau'_g \right)_{zz} \\
&+ \frac{\partial}{\partial x} \rho_g (U_{mz} - U_{gz})(U_{mx} - U_{gx}) \\
&+ \frac{\partial}{\partial y} \rho_g (U_{mz} - U_{gz})(U_{my} - U_{gy}) + \frac{\partial}{\partial z} \rho_g (U_{mz} - U_{gz})^2 + \Gamma_g U_{mz} \\
&- \sum_k \rho_{ck} F_{ckg} (U_{gz} - U_{ckg}) - \sum_k \rho_{kg} F_{dkg} (U_{gz} - U_{dkz}) \\
&- \sum_k \rho_{bk} F_{bkg} (U_{gz} - U_{bkz}) - \rho_g F_{gwz} U_{gz} - \rho_g g \\
&+ \sum I'_{lkz}, \quad (6.12)
\end{aligned}$$

where $\tau'_{jj} \sim 0$ because of lack of knowledge on bulk viscosity ζ_m ;

and

$$\begin{aligned}
 (\tau_g)_{yx} &= \mu_m \frac{\rho_g}{\rho_m} \left[\frac{\partial U_{gy}}{\partial x} + \frac{\partial U_{gx}}{\partial y} \right] \\
 &+ \frac{\mu_m}{\rho_m} \left[(U_{gy} - U_{my}) \frac{\partial \rho_g}{\partial x} + (U_{gx} - U_{mx}) \frac{\partial \rho_g}{\partial y} \right] \quad (6.13)
 \end{aligned}$$

$$\begin{aligned}
 (\tau_g)_{zx} &= \mu_m \frac{\rho_g}{\rho_m} \left[\frac{\partial U_{gz}}{\partial x} + \frac{\partial U_{gx}}{\partial y} \right] \\
 &+ \frac{\mu_m}{\rho_m} \left[(U_{gz} - U_{mz}) \frac{\partial \rho_g}{\partial x} + (U_{gx} - U_{mx}) \frac{\partial \rho_g}{\partial z} \right] \quad (6.14)
 \end{aligned}$$

Similar permutation is applicable to $(\tau_g)_{zy}$, and $(\tau_g)_{yz}$.

Also, we have

$$(\tau_{ck})_{ji}, \quad (\tau_{dk})_{ji}, \quad (\tau_{bk})_{ji}$$

Note that both τ_{bk} and τ_g are small in the fluidized bed (dense phase), but significant in the free board (dilute phase).

For other ℓ 's, $\ell = c, d, b$, we have

$$\begin{aligned}
 &\frac{\partial \rho_{\ell k} U_{\ell kx}}{\partial t} + \frac{\partial \rho_{\ell k} U_{\ell kx}^2}{\partial x} + \frac{\partial \rho_{\ell k} U_{\ell kx} U_{\ell ky}}{\partial y} + \frac{\partial \rho_{\ell k} U_{\ell kx} U_{\ell kz}}{\partial z} \\
 &= - \frac{\partial \phi_{\ell k}^P}{\partial x} + \frac{\partial}{\partial x} \left(\tau'_{\ell k} \right)_{xx} + \frac{\partial}{\partial y} \left(\tau_{\ell k} \right)_{yx} + \frac{\partial}{\partial z} \left(\tau_{\ell k} \right)_{zx} + \Gamma_{\ell k} U_{mx} \\
 &+ \frac{\partial}{\partial x} \rho_{\ell k} (U_{mx} - U_{\ell kx})^2 + \frac{\partial}{\partial y} \rho_{\ell k} (U_{mx} - U_{\ell kx}) (U_{my} - U_{\ell ky}) \\
 &+ \frac{\partial}{\partial z} \rho_{\ell k} (U_{mx} - U_{\ell kx}) (U_{mz} - U_{\ell kz}) + \rho_{\ell k} F_{\ell kg} (U_{gx} - U_{\ell kx}) \\
 &+ \sum_{\ell'} \sum_{(\ell')k'} \rho_{\ell k} F_{(\ell k)(\ell' k')} (U_{\ell' k'x} - U_{\ell kx}) - \rho_{\ell k} F_{\ell kwx} U_{\ell kx} \\
 &- \rho_{\ell k} F_{\ell k\sigma} U_{\ell kx} + I'_{\ell kx} \quad (6.15)
 \end{aligned}$$

$F_{\ell kw}$ and $F_{\ell k\sigma}$ are the relaxation times due to flow resistance and surface resistance. It is to be noted that only $F_{bk\sigma}$ exists.

$$\frac{\partial \rho_{\ell k} U_{\ell ky}}{\partial t} + \frac{\partial \rho_{\ell k} U_{\ell ky} U_{\ell kx}}{\partial x} + \frac{\partial \rho_{\ell k} U_{\ell ky}^2}{\partial y} + \frac{\partial \rho_{\ell k} U_{\ell ky} U_{\ell kz}}{\partial z}$$

$$\begin{aligned}
&= - \frac{\partial \phi_{lk}^P}{\partial y} + \frac{\partial}{\partial x} (\tau_{lk})_{xy} + \frac{\partial}{\partial y} (\tau'_{lk})_{yy} + \frac{\partial}{\partial z} (\tau_{lk})_{zy} + \Gamma_{lk} U_{my} \\
&+ \frac{\partial}{\partial x} \rho_{lk} (U_{my} - U_{lky}) (U_{mx} - U_{lkx}) + \frac{\partial}{\partial y} \rho_{lk} (U_{my} - U_{lky})^2 \\
&+ \frac{\partial}{\partial z} \rho_{lk} (U_{my} - U_{lky}) (U_{mz} - U_{lkz}) + \rho_{lk} F_{lkg} (U_{gy} - U_{lky}) \\
&+ \sum_{l'} \sum_{(l')k'} \rho_{lk} F_{(lk)(lk)'} (U_{l'k'y} - U_{lky}) - \rho_{lk} F_{lkwy} U_{lky} \\
&- \rho_{lk} F_{lk\sigma} U_{lky} + I'_{lky}
\end{aligned} \tag{6.16}$$

$$\begin{aligned}
&\frac{\partial \rho_{lk} U_{lkz}}{\partial t} + \frac{\partial \rho_{lk} U_{lkz} U_{lkx}}{\partial x} + \frac{\partial \rho_{lk} U_{lkz} U_{lky}}{\partial y} + \frac{\partial \rho_{lk} U_{lkz}^2}{\partial z} \\
&= - \frac{\partial \phi_{lk}^P}{\partial z} + \frac{\partial}{\partial x} (\tau_{lk})_{zx} + \frac{\partial}{\partial y} (\tau_{lk})_{zy} + \frac{\partial}{\partial z} (\tau'_{lk})_{zz} + \Gamma_{lk} U_{mz} \\
&+ \frac{\partial}{\partial x} \rho_{lk} (U_{mz} - U_{lkz}) (U_{mx} - U_{lkx}) + \frac{\partial}{\partial y} \rho_{lk} (U_{mz} - U_{lkz}) (U_{my} - U_{lky}) \\
&+ \frac{\partial}{\partial x} \rho_{lk} (U_{mz} - U_{lkz})^2 + \rho_{lk} F_{lkg} (U_{gz} - U_{lkz}) \\
&+ \sum_{l'} \sum_{(l')k'} \rho_{lk} F_{(lk)(lk)'} (U_{l'k'z} - U_{lkz}) - \rho_{lk} F_{lk wz} U_{lkz} \\
&- \rho_{lk} F_{lk\sigma} U_{lkz} - \rho_{lk} g + I'_{lkz}
\end{aligned} \tag{6.17}$$

In the above relation $\sum_{(l')k'}$ means summing over all k's of each l' for $lk \neq l'k'$ and $\sum_{l'}$ means summing over all l's. Subscript s relates to tube bundle (immersed solid surfaces) and subscript σ relates to interface forces $R_{bkw} = 0$ in the multiphase range, $a_{bk} < a_m$. F_{bkwj} is the jth component of inverse relaxation time of momentum transfer in the heterogeneous phase range when a bubble covers one or more tubes. Dynamic interaction among bubbles themselves are neglected because of the large ϕ_s .

When applied to bubbles, the ϕ_{bk}^P , τ_{bk} , and $\frac{\partial}{\partial x_j} \rho_{bk} (U_{mj} - U_{bkj}) (U_{mk} - U_{bki})$ terms have negligible contribution; the I'_{bk} terms are important.

Summing up for the momentum equations, we have 3 (g) + 3 (ck) + 3 (dk) + 3 (bk) independent equations.

When applied to the free board, the above momentum equations will be retained only for the three equations of gas phase and three (ck)' equations of the range of fines of solid phase only.

6.3 Energy Equations

The kinetic energy is neglected because of low velocities and large heat release rates. The enthalpy of the mixture is given by:

$$\begin{aligned}\rho_m h_m &= \sum_k \rho_{gk} h_{gk} + \sum_l \sum_k \rho_{lk} h_{lk} \\ &= \rho_{mg} h_g + \sum_l \sum_k \rho_{lk} h_{lk}\end{aligned}\quad (6.18)$$

For the gas phase, we have:

$$\begin{aligned}&\frac{\partial}{\partial t} (\rho_g h_g) + \frac{\partial}{\partial x} (\rho_g U_{gx} h_g) + \frac{\partial}{\partial y} (\rho_g U_{gy} h_g) + \frac{\partial}{\partial z} (\rho_g U_{gz} h_g) \\ &= - \left(\frac{\partial}{\partial x} J_{mgx} + \frac{\partial}{\partial y} J_{mgy} + \frac{\partial}{\partial z} J_{mgyz} \right) + \phi_g \frac{\partial P}{\partial t} \\ &+ \frac{\partial}{\partial x} \rho_g (U_{mx} - U_{gx}) (h_m - h_g) + \frac{\partial}{\partial y} \rho_g (U_{my} - U_{gy}) (h_m - h_g) \\ &+ \frac{\partial}{\partial z} \rho_g (U_{mz} - U_{gz}) (h_m - h_g) + \Gamma_g h_m \\ &- \sum_{ck} \rho_{ck} c_{pck} G_{ckg} (T_g - T_{ck}) \\ &- \sum_{dk} \rho_{dk} c_{pdk} G_{dkg} (T_g - T_{dk}) \\ &- \sum_{bk} \rho_{bk} c_{pbk} G_{bkg} (T_g - T_{bk}) \\ &+ A_w \hat{h}_{gw} (T_w - T_g) + J_{Eg}\end{aligned}\quad (6.19)$$

where $\hat{h}_{gw}$ is the heat transfer coefficient at the tube wall (w), A_w denotes tube surface area per unit volume, and J_{Eg} is the heat source in the gas phase. Details relating to tube banks or tube bundles (submerged solid surfaces) are given in Section 5. $c_{plk} \approx c_{lk}$ for solids. Pending further research, we take $A_w \hat{h}_{gw} = c_{pg} \rho_g (G_{gwx} + G_{gwy} + G_{gwz})$ as a sufficient approximation.

For phase ℓk ($\ell = c, d$ only):

$$\begin{aligned}
 & \frac{\partial}{\partial t} (\rho_{\ell k} h_{\ell k}) + \frac{\partial}{\partial x} (\rho_{\ell k} U_{\ell kx} h_{\ell k}) + \frac{\partial}{\partial y} (\rho_{\ell k} U_{\ell ky} h_{\ell k}) + \frac{\partial}{\partial z} (\rho_{\ell k} U_{\ell kz} h_{\ell k}) \\
 &= - \left(\frac{\partial}{\partial x} J_{\ell kx} + \frac{\partial}{\partial y} J_{\ell ky} + \frac{\partial}{\partial z} J_{\ell kz} \right) + \phi_{\ell k} \frac{\partial P}{\partial t} \\
 &+ \frac{\partial}{\partial x} \rho_{\ell k} (U_{mx} - U_{\ell kx}) (h_m - h_{\ell k}) + \frac{\partial}{\partial y} \rho_{\ell k} (U_{my} - U_{\ell ky}) (h_m - h_{\ell k}) \\
 &+ \frac{\partial}{\partial z} \rho_{\ell k} (U_{mz} - U_{\ell kz}) (h_m - h_{\ell k}) + \Gamma_{\ell k} h_m \\
 &+ \rho_{\ell k} c_{\ell k} G_{\ell kg} (T_g - T_{\ell k}) + \sum_{\ell'} \sum_{(k')} \rho_{\ell k} c_{\ell k} F_{\ell k(\ell k)'} (T_{(\ell k)'} - T_{\ell k}) \\
 &+ A_w \hat{h}_{\ell kw} (T_w - T_{\ell k}) + J_{E\ell k}, \tag{6.20}
 \end{aligned}$$

where $J_{E\ell k}$ is given for the diffused radiation, with Eq. (4.45) as an approximation.

The temperature of the tube walls is given by the heat conduction equation, neglecting the circumferential variation of temperature:

$$\frac{\partial}{\partial z} (\kappa_w \pi b \Delta b \frac{\partial T_w}{\partial z}) + 2\pi b q - \hat{h}_m 2\pi b (T_w - T_m) = c_w \bar{\rho}_w \pi b \Delta b \frac{\partial T_w}{\partial t}, \tag{6.21}$$

where subscript w refers to tube properties. Distribution of T_w in the x, y directions is given via local values of mean temperature, T_m ; $\hat{h}_m$ is the heat transfer coefficient based on the mixture which is that of the dense phase for a fluidized bed; q is the heat removed by the coolant per unit length of the tube; and b and Δb are tube radius and tube thickness respectively.

For constant values of b and κ_b , Eq. (6.21) is simplified to:

$$\frac{\partial^2 T_w}{\partial z^2} + \frac{1}{\Delta b} \left(\frac{2q}{\kappa_b} \right) - \frac{1}{\Delta b} \left(\frac{2\hat{h}_m}{\kappa_w} \right) (T_w - T_m) = \frac{c_w \bar{\rho}_w}{\kappa_w} \frac{\partial T_w}{\partial t}, \tag{6.22}$$

where $\kappa_w / c_w \bar{\rho}_w$ is the thermal diffusivity of the tube material.

The heat fluxes are given by [p. 253 of [35]]

$$J_{mgx} = - \kappa_m \frac{\rho_g c_g}{\rho_m c_m} \frac{\partial T_g}{\partial x} - \kappa_m T_g \frac{\partial}{\partial x} \left(\frac{\rho_g c_g}{\rho_m c_m} \right), \tag{6.23}$$

where c 's are the specific heat at constant volume, and

$$\rho_m c_m = \sum \rho_{gk} c_{gk} + \sum \sum \rho_{lk} c_{lk} \quad (6.24)$$

and, similarly, for y, z component, and alternately, we write for species lk:

$$J_{lkx} = - \kappa_m \frac{\partial}{\partial x} \left[\frac{\rho_{lk} c_{lk}}{\rho_m c_m} T_{lk} \right] \quad (6.25)$$

We have altogether (g) + (ck) + (dk) energy equations of the fluidized bed.

The above specific heats at constant volume (c) are related to specific heats at constant pressure (c_p) discussed in the next section:

For gases,

$$M_k c_k = M_k c_{pk} - R = \overline{c_{pk}} - R, \quad (6.26)$$

where $\overline{c_{pk}}$ is the molal specific heat at constant pressure and R is the universal gas constant ($R = 8314 \text{ J/kg} \cdot \text{mole} \cdot \text{K}$).

For solids,

$$c_k = c_{pk}. \quad (6.27)$$

For a mixture,

$$n_m \overline{c_m} = \rho_m c_m = n_m (\overline{c_{pm}} - R) = \rho_m c_{pm} - \left(\sum \frac{\rho_k}{M_k} \right) R. \quad (6.28)$$

In the tube bundle region, for heat source q in W/m^2 of the tube surface,

$$\begin{aligned} J_{Egk} &= q (\text{tube area/bubble}) (\text{number of bubbles/volume}) \\ &= q (\pi b / 2\sqrt{3} \text{ s}^2) \phi_{lk} \\ &= \hat{h}_{w\ell k} (T_w - T_k) (\pi b / 2\sqrt{3} \text{ s}^2) \phi_{lk}, \end{aligned} \quad (6.29)$$

where $\hat{h}_{w\ell k}$ is the heat transfer coefficient at the interface of bubble and dense phase.

In the dense phase (e), the tubes act as distributed heat sinks according to:

$$\begin{aligned}
 J_{E_e} &= (\pi b / 2\sqrt{3} \text{ s}^2) q \phi_e \\
 &= (\pi b / 2\sqrt{3} \text{ s}^2) \hat{h}_{we} (T_w - T_p) \phi_e
 \end{aligned} \tag{6.30}$$

where $\hat{h}_{we}$ is the heat transfer coefficient of the dense phase at the solid surface.

6.4 Standard Heats of Reaction and Enthalpies

Conversion from molal enthalpy ($\bar{h}$) to specific enthalpy (h) is readily made via the equality:

$$n_k \bar{h}_k = \rho_k h_k \tag{6.31}$$

The heats of reaction are related to enthalpies at standard state (25°C) according to, for reactions in Eqs. (2.3) to (2.9) according to:

$$\begin{aligned}
 \bar{h}_{30} + \bar{h}_{40} - \bar{h}_{10} - \bar{h}_{20} &= \Delta H_I \\
 \bar{h}_{30} - \bar{h}_{20} - \bar{h}_{40} &= \Delta H_{II} \\
 2 \bar{h}_{20} - \bar{h}_{00} - \bar{h}_{30} &= \Delta H_{III} \\
 \bar{h}_{30} - \bar{h}_{00} - \bar{h}_{10} &= \Delta H_{IV} \\
 \bar{h}_{60} + \bar{h}_{20} - \bar{h}_{10} - \bar{h}_{50} &= \Delta H_V \\
 \bar{h}_{70} - \bar{h}_{10} - \bar{h}_{s0} &= \Delta H_{VI} \\
 \bar{h}_{d0} + \bar{h}_{30} - \frac{1}{2} \bar{h}_{10} - \bar{h}_{70} - \bar{h}'_{d0} &= \Delta H_{VII}
 \end{aligned} \tag{6.32}$$

We choose the datum states according to: [52]

$$\begin{aligned}
 \bar{h}_{00} &= - \Delta H_{IV} \\
 \bar{h}_{20} &= - \frac{1}{2} (\Delta H_I + \Delta H_{II}) \\
 \bar{h}_{40} &= \frac{1}{2} (\Delta H_I - \Delta H_{II})
 \end{aligned}$$

$$\left. \begin{aligned}
 \bar{h}_{50} &= - \left(\frac{1}{2} \Delta H_I + \frac{1}{2} \Delta H_{II} + \Delta H_V \right) \\
 \bar{h}_{s0} &= - \Delta H_{VI} \\
 \bar{h}'_{d0} &= - \Delta H_{VII}
 \end{aligned} \right\} \quad (6.33)$$

and

$$\bar{h}_{10} = \bar{h}_{30} = \bar{h}_{60} = \bar{h}_{70} = \bar{h}_{d0} = 0$$

The enthalpies in Eqs. (6.18) to (6.20) are now given by:

$$h_{ck} = \int_{T_o}^{T_{ck}} c_{po} dT - (\Delta H_{IV}/M_o)$$

$$h_{g1} = \int_{T_o}^{T_g} c_{p1} dT$$

$$h_{g2} = \int_{T_o}^{T_g} c_{p2} dT - \frac{1}{2} (\Delta H_I + \Delta H_{II}) M_2^{-1}$$

$$h_{g3} = \int_{T_o}^{T_g} c_{p3} dT$$

$$h_{g4} = \int_{T_o}^{T_g} c_{p4} dT + \frac{1}{2} (\Delta H_I - \Delta H_{II}) M_4^{-1}$$

$$h_{g5} = \int_{T_o}^{T_g} c_{p5} dT - \left(\frac{1}{2} \Delta H_I + \frac{1}{2} \Delta H_{II} + \Delta H_V \right) M_5^{-1}$$

$$h_{g6} = \int_{T_o}^{T_g} c_{p6} dT$$

$$h_{g7} = \int_{T_o}^{T_g} c_{p7} dT$$

$$h_{g8} = \int_{T_o}^{T_g} c_{p8} dT$$

$$\begin{aligned}
 h_{sk} &= \int_{T_o}^{T_{sk}} c_{ps} dT - \Delta H_{VI} M_s^{-1} \\
 h_{dk} &= \int_{T_o}^{T_{dk}} c_{pd} dT \\
 h'_{dk} &= \int_{T_o}^{T_{dk}} c_{pd'} dT - \Delta H_{VII} M_{d'}^{-1}
 \end{aligned} \tag{6.34}$$

where c_{pk} is the specific heat at constant pressure, and is equal to $(\bar{c}_{pk}/M_k)$; and $\bar{c}_{pk}$ is the molal specific heat at constant pressure.

We note that for a fluidized bed, there are altogether

(gk) + (ck) + (dk) + (bk) continuity equations

3 + 3 [(ck) + (dk) + (bk)] momentum equations

1 + (ck) + (dk) energy equations

and

1 equation of state (Sec. 6.6),

or a total of

1 + 4 + (gk) + 5 [(ck) + (dk)] + 4 (bk) equations.

The dependent variables consist of:

gk of ρ_{gk}	3 U_{gj}	1 T_g	1 P
ck of ρ_{ck}	3 ck of U_{ckj}	1 ck of T_{ck}	
dk of ρ_{dk}	3 dk of U_{dkj}	1 dk of T_{dk}	
bk of ρ_{bk}	3 bk of U_{bkj}		

or a total of

$$5 + (gk) + 5 [(ck) + (dk)] + 4 bk$$

quantities to be determined at each spatial point. (55 quantities for $gk = 8$, $ck = dk = bk = 3$.)

Derivations of basic equations are given in [1], and with immersed solid surfaces in [53].

6.5 Interface

The initial approach is to treat the free surface as a simple discontinuity of particle concentration with background elutriation of fine particles whose terminal velocity is lower than superficial velocity of the gas entering the bed. In this case, at the surface, we have

$$\rho_g U_{gz} = \rho_{gf} U_{gf} \quad (6.35)$$

$$\rho_{ck} U_{ckz} = \rho_{ckf} U_{ckf} \quad (6.36)$$

for the background elutriation of species $(ck)'$, where $U_{gzf} = g/F_{(ck)'} g$, and

$$U_{lkzf} = 0 \quad (6.37)$$

for other species lk 's. Conservation of momentum across and at the interface gives:

$$\rho_g U_{gz}^2 + \sum \rho_{lk} U_{lk}^2 = \rho_{gf} U_{gzf}^2 + \sum \rho_{lkf} U_{lkf}^2 \quad (6.38)$$

Further, we have

$$T_g = T_{gf} \quad (6.39)$$

$$\bar{\rho}_g = \bar{\rho}_{gf} \quad (6.40)$$

For the dilute phase due to background elutriation in the free board, we repeat the conservation equations without dk , bk , and some ck 's. The effect of bk , if present, has to be specially identified next.

Simultaneous with background elutriation by the superficial velocity above the bed, bursting bubbles, when present, produce pulses of gas jets

ejecting other particles in addition to the background elutriation. These particles differ from those in the background elutriation in that they will fall back to the bed after rising to a certain height in the free board. This height of rise constitutes a transition region from the bed to the true free board having background elutriation and unagitated gas flow only. Within this transition region, particles of different size will rise to different heights around pulses of gas jets which can be identified as phases or domains, depending on the population of the bursting bubbles. Knowledge of the transition region is important because it determines the free board height needed to eliminate carryover of particles larger than background elutriation.

As discussed in Sec. 3.5, and demonstrated in Appendix F, details of the pulses carrying solid particles remain to be determined in order that this new phase can be formulated. For the present, it appears valid to approximate the condition illustrated in Appendix F according to the following specifications:

(a) Of the amount ejected, each species rises to the height Δz above the bed where the jet velocity ($U_{bz f}$) is equal to its terminal velocity (Eq. 3.38). Δz is given by:

$$U_{Jz f} = (3/8) U_{Jz f o} (a_b U_{Jz f o} / v_g) [(\Delta z / a_b) + (3/2) a_b (a_b U_{Jz f} / v_g)]^{-1}$$

$$= g / F_{(ck)} n_g \quad (6.41)$$

$U_{Jz f o}$ is given by Eq. (3.37) at the free surface. From Eq. (6.41), Δz can be solved.

(b) Because of the diffuse nature of the spray of particles via ejection, we postulate that $\rho_{(ck)} n_f$ diminishes exponentially [41] to zero at $(\Delta z)_{(ck)}$

$$\rho_{(ck)} n_f = \rho_{(ck)} n_{f o} \frac{\exp [-g(z - \Delta z) / D_{(ck)} n_{(ck)} n_g] - 1}{\exp [g(\Delta z) / D_{(ck)} n_{(ck)} n_g] - 1} \quad (6.42)$$

where $\rho_{(ck)} n_{f o}$ is given by Eq. (3.43) as:

$$\rho_{(ck)} n_{f o} = \hat{k}_D \frac{\rho_b}{\rho_c} \frac{\rho_{(ck)} n}{\sum \rho_{ck}} \quad (6.43)$$

and $D_{(ck)} n$ is given in Appendix G of [1].

(c) At a height Δz above the bed where $U_{Jz f} = U_{gz f}$, the jet effect is completely dissipated. Above this level, only background gas flow and elutriation exist.

In the tube bundle section, because of the surface provided by the tubes, the interaction between the tubes and the interface tends to predominate.

The continuity at the interface (large bubble) is given by: (Fig. 11)

$$\rho_e (U_{ei} - U_{si}) + \rho_g (U_{gi} - U_{si}) = 0 \quad (6.44)$$

across the interface of a discrete domain; m is for the dense phase.

The momentum equation is reduced to: (Fig. 11) [1]

$$\rho_e U_{ei} (U_{ei} - U_{si}) + \rho_g U_{gi} (U_{gi} - U_{si}) + P_e - P_g - \hat{p}_{si} \left(\frac{U_{si}}{|U_{si}|} \right) + 2H_{ge}\sigma = 0 \quad (6.45)$$

where $\hat{p}_{si}$ is given in Sec. 5.3. This simplification is made because $s \ll R_d$, the radius of curvature of the discrete domain. H_{ge} is the mean curvature at the interface; $H_{ge} > 0$ if the interface is a convex surface in the dense phase, i.e. the case of a bubble.

The energy equation is again simplified because the dynamic energies are not significant and we have at the interface

$$T_e = T_g = T_s, \quad (6.46)$$

where T_s is the temperature of the interface.

Additional specification will be given by the boundary condition of the interface to give the temperature distribution inside a discrete domain.

Again, in this case, the cooling by the tubes tends to predominate the interface heat transfer.

6.6 Equation of State

The variable P calls for another independent relation, the equation of state

$$\frac{P}{\sum (\rho_{gk}/M_k)} = RT_g, \quad (6.47)$$

where R is the universal gas constant (8314 J/kg mole K). We also have for each component:

$$\rho_{gk} = \frac{P_k}{\left(\frac{R}{M_k} \right) T} = \frac{P(n_{gk}/\sum n_{gk})}{(R/M_k) T} \quad (6.48)$$

Fig. 11. Interface Across a Tube Bundle

Since

$$\frac{P}{\rho_g} = \frac{R}{M_g} T = \frac{P}{\rho_g} ,$$

and

$$\rho_g = \sum_{k=1}^8 \rho_{gk} , \quad (6.49)$$

$$\frac{\rho_g}{M_g} = \sum_{k=1}^8 \frac{\rho_{gk}}{M_k}$$

and

$$P\phi_g = R \left(\sum_{k=1}^8 \frac{\rho_{gk}}{M_k} \right) T_g . \quad (6.50)$$

6.7 Boundary Conditions and Initial Condition

For the system defined in Fig. 5, the boundary conditions can be outlined as follows:

(a) At the top of the distributor plate (total air flow, $\dot{m}_a$, through the distributor):

$$z = 0, \quad U_{gz} = U_{ao}(\text{air}), \quad U_{gx} = U_{gy} = 0 \quad (6.51)$$

$$\bar{\rho}_g = \bar{\rho}_{ao} \quad (6.52)$$

$$T_g = T_{ao} \quad (6.53)$$

(including heat transfer from the plate at $z < 0$)

$$U_{lkx} = U_{lky} = U_{lkz} = 0 \quad l = c, d \quad (6.54)$$

$$U_{bz} = U_{bo} \quad (\text{bubble departure velocity}) \quad (6.55)$$

$$N_b = N_{bo} = N'_b \hat{f}/U_{bo} \quad (\text{bubble number density}) \quad (6.56)$$

(b) At the vertical walls:

$$U_{gz} = U_{gx} = U_{gy} = 0 \quad (6.57)$$

$$U_{lkz} = U_{lkx} = U_{lky} = 0 \quad (l = c, d) \quad (6.58)$$

$$\frac{\partial \rho_{lk}}{\partial \hat{n}} = 0 \quad (6.59)$$

$$\frac{\partial P}{\partial \hat{n}} = 0 \quad (6.60)$$

In the case of an insulated wall: $\frac{\partial T_g}{\partial \hat{n}} = 0 \quad (6.61)$

In the case of a cooled wall (or initial heating by calrod heater [25]):

$$(\kappa_m + \kappa_{rad}) \frac{\partial T_m}{\partial \hat{n}} = h_m (T_m - T_w) \quad (6.62)$$

where from Eq. (6.24), based on specific heat at constant volume:

$$\rho_m c_m T_m = \rho_g c_g T_g + \sum_l \sum_k \rho_{lk} c_{lk} T_{lk} \quad (6.63)$$

(c) At the coal feed conduit

$$\dot{m}_{coal} = \dot{m}_F = \int_{A_F} \rho_F \underline{U}_{Fo} \cdot \underline{ndA}_F = \int_{A_F} \bar{\rho}_F \underline{U}_{Fo} \cdot \underline{ndA}_F \quad (6.64)$$

where $\underline{n}$ is unit normal vector to area A.

The air entrained with the coal feed is given by:

$$\begin{aligned} \dot{m}_{aF} &= \int (1 - \phi_{Fo}) \bar{\rho}_{a-Fo} \underline{U}_{Fo} \cdot \underline{ndA}_F \\ &= \frac{\dot{m}_{aF}}{M_a} \left[\frac{3.76}{4.76} M_8 + \frac{1}{4.76} M_1 \right] = \dot{m}_{8F} + \dot{m}_{1F} \\ &= \int \rho_{8-Fo} \underline{U}_{Fo} \cdot \underline{ndA}_F + \int \rho_{1-Fo} \underline{U}_{Fo} \cdot \underline{ndA}_F \end{aligned} \quad (6.65)$$

where $\underline{U}_F$ and ϕ_{Fo} denote feeding velocity and volume fraction of coal respectively. Both are given quantities.

Devolatilization occurs so that:

$$\dot{n}_F \rightarrow \dot{n}_c + \dot{n}_c \frac{\delta}{2} N_2 + \dot{n}_c \gamma H_2O + \dot{n}_c \frac{\nu}{4} \frac{1}{n} (CH_2)_n \quad (6.66)$$

with $\dot{n}_F = \dot{n}_c$, $M_F = 100$ can be taken from coal analysis.

During the process

$$\dot{n}_F M_F = \Gamma_F \quad (6.67)$$

$$\dot{n}_c [\alpha M_c + \epsilon M_s + M_A] = \Gamma'_c \quad (6.68)$$

$$\dot{n}_c \frac{v}{4} [M_5] = \Gamma'_5 \quad (6.69)$$

$$\dot{n}_c \gamma M_6 = \Gamma'_6 \quad (6.70)$$

all the above Γ 's are due to devolatilization in the bed. The species F (fuel or coal) needs to be identified. Because of incomplete knowledge on the rates of devolatilization, we can use either of the following approximations:

(1) Instantaneous devolatilization at the coal inlet

The feed ρ_F is replaced by:

$$\rho_c = \rho_F \frac{1}{100} [\alpha M_c + \epsilon M_s + M_A] \quad (6.71)$$

$$\rho_5 = \rho_F \frac{1}{100} \frac{v}{4} M_5 \quad (6.72)$$

$$\rho_6 = \rho_F \frac{1}{100} \gamma M_6 \quad (6.73)$$

$$\rho_8 = \left[\rho_F \frac{1}{100} \frac{\delta}{2} + \frac{3.76}{4.76} \frac{\rho_a}{M_a} \right] M_8 \quad (6.74)$$

$$\rho_1 = \frac{1}{4.76} \frac{\rho_a}{M_a} M_1 \quad (6.75)$$

(2) Transition at 1085 K: [22]

Treat the above conversion as the feed is distributed in the bed and reaches 1085 K by heat transfer and mixing. A set of equations for species F will have to be added.

(d) At the dolomite feed conduit:

$$\dot{m}'_d = \int_{A_d} \rho'_d \underline{U}'_{do} \cdot d\underline{A}_d = \int_{A_d} \bar{\rho}'_d \phi_{do} \underline{U}'_{do} \cdot d\underline{A}_d \quad (6.76)$$

The accompanying air in the feed is:

$$\dot{m}'_{ad} = \int_{A_d} (1 - \phi_{do}) \bar{\rho}'_a \underline{U}'_{do} \cdot d\underline{A}_d \quad (6.77)$$

where ϕ_{do} and $\underline{U}'_{do}$ are given.

(e) At the interface between bed and free board:

In the transition from the visible bed surface to the free board, there are basically two superposed phenomena: (1) bed movement and background elutriation of fine particles, if any, in the quiescent part of the bed surface during the interval between passage of bursting bubbles; and (2) pulses of jets from bubble bursts tossing large and small particles upward until the jet dissipates.

(1) Background elutriated particles have terminal velocities below the gas velocity immediately at the surface. Other particles have the boundary condition of

$$U_{lkz} = 0 , \quad (6.78)$$

giving the surface of the fluidized bed (see Appendix C).

(2) When bubbles exist and burst at the surface defined in (1), the background elutriation decreases because of reduced background velocity as part of the total gas flow goes through the bubbles. These bubble bursts raise particles to various heights given by Eqs. (6.41) to (6.43). The uppermost level reached by a given particle species again has the boundary condition of

$$U_{(ck)z} = 0 , \quad (6.79)$$

This describes a "stream surface" of species (ck)" in the dilute phase in the free board (Fig. 5). Small particles will reach a higher $(\Delta z)_{(ck)}$ than large particles. A finite number of particle species will have a finite number of heights (Δz) 's. The species of particles among those raised by the bubble bursts but having the same size of the background elutriation will join the elutriated particles as the jets are dissipated while increasing the background gas velocity. In general, bubble bursts will increase the total background elutriation as well as set the minimum free board height for limiting the carryover to only the particles belonging to the background elutriation into the exit of the fluidized bed system.

(f) Overflow tube

For a given feed ratio of coal, dolomite, and air, the bed height is controlled by the overflow tube as shown in Figs. 6(d) and 6(f), and 12. The flow rate into this overflow tube [or withdrawal gate as shown in Fig. 6(e)] is determined by the flow condition inside and downstream of the tube or the static pressure at the plane of the tube inlet. The bed height and flow rate is iterated so that the flow

Fig. 12 Detail Drawing of 6-In.-Dia. Pressurized, Fluidized-Bed Combustor (Reproduced from Ref. 25)

rate into the overflow tube is given by:

$$\dot{m}_{eu} = \int_{A_u} \rho_e \underline{U}_e \cdot \underline{n} dA_u \quad (6.80)$$

where A_u is the area at the inlet to the overflow tube, $\rho_e \underline{U}_e$ is the mass flow of the dense phase at that point.

The balance of input $\dot{m}_F$, $\dot{m}_d$, $\dot{m}_{aF}$, $\dot{m}_{ad}$, and $\dot{m}_a$, and the output $\dot{m}_g$, $\dot{m}_{lk}$ (elutriated), to the gas exit, and $\dot{m}_{eu}$ determines the bed height at a given moment of operation. At steady operating condition, we have

$$\begin{aligned} \dot{m}_F + \dot{m}_d + \dot{m}_{aF} + \dot{m}_{ad} + \dot{m}_a &= \dot{m}_g + \dot{m}_{lk} \text{ (elutriated)} + \dot{m}_{eu} \\ \text{(all in flows)} &\qquad \qquad \text{(all out flows)} \end{aligned} \quad (6.81)$$

(g) Initial Conditions

The initial conditions must be specified so that numerical computation can be started. Normally, the computation will start with a non-reacting fluidized bed (Appendix A) with external heating and subsequent introduction of input of fuel and dolomite, and exit flows (Fig. 12). The starting condition of numerical computation is expected to parallel the experimental procedure at ANL [25]:

"Although the experimental procedure was subject to minor variations, it was basically as follows: a preweighed amount (15 kg) of either partially sulfated sorbent from a previous experiment or fresh unsulfated sorbent was charged to the reactor to provide an initial bed of material. The starting bed temperature was then raised to about 430°C by passing fluidizing air (pre-heated to 430-480°C) through the combustor and simultaneously employing the resistance heaters on the combustor wall. Once the bed temperature reached 430°C, the system was brought to the desired operating pressure, and coal (entrained in a transport air stream) was injected into the bed. To prevent carbon accumulation in the fluidized bed during startup, coal was initially injected in small amounts intermittently until a rapidly increasing temperature and a changing flue-gas composition confirmed ignition and sustained combustion. Continuous injection of coal was then initiated, and the bed temperature was raised to a selected combustion temperature. The desired temperature was maintained by the use of external and internal cooling coils.

"Injection of the sulfur-accepting sorbent was begun when the bed reached operating temperatures. The air, coal, and sorbent feed rates were adjusted to give a specified mole ratio of calcium in the sorbent to sulfur in the coal, a specified superficial gas velocity, and a specified level of oxygen in the flue gas leaving the combustor. Sulfated sorbent was removed from the combustor by means of a standpipe to maintain a constant fluidized-bed level."

Detailed formulation of these steps will be given after choosing the system for computation.

The simplest non-trivial formulation is given in Appendix A together with the necessary and sufficient boundary conditions. The deterministic nature of the formulation is shown. Appendix B, through nondimensionalizing, further shows the relations of parameters and variables. Appendix C clarifies the nature of the stream surfaces of the solid phase.

When a steady state is reached, species in the inlet and the outlet streams will, in addition to other conservative relations, include conservation of chemical species according to Eqs. (2.14).

7.0 Summary of Relations for Computation

We now are in the position to state, at least in a preliminary sense, a formulation of the fluidized bed combustion system has been completed. For practical purposes, it is desirable to identify the basic equations, the transport properties, material properties, and input conditions which are directly related to the numerical modeling.

7.1 Governing Equations

Continuity Equations (6.5), (6.6), (6.7)

Momentum Equations (6.8) - (6.17), including substitutions

Energy Equations (6.19) - (6.34), including substitutions

7.2 Transport Relations

(a) Chemical Reactions

Chemical species $n_o, n_1, n_2, n_3, n_4, n_d'$, (Eqs. 2.14) to give n_5, n_6, n_7, n_s, n_d .

Rates k_I to k_{VII} (Table 2) $R = 1.98587 \times 10^{-3}$, $T = T_g$

Γ_v or dn_v/dt in Eqs. (2.60) to (2.72) into Eqs. (6.5), (6.6)

Heats of reaction Eq. (6.34) and Table 2

(b) Bubbles

Eqs. (3.20) to (3.23) coalescence use $k^* = 10^{-3} \text{ m}^3/\text{s}$ as average

(c) Free Board

Background elutriation by Eqs. (6.35) to (6.40). Bubble burst by:

ΔP Eq. (3.35)

$\hat{k}_D = 10^{-3}$

ρ_{ckf} Eq. (6.42)

U_{bzf} Eq. (6.41)

(d) Transport Properties

F_{lkg} Eqs. (4.8), (4.9), (4.10)

$F_{lk(lk)}$ Eqs. (4.11), (4.12), (4.14), (4.15), (4.16)

G_{lkg} Eqs. (4.20), (4.23), (4.24), (4.26), (4.31)

$G_{lk(lk)}$ Eqs. (4.27), (4.28), (4.11), (4.12), (4.14)

μ_m Eqs. (4.36), (4.37)

$$\begin{aligned} \mu_g &= 1.8 \times 10^{-5} \left(\frac{T}{300}\right)^{0.68} \text{ kg/m}\cdot\text{s} \\ \kappa_m &= \text{Eqs. (4.39)} \\ \kappa_g &= 0.0269 \left(\frac{T}{300}\right)^{0.85} \text{ W/m}^{\circ}\text{K} \\ \kappa_{\text{rad}} &= \text{Eqs. (4.43), (4.44)} \\ \alpha &= 0.8, a_p^2 n_p = \sum_{\ell k} a_{\ell k}^2 N_{\ell k} \quad \text{Eq. (4.40)} \\ &\ell k \text{ species of particles} \\ n_m &= \text{index of refraction of gas} \\ &\sim 1 + 3 \times 10^{-4} \\ \sigma_r &= 56.7 \times 10^{-9} \text{ W/m}^2\cdot\text{K}^4 \\ \kappa_p &= (\text{mean of coal and dolomite}) \sim 2 \text{ W/m}\cdot\text{K} \end{aligned}$$

7.3 Properties of Materials

(a) Coal in ANL-FBC

	<u>M</u>	<u>Wt. %*</u>	<u>Wt. %/M</u>
C	12.01	77.14	0.06423 = α'
H	1.008	5.23	5.188 = β
S	32.06	2.90	0.09046 = ϵ
N	14.01	1.66	0.1185 = δ
O	16	4.97	0.3106 = γ
A	"8.10"	8.10	1

*Weight % based on ultimate analysis.

We take

$$M_{\text{coal}} = 100 = M_F$$

and

$$M_A = 8.1$$

We thus have:

$$\alpha = 4.140$$

$$\epsilon = 0.09046$$

$$\frac{\delta}{2} = 0.05925$$

$$\gamma = 0.3106$$

$$\frac{\nu}{4} = 2.283$$

(b) Mechanical Properties of Solids [For Eqs. (4.11), (4.12), (4.15), (4.16), and (4.22)]

Coal

$$\bar{\rho} = 1440 \text{ kg/m}^3$$

$$E = 10^{10} \text{ N/m}^2$$

$$\nu = 0$$

$$k = 3.183 \times 10^{-11}$$

$$\begin{aligned} \text{Dolomite } \bar{\rho} &= 2900 \text{ kg/m}^3 \\ E &= 5.9 \times 10^{10} \text{ N/m}^2 \\ \nu &\sim 0 \quad k = 5.395 \times 10^{-12} \text{ m}^2/\text{N} \end{aligned}$$

$$\begin{aligned} \text{Steel } \bar{\rho} &= 7860 \text{ kg/m}^3 \\ (\text{SAE 1112}) E &= 20 \times 10^{10} \text{ N/m}^2 \\ \nu &= 0.305 \quad k = 1.443 \times 10^{-12} \text{ m}^2/\text{N} \end{aligned}$$

(c) Molal Specific Heats of Gases at Constant Pressure

$$\bar{c}_p \text{ in J/kg}\cdot\text{mole}\cdot\text{K}$$

$$\theta = T(\text{K})/100$$

$$\begin{aligned} \text{N}_2: \quad \bar{c}_{p8} &= (39.060 - 512.79 \theta^{-1.5} + 1072.7 \theta^{-2} \\ &\quad - 820.40 \theta^{-3}) \times 10^3 \\ \text{O}_2: \quad \bar{c}_{p1} &= (37.432 + 0.020102 \theta^{1.5} - 178.57 \theta^{-1.5} \\ &\quad + 236.88 \theta^{-2}) \times 10^3 \\ \text{CO}: \quad \bar{c}_{p2} &= (69.145 - 0.70463 \theta^{0.25} - 200.77 \theta^{-0.5} \\ &\quad + 176.76 \theta^{-0.75}) \times 10^3 \\ \text{H}_2\text{O}: \quad \bar{c}_{p6} &= (143.05 - 183.54 \theta^{0.25} + 82.751 \theta^{0.5} \\ &\quad - 3.6989 \theta) \times 10^3 \\ \text{CO}_2: \quad \bar{c}_{p3} &= -3.7357 + 30.529 \theta^{0.5} - 4.1034 \theta \\ &\quad + 0.024198 \theta^2 \times 10^3 \\ \frac{1}{n}(\text{CH}_2)_n: \quad \bar{c}_{p5} &= (-47.697 + 61.575 \theta^{0.5} - 17.821 \theta^{0.75} \\ &\quad + 91.385 \theta^{-3}) \times 10^3 \\ \text{O}: \quad \bar{c}_{p4} &= 20778.8 \\ \text{SO}_2: \quad \bar{c}_{p7} &= 17983 \end{aligned}$$

(d) Densities and Specific Heats:

$$\begin{aligned} \text{Density of flyash } 800 \text{ kg/m}^3 &= \\ \text{coal } 1300 \text{ kg/m}^3 &= \bar{\rho}_{\text{coal}} = \bar{\rho}_F \\ \text{char } 1440 \text{ kg/m}^3 &= \bar{\rho}_c \\ \text{dolomite } 2000 \text{ kg/m}^3 &= \bar{\rho}_d \end{aligned}$$

Specific heats of:

$$\begin{aligned} \text{dolomite} & 0.222 \text{ kcal/kg}^\circ\text{K} = 929.3 \text{ J/kg}\cdot\text{K} \\ \text{coal} & 0.3 \text{ kcal/kg}^\circ\text{K} = 1256 \text{ J/kg}\cdot\text{K} \\ \text{ash} & 0.2 \text{ kcal/kg}^\circ\text{K} = 837 \text{ J/kg}\cdot\text{K} \\ \text{Sulfur (solid)} & 0.18 \text{ kcal/kg}^\circ\text{K} = 753 \text{ J/kg}\cdot\text{K} \\ (\text{Sulfur (liquid)} & 0.331 \text{ kcal/kg}^\circ) \end{aligned}$$

7.4 Typical Data for Fluidized Bed Combustor (ANL)

Superficial gas velocity: 1.1 m/s
 Bed temperature: 800°C
 Pressure: 8.3 atm = $8.408 \times 10^5 \text{ N/m}^2$
 Bed Height: 1 m
 Bed Diameter: 0.15 m
 Coal Particle: $300 \times 10^{-6} \text{ m}$
 Dolomite particle: $700 \times 10^{-6} \text{ m}$
 Coal/dolomite flow ratio: 2000 kg/700 kg
 Excess O_2 : 17 %
 Feed: Air 136 kg/hr $n_1' = 0.0754 \text{ kg.mole/h}$
 Coal 10.4 kg/hr $n_0' = 1 \text{ kg.mole/h}$
 Dolomite 3.6 kg/hr $n_d' = 0.0256 \text{ kg.mole/h}$
 Bed content: coal 2.1 kg
 dolomite 4.0 kg
 Removal: Ash 0.1 kg
 Dolomite 5.0 kg
 Char
 Heat removed by cooling water (wall and inside tube bundle): $2.64 \times 10^8 \text{ J/h}$
 Initial condition:
 $2 a_c = 300 \times 10^{-6} \text{ m}$
 $2 a_d = 700 \times 10^{-6} \text{ m}$
 $2 a_b = 5 \times 10^{-3} \text{ m}$
 Recommend: Start computation from steady-state condition with a bed of dolomite at constant temperature and at $U_{z0} = 0.5 \text{ m/s}$, and gradually add coal and dolomite (Sec. 6.7(f)).
 Further details on substitutions are given in Appendix E.

8.0 Discussion

In spite of its length, this report deals with an adequate description of all the phenomena of a reacting fluidized bed in the simplest form. Feasibility of numerical modeling has been demonstrated.

Complexity occurs even with the input of one size of coal, one size of dolomite, and air, and even with the simplified identification of transition of char to ash in three steps (sizes), from dolomite to sulfated dolomite in three steps

(masses), bubble expansion and coalescence in three steps (masses), and eight chemical species. For three-dimensional analysis, we have a minimum of 55 independent equations in the bed, and 16 in the free board (Appendix E).

The areas needing refinements in our continuing study are:

- (1) Calibrating reaction rate data and mechanisms with experimental results such as gas analysis or heat balance or both.
- (2) Introducing the coking mechanism into the computation.
- (3) Bubble mechanics and coalescence.
- (4) Accounting for the non-Newtonian nature of the bed [54].
- (5) Performing stability analyses for both large shallow beds and deep beds.
- (6) Formulations of bubble burst and transition region in the free board.
- (7) Formulating large single bubbles, slugging, and sloshing.
- (8) Effects of various types of bed support.

Appendix A

Simplest Non-Trivial Solution and Boundary Conditions

A.1 Fluidized Bed

When applied to a simple incompressible fluid, non-reactive, isothermal system (Fig. 13), the basic equations are reduced to simple forms, with

$$\rho = \bar{\rho} (1 - \phi), \quad \rho_p = \bar{\rho}_p \phi$$

where $\bar{\rho} = \text{constant}$, $\bar{\rho}_p = \text{constant}$ for the gas and the solid phases.

The equations are:

Continuity Equations (2)

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_x}{\partial x} + \frac{\partial \rho U_y}{\partial y} + \frac{\partial \rho U_z}{\partial z} = 0 \quad (\text{A.1})$$

$$\frac{\partial \rho_p}{\partial t} + \frac{\partial \rho_p U_{px}}{\partial x} + \frac{\partial \rho_p U_{py}}{\partial y} + \frac{\partial \rho_p U_{pz}}{\partial z} = 0 \quad (\text{A.2})$$

Momentum Equations

Gas phase $\bar{\rho} \ll \bar{\rho}_p$, $\rho \ll \rho_p$ and $\rho_p U_p \gg \rho U$

$$\begin{aligned} & \frac{\partial \rho U_x}{\partial t} + \frac{\partial}{\partial x} \rho U_x^2 + \frac{\partial}{\partial y} \rho U_x U_y + \frac{\partial}{\partial z} \rho U_x U_z - \frac{\partial}{\partial x} \rho (U_x - U_{px})^2 \\ & - \frac{\partial}{\partial y} \rho (U_x - U_{py})(U_y - U_{py}) - \frac{\partial}{\partial z} \rho (U_x - U_{px})(U_z - U_{pz}) \\ & = - \frac{\partial}{\partial x} P(1 - \phi) - \rho_p F (U_x - U_{px}) \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} & \frac{\partial \rho U_y}{\partial t} + \frac{\partial}{\partial x} \rho U_y U_x + \frac{\partial}{\partial y} \rho U_y^2 + \frac{\partial}{\partial z} \rho U_y U_z - \frac{\partial}{\partial x} \rho (U_y - U_{py})(U_x - U_{px}) \\ & - \frac{\partial}{\partial y} \rho (U_y - U_{py})^2 - \frac{\partial}{\partial z} \rho (U_y - U_{py})(U_z - U_{pz}) \\ & = - \frac{\partial}{\partial y} P(1 - \phi) - \rho_p F (U_y - U_{py}) \end{aligned} \quad (\text{A.4})$$

Fig. 13. Geometry of Simplest Fluidized Bed

$$\begin{aligned}
 & \frac{\partial \rho U_z}{\partial t} + \frac{\partial}{\partial x} \rho U_z U_x + \frac{\partial}{\partial y} \rho U_z U_y + \frac{\partial}{\partial z} \rho U_z^2 - \frac{\partial}{\partial x} \rho (U_z - U_{pz}) (U_x - U_{px}) \\
 & - \frac{\partial}{\partial y} \rho (U_z - U_{pz}) (U_y - U_{py}) - \frac{\partial}{\partial z} \rho (U_z - U_{pz})^2 \\
 & = - \frac{\partial}{\partial z} P(1 - \phi) - \rho_p F (U_z - U_{pz}) - \rho g
 \end{aligned} \tag{A.5}$$

Particle phase ("boundary layer" model)

$$\begin{aligned}
 & \frac{\partial \rho_p U_{px}}{\partial t} + \frac{\partial}{\partial x} \rho_p U_{px}^2 + \frac{\partial}{\partial y} \rho_p U_{px} U_{py} + \frac{\partial}{\partial z} \rho_p U_{px} U_{pz} \\
 & = - \frac{\partial}{\partial x} P\phi + \rho_p F (U_x - U_{px}) + \frac{\partial}{\partial y} \mu_m \frac{\partial U_{px}}{\partial y} + \frac{\partial}{\partial z} \mu_m \frac{\partial U_{px}}{\partial z}
 \end{aligned} \tag{A.6}$$

$$\begin{aligned}
 & \frac{\partial \rho_p U_{py}}{\partial t} + \frac{\partial}{\partial x} \rho_p U_{py} U_{px} + \frac{\partial}{\partial y} \rho_p U_{py}^2 + \frac{\partial}{\partial z} \rho_p U_{py} U_{pz} \\
 & = - \frac{\partial}{\partial y} P\phi + \rho_p F (U_y - U_{py}) + \frac{\partial}{\partial x} \mu_m \frac{\partial U_{py}}{\partial x} + \frac{\partial}{\partial z} \mu_m \frac{\partial U_{py}}{\partial z}
 \end{aligned} \tag{A.7}$$

$$\begin{aligned}
 & \frac{\partial \rho_p U_{pz}}{\partial t} + \frac{\partial}{\partial x} \rho_p U_{pz} U_{px} + \frac{\partial}{\partial y} \rho_p U_{pz} U_{py} + \frac{\partial}{\partial z} \rho_p U_{pz}^2 \\
 & = - \frac{\partial}{\partial z} P\phi + \rho_p F (U_z - U_{pz}) + \frac{\partial}{\partial x} \mu_m \frac{\partial U_{pz}}{\partial x} + \frac{\partial}{\partial y} \mu_m \frac{\partial U_{pz}}{\partial y} - \rho_p g
 \end{aligned} \tag{A.8}$$

Independent boundary conditions:

- (1) at $z = 0$ $U_z = U_o$, $U_x = U_y = 0$, $U_{px} = U_{py} = 0$
- (2) at $x = x_o$ $U_x = U_y = U_z = 0 = U_{px} = U_{py} = U_{pz}$
(strong particle-particle interaction)
 $\partial \rho_p / \partial x = 0$, $\partial P / \partial x = 0$
- (3) at $y = y_o$ $U_x = U_y = U_z = 0 = U_{px} = U_{py} = U_{pz}$
(strong particle-particle interaction)
 $\partial \rho_p / \partial y = 0$, $\partial P / \partial y = 0$
- (4) at $x = 0$ $\partial / \partial x = 0$ for all eight dependent variables
- (5) at $y = 0$ $\partial / \partial y = 0$ for all eight dependent variables
- (6) at surface S or $z = h$, h to be determined by

$$\int_0^h \int_0^{y_0} \int_0^{x_0} \rho_p dx dy dz = \frac{m_p}{4}$$

m_p is the total particle charge

$$(7) \text{ at } z = h \quad U_{pz} = 0$$

$$P = P_o \text{ (given)}$$

$$\partial \rho_p / \partial z = 0$$

Total data: (Fig. 14)

$$\begin{aligned} & 8 (n_x + 1)(n_y + 1)(n_z + 1) + 1 \\ & = 8 n_x n_y n_z + 8 n_x n_y + 8 n_y n_z + 8 n_z n_x + 8 n_x + 8 n_y + 8 n_z + 9 \end{aligned}$$

No. of Equations :

No. of Interior points $8 n_x n_y n_z$

Boundary conditions

$$(1) \quad 5 (n_x + 1)(n_y + 1)$$

$$(2) \quad 8 (n_z)(n_x)$$

$$(3) \quad 8 (n_z)(n_y - 1) \quad (\text{excluding redundancy})$$

$$(4) \quad 8 n_z \quad (\text{excluding top})$$

$$(5) \quad 8 n_z \quad (\text{excluding top})$$

$$(6) \quad 1$$

$$(7) \quad 3 (n_x + 1)(n_y + 1)$$

$$\text{Sum: } 8 n_x n_y n_z + 8 (n_x + 1)(n_y + 1) + 8 n_x n_z + 8 n_y n_z - 8 n_z + 8 n_z + 8 n_z + 1$$

$$= 8 n_x n_y n_z + 8 n_x n_y + 8 n_y n_z + 8 n_z n_x + 8 n_x + 8 n_y + 8 n_z + 9$$

which checks with total number of data

A.2 Free Board:

In the free board (f) (Fig. 13) (Laminar boundary layer approximation)

$$z = h, \quad U_{zf} = U_z (1 - \phi)$$

$$P_{o+} + \frac{\rho U_{zf}^2}{2} = P_{o-} + \frac{\rho U_{z=h}^2}{2}$$

$$(U_p = 0)$$

Fig. 14 . Coordinates of a Fluidized Bed for Finite Difference Computation

$$\begin{aligned} P_{o-} &= P_{o+} - \frac{\bar{\rho}}{2} \left[U_{zh}^2 - U_{zh}^2 (1 - \phi)^2 \right] \\ &= P_{o+} - \frac{\bar{\rho}}{2} U_{zh}^2 \left[1 - (1 - \phi)^2 \right] \end{aligned}$$

$z > h$

$$\frac{\partial \rho U_x}{\partial x} + \frac{\partial \rho U_y}{\partial y} + \frac{\partial \rho U_z}{\partial z} = 0 \quad (A.9)$$

$$\begin{aligned} \frac{\partial \rho U_x}{\partial t} + \frac{\partial}{\partial x} \rho U_x^2 + \frac{\partial}{\partial y} \rho U_x U_y + \frac{\partial}{\partial z} \rho U_x U_z \\ = - \frac{\partial P}{\partial x} + \mu \frac{\partial^2 U_x}{\partial y^2} + \mu \frac{\partial^2 U_x}{\partial z^2} \end{aligned} \quad (A.10)$$

$$\begin{aligned} \frac{\partial \rho U_y}{\partial t} + \frac{\partial}{\partial x} \rho U_y U_x + \frac{\partial}{\partial y} \rho U_y^2 + \frac{\partial}{\partial z} \rho U_y U_z \\ = - \frac{\partial P}{\partial y} + \mu \frac{\partial^2 U_y}{\partial x^2} + \mu \frac{\partial^2 U_y}{\partial z^2} \end{aligned} \quad (A.11)$$

$$\begin{aligned} \frac{\partial \rho U_z}{\partial t} + \frac{\partial}{\partial x} \rho U_z U_x + \frac{\partial}{\partial y} \rho U_z U_y + \frac{\partial}{\partial z} \rho U_z^2 \\ = - \frac{\partial P}{\partial z} + \mu \frac{\partial^2 U_z}{\partial x^2} + \mu \frac{\partial^2 U_z}{\partial y^2} - \rho g \end{aligned} \quad (A.12)$$

$$\rho = \bar{\rho} = \text{constant}$$

Boundary Conditions:

$$x = x_o, y = y_o, U_x = U_y = U_z = 0, \frac{\partial \rho}{\partial x} = \frac{\partial \rho}{\partial y} = 0;$$

$$x = 0, y = 0, \frac{\partial}{\partial x} = 0: U_x, U_y, U_z, P$$

The unknowns are: U_x, U_y, U_z, P calling for:

four equations and $4(n_x + 1)(n_y + 1)(n_z + 1)$ data

Interior points: $4(n_x n_y n_z)$

Boundary condition: at $z = h, U_{zf}, U_x, U_y, P_{ox}$ — $4(n_x + 1)(n_y + 1)$

$$x = x_o, U_x = U_y = U_z = 0, \frac{\partial P}{\partial y} = 0$$

$$\text{— } 4n_z n_x$$

$$y = y_o, U_x = U_y = U_z = 0 \quad \frac{\partial P}{\partial x} = 0$$

$$\frac{\partial}{\partial x} = 0 \quad 4 n_z (n_y - 1)$$

$$x = 0 \quad \frac{\partial}{\partial x} = 0 \quad 4 n_z$$

$$y = 0 \quad \frac{\partial}{\partial y} = 0 \quad 4 n_z$$

$$\begin{aligned} & 4 n_x n_y n_z + 4 (n_x + 1)(n_y + 1) + 4 n_z n_x + 4 n_z (n_y - 1) + 8 n_z \\ & = 4 n_x n_y n_z + 4 n_x n_y + 4 n_y n_z + 4 n_z n_x \\ & + 4 n_x + 4 n_y + 4 n_z + 4 \end{aligned}$$

Typical properties and input data for this calculation are:

$$F = \frac{75}{2} \frac{\phi}{(1 - \phi)^2} \frac{\bar{\mu}_g}{\bar{\rho}_p a^2} + \frac{1.75}{2(1 - \phi)} \frac{\bar{\rho}}{\bar{\rho}_p} \frac{|\underline{U} - \underline{U}_p|}{a} s^{-1}$$

$$\mu_m = \bar{\mu}_g + 150 a^2 \bar{\rho}_p \mu_s^* \text{ kg/m}\cdot\text{s}$$

$$\mu_s^* = 1.650 \left(\frac{\phi}{\phi_o - \phi} \right)^2 - 0.2709 \left(\frac{\phi}{\phi_o - \phi} \right)^3 + 0.01114 \left(\frac{\phi}{\phi_o - \phi} \right)^4$$

$$\phi_o = 0.52.$$

Use $\bar{\rho}_p = 1500 \text{ kg/m}^3$, $\bar{\rho} = 1 \text{ kg/m}^3$, $P_o = 1 \text{ atm}$, $a = 50 \times 10^{-6} \text{ m}$; also

$\mu_g = 1.4 \times 10^{-5} \text{ kg/m}\cdot\text{s}$ at room temperature.

To avoid the complication of movement of particles in the packed bed in this simple solution, start with the steady-state condition at

$$z = 0, U_z = U_o = 0.07 \text{ m/s},$$

$$z = h, P_o = 1 \text{ atm} = 1.013 \times 10^5 \text{ N/m}^2,$$

$$x_o = 0.1 \text{ m} = y_o,$$

and

$$\frac{m_p}{4} = (0.52) (0.1)^3 (1500)$$

$$= 0.78 \text{ kg} \quad \text{or} \quad m_p = 3.12 \text{ kg}$$

If $h > 0.15 \text{ m}$, try a smaller U_o .

After determining the initial steady-state condition, begin transient computations by increasing U_o with time until $\phi = 0.02$, above which F should be modified.

A.3 Dynamics of bubbles. (bubble cloud)

In treating bubbles of fixed size, replace $1 - \phi$ in A.1 by $1 - \phi - \phi_b$.

Continuity:

$$\frac{\partial \rho_b}{\partial t} + \frac{\partial \rho_b U_{bx}}{\partial x} + \frac{\partial \rho_b U_{by}}{\partial y} + \frac{\partial \rho_b U_{bz}}{\partial z} = 0$$

Momentum: (resistance mainly from particle cloud)

$$\begin{aligned} \frac{\partial \rho_b U_{bx}}{\partial t} + \frac{\partial \rho_b U_{bx}^2}{\partial x} + \frac{\partial \rho_b U_{bx} U_{by}}{\partial y} + \frac{\partial \rho_b U_{bx} U_{bz}}{\partial z} - I_{bx} \\ = - \frac{\partial}{\partial x} P \phi_b + \rho_b F_{be} (U_{ex} - U_{bx}) + I'_{bx} + V'_{bx}, \end{aligned}$$

$$\begin{aligned} \frac{\partial \rho_b U_{by}}{\partial t} + \frac{\partial \rho_b U_{by} U_{bx}}{\partial x} + \frac{\partial \rho_b U_{by}^2}{\partial y} + \frac{\partial \rho_b U_{by} U_{bz}}{\partial z} - I_{by} \\ = - \frac{\partial}{\partial y} P \phi_b + \rho_b F_{be} (U_{ey} - U_{by}) + I'_{by} + V'_{by}, \end{aligned}$$

and

$$\begin{aligned} \frac{\partial \rho_b U_{bz}}{\partial t} + \frac{\partial \rho_b U_{bz} U_{bx}}{\partial x} + \frac{\partial \rho_b U_{bz} U_{by}}{\partial y} + \frac{\partial \rho_b U_{bz}^2}{\partial z} - I_{bz} \\ = - \frac{\partial}{\partial z} P \phi_b + \rho_b F_{be} (U_{ez} - U_{bz}) + I'_{bz} + V'_{bz}, \end{aligned}$$

where

$$\begin{aligned} I_{bx} &= \frac{\partial}{\partial x} \rho_b (U_{bx} - U_{ex})^2 + \frac{\partial}{\partial y} \rho_b (U_{bx} - U_{ex})(U_{by} - U_{ey}) \\ &+ \frac{\partial}{\partial z} \rho_b (U_{bx} - U_{ex})(U_{bz} - U_{ez}), \end{aligned}$$

$$V'_{bx} = \frac{9}{2\sqrt{\pi}} \frac{\rho_b}{a_b} \sqrt{\frac{\mu_m}{\rho_e}} \frac{\rho_b}{\rho_b} \int^t \frac{(\partial/\partial t)(U_{ex} - U_{bx})}{\sqrt{t - \tau}} d\tau,$$

and

$$I'_{bx} = \frac{1}{2} \rho_b \frac{\rho_e}{\rho_b} \left[\frac{\partial}{\partial t} (U_{ex} - U_{bx}) + U_{bx} \frac{\partial}{\partial y} (U_{ex} - U_{bx}) \right. \\ \left. + U_{by} \frac{\partial}{\partial y} (U_{ex} - U_{bx}) + U_{bx} \frac{\partial}{\partial z} (U_{ex} - U_{bx}) \right].$$

Similar permutation for I'_{by} , I'_{bz} ; V'_{by} , V'_{bz}

Since bubbles are dilute

$$I' \gg I,$$

$\phi_b \frac{\partial P}{\partial x_j}$ is negligible, and

$$F_{bp} = \frac{9\mu_m}{2a_b^2 \rho_b} \sim \frac{9\mu_m}{2a_b^2 \rho}.$$

Further modification of free board equations will include solid particles.

Appendix B

Nondimensionalized Forms of Relations in Appendix A

Some general relations among interacting parameters and flow properties are seen from non-dimensionalizing. In the simplest non-trivial form, the latter can be made based on x_o , U_o , and $\bar{\rho}$, $\bar{\rho}_p$, with

$$\begin{aligned} U_x^+ &= \frac{U}{U_o} x, & U_y^+ &= \frac{U}{U_o} y, & U_z^+ &= \frac{U}{U_o} z \\ U_{px}^+ &= \frac{U}{U_o} p_x, & U_{py}^+ &= \frac{U}{U_o} p_y, & U_{pz}^+ &= \frac{U}{U_o} p_z \\ P^+ &= \frac{P}{\bar{\rho} U_o^2}, & R^+ &= \frac{\bar{\rho} U_o x_o}{\mu_m}, & F^+ &= \frac{\bar{\rho}}{\rho} \frac{F x_o}{U_o} \\ x^+ &= \frac{x}{x_o}, & y^+ &= \frac{y}{x_o}, & z^+ &= \frac{z}{x_o} \\ f^+ &= \frac{g x_o}{U_o^2}, & t^+ &= t U_o / x_o \end{aligned}$$

B.1 Bed: Gas Phase

Continuity:

$$-\frac{\partial \phi}{\partial t^+} + \frac{\partial(1-\phi)U_x^+}{\partial x^+} + \frac{\partial(1-\phi)U_y^+}{\partial y^+} + \frac{\partial(1-\phi)U_z^+}{\partial z^+} = 0, \quad (B.1)$$

and

$$\frac{\partial \phi}{\partial t^+} + \frac{\partial \phi U_{px}^+}{\partial x^+} + \frac{\partial \phi U_{py}^+}{\partial y^+} + \frac{\partial \phi U_{pz}^+}{\partial z^+} = 0. \quad (B.2)$$

Momentum Equations, gas:

$$\begin{aligned} &\frac{\partial(1-\phi)U_x^+}{\partial t^+} + \frac{\partial(1-\phi)U_x^{+2}}{\partial x^+} + \frac{\partial(1-\phi)U_x^+U_y^+}{\partial y^+} + \frac{\partial(1-\phi)U_x^+U_z^+}{\partial z^+} \\ &- \frac{\partial}{\partial x^+} (1-\phi)(U_x^+ - U_{px}^+)^2 - \frac{\partial}{\partial y^+} (1-\phi)(U_x^+ - U_{px}^+)(U_y^+ - U_{py}^+) \\ &- \frac{\partial}{\partial z^+} (1-\phi)(U_x^+ - U_{px}^+)(U_z^+ - U_{pz}^+) = -\frac{\partial}{\partial x^+} P^+ (1-\phi) - F^+ \phi (U_x^+ - U_{px}^+), \quad (B.3) \end{aligned}$$

where

$$F^+ = \frac{\bar{\rho}}{\rho} F \frac{x_o}{U_o} = \frac{75}{2} \frac{\phi}{(1-\phi)^2} \frac{\bar{\mu}_g x_o}{\rho a^2 U_o} + \frac{1.75}{2(1-\phi)} \frac{|U^+ - U_p^+|}{a} x_o,$$

$$\frac{1}{R^+} = \frac{\bar{\mu}_g + 150 a^2 \bar{\rho}_p \mu_s^*}{\bar{\rho}_p U_o x_o} \sim \frac{150 a^2}{U_o x_o} \mu_s^*,$$

and

$$Re = \bar{\rho} U_o x_o / \bar{\mu}_g.$$

Other components are given by:

$$\begin{aligned} & \frac{\partial}{\partial t^+} (1-\phi) U_y^+ + \frac{\partial}{\partial x^+} (1-\phi) U_y^+ U_x^+ + \frac{\partial}{\partial y^+} (1-\phi) U_y^{+2} + \frac{\partial}{\partial z^+} (1-\phi) U_y^+ U_z^+ \\ & - \frac{\partial}{\partial x^+} (1-\phi) (U_y^+ - U_{py}^+) (U_x^+ - U_{px}^+) - \frac{\partial}{\partial y^+} (1-\phi) (U_y^+ - U_{py}^+)^2 \\ & - \frac{\partial}{\partial z^+} (1-\phi) (U_y^+ - U_{py}^+) (U_z^+ - U_{pz}^+) = - \frac{\partial}{\partial y^+} P^+ (1-\phi) - \phi F^+ (U_y^+ - U_{py}^+), \end{aligned} \quad (B.4)$$

and

$$\begin{aligned} & \frac{\partial}{\partial t^+} (1-\phi) U_z^+ + \frac{\partial}{\partial x^+} (1-\phi) U_z^+ U_x^+ + \frac{\partial}{\partial y^+} (1-\phi) U_z^+ U_y^+ + \frac{\partial}{\partial z^+} (1-\phi) U_z^{+2} \\ & - \frac{\partial}{\partial x^+} (1-\phi) (U_z^+ - U_{pz}^+) (U_x^+ - U_{px}^+) - \frac{\partial}{\partial y^+} (1-\phi) (U_z^+ - U_{pz}^+) (U_y^+ - U_{py}^+) \\ & - \frac{\partial}{\partial z^+} (1-\phi) (U_z^+ - U_{pz}^+)^2 = - \frac{\partial}{\partial z^+} P^+ (1-\phi) - \phi F^+ (U_z^+ - U_{pz}^+) - (1-\phi) f^+. \end{aligned} \quad (B.5)$$

Particles:

$$\begin{aligned} & \frac{\partial}{\partial t^+} \phi U_{px}^+ + \frac{\partial}{\partial x^+} \phi U_{px}^{+2} + \frac{\partial}{\partial y^+} \phi U_{px}^+ U_{py}^+ + \frac{\partial}{\partial z^+} \phi U_{px}^+ U_{pz}^+ \\ & = - \frac{\bar{\rho}}{\rho} \frac{\partial}{\partial x^+} P^+ \phi + \phi \frac{\bar{\rho}}{\rho_p} F^+ (U_x^+ - U_{px}^+) + \frac{\partial}{\partial y^+} \left(\frac{1}{R^+} \frac{\partial U_{px}^+}{\partial y^+} \right) + \frac{\partial}{\partial z^+} \left(\frac{1}{R^+} \frac{\partial U_{px}^+}{\partial z^+} \right), \end{aligned} \quad (B.6)$$

$$\begin{aligned} & \frac{\partial}{\partial t^+} \phi U_{py}^+ + \frac{\partial}{\partial x^+} \phi U_{py}^+ U_{px}^+ + \frac{\partial}{\partial y^+} \phi U_{py}^{+2} + \frac{\partial}{\partial z^+} \phi U_{py}^+ U_{pz}^+ \\ & = - \frac{\bar{\rho}}{\rho_p} \frac{\partial}{\partial y^+} P^+ \phi + \phi \frac{\bar{\rho}}{\rho_p} F^+ (U_y^+ - U_{py}^+) + \frac{\partial}{\partial x^+} \left(\frac{1}{R^+} \frac{\partial U_{py}^+}{\partial x^+} \right) + \frac{\partial}{\partial z^+} \left(\frac{1}{R^+} \frac{\partial U_{py}^+}{\partial z^+} \right), \end{aligned} \quad (B.7)$$

and

$$\begin{aligned} & \frac{\partial}{\partial t^+} \phi U_{pz}^+ + \frac{\partial}{\partial x^+} \phi U_{pz}^+ U_{px}^+ + \frac{\partial}{\partial y^+} \phi U_{pz}^+ U_{py}^+ + \frac{\partial}{\partial z^+} \phi U_{pz}^{+2} \\ & = - \frac{\bar{\rho}}{\rho_p} \frac{\partial}{\partial z^+} P^+ \phi + \phi \frac{\bar{\rho}}{\rho_p} F^+ (U_z^+ - U_{pz}^+) + \frac{\partial}{\partial x^+} \left(\frac{1}{R^+} \frac{\partial U_{pz}^+}{\partial x^+} \right) + \frac{\partial}{\partial y^+} \left(\frac{1}{R^+} \frac{\partial U_{pz}^+}{\partial y^+} \right) - \phi f^+, \end{aligned} \quad (B.8)$$

Boundary Conditions:

$$(1) \text{ at } z^+ = 0: \quad U_z^+ = 1, \quad U_x^+ = U_y^+ = 0, \quad U_{px}^+ = U_{py}^+ = 0$$

$$(2) \text{ at } x^+ = 1: \quad U_x^+ = U_y^+ = U_z^+ = U_{px}^+ = U_{py}^+ = U_{pz}^+ = 0$$

$$\partial\phi/\partial y^+ = 0, \quad \partial P^+/\partial y^+ = 0$$

$$(3) \text{ at } y^+ = y_0/x_0: \quad U_x^+ = U_y^+ = U_z^+ = 0 = U_{px}^+ = U_{py}^+ = U_{pz}^+$$

$$\partial\phi/\partial x^+ = 0, \quad \partial P^+/\partial x^+ = 0$$

$$(4) \text{ at } x^+ = 0: \quad \partial/\partial x^+ = 0, \quad \text{all } \phi, P^+, \underline{U}^+, \underline{U}_p^+ \quad (8 \text{ variables})$$

$$(5) \text{ at } y^+ = 0: \quad \partial/\partial y^+ = 0 \quad (8 \text{ variables})$$

$$(6) \text{ at } S \text{ or } z_0^+ = h/x_0:$$

$$\int_0^{h/x_0} \int_0^{y_0/x_0} \int_0^1 \phi dx^+ dy^+ dz^+ = m_p/4 \bar{\rho}_p x_0^3$$

$$(7) \text{ at } z^+ = h/x_0: \quad U_{pz}^+ = 0$$

$$P^+ = P_0/\bar{\rho} U_0^2$$

$$\partial\phi/\partial z^+ = 0$$

B.2 Free Board:

$$Z \geq h$$

$$P^+ = P_0^+ - \frac{1}{2} U_{zh}^{+2} (2\phi - \phi^2),$$

$$\frac{\partial U_x^+}{\partial x^+} + \frac{\partial U_y^+}{\partial y^+} + \frac{\partial U_z^+}{\partial z^+} = 0,$$

(B.9)

$$\frac{\partial U_x^+}{\partial t^+} + \frac{\partial U_x^{+2}}{\partial x^+} + \frac{\partial U_x^+ U_y^+}{\partial y^+} + \frac{\partial U_x^+ U_z^+}{\partial z^+} = - \frac{\partial P^+}{\partial x^+} + \frac{1}{Re} \left(\frac{\partial^2 U_x^+}{\partial x^{+2}} + \frac{\partial^2 U_x^+}{\partial y^{+2}} \right),$$

(B.10)

where

$$Re = \bar{\rho} U_0 x_0 / \bar{\mu}$$

$$\text{and } \frac{\partial U^+}{\partial t^+} + \frac{\partial U^+ U^+}{\partial x^+} + \frac{\partial U^{+2}}{\partial y^+} + \frac{\partial U^+ U^+}{\partial z^+} = - \frac{\partial P^+}{\partial y^+} + \frac{1}{\text{Re}} \left(\frac{\partial^2 U^+}{\partial x^{+2}} + \frac{\partial^2 U^+}{\partial z^{+2}} \right), \quad (\text{B.11})$$

$$\frac{\partial U^+}{\partial t^+} + \frac{\partial U^+ U^+}{\partial x^+} + \frac{\partial U^+ U^+}{\partial y^+} + \frac{\partial U^{+2}}{\partial z^+} = - \frac{\partial P^+}{\partial z^+} + \frac{1}{\text{Re}} \left(\frac{\partial^2 U^+}{\partial x^{+2}} + \frac{\partial^2 U^+}{\partial y^{+2}} \right) - f^+. \quad (\text{B.12})$$

Boundary Conditions:

$$z^+ = h/x_o \quad U_j^+ = U_{j\text{bed}}^+ (1 - \phi) \quad j = x, y, z$$

$$P^+ = P_o^+ + \frac{1}{2} U_z^{+2} (\text{bed}) [2\phi - \phi^2]$$

$$x^+ = 1 \quad U_x^+ = U_y^+ = U_z^+ = 0 \quad \frac{\partial P^+}{\partial y^+} = 0$$

$$y^+ = y_o/x_o \quad U_x^+ = U_y^+ = U_z^+ = 0 \quad \frac{\partial P^+}{\partial x^+} = 0$$

$$x^+ = 0 \quad \frac{\partial}{\partial x^+} = 0$$

$$y^+ = 0 \quad \frac{\partial}{\partial y^+} = 0$$

B.3 Bubbles and Bubble Motion

Replace $1 - \phi$ in Eqs. (B.1), and (B.3) - (B.5) by $1 - \phi - \phi_b$, and obtain

$$\rho_b = N_b \frac{4\pi}{3} a_b^3 \bar{\rho}_b \sim N_b \frac{4\pi}{3} a_b^3 \bar{\rho},$$

$$N_{bo} = N_b' f/U_{bo}, \quad \underline{U}_b = \underline{U}_b/U_o,$$

and

$$\phi_b = N_b \frac{4\pi}{3} a_b^3, \quad F_b^+ = F_{bp} x_o/U_o.$$

also take $\rho_e \sim \rho_p$, namely dense phase properties are represented by that of the solid phase.

Continuity:

$$\frac{\partial \phi_b}{\partial t^+} + \frac{\partial \phi_b U_{bx}^+}{\partial x^+} + \frac{\partial \phi_b U_{by}^+}{\partial y^+} + \frac{\partial \phi_b U_{bz}^+}{\partial z^+} = 0. \quad (\text{B.13})$$

Momentum:

$$\begin{aligned} & \frac{\partial \phi_b U_{bx}^+}{\partial t^+} + \frac{\partial \phi_b U_{bx}^+}{\partial x^+} + \frac{\partial \phi_b U_{bx}^+ U_{by}^+}{\partial y^+} + \frac{\partial \phi_b U_{bx}^+ U_{bz}^+}{\partial z^+} \\ & = \phi_b F_b^+ (U_{nx}^+ - U_{bx}^+) + \frac{1}{2} \phi_b \phi \frac{\bar{\rho}_p}{\bar{n}} \left[\frac{\partial}{\partial x^+} (U_{nx}^+ - U_{bx}^+) \right] \end{aligned}$$

$$\begin{aligned}
 & + U_{bx}^+ \frac{\partial}{\partial x^+} (U_{px}^+ - U_{bx}^+) + U_{by}^+ \frac{\partial}{\partial y^+} (U_{px}^+ - U_{bx}^+) \\
 & + U_{bz}^+ \frac{\partial}{\partial z^+} (U_{px}^+ - U_{bx}^+) \Big] + v_{bx}'^+ , \tag{B.14}
 \end{aligned}$$

$$\begin{aligned}
 & \frac{\partial \phi_b U_{by}^+}{\partial t^+} + \frac{\partial \phi_b U_{by}^+ U_{bx}^+}{\partial x^+} + \frac{\partial \phi_b U_{by}^{+2}}{\partial y^+} + \frac{\partial \phi_b U_{by}^+ U_{bz}^+}{\partial z^+} \\
 & = \phi_b F_b^+ (U_{py}^+ - U_{by}^+) + \frac{1}{2} \phi_b \phi \frac{\bar{\rho}_p}{\bar{\rho}} \left[\frac{\partial}{\partial t^+} (U_{py}^+ - U_{by}^+) \right. \\
 & + U_{bx}^+ \frac{\partial}{\partial x^+} (U_{py}^+ - U_{by}^+) + U_{by}^+ \frac{\partial}{\partial y^+} (U_{py}^+ - U_{by}^+) \\
 & \left. + U_{bz}^+ \frac{\partial}{\partial z^+} (U_{py}^+ - U_{by}^+) \right] + v_{by}'^+ , \tag{B.15}
 \end{aligned}$$

and

$$\begin{aligned}
 & \frac{\partial \phi_b U_{bz}^+}{\partial t^+} + \frac{\partial \phi_b U_{bz}^+ U_{bx}^+}{\partial x^+} + \frac{\partial \phi_b U_{bz}^+ U_{by}^+}{\partial y^+} + \frac{\partial \phi_b U_{bz}^{+2}}{\partial z^+} \\
 & = \phi_b F_b^+ (U_{pz}^+ - U_{bz}^+) + \frac{1}{2} \phi_b \phi \frac{\bar{\rho}_p}{\bar{\rho}} \left[\frac{\partial}{\partial t^+} (U_{pz}^+ - U_{bz}^+) \right. \\
 & + U_{bx}^+ \frac{\partial}{\partial x^+} (U_{pz}^+ - U_{bz}^+) + U_{by}^+ \frac{\partial}{\partial y^+} (U_{pz}^+ - U_{bz}^+) \\
 & \left. + U_{bz}^+ \frac{\partial}{\partial z^+} (U_{pz}^+ - U_{bz}^+) \right] - \phi_b f^+ + v_{bz}'^+ , \tag{B.16}
 \end{aligned}$$

with

$$\begin{aligned}
 v_b'^+ &= \frac{g}{\sqrt{\pi}} \left(\frac{x_o}{2a_b} \right) \sqrt{\frac{\rho_p}{\bar{\rho}}} \sqrt{\frac{\mu_m}{\rho U_o x_o}} \phi_b \sqrt{\phi} \\
 & \int_{\tau^+}^{t^+} \frac{(\partial/\partial \tau^+) (U_p^+ - U_b^+)}{\sqrt{t^+ - \tau^+}} d\tau^+ ,
 \end{aligned}$$

$$F_{bp} = \frac{9\mu_m}{2a_b^2 \bar{\rho}} ,$$

and

$$f_b^+ = \frac{x_o \mu_m}{2a_b^2 U_o \bar{\rho}} = \left(\frac{x_o}{2a_b} \right) \left(\frac{\mu_m}{a_b U_o \bar{\rho}} \right) .$$

Boundary Conditions:

$$z^+ = 0 ; \quad 2a_{bo}, N_{bo}, U_{bzo} \text{ given} .$$

$$\phi_{bo} = N_{bo} \frac{4\pi}{3} a_{bo}^3 .$$

Bubble Burst at:

$$p_b^+ - p^+ = \frac{1}{2} U^{+2} [1 - (1 - \phi)^2]$$

Appendix C

Streamlines and Particle Lines

The ideal condition at the bed surface is readily visualized in a 2-D case.

The continuity equations are satisfied by introducing stream functions ψ and ψ_p

For gas:

$$\frac{\partial \psi}{\partial z} = -\rho U_x, \quad \frac{\partial \psi}{\partial x} = \rho U_z,$$

giving

$$\frac{U_z}{U_x} = -\frac{(\partial \psi / \partial x)}{(\partial \psi / \partial z)} = \left(\frac{\partial z}{\partial x} \right)_{\psi}.$$

For the particles:

$$\frac{\partial \psi_p}{\partial z} = -\rho_p U_{px}, \quad \frac{\partial \psi_p}{\partial x} = \rho_p U_{pz},$$

giving

$$\frac{U_{pz}}{U_{px}} = -\frac{(\partial \psi_p / \partial x)}{(\partial \psi_p / \partial z)} = \left(\frac{\partial z}{\partial x} \right)_{\psi_p}.$$

The general situations are illustrated in Fig. 15. The streamline at the top surface (where $U_{pz} = 0$) is a horizontal line. An ideal fluidized bed, therefore, has a flat surface on top.

The vector of the outer streamline ψ_p is readily seen in that:

At the center; $U_{pz} > 0$, $U_{px} = 0$, $\frac{\partial z}{\partial x} \rightarrow \infty$; hence the streamline ab points upward.

At the top; $U_{pz} = 0$, U_{px} finite, $\frac{\partial z}{\partial x} = 0$; the streamline points away from the centerline continuing from b to c.

At the outer wall; $U_{pz} < 0$, $U_{px} = 0$, $\frac{\partial z}{\partial x} \rightarrow -\infty$; hence stream line cd points downward.

At the bottom; $U_{pz} = 0$, U_{px} finite, $\frac{\partial z}{\partial x} = 0$, thus completing the outer streamline of a nonelutriating bed.

Other streamlines of particle paths can be similarly deduced.

(a) Gas

(b) Solid

Fig. 15. Two-dimensional Fluidized Bed and Streamlines of Phases

Appendix D

Simplified Rate Computation

In the simplified form of Avedesian and Davidson [29] for stoichiometric reaction $2CO + O_2 \rightarrow 2CO_2$, we have

$$\begin{aligned} \frac{dn_1}{dt} &= - \frac{1}{32} D_1 \text{ (Sh)} \frac{4\pi a^2}{2a} \rho_1 N_c = - D_1 \text{ (Sh)} \frac{4\pi a^2}{2a} n_1 N_c \\ &= \frac{1}{2} \frac{dn_2}{dt} = - \frac{1}{2} \frac{dn_3}{dt} = - D_1 \text{ (Sh)} \frac{3M_c}{2a^2 \rho_c} n_o n_1 \end{aligned}$$

for N_c char particles per unit volume outside of the flame surface; and for reaction Eq. (2.5) $C + CO_2 \rightarrow 2CO$

$$\frac{dn_o}{dt} = \frac{dn_3}{dt} = - \frac{1}{2} \frac{dn_2}{dt} = - D_3 \text{ (Sh)} \frac{4\pi a^2}{2a} n_3 N_c$$

inside the flame surface. The net gas generation is:

$$\begin{aligned} \frac{dn_1}{dt} = - \frac{dn_3}{dt} = \frac{dn_o}{dt} &= - D_1 \text{ (Sh)} \frac{4\pi a^2}{2a} n_1 N_c \\ &\equiv - k_D n_1 A_c^* \end{aligned}$$

in place of reaction Eqs. (2.3) to (2.6) and retaining Eqs. (2.7) to (2.9), we have [assuming excess air, and including $CO + \frac{1}{2} O_2 \rightarrow CO_2$ in Eq. (2.7) to give $\frac{1}{n} (CH_2)_n + \frac{3}{2} O_2 \xrightarrow{k_V} CO_2 + H_2O$]:

$$\begin{aligned} C: \quad \frac{dn_o}{dt} &= - k_D n_1 A_c^* \\ O_2: \quad \frac{dn_1}{dt} &= - k_D n_1 A_c^* - \frac{3}{2} k_V' n_5 n_1^{3/2} - k_{VI} A_s^* n_1 - \frac{1}{2} k_{VII} A_d^* n_7 n_1^{1/2} \end{aligned}$$

CO: ----

$$CO_2: \quad \frac{dn_3}{dt} = k_D n_1 A_c^* + k_V' n_5 n_1^{3/2} + k_{VII} A_d^* n_7 n_1^{1/2}$$

O: ----

$$\begin{aligned}
 \frac{1}{n}(\text{CH}_2)_n: \quad & \frac{dn_5}{dt} = -k'_{V1} n_5^{3/2} \\
 \text{H}_2\text{O}: \quad & \frac{dn_6}{dt} = k'_{V1} n_5^{3/2} \\
 \text{SO}_2: \quad & \frac{dn_7}{dt} = k_{VI}^* n_1 - k_{VII}^* n_7 n_1^{1/2} \\
 \text{Dolomite}: \quad & \frac{dn'_d}{dt} = -k_{VII}^* n_7 n_1^{1/2} = -\frac{dn_d}{dt} \\
 \text{S} \quad & \frac{dn_s}{dt} = -k_{VI}^* n_1
 \end{aligned}$$

Using single species of particle for our illustration, we now have

$$\begin{aligned}
 \Gamma_{\text{gas}} &= 32 \left[-k_{D1c}^* n_1 - \frac{3}{2} k'_{V5} n_1^{3/2} - k_{VI}^* n_1 - \frac{1}{2} k_{VII}^* n_7 n_1^{1/2} \right] \\
 &+ 44 \left[k_{D1c}^* n_1 + k'_{V5} n_1^{3/2} + k_{VII}^* n_7 n_1^{1/2} \right] \\
 &+ 14 \left[-k'_{V1} n_5^{3/2} \right] + 18 \left[k'_{V1} n_5^{3/2} \right] \\
 &+ 64 \left[k_{VI}^* n_1 - k_{VII}^* n_7 n_1^{1/2} \right] \\
 &= k_{D1c}^* (-32 + 44.01) \\
 &+ k'_{V5} n_1^{3/2} \left(-32 \left(\frac{3}{2} \right) + 44.01 - 14.026 + 18.016 \right) \\
 &+ k_{VI}^* n_1 (-32 + 64.06) + k_{VII}^* n_7 n_1^{1/2} (44.01 - 64.06 - 16) \\
 &= k_{D1c}^* (12.01) + k_{VII}^* n_7 n_1^{1/2} (-36.05) + k_{VI}^* n_1 (32.06), \\
 \Gamma_{\text{coal}} &= -k_{D1c}^* (12.01) - k_{VI}^* n_1 (32.06), \\
 \text{and} \\
 \Gamma_{\text{dolomite}} &= 36.05 (k_{VII}^* n_7 n_1^{1/2}).
 \end{aligned}$$

Appendix E

Simplified Input for Computation

For simplified computation: 3 phases of char
 3 phases of dolomite
 3 phases of bubbles
 8 components of gas

Input - Coal (Subscript F)

Initial condition

$$\rho_{F(in)} U_{(in)} A_{(in)} = \text{coal feed rate}$$

where U_{in} is the velocity and A_{in} is the flow area

$$\rho_{c10} = \frac{\rho_F}{100} [\alpha M_o + \epsilon M_s + M_A] \equiv \frac{\rho_F}{100} M_c = n_o' M_c$$

where 0 stands for Initial

1 stands for size 1 of char

c stands for char, and

$$\rho_{g80} = \frac{\rho_{c10}}{M_c} \frac{\delta}{2} M_8 = \frac{\delta}{2} n_o' M_8$$

$$\rho_{g60} = \frac{\rho_{c10}}{M_c} \gamma M_6 = \gamma n_o' M_6$$

$$\rho_{g50} = \frac{\rho_{c10}}{M_c} \frac{v}{4} M_5 = \frac{v}{4} n_o' M_5$$

(typical input data of γ , ϵ , etc. on p. 102)

$$\rho_F = 720 \text{ kg/m}^3$$

Input - Dolomite

$$\rho_{d(in)} U_{d(in)} A_{d(in)} = \text{dolomite feed rate}$$

$$\rho_{d(in)} = \rho_{d(in)} = 1450 \text{ kg/m}^3$$

Input - Air (at Z = 0)

$$\rho_{a(in)} U_{a(in)} A_{a(in)} = \text{Air flow rate}$$

$$\rho_{g10} = \frac{\rho_{a(in)}}{28.97} \frac{1}{4.76} M_1 = n_1' M_1$$

$$\rho_{g80} = \frac{\rho_{a(in)}}{28.97} \frac{3.76}{4.76} M_8 = 3.76 n_1' M_8$$

Gases

$$\rho_{g1} = n_1 M_1$$

$$\rho_{g5} = n_5 M_5$$

$$\rho_{g2} = n_2 M_2$$

$$\rho_{g6} = n_6 M_6$$

$$\rho_{g3} = n_3 M_3$$

$$\rho_{g7} = n_7 M_7$$

$$\rho_{g4} = n_4 M_4$$

$$\rho_{g8} = n_8 M_8$$

Carbon

$$\rho_{o1} = N_{c1} \frac{m_F}{100} \propto M_o$$

$$\rho_{o2} = N_{c2} \frac{m_F}{100} \frac{\alpha}{2} M_o$$

Sulfur (Simplification: assume S removed at the same fraction as C)

$$\rho_{s1} = N_{c1} \frac{m_F}{100} \epsilon M_s = \frac{\rho_{o1}}{\alpha M_o} \epsilon M_s$$

$$\rho_{s2} = \frac{\rho_{o2}}{\alpha M_o} \epsilon M_s$$

Molecular Weights

$$C: \quad M_o = 12.01$$

$$O_2: \quad M_1 = 32$$

$$CO: \quad M_2 = 28.01$$

$$CO_2: \quad M_3 = 44.01$$

$$O: \quad M_4 = 16$$

$$\text{Dolomite } M_d' = 140.41$$

$$\text{Sulfated Dolomite } M_d = 176.46$$

$$\frac{1}{n} (CH_2)_n: \quad M_5 = 14.026$$

$$H_2O: \quad M_6 = 18.016$$

$$SO_2: \quad M_7 = 64.06$$

$$N_2: \quad M_8 = 28.02$$

$$S: \quad M_s = 32.06$$

Phases and Species

$$\text{Coal (Initial)} \quad \rho_F = N_c m_F = N_c \frac{4\pi}{3} a_{cl}^3 \bar{\rho}_F, \quad \bar{\rho}_F = 1300 \text{ kg/m}^3$$

$$\text{Char} \quad \rho_{cl} = N_{cl} \frac{4\pi}{3} a_{cl}^3 \bar{\rho}_c = N_{cl} m_{chl} = N_{cl} \frac{m_F}{100} (\alpha M_o + \epsilon M_s + M_A)$$

$$\rho_{c2} = N_{c2} \frac{4\pi}{3} a_{c2}^3 \bar{\rho}_c = N_{c2} m_{ch2} = N_{c2} \frac{m_F}{100} \left(\frac{\alpha}{2} M_c + \frac{\epsilon}{2} M_s + M_A \right)$$

$$\rho_{c3} = N_{c3} \frac{4\pi}{3} a_{c3}^3 \bar{\rho}_c = N_{c3} m_{ch3} = N_{c3} \frac{m_F}{100} (M_A)$$

$$A_{ck}^* = N_{ck} 4\pi a_{ck}^2 = (4\pi)^{1/3} 3^{2/3} \left(\frac{\rho_{ck}}{\bar{\rho}_c} \right)^{2/3} (N_{ck})^{1/3} (= A_{sk}^*)$$

$$\bar{\rho}_c = 1440 \text{ kg/m}^3$$

Dolomite:

$$\rho_{d1} = N_{d1} \frac{4\pi}{3} a_d^3 \bar{\rho}_{d1} = N_{d1} m_{d1} = N_{d1} \frac{m_{d1}}{M_d'} M_d'$$

$$k_{VII} (1) = 3 \left(0.075 + 10^3 \frac{\rho_6}{M_6} \right) \frac{\bar{\rho}_{d1}}{\rho_{d1}}$$

$$\rho_{d2} = N_{d2} \frac{4\pi}{3} a_d^3 \bar{\rho}_{d2} = N_{d2} m_{d2} = N_{d2} \frac{m_{d1}}{M_d'} \left(\frac{1}{2} M_d' + \frac{1}{2} M_d \right)$$

$$k_{VII} (2) = 4 \left(0.075 + 10^3 \frac{\rho_6}{M_6} \right) \frac{\bar{\rho}_{d2}}{\rho_{d2}}$$

$$\rho_{d3} = N_{d3} \frac{4\pi}{3} a_d^3 \bar{\rho}_{d3} = N_{d3} m_{d3} = N_{d3} \frac{m_{d1}}{M_d'} \left(\frac{1}{10} M_d' + \frac{9}{10} M_d \right)$$

$$k_{VII} (3) = 5.45 \left(0.075 + 10^3 \frac{\rho_6}{M_6} \right) \frac{\bar{\rho}_{d3}}{\rho_{d3}}$$

$$A_{dk}^* = N_{dk} 4\pi a_d^2 = (4\pi)^{1/3} 3^{2/3} \left(\frac{\rho_{dk}}{\bar{\rho}_{dk}} \right)^{2/3} N_{dk}^{1/3}$$

Bubbles

$$\rho_{b1} = N_{b1} \frac{4\pi}{3} a_{b1}^3 \bar{\rho}_g$$

$$\rho_{b2} = N_{b2} \frac{4\pi}{3} a_{b2}^3 \bar{\rho}_g$$

$$\rho_{b3} = N_{b3} \frac{4\pi}{3} a_{b3}^3 \bar{\rho}_g$$

Generation Rates (Simplified)

Gases:

$$\Gamma_{g1} = M_1 \left\{ -k_I \frac{\rho_{g1}}{M_1} \frac{\rho_{g2}}{M_2} - k_{IV} \left(\sum_1^2 A_{ck}^* \right) \frac{\rho_{g1}}{M_1} \left(1 + \frac{\epsilon}{\alpha} \right) \right\}$$

$$\begin{aligned}
 & -k_V \frac{\rho_{g5}}{M_5} \frac{\rho_{g1}}{M_1} - \frac{1}{2} \left(\sum_1^3 k_{VII(k)} A_{dk}^* \right) \frac{\rho_{g7}}{M_7} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \Bigg\} \\
 \Gamma_{g2} = M_2 & \left\{ -k_I \frac{\rho_{g1}}{M_1} \frac{\rho_{g2}}{M_2} - k_{II} \frac{\rho_{g2}}{M_2} \frac{\rho_{g4}}{M_4} + k'_{II} \frac{\rho_{g3}}{M_3} \right. \\
 & \left. + 2k_{III} \left(\sum_1^2 A_{ck}^* \right) \frac{\rho_{g3}}{M_3} + k_V \frac{\rho_{g1}}{M_1} \frac{\rho_{g5}}{M_5} \right\} \\
 \Gamma_{g3} = M_3 & \left\{ k_I \frac{\rho_{g1}}{M_1} \frac{\rho_{g2}}{M_2} + \left(\sum_1^3 k_{VII(k)} A_{dk}^* \right) \frac{\rho_{g7}}{M_7} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} + k_{II} \frac{\rho_{g2}}{M_2} \frac{\rho_{g4}}{M_4} \right. \\
 & \left. - k_{II} \frac{\rho_{g3}}{M_3} - k_{III} \left(\sum_1^3 A_{ck}^* \right) \frac{\rho_{g3}}{M_3} + k_{IV} \left(\sum_1^2 A_{ck}^* \right) \frac{\rho_{g1}}{M_1} \right\} \\
 \Gamma_{g4} = M_4 & \left\{ k_I \frac{\rho_{g1}}{M_1} \frac{\rho_{g2}}{M_2} - k_{II} \frac{\rho_{g2}}{M_2} \frac{\rho_{g4}}{M_4} + k'_{II} \frac{\rho_{g3}}{M_3} \right\} \\
 \Gamma_{g5} = M_5 & \left\{ -k_V \frac{\rho_{g1}}{M_1} \frac{\rho_{g5}}{M_5} \right\} = -\Gamma_{g6} \frac{M_5}{M_6} \\
 \Gamma_{g7} = M_7 & \left\{ \Gamma_{g1} \frac{\epsilon M}{\alpha M_o} - \left(\sum_1^3 k_{VII(k)} A_{dk}^* \right) \frac{\rho_{g7}}{M_7} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \right\}
 \end{aligned}$$

For the continuity equations of the gas phase

$$\Gamma_{g8} = 0 .$$

For the momentum and energy equations of the gas phase

$$\begin{aligned}
 \Gamma_{gas} = & \left\{ M_1 k_{III} \left(\sum_1^2 A_{ck}^* \right) \frac{\rho_{g3}}{M_3} + M_1 k_{IV} \left(\sum_1^2 A_{ck}^* \right) \frac{\rho_{g1}}{M_1} \right\} \left(1 + \frac{\epsilon M}{\alpha M_p} \right) \\
 & + \left\{ -M_7 + M_3 - \frac{1}{2} M_1 \right\} \left(\sum_1^3 k_{VII(k)} A_{dk}^* \right) \frac{\rho_{g7}}{M_7} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \Bigg\}
 \end{aligned}$$

Char:

$$\begin{aligned}
 \Gamma_{c1} = (M_o + \frac{\epsilon}{\alpha} M_s) & \left\{ -k_{III} A_{c1}^* \frac{\rho_{g3}}{M_3} - k_{IV} A_{c1}^* \frac{\rho_{g1}}{M_1} \right\} \\
 \Gamma_{c2} = -\Gamma_{c1} \frac{m_{c2}}{m_{c1}} + (M_o + \frac{\epsilon}{\alpha} M_s) & \left\{ -k_{III} A_{c2}^* \frac{\rho_{g3}}{M_3} - k_{IV} A_{c2}^* \frac{\rho_{g7}}{M_1} \right\} \\
 \Gamma_{c3} = -\left(\Gamma_{c2} + \Gamma_{c1} \frac{m_{c2}}{m_{c1}} \right) \frac{m_{c3}}{m_{c2}}
 \end{aligned}$$

Dolomite:

$$\Gamma_{d1} = M_d \left\{ -k_{VII(1)} A_{d1}^* \frac{\rho_{g7}}{M_7} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \right\}$$

$$\Gamma_{d2} = -\Gamma_{d1} \frac{m_{d2}}{m_{d1}} + M_d \left\{ -k_{VII(2)} A_{d2}^* \frac{\rho_{g7}}{M_7} \left(\frac{\rho_{g1}}{M_1} \right)^{1/2} \right\}$$

$$\Gamma_{d3} = -\left(\Gamma_{d2} + \Gamma_{d1} \frac{m_{d2}}{m_{d1}} \right) \frac{m_{d3}}{m_{d2}}$$

where:

$$\frac{m_{c2}}{m_{c1}} = \frac{\frac{1}{2} (M_o + \frac{\varepsilon}{\alpha} M_s) + \frac{M_A}{\alpha}}{(M_o + \frac{\varepsilon}{\alpha} M_s) + \frac{M_A}{\alpha}}$$

$$\frac{m_{c3}}{m_{c2}} = \frac{\frac{M_A}{\alpha}}{\frac{1}{2} (M_o + \frac{\varepsilon}{\alpha} M_s) + \frac{M_A}{\alpha}}$$

$$\frac{m_{d2}}{m_{d1}} = \frac{\frac{1}{2} M'_d + \frac{1}{2} M_d}{M'_d}$$

$$\frac{m_{d3}}{m_{d2}} = \frac{\frac{1}{10} M'_d + \frac{9}{10} M_d}{\frac{1}{2} M'_d + \frac{1}{2} M_d}$$

Bubbles: $\hat{k}_k = 10^{-3} \left(\frac{N_{bk}}{N_{bo}} \right)^{-1/3}$, based on reasoning of Eq. (3.26)
($k^* = 10^{-3}$)

$$\Gamma_{(N)b1} = \Gamma_{(N)bo} - \hat{k}_1 N_{b1}^2,$$

with a_b^*

$$\Gamma_{(N)b2} = \hat{k}_1 N_{b1}^2 - \hat{k}_2 N_{b1} N_{b2},$$

with $2^{1/3} a_b^*$

$$\Gamma_{(N)b3} = \hat{k}_2 N_{b1} N_{b2},$$

with $3^{1/3} a_b^*$

at $z = 0$

$$\Gamma_{(N)bo} = 2000 \text{ bubbles/m}^3 \cdot \text{s}$$

$$N_{bo} = 2 \times 10^4 \text{ bubbles/m}^3$$

$$\bar{U}_{bo} = 0.1 \text{ m/s}$$

$$a_{bo} = a_b^* = 5 \times 10^{-3} \text{ m}$$

$$\bar{\rho}_{bo} = \bar{\rho}_{go}$$

At other positions,

$$a_{b1} = a_b^* \left(\frac{\bar{\rho}_{go}}{\bar{\rho}_g} \right)^{1/3},$$

$$\rho_{b1} = N_{b1} \frac{4\pi}{3} a_{b1}^3 \bar{\rho}_g$$

$$\phi_{b1} = N_{b1} \frac{4\pi}{3} a_{b1}^3$$

$$a_{b2} = 2^{1/3} a_b^* \left(\frac{\bar{\rho}_{go}}{\bar{\rho}_g} \right)^{1/3},$$

$$\rho_{b2} = N_{b2} \frac{4\pi}{3} a_{b2}^3 \bar{\rho}_g$$

$$\phi_{b2} = N_{b2} \frac{4\pi}{3} a_{b2}^3$$

$$a_{b3} = 3^{1/3} a_b^* \left(\frac{\bar{\rho}_{go}}{\bar{\rho}_g} \right)^{1/3},$$

$$\rho_{b3} = N_{b3} \frac{4\pi}{3} a_{b3}^3 \bar{\rho}_g$$

$$\phi_{b3} = N_{b3} \frac{4\pi}{3} a_{b3}^3$$

Continuity equation of bubbles is based on the conservation of the number of bubbles (Eq. 6.7)

The computations might be simplified by taking the mean values of molal specific heats of gases at constant pressure c_p (in J/kg · K) at 500°C:

$$N_2: \quad c_{p8} = 1117.5$$

$$O_2: \quad c_{p1} = 1049.3$$

$$CO: \quad c_{p2} = 1133.3$$

$$\text{H}_2\text{O}: \quad c_{p6} = 2134.4$$

$$\text{CO}_2: \quad c_{p3} = 1160.6$$

$$\frac{1}{n}(\text{CH}_2)_n: \quad c_{p5} = 1548.2$$

$$\text{O}: \quad c_{p4} = 1298.7$$

$$\text{SO}_2: \quad c_{p7} = 664.6$$

$$\text{Char}: \quad c_{pc} = 1256$$

$$\text{Dolomite}: \quad c_{pd} = 929$$

Enthalpies (for Eqs. 6.18 to 6.20); $T_o = 298.16 \text{ K}$

$$h_{c1} = c_{pc} (T_{c1} - T_o) + 3.937 \times 10^8 + \frac{\epsilon}{\alpha} 2.969 \times 10^8$$

$$h_{c2} = c_{pc} (T_{c2} - T_o) + 1.969 \times 10^8 + \frac{\epsilon}{\alpha} 1.485 \times 10^8$$

$$h_{c3} = c_{pc} (T_{c3} - T_o)$$

$$h_{d1} = c_{pd} (T_{d1} - T_o) + 6.091 \times 10^8$$

$$h_{d2} = c_{pd} (T_{d2} - T_o) + 3.046 \times 10^8$$

$$h_{d3} = c_{pd} (T_{d3} - T_o) + 6.091 \times 10^9$$

$$h_1 = 1049.3 (T - T_o)$$

$$h_2 = 1133.3 (T - T_o) + 2.8465 \times 10^8$$

$$h_3 = 1160.6 (T - T_o)$$

$$h_4 = 1298.7 (T - T_o) + 2.4626 \times 10^8$$

$$h_5 = 1548.2 (T - T_o) + 6.7955 \times 10^8$$

$$h_6 = 2134.4 (T - T_o)$$

$$h_7 = 644.6 (T - T_o) - 2.969 \times 10^8$$

$$h_8 = 1117.5 (T - T_o)$$

Equations (6.23) - (6.25)

$$\rho_g c_g = \rho_{g1} \frac{\bar{c}_{p1}}{M_1} + \rho_{g2} \frac{\bar{c}_{p2}}{M_2} + \rho_{g3} \frac{\bar{c}_{p3}}{M_3} + \rho_{g4} \frac{\bar{c}_{p4}}{M_4} + \rho_{g5} \frac{\bar{c}_{p5}}{M_5} + \rho_{g6} \frac{\bar{c}_{p6}}{M_6} \\ + \rho_{g7} \frac{\bar{c}_{p7}}{M_7} + \rho_{g8} \frac{\bar{c}_{p8}}{M_8}$$

$$\rho_m c_m = \left(\sum_1^3 \rho_{ck} \right) c_{pc} + \left(\sum_1^3 \rho_{dk} \right) c_{pd} + \left(\sum_1^3 \rho_{bk} \right) c_g + \rho_g c_g$$

$$\rho_g = \rho_{g1} + \rho_{g2} + \rho_{g3} + \rho_{g4} + \rho_{g5} + \rho_{g6} + \rho_{g7} + \rho_{g8}$$

$$\rho_m = \rho_g + \sum_1^3 \rho_{ck} + \sum_1^3 \rho_{dk} + \sum_1^3 \rho_{bk}$$

$$\rho_g h_g = \sum_1^8 \rho_{gk} h_{gk}$$

$$\rho_m h_m = \rho_g h_g + \sum_1^3 \rho_{ck} h_{ck} + \sum_1^3 \rho_{dk} h_{dk} + \sum_1^3 \rho_{bk} h_{bk}$$

for the bubbles

$$T_b = T_g \quad \text{No separate energy equation of bubble phases}$$

$$\rho_g h_g = (\sum \rho_{gk} c_{pgk}) T_g - (\sum \rho_{gk} c_{pgk}) T_o + [\rho_{g2} 2.8465 + \rho_{g4} 2.4626 \\ + \rho_{g5} 6.7985 - \rho_{g7} 2.969] \times 10^8$$

A typical fluidized bed with the simplest configuration and input for computation is shown in Fig. 16. Only background elutriation is illustrated.

Fig. 16. Parameters of a Fluidized Bed for Test Computation

Summary of Equations and Variables (using 8 gas components)

In Fluidized Bed

Equation of State	1		P
Continuity Equations	3	for char phases c_k	3 ρ 's
	3	for dolomite dk	3 ρ 's
	3	for bubbles bk (in N_b)	3 ρ 's
	8	for gases gk $k = 1,$	8 ρ_k 's
		(6 Γ 's, 1 $\underline{U}_g$)	
	<u>17</u>		<u>17</u>
Momentum Equations	3 x 3	for char phases $ck, j = x, y, z$	9 U_j 's
	3 x 3	for dolomite $dk, j = x, y, z$	9 U_j 's
	3 x 3	for bubbles $bk, j = x, y, z$	9 U_j 's
	<u>3</u>	for gas phase $g, j = x, y, z$	<u>3</u> U_j 's
	30		30
Energy Equations	3	for char phases $ck, k = 1, 2, 3$	3 T_{ck} 's
	3	for dolomite $dk, k = 1, 2, 3$	3 T_{dk} 's
	<u>1</u>	for gas phase	<u>1</u> T_g
	7		7
	<u><u>55</u></u>		<u><u>55</u></u>
	55 Equations		55 Quantities

In Free Board

Equation of State	1		1
Continuity Equation	2	from elutriated and ejected solid $c3$	2
	<u>1</u>	for gas g	<u>1</u>
	3		3
Momentum Equations	3 x 2	for solids $c3$	6 U_j
	<u>3</u>	for gas g	<u>3</u> U_j
	9		9
Energy Equations	2	for solids $c3$	1 T_{c3}
	<u>1</u>	for gas	<u>1</u> T_g
	3		3
	<u><u>16</u></u>		<u><u>16</u></u>

If we use relations given in Appendix D for the gas composition and further simplify, we have:

$1 + 15 + 30 + 7 = 53$ equations and 53 variables in the bed, and 15 in the free board.

Appendix F

Elutriation by a Jet in the Gravitational Field

Each bubble burst is visualized as a quasi-steady jet of gas produced at the surface of a fluidized bed, ejecting solid particles of various sizes whose terminal velocities are below the initial gas velocity produced by bubble rise and bubble burst. This velocity corresponds to the initial jet velocity U_{bzf} .

The jets and the particles which they elutriate constitute a phase in the free board of a fluidized bed. As long as the jets are far apart, the phase of jets consists of individual non-interacting jets.

For the computations in this appendix, we introduce the coordinates z along the jet axis and r radial from it, and their conjugate velocity components w and u , with gravitational acceleration g opposite to w . The jet of radius r_1 has an initial velocity w_1 at the free surface which is located at $z = (\sqrt{3}/2)\gamma r_1$ (see Fig. 17).

Since the suspension is dilute, local distribution of the density ρ_k of particle species k is given by [35]:

$$\frac{D_k}{r} \frac{\partial}{\partial r} r \frac{\partial \rho_k}{\partial r} = u \frac{\partial \rho_k}{\partial r} + \left(w - \frac{g}{F_k} \right) \frac{\partial \rho_k}{\partial z}, \quad (F.1)$$

where D_k is the diffusivity of particle k in the jet flow field, and F_k is the inverse relaxation time for momentum transfer from the gas to the particle of species k . For all species of particles whose terminal velocities are smaller than w_1 , we have one equation for each species k .

Equation (F.1) is readily solved by extending the procedure in [35]; i.e., by changing the independent variables from r, z to η, z , with $\eta = r/z$; u, w were given before:

Fig. 17. Idealized Motion of Gas Jet and Trends of Particle Ejection Via Bubble Velocity and Bubble Burst

$$u = \frac{\bar{v}}{z\eta} (\eta f' - f) = \frac{\gamma \bar{v}}{z} \eta (1 - \frac{1}{4} \gamma^2 \eta^2) X^{-3}, \quad (F.2)$$

and

$$w = \frac{\bar{v}}{z\eta} f' = 2 \frac{\gamma \bar{v}}{z} X^{-2}, \quad (F.3)$$

where $\bar{v}$ is the kinematic viscosity of the fluid, and

$$X = 1 + \frac{\gamma}{4} \eta^2, \quad (F.4)$$

and

$$f = \gamma^2 \eta^2 X^{-1}, \quad (F.5)$$

where $\gamma = (\sqrt{3}/8) 2r_1 w_1 / \bar{v}$.

We now express Eq. (F.1) in the following manner:

$$\frac{\partial}{\partial \eta} \eta \frac{\partial \rho_k}{\partial \eta} = \left[- \left(\frac{\bar{v}}{D_k} \right) f + \eta^2 \frac{gz}{FD} \right] \frac{\partial \rho_k}{\partial \eta} + \left(\frac{\bar{v}}{D_k} f' - \eta \frac{gz}{FD_k} \right) z \frac{\partial \rho_k}{\partial z} \quad (F.6)$$

which is solved by postulating

$$\rho_k = z^{-1} h_{-1} + h_0 + z h_1 + z^2 h_2 + \dots \quad (F.7)$$

Substituting into Eq. (F.6) and separating into different orders of z gives:

((') denotes $d/d\eta$)

$$(\eta h_{-1}')' = - (Sc) (f h_{-1}' + f' h_{-1}), \quad (F.8)$$

$$(\eta h_0')' = - (Sc) (f h_0') + (Sc) \frac{g}{\bar{v} F_k} \eta (\eta h_{-1}')', \quad (F.9)$$

$$(\eta h_1')' = - (Sc) [\eta f' h_1' + (f h_1)'] + (Sc) \frac{g}{\bar{v} F_k} \eta^2 h_0', \quad (F.10)$$

which can be solved in succession to determine h_{-1} , h_0 , ... $Sc_k = \bar{v}/D_k$ is the Schmidt number of species k ; for simplicity we shall use Sc .

Equation (F.8) has been solved before [35] to give:

$$h_{-1} = \rho_{k1} \left(\frac{w_1 r_1}{v} \right) (1 + 2Sc) r_1 \frac{1}{8} X^{-2Sc} . \quad (F.11)$$

Equation (F.9) is solved by writing

$$h''_0 + h'_0 \left(\frac{1 + Sc f}{\eta} \right) = \frac{g}{D_k F_k} (\eta h_{-1})' . \quad (F.12)$$

Integrating once gives

$$\eta h'_0 = \frac{g}{D_k F_k} \left[\frac{\eta^2}{z} (1 - 4Sc) + \frac{8(Sc)}{\gamma^2} \ln X \right] h_{-1} \quad (F.13)$$

for substitution into Eq. (F.10), and further integration gives

$$h_0 = \rho_{k1} (1 + 2 Sc) (Sc) \left(\frac{g}{w_1 F_k} \right) \left[\frac{4}{3} (1 - 4 Sc) \int_1^x \frac{dX}{X^{2Sc}} + \frac{8}{3} (Sc) \int_1^x \frac{\ln X dX}{(X - 1) X^{2Sc}} \right] \quad (F.14)$$

which gives the increase in particle density ρ_k due to gravity effect via parameter $(g/w_1 F_k)$.

Equation (F.10) is solved in an analogous manner by substituting Eq. (F.13)

$$h''_1 + \frac{h_1}{\eta} \left[1 + 4 Sc \left(1 + \frac{1}{X} - \frac{2}{X^2} \right) \right] + (Sc) \frac{2\gamma^2}{2} h_1 = \frac{g}{F_k D_k} \eta h'_0 . \quad (F.15)$$

Numerical solution is probably needed from here on. h_1 takes the form:

$$h_1 = \rho_{k_1} (1 + 2Sc)(Sc)^2 \left(\frac{g}{w_1 F_k} \right)^2 \left(\frac{v}{2r_1 w_1} \right) \frac{1}{r_1} [\text{function of } Sc \text{ and } \eta] \quad (F.16)$$

h_0 is integrable in a reasonably simple form for $Sc = \frac{1}{2}$, giving:

$$h_0 = \frac{2}{3} \rho_{k_1} \left(\frac{g}{w_1 F_k} \right) \left[\frac{1}{2} \ln X - (\ln X)^2 + 2 \int_1^X \frac{\ln X dX}{X - 1} \right] \quad (F.17)$$

For $y = \frac{Y^2}{4}$ $\eta^2 = X - 1$, the last term of Eq. (F.17) is given by [55]

$$\begin{aligned} \int \frac{\ln(y+1)}{y} dy &= y - \frac{y^2}{2^2} + \frac{y^3}{3^2} - \frac{y^4}{4^2} + \dots \quad \text{for } 0 < y \leq 1 \\ &\quad (= \pi^2/12 \text{ at } y = 1) \\ &= \frac{(\ln y)^2}{2} - \frac{1}{y} + \frac{1}{2^2 y^2} - \frac{1}{3^2 y^3} + \dots \quad \text{for } y \rightarrow \infty \end{aligned}$$

at $y = 1$, $x = 2$, $[] = 1.511$

$y = 0$, $x = 1$, $[] = 0$

$y \rightarrow \infty$, $x \rightarrow \infty$ $[] \rightarrow \frac{1}{2} \ln X$

for term in $[]$ (bracket) in Eq. (F.17) within the limit of the jet boundary [35]. The trend shows an increase in particle density as the particles are slowed down or falling back by gravity. Continuation of this analysis will be reported later.

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