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SIMULATION OF FLUIDIZED BED COAL COMBUSTORS

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16. Abstract

A comprehensive model for the simulation of fluidized bed coal combustors (FBC) is developed taking into account (i) devolatilization of coal and subsequent combustion of char and volatiles; (ii) kinetics of char combustion; SO_2 absorption by limestone; (iv) release of NO_x and reduction of NO_x by char; (v) attrition and entrainment of particles; (vi) hydrodynamics of gas and solids; (vii) freeboard reactions; (viii) heat transfer between bed and cooling tubes. The model is capable of simulating combustion efficiency, char and limestone elutriation and the corresponding particle size distribution in the bed, bed temperature profile, O_2, CO, CO_2, SO_2, and NO_x concentration profiles along the combustor. Agreement between the computed results and the observed data is good.

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FORTRAN Symbol	Mathematical Symbol	Description
G	g	Acceleration due to gravity, cms/sec^2
REP	$R_{e,p}$	Particle Reynolds number
RHOGAS	ρ_g	Density of gas, gm/cm^3
RHOS	ρ_s	Density of solids, gm/cm^3
UM	U_{mf}	Minimum fluidization velocity, cm/sec
UT	U_t	Terminal velocity of the particle, cms/sec
VISC	μ	Viscosity of gas, gm/cm.sec

SUBPROGRAM VOLUME

FORTRAN Symbol	Mathematical Symbol	Description
DVBEFF	-	Volume of each compartment excluding the tubes, cm^3
DZAV	-	Average compartment size used in design calculations, cm
VOLUME	-	Volume of bed (excluding tubes) at any height ZZ, cm^3
ZZ	-	Height above the distributor, cms

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NOMENCLATURE

A	Defined by equation (V.2)
A_t	Cross sectional area of the bed, cm^2
$a_{B,NO}$	Defined by equation (VI.51)
a_{B,SO_2}	Defined by equation (VI.49)
$a_{E,NO}$	Defined by equation (VI.47)
a_{E,SO_2}	Defined by equation (VI.45)
a_{HE}	Specific heat transfer area of the tubes, cm^2/cm^3 FBC volume
a_{HEW}	Specific heat transfer area of the walls, cm^2/cm^3 FBC volume
a_{NO}	Defined by equation (VI.55)
a_{SO_2}	Defined by equation (VI.53)
a_m	Defined by equation (VI.12)
a_x	Proportion of total abrasion fines in the xth size fraction
a_1	Defined by equation (VI.9)
a_2	Defined by equation (VI.15)
a_3	Defined by equation (VI.25)
a_4	Defined by equation (VI.11)
a_2'	Defined by equation (VI.33)
a_4'	Defined by equation (VI.20)
B	Defined by equation (V.3)
b_x	Weight fraction of bed material in the xth size fraction
C_{cf}	Heat capacity of coal feed, cals/gm·°C
C_{CO_2}	Concentration of carbon dioxide, $gmole/cm^3$

C_{NO}	Concentration of nitric oxide, $gmole/cm^3$
C_S	Heat capacity of solids, cals/gm. °C
C_{Sf}	Heat capacity of feed additives, cals/gm.°C
C_{SO_2}	Concentration of sulfur dioxide, $gmole/cm^3$
C_{ch}	Carbon content in char, gm carbon/gm char
C_{gm}	Molar heat capacity of gas at constant pressure, cals/gmole °C
CH_4	Wt. fraction CH_4 in the volatiles
CO	Wt. fraction CO in the volatiles
CO_2	Wt. fraction CO_2 in the volatiles
D	Molecular diffusivity for O_2-N_2, cm^2/sec
D_B	Bubble diameter, cm
D_{BO}	Bubble diameter at the distributor level, cm
D_{BM}	Fictitious maximum bubble diameter, cm
D_t	Diameter of the FBC as a function of height above the distributor, cm
d_c	Diameter of char particle in the bed, cm
d_{ce}	Diameter of char particle entrained in the freeboard, cm
d_ℓ	Diameter of limestone particle in the bed, cm
$d_{\ell e}$	Diameter of limestone particle entrained in the freeboard, cm
d_o	Diameter of cooling tubes, cm
d_p	Particle diameter, cm
d_x	Mean diameter of the particles of xth size fraction, cm
E_x	Elutriation rate constant, gm/sec
E_z	Dispersion coefficient in the freeboard, 1/sec
F_{BM}	Molar flow rate of gas in the bubble phase, gmole/sec
F_{EM}	Molar flow rate of gas in the emulsion phase, gmole/sec
F_{MT}	Total molar flow rate of gas in the combustor, gmole/sec
F_0	Solids entrainment rate at the bed surface, gms/sec

f_ℓ Fractional conversion of limestone

f_{sw} Fraction of wake solids thrown into the freeboard

f_w Solids mixing parameter, ratio of wake volume to the bubble volume including the wakes

G Gas flow rate, gms/sec

g Acceleration due to gravity, cms/sec^2

g_B Volatiles burning rate in the bubble phase, gmole/sec

g_{CO} Carbon monoxide burning rate, gmole/sec

g_E Volatiles burning rate in the emulsion phase, gmole/sec

H_2 Wt. fraction hydrogen in the volatiles

H_2O Wt. fraction H_2O in the volatiles

h Height above the bed surface, cm

K Attrition rate constant, 1/cm

K_{BE} Gas exchange coefficient, 1/sec

k Defined by Equation (VI.24)

$k_{B,NO}$ NO reduction rate constant in the bubble phase, cm/sec

k_{CO_2} C-CO_2 chemical reaction rate constant, cm/sec

$k_{E,NO}$ NO reduction rate constant in the emulsion phase, cm/sec

k_{NO} NO reduction rate constant, cm/sec

k_c Overall rate constant for char combustion, cm/sec

$k_{c,B}$ Overall rate constant for char combustion in bubble phase, cm/sec

$k_{c,E}$ Overall rate constant for char combustion in emulsion phase, cm/sec

k_{cf} Gas film diffusion rate constant, gm/cm^2·sec.atm

k_{cR} Chemical reaction rate constant for char combustion, gm/cm^2. sec.atm

k_{vl} Overall volume reaction rate constant for limestone-SO_2 reaction, 1/sec

k_x Abrasion rate constant for the xth size fraction, 1/sec

k'	Defined by Equation (VI.32)
k'_{v1}	Chemical reaction rate constant for limestone-SO_2 reaction, 1/sec
M	Weight of particles remaining in the bed after the size reduction from the original size to d_x
M_b	Weight of bed material, gms
M_c	Atomic weight of carbon, gms/gm atom
M_x	Weight of bed material in the xth size fraction
N_A	Number of limestone particles in the ith compartment in the freeboard
N_{Pe}	Peclet number, defined by Equation (V.43)
N_{Re}	Reynolds number, defined by Equation (V.42)
N_{Sc}	Schmidt number, defined by Equation (V.44)
N_c	Number of char particles in the ith compartment in the freeboard
N_d	Number of orifices in the distributor
P	Average pressure of the FBC, atm
P_H	Horizontal pitch distance between the tubes, cms
P_v	Vertical pitch distance between the tubes, cms
p	Defined by Equation (V.16)
p_{O_2}	Partial pressure of oxygen, atm
p_1	Proportion of fines recycled to the bed from the primary cyclone
p_2	Proportion of fines recycled to the bed from the secondary cyclone
q_{cal}	Heat of calcination of limestone, cals/gm
q_{ch}	Heat of combustion of char, cals/gm
q_v	Heat of combustion of volatiles (complete burning), cals/gmole
$q_{v,CO}$	Heat of combustion of volatiles (partial burning), cals/gmole

q_{1x}	Collection efficiency of the primary cyclones for the xth size fraction
q_{2x}	Collection efficiency of the secondary cyclones for the xth size fraction
R	Gas constant, 1.987 cals/gmole °K
$R_{B,NO,c}$	NO release rate in the bubble phase due to char combustion, gmole/sec
$R_{B,NO,V}$	NO release rate in the bubble phase due to volatiles combustion, gmole/sec
$R_{B,SO_2,c}$	SO_2 release rate in the bubble phase due to char combustion, gmole/sec
$R_{B,SO_2,V}$	SO_2 release rate in the bubble phase due to volatiles combustion, gmole/sec
R_{CO}	CO released during devolatilization, gmole/sec
R_{CO_2}	CO_2 released during devolatilization, gmole/sec
$R_{E,NO,c}$	NO release rate in the emulsion phase due to char combustion, gmole/sec
$R_{E,NO,V}$	NO release rate in the emulsion phase due to volatiles combustion, gmole/sec
$R_{E,SO_2,c}$	SO_2 release rate in the emulsion phase due to char combustion, gmole/sec
$R_{E,SO_2,V}$	SO_2 release rate in the emulsion phase due to volatiles combustion, gmole/sec
$R_{e,p}$	Particle Reynolds number, defined by equations (A.VII.22-24)
R_{NO}	NO release rate, gmole/sec
R_{SO_2}	SO_2 release rate, gmole/sec
R_a	Attrition rate, gms/sec
R_{ch}	Char produced per unit gm of coal fed, gm/gm
R_v	Volatiles released, gmole/sec
R_g	Gas constant, 82.06 atm.cm^3/gmole °K
r_{CO}	Rate of combustion of CO, gmole/cm^3 sec
r_i	Char combustion rate in ith compartment, gms/sec

r_c^*	Char combustion rate, gmole/sec·particle
S_g	Effective specific surface area of limestone, cm^2/gm
T	Temperature in the bed, °K
T_B	Mean temperature in the boundary layer of the char particle in the bubble phase, °K ; also in the freeboard, °K
TDH	Transport Disengaging Height, cms
T_E	Mean temperature in the boundary layer of the char particle in the emulsion phase, °K
Tar	Wt. fraction tar in the volatiles
T_c	Char particle temperature, °K
T_m	Mean temperature in the boundary layer of the char particle, °K
T_{sf}	Solids feed temperature, °K
T_w	Cooling water temperature, °K
T_{wall}	Average FBC wall temperature, °K
t	Temperature, °C
t_b	Burning time of a char particle, sec
U	Bed to tube heat transfer coefficient, $cals/sec \cdot cm^2 \, °C$
U_B	Bubble velocity, cms/sec
U_{mf}	Minimum fluidization velocity, cms/sec
U_o	Superficial gas velocity or fluidization velocity, cms/sec
$\overline{U}_o$	Average superficial gas velocity in the freeboard, cms/sec
U_t	Terminal velocity of the particle, cms/sec
U_w	Bed to wall heat transfer coefficient, $cals/sec \cdot cm^2 \, °C$
V	Volatiles yield during devolatilization, % of coal daf
VM	Proximate volatile matter in the coal, % of coal daf
V_{CO}	CO produced due to volatiles burning, gmole CO/gmole volatile

V_{CO_2}	CO_2 produced due to volatiles burning, gmole CO_2/gmole volatile
V_N	Volatile nitrogen in coal, gm/gm, dry basis (d.b.)
V_S	Volatile sulfur in coal, gm/gm, dry basis (d.b.)
W_D	Solids withdrawal rate, gms/sec
W_{ent}	Solids entrainment rate, gms/sec
$W_{f,a}$	Additives feed rate, gms/sec
$W_{f,c}$	Coal feed rate, gms/sec
$W_{f,x}$	Solids feed rate of xth size fraction, gms/sec
W_{mix}	Solids mixing rate, gms/sec
W_{net}	Net flow rate of solids, gms/sec
W_x	Rate of transfer of particles from size fraction x to fraction x + 1 by size reduction, gms/sec
X	Weight fraction carbon in the bed
X_{O_2}	Oxygen required for partial combustion of volatiles, gmole O_2/gmole volatile.
$X_{O_2,c}$	Oxygen required for complete combustion of volatiles, gmole O_2/mole volatile
X_{VM}	Proximate volatile matter content of coal, gms/gm coal (daf)
Y_B	Mole fraction O_2 in the bubble phase
Y_{B,CO_2}	Mole fraction CO_2 in the bubble phase
$Y_{B,NO}$	Mole fraction NO in the bubble phase
Y_{B,SO_2}	Mole fraction SO_2 in the bubble phase
Y_{CO}	Mole fraction CO
Y_{CO_2}	Mole fraction CO_2
Y_E	Mole fraction O_2 in the emulsion phase
$Y_{E,CO}$	Mole fraction CO in the emulsion phase
Y_{E,CO_2}	Mole fraction CO_2 in the emulsion phase

$Y_{E,NO}$	Mole fraction NO in the emulsion phase
Y_{E,SO_2}	Mole fraction SO_2 in the emulsion phase
$Y_{E,v}$	Mole fraction volatiles in the emulsion phase
Y_{H_2O}	Mole fraction H_2O
Y_O	Mole fraction O_2
Y_{NO}	Mole fraction NO
Y_{SO_2}	Mole fraction SO_2
Y_v	Mole fraction volatiles
Z	Height above the distributor, cms; ΔZ compartment size, cms

Greek Symbols

ε_B	Bubble fraction
ε_c	Cloud fraction including bubble
ε_m	Emissivity of the char particle
ε_{mf}	Void fraction at minimum fluidization
ε_{tube}	Volume fraction of tubes
Θ	Time, sec
λ	Thermal conductivity of the gas, cals/sec.cm°C
λ_ℓ	Reactivity of limestone
μ	Viscosity of gas, gm/cm·sec
Π	3.14159265
ρ_b	Density of the bed materials, gms/cm^3
$\rho_{c,ch}$	Density of carbon in char, gms/cm^3
ρ_{ch}	Density of char, gms/cm
ρ_g	Density of gas, gms/cm^3
ρ_s	Density of solids, gms/cm^3
σ	Stefan-Boltzman constant, 1.36×10^{-12}, $cals/sec{\cdot}cm^2{\cdot}{}^\circ K^4$
ϕ	Mechanism factor of char combustion

ϕ_B	Mechanism factor in the freeboard
ϕ_E	Mechanism factor in the emulsion phase

Subscript

x	xth size fraction
i	ith compartment

Abbreviation

d.b.	dry basis
daf	dry ash free basis

I. INTRODUCTION

Among the various ways of direct burning of coal, fluidized bed combustion appears to be the most attractive, both from an economic and environmental standpoint. By carrying out combustion in a fluidized bed combustor (FBC) operating at relatively low temperature (750°C-950°C; 1382°F-1742°F), both SO_2 and NO_x emissions can be maintained at environmentally acceptable levels. In addition, the FBC is well suited for burning low grade, high sulfur coal.

Fluidized bed combustion involves the burning of coal particles in a bed containing limestone/dolomite additives and coal ash. Under normal operating conditions the coal particles constitute less than 4 percent of the total solids in the bed. The limestone/dolomite is added to absorb the sulfur dioxide released from coal during combustion. Sulfur dioxide reacts with calcined limestone/dolomite according to the following reaction:

$$CaO + SO_2 + 1/2\ O_2 \longrightarrow CaSO_4$$

NO_x emission is kept low due to low combustion temperature and by the NO_x reduction reaction with carbon present in the fluidized bed. The low temperature operation of the fluidized bed offers little, if any, clinker formation of the ash. The heat of combustion is removed by steam coils immersed in the bed. The steam coils also control the temperature of the bed with minimum hinderance to the solids mixing and circulation in the bed. The high heat transfer coefficients between the bed material and the heat exchange surfaces [250 to 420 W/m^2 °K (45 to 75 Btu/hr ft^2°F)] and the large heat generation rates

[2.0 to 5.0 MW/m^3 (0.193 to 0.483 x 10^6 Btu/hr ft^3)] in FBC result in a smaller boiler volume for a given duty than the conventional pulverized coal burning boilers.

Pressurized fluidized bed combustion is also being investigated because of its potential for power generation in gas turbines combined with conventional steam turbines. In pressurized FBC, the combustion is carried out at elevated pressures, generally in the range of 600 to 1000 kPa (6 to 10 atm abs.). The hot, high pressure flue gas is cleaned to remove the particulates and expanded through a gas turbine to generate additional electricity.

Although the FBC offers several advantages, it is not free from shortcomings. Problem areas include erosion of immersed heat-transfer coils, continuous feeding of solids into the bed, agglomeration of solids, formation of stagnant zones on the distributor plate, carry-over of unburnt char particles in the flue gas, high particulate emissions, and in the case of pressurized fluid bed combustor (PFBC), the difficulty in hot gas clean-up. The extent of these problems has to be evaluated and resolved before any large-scale commercialization is ventured.

II. LITERATURE REVIEW

A considerable amount of investigation on the performance of fluidized bed combustion system has been under way particularly in the U.S. and U.K. (Argonne National Laboratory (ANL), Combustion Power Company (CPC), Pope, Evans and Robbins (PER), Westinghouse Research Laboratories (WRL), Exxon Research and Engineering Company (ER&E), Morgantown Energy Technology Center (METC), National Coal Board (NCB), British Coal Utilization Research Association (BCURA). Most of the experimental tests have concentrated on feasibility evaluation of FBC. As a result of these studies, a considerable amount of pilot plant data related to FBC performance has become available in recent years.

A systematic, theoretical examination of these data has been initiated only recently, and attempts are presently being made to develop theoretical models for predicting the performance of FBC under various operating conditions. A review of the modeling efforts in fluidized bed combustion has been presented by Caretto (1977). The fundamental and engineering aspects of fluidized bed coal combustion have been discussed by Beer (1977). Almost all of the FBC models proposed to date are based on the two phase theory of fluidization (Davidson and Harrison (1963)). According to this theory, the fluidized bed is assumed to consist of two phase, viz., a continuous, dense particulate phase (emulsion phase) and a discontinuous, lean gas phase (bubble phase) with exchange of gas between the bubble phase and the emulsion phase. The gas flow rate through the emulsion phase is assumed to be that corresponding to minimum fluidization, and that in excess of the minimum fluidization velocity goes through the bubble phase in the form of bubbles. However, as pointed out by Horio and Wen (1977), Rowe (1978), Catipovic et al. (1978), this assumption may be an oversimplification for particles smaller than 50 μm and larger than 2000 μm. Experiments with fine powders (d_p < 50 μm) conducted by Rowe (1978) show that the dense phase voidage changes with gas velocity, and that as much as 30 percent of the gas flow may occur interstitially. Catipovic, et al. (1978) have pointed out qualitatively the difference in the fluidization of larger particles.

Avedesian and Davidson (1973) developed a combustion model based on the two phase theory. Their objective was to study the mechanism of combustion of carbon particles in a fluidized bed of ash particles at 1173°K. The combustion was assumed to be controlled by two diffusional resistances, namely:

(i) Interphase transfer of oxygen from bubbles of air to the surrounding ash particles.

(ii) Diffusion of oxygen through the ash phase towards each burning carbon particle.

Campbell and Davidson (1975) later modified the Avedesian and Davidson model to include the presence of carbon dioxide in the particulate phase and applied the model to predict the carbon particle size distribution in a continuously operated fluidized bed combustor.

Baron, et al. (1977) proposed a model for the FBC based on the two phase theory for predicting the combustion efficiency and carbon concentration in the bed. In their model, they took into account the carbon loss due to elutriation and attrition of bed particles, employing the correlations developed by Merrick and Highley (1974). Borghi, et al. (1977) have proposed a mathematical model for the combustion of coal particles in fluidized bed which takes into account the evolution and burning of volatiles in addition to the combustion of residual char. Their conclusions indicate that (i) the devolatilization times for coal particles are commensurable with the solids mixing time and (ii) the homogeneous release of volatiles in the bed, as opposed to instantaneous devolatilization is close to reality. Gibbs (1975) derived a mechanistic model for the combustion of coal in a fluidized bed capable of predicting the combustion efficiency, carbon hold-up and spatial distribution of oxygen in the bed. The carbon loss due to elutriation, attrition and splashing of coal from bursting of bubbles on the bed surface was taken into account in the model formulation. The burning rate of coal was assumed to be diffusion controlled. The carbon loss predicted by the model was strongly dependent on the mean bubble diameter which is an adjustable parameter.

Gordon and Amundson (1976) examined the influence of several operating variables on the steady state performance of a FBC. Based on the model calculations, they found that multiple steady state solutions exist in the typical range of operating variables. In particular, it was noted that one of the key factors in determining the state of the bed, as well as the multiplicity of the system was the gas interchange coefficient between the bubble phase and emulsion phase.

Horio and Wen (1978) have proposed a model based on the population balance technique to calculate the char elutriation loss, particle size distribution in the bed and size distribution of the elutriated char.

In the FBC models described so far, they have at least one of the following deficiencies:

(1) The bubble diameter was taken as a constant and an adjustable parameter. In reality, bubbles coalesce as they ascend through the bed. The bubble diameter changes with the height above the distributor. Bubble size is also affected by the immersed cooling coils. (Baron, et al. 1977; Gibbs, 1975).

(2) Devolatilization of coal is not considered. (Horio and Wen, 1978; Avedesian and Davidson, 1973; Campbell and Davidson, 1975; Baron, et al. 1977; Gibbs, 1975; Gordon and Amundson, 1976).

(3) The mechanism of carbon combustion was assumed to be diffusion controlled. This is true only for large particles at high temperatures. (Avedesian and Davidson, 1973; Campbell and Davidson, 1975; Borghi, et al. 1977; Baron, et al. 1977).

(4) Solids mixing in the emulsion phase was assumed to be uniform. Hence the bed was assumed to be under isothermal conditions. This is not true because the experimental data show a non-uniform temperature profile across the bed. (Avedesian and Davidson, 1973; Borghi, et al. 1977; Baron, et al. 1977; Horio and Wen, 1977).

Bethell, et al. (1973) presented a model for sulfur dioxide retention by limestone in a fluidized bed combustor. Horio and Wen (1975) have also formulated a model for the removal of sulfur dioxide by limestone in a FBC. In their model, the hydrodynamics of the fluidizing gas is based on the bubble assemblage model developed by Kato and Wen (1975). Chen and Saxena (1977) used a three phase bubbling bed model (bubble phase, cloud-wake phase and emulsion phase) for predicting the sulfur retention efficiency in a FBC. The model predictions were compared with some experimental data. However, a limitation of the model is that it assumes isothermal conditions in the bed. The models described above for SO_2 absorption do not take into account the char and volatiles combustion in the bed. (Bethell, et al. 1973; Horio and Wen, 1975; Chen and Saxena, 1977).

Recently, Horio, et al. (1977) presented a model for fluidized bed coal combustion that can estimate the performance of a FBC under fuel rich operation and also predict the NO_x emissions from the combustor. This model does not deal with the NO_x release from volatiles and char during the combustion. Char particle temperature is assumed as a constant, 100°C above the bed temperature. Char particle temperature is actually dependent on the oxygen concentration and is different in the bubble and emulsion phases. Also, the char temperature affects the carbon concentration in the bed which in turn affects the NO_x reduction rate. Perira and Beer (1978) have proposed a mechanism for the formation of NO (nitric oxide) from fuel nitrogen and the subsequent reduction of NO by volatiles. However, they have not dealt with the reduction of NO by char subsequent to the completion of devolatilization in the bed which has been established by other workers (Oguma, et al., 1977).

A general methematical model for FBC has been developed (Rengarajan, et al. 1977, Rajan, et al. 1978) employing the modified version of the bubble assemblage model (Kato and Wen, 1969, Mori and Wen, 1975). The model includes the devolatilization of coal, char combustion and SO_2 absorption. Predictions of the combustion efficiency, axial temperature profile and sulfur retention efficiency in the bed were compared with experimental data. A deficiency of the model is that the elutriation of char and limestone is not considered. Experimental values are used for elutriation losses in the calculation.

All of the models proposed so far do not take into account the char combustion, SO_2 absorption and NO_x reduction in the freeboard, which may be substantial. A classification of the fluidized bed combustion models discussed above is presented in Table I.

TABLE 1. CLASSIFICATION OF FBC MODELS

		Gas Flow Pattern			
Model Description	Investigators	Bubble Phase	Emulsion Phase	Solids mixing in the bed	Remarks
Two phase bubbling bed model	Avedesian and Davidson (1973) Gibbs (1975) Campbell and Davidson (1975) Gordon and Amundson (1976) Baron, et al. (1977)	a) Plug Flow b) Plug Flow c) Complete Mixing	Plug Flow Complete Mixing Complete Mixing	Complete Mixing	1) Bubble diameter is assumed to be uniform throughout the bed in most cases and is an adjustable parameter 2) Cloud and wake are combined in the emulsion phase. 3) No reactions in the bubble phase. 4) Char combustion is assumed to be diffusion controlled at all temperatures.
Two phase compartment in series model	Horio, et al. (1977) Rengarajan, et al. (1977) Horio and Wen (1978) Rajan, et al. (1978)	Complete mixing within each compartment	Complete mixing within each compartment	Complete mixing within each compartment with backflow of solids from one compartment to another	1) Bubbles grow along the bed height. 2) The backflow solid mixing is considered using an adjustable parameter. 3) Cloud is combined with the bubble phase. 4) Reactions take place in the bubble phase.
Three phase bubbling bed model	Chen and Saxena (1977)	Plug Flow	Plug Flow	Complete mixing	1) Cloud-wake is treated as a separate phase and is in plug flow 2) Isothermal condition throughout the bed for solids, char and gas. 3) Bubble growth is considered. 4) Combustion occurs in cloud-wake and emulsion phases only.

III. OBJECTIVES OF PRESENT WORK

Most of the modeling work performed to date has concentrated on a few specific aspects of the fluid bed combustion process. The many deficiencies of the previous work have been pointed out earlier. It is the aim of the present work to reduce these deficiencies, and to formulate a comprehensive FBC model taking into account the following elements which were either partially considered or not considered at all in the previous work.

(1) Devolatilization of coal and the subsequent combustion of volatiles and residual char.

(2) Sulfur dioxide capture by limestone.

(3) NO_x release and reduction of NO_x by char.

(4) Attrition and elutriation of char and limestone.

(5) Bubble hydrodynamics.

(6) Solids mixing.

(7) Heat transfer between gas and solid, and solids and heat exchange surfaces.

(8) Freeboard reactions.

This model will be able to simulate most of the important performance characteristics, viz.,

(1) Combustion efficiency of coal.

(2) Sulfur dioxide retention efficiency.

(3) SO_2 and NO_x emissions.

(4) Particulates emission.

(5) Attrition and elutriation of char and limestone.

(6) Size distribution of char and limestone in the bed and in the elutriated material.

(7) Axial bed temperature profile.

(8) O_2, CO, CO_2, SO_2 and NO_x concentration profiles.

(9) Pressure drop across the distributor and the bed.

The present work will aid in the understanding of the performance of FBC under a range of operating conditions. For example, SO_2, NO_x and particulates emissions from the FBC can be estimated for a range of operating conditions. The optimum operating temperature and gas residence time in the bed, which would give maximum combustion efficiency and lower SO_2 and NO_x emissions, can be estimated. The temperature profile simulated based on the model will help identify the proper location of cooling coils in the bed to avoid steep temperature gradients for design of coils configuration and packing density.

The uniqueness of the proposed model is its capability to account for (i) the freeboard reactions which may be substantial; (ii) the solids mixing within the bed; (iii) the devolatilization of coal; (iv) SO_2 and NO_x release during the combustion of char and volatiles and the simultaneous absorption of SO_2 by limestone and reduction of NO_x by char, and (v) the entrainment of char and limestone from the bed.

IV. MODEL ASSUMPTIONS

The following assumptions are made in constructing the FBC model:

1. Single phase backflow cell model is used for solids mixing calculation.

2. Two phase bubble assemblage model is adopted for gas phase material balances.

3. Solids exchange between the bubble phase and emulsion phase is assumed to be rapid.

4. Bubble size is a function of bed diameter and height above the distributor. When cooling tubes are present, bubble size in the tubes region of the bed is based on the horizontal pitch distance between the tubes.

5. Bubbles and clouds are both combined into the bubble phase. The gas interchange coefficient between the bubble and emulsion phases is a function of the bubble size and is distributed axially.

6. The gas flow rate through the emulsion phase corresponds to minimum fluidization velocity.

7. Devolatilization of coal is neither instantaneous nor uniform in the bed. It is assumed that volatiles release rate is proportional to the solids mixing rate.

8. Volatiles are assumed to be released in the emulsion phase.

9. Volatile nitrogen and sulfur in coal increase as a function of bed temperature. (Fine, et al. 1974).

10. Sulfur and nitrogen in the residual char are assumed to be released as SO_2 and NO_x during the combustion of char.

V. MODEL BACKGROUND

The various physico-chemical processes occurring in the FBC are shown in Fig. 1. The basic elements of the overall combustion process are described as follows:

1. Devolatilization and Combustion of Char:

Coal particle fed to the hot combustor is rapidly heated while undergoing devolatilization (or pyrolysis). The volatile matter of coal is evolved into the particulate phase or emulsion phase of the bed. The bed temperature and the proximate volatile matter content of coal determine the yield of volatiles. Volatile yield is estimated by the following empirical correlations (Gregory and Littlejohn, 1965):

$$V = VM - A - B \tag{V.1}$$

$$A = \exp(26.41 - 3.961 \ln t + 0.0115\, VM) \tag{V.2}$$

$$B = 0.2(VM - 10.9) \tag{V.3}$$

where V = yield of volatiles, % of coal, daf

VM = proximate volatile matter in coal, daf %

t = devolatilization temperature, °C

The compositions of the products of devolatilization in weight fractions are estimated from the correlations developed using the data of Loison and Chauvin (1964):

$$CH_4 = 0.201 - 0.469\, X_{VM} + 0.241\, X_{VM}^2 \tag{V.4}$$

$$H_2 = 0.157 - 0.868\, X_{VM} + 1.388\, X_{VM}^2 \tag{V.5}$$

$$CO_2 = 0.135 - 0.900\, X_{VM} + 1.906\, X_{VM}^2 \tag{V.6}$$

$$CO = 0.428 - 2.653\, X_{VM} + 4.845\, X_{VM}^2 \tag{V.7}$$

$$H_2O = 0.409 - 2.389\, X_{VM} + 4.554\, X_{VM}^2 \tag{V.8}$$

$$Tar = -0.325 + 7.279\, X_{VM} - 12.880\, X_{VM}^2 \tag{V.9}$$

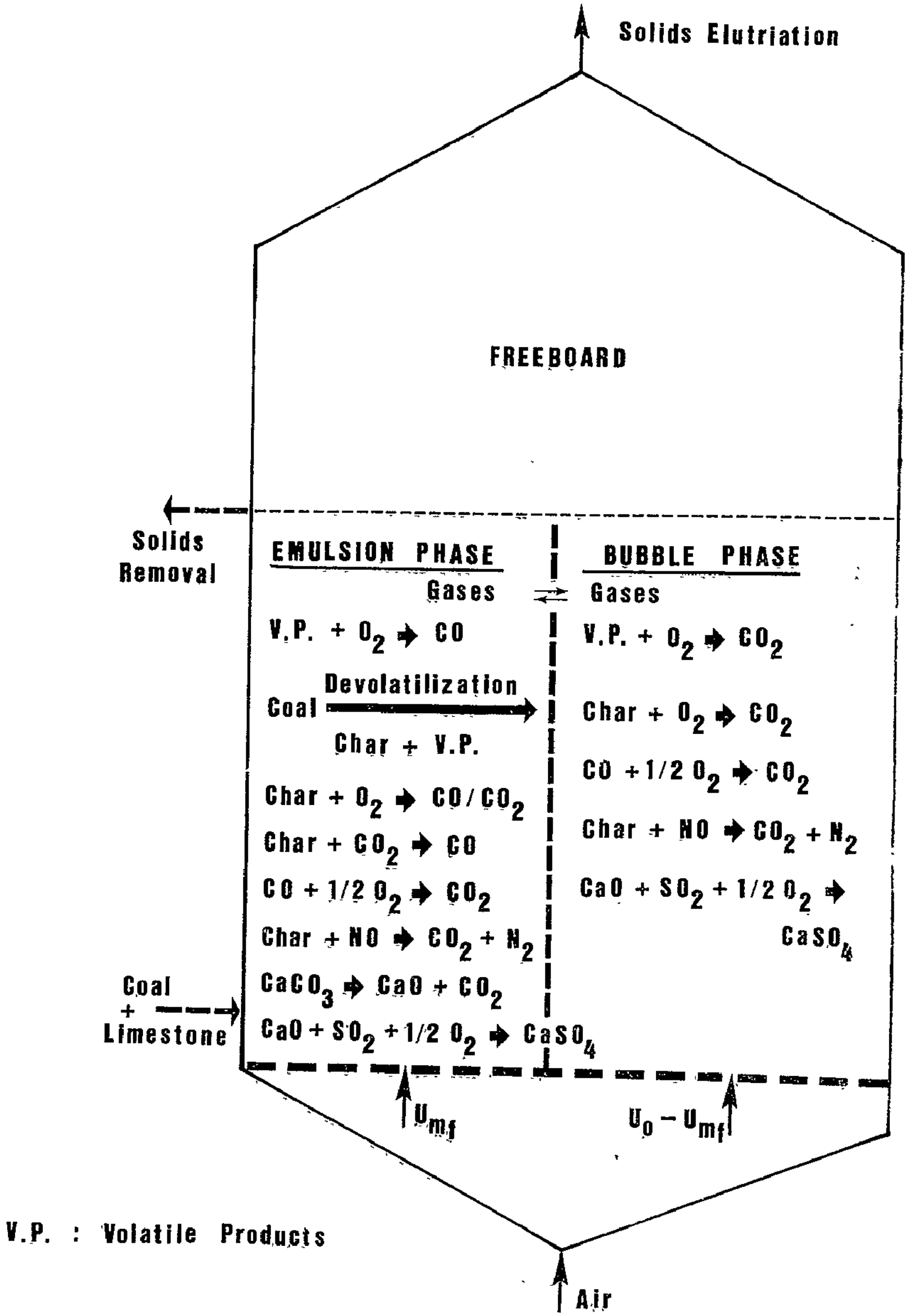


Fig. 1 Schematic Illustration of the FBC

Volatile nitrogen released during devolatilization is expressed as (Fine, et al. 1974):

$$V_N = 0.001\ T - 0.6 \quad \text{gm/gm coal, (d.b.)} \qquad (V.10)$$

and volatile sulfur is expressed as:

$$V_S = 0.001T - 0.6 \quad \text{gm/gm coal (d.b.)} \qquad (V.11)$$

Despite the extensive research in the area of coal devolatilization, accurate rate expressions describing the rate of devolatilization of coal are unavailable to date. However, it is estimated that the time needed for the devolatilization of a 1 mm coal particle is 0.5-1 sec under the conditions existing in the FBC (Beer, 1977). Solids mixing time for a 2 ft. combustor with a bed height of 4 ft. and a superficial gas velocity of 4 ft/sec lies in the range of 2 to 10 secs depending on whether solids mixing is good or poor. Hence it is more likely that a major portion of the volatiles will be released near the coal feed point. In the model, f_w, the solid mixing coefficient will represent the amount of volatiles released uniformly and $(1-f_w)$ will represent the proportion of volatiles released near the coal feed point.

At temperatures above 650°C and in an oxidizing atmosphere the rate of burning of volatiles is fast compared to the time required for volatiles evolution. However, the combustion of volatiles released in the emulsion phase is controlled by the availability of oxygen in the emulsion phase. Since the oxygen concentration in the emulsion phase is low, the volatile gases in the emulsion phase first tend to form CO by partial combustion; whereas, the volatiles exchanged to the bubble phase burns completely to CO_2 because of excess oxygen present in the bubble phase.

The rate of burning of CO is expressed as (Hottel, et al 1965)

$$CO + \frac{1}{2} O_2 \longrightarrow CO_2, \quad r_{CO} = 3 \times 10^{10} \left(\frac{P}{R_g T}\right)^{1.8} \exp(-16000/RT)\, Y_{H_2O}^{0.5} \times$$

$$Y_{CO} \frac{17.5\ Y_O}{1 + 24.7\ Y_O} \quad \text{gmole/cm}^3\text{sec} \qquad (V.12)$$

Residual char burns according to the reaction:

$$C + \frac{1}{2} O_2 \longrightarrow (2 - \frac{2}{\phi})CO + (\frac{2}{\phi} - 1)CO_2 \qquad (V.13)$$

where ϕ is a mechanism factor, which takes the value 1 when CO_2 is transported away from the char particle and 2 when CO is transported away (Field, et al. 1967) during char combustion. The factor, ϕ, is a function of char particle diameter and temperature. For small particles, CO formed during char combustion diffuses out fast because of rapid mass transfer and burns to form CO_2 outside the particle; whereas, for large particles, because of slower mass transfer, CO burns within the particle and CO_2 is transported out. ϕ is expressed as:

$$\phi = \frac{2p + 2}{p + 2} \qquad \text{for } d_c \leqslant 0.005 \text{ cm} \qquad (V.14)$$

$$\phi = \frac{(2p + 2) - p(d_c - 0.005)/0.095}{p + 2} \qquad \text{for } 0.005 < d_c < 0.1, \text{ cm} \qquad (V.15)$$

where p is the ratio of carbon monoxide to carbon dioxide formed during char combustion and is given by (Arthur, 1951).

$$p = CO/CO_2 = 2500 \exp(-12400/RT) \qquad (V.16)$$

The rate expression for char combustion is estimated by Field et al. (1967)

$$r_c^* = \pi\, d_c^2\, k_c\, C_{O_2} \qquad \text{gmole/sec particle} \qquad (V.17)$$

where k_c is the overall rate constant, and is given by:

$$k_c = \frac{R_g T_m/M_c}{\frac{1}{k_{cR}} + \frac{1}{k_{cf}}} \qquad \text{cm/sec} \qquad (V.18)$$

k_{cR} = chemical reaction rate constant

$$= 8710 \exp(-35700/RT_c) \qquad \text{gm/cm}^2 \cdot\text{sec}\cdot\text{atm} \qquad (V.19)$$

k_{cf} = diffusion rate constant

$$= 24\, \phi\, D/d_c\, R_g\, T_m, \quad \text{gm/cm}^2\cdot\text{sec}\cdot\text{atm} \qquad (V.20)$$

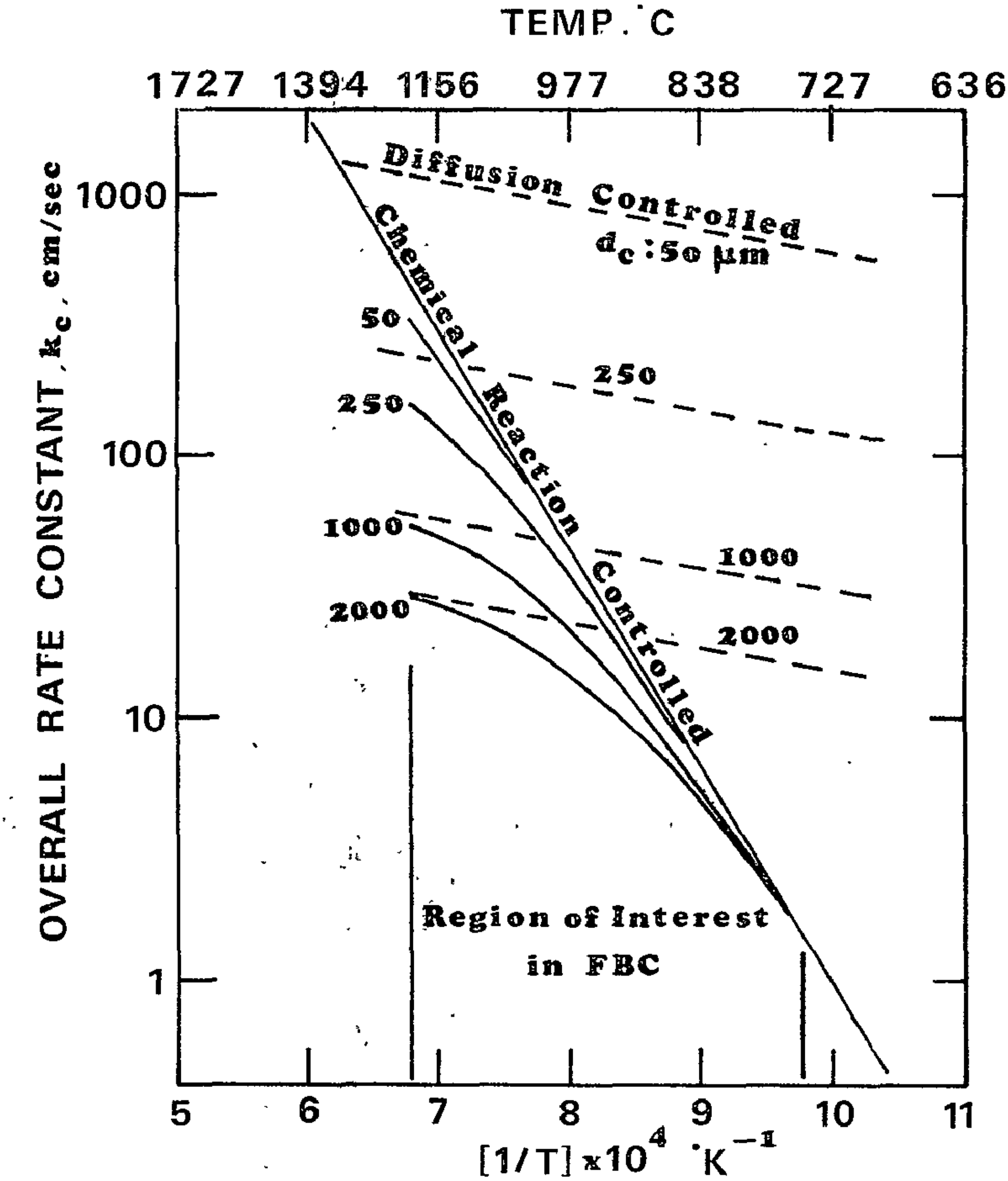


Fig. 2 Rate Controlling Regimes in FBC

For smaller particles, diffusion of oxygen to the surface of the char particle is faster than the chemical reaction rate of combustion while for larger particles, diffusion of oxygen is slower than the chemical rate. Thus, the diffusional term tends to dominate for larger particles at high temperatures, while the chemical term tends to dominate at low temperatures (Fig. 2). CO_2 formed during combustion reacts with char according to the following reaction:

$$C + CO_2 \longrightarrow 2\ CO \qquad (V.21)$$

and the rate expression for the above reaction is $r_{CO_2} = \pi\, d_c^2\, k_{CO_2}\, C_{CO_2}$ gmole/sec · particle, where $k_{CO_2} = 4.1 \times 10^8 \exp(-59200/RT)$ cm/sec (Caram and Amundson, 1977).

2. <u>Sulfur Dioxide - Limestone Reaction</u>:

When limestone is added to a fluidized bed burning coal, the SO_2 released from the combustion of coal reacts with calcined limestone according to the reaction:

$$CaO + SO_2 + \frac{1}{2} O_2 \longrightarrow CaSO_4 \qquad (V.22)$$

The reaction rate of a limestone particle can be expressed as (Borgwardt, 1970)

$$r_\ell = \frac{\pi}{6} d_\ell^3\, k_{v\ell}\, C_{SO_2} \quad \text{gmole/sec particle} \qquad (V.23)$$

where $k_{v\ell}$ is the overall volumetric reaction rate constant and is a rapidly decreasing function of limestone conversion, f_ℓ. The overall reaction rate constant, $k_{v\ell}$, is calculated by the equation:

$$k_{v\ell} = k'_{v\ell}\, S_g\, \lambda_\ell \qquad (V.24)$$

where $k'_{v\ell}$ is equal to 490 exp(-17500/RT) gm/cm^3 sec. The value of activation energy was obtained by Wen and Ishida (1973). By using Borgwardt's data (1971), the specific surface area, S_g, is correlated with calcination temperature as:

$$S_g = -38.4\ T + 5.6 \times 10^4,\ cm^2/gm \text{ for } T \geq 1253°K \qquad (V.25)$$

$$= 35.9\ T - 3.67 \times 10^4,\ cm^2/gm \text{ for } T < 1253°K \qquad (V.26)$$

λ_ℓ , the reactivity of limestone, is a function of conversion, temperature and particle size. $CaSO_4$ formed due to the sulfation of calcined limestone tends to block the pores formed during limestone calcination, building an impervious layer on the particle surface, thus reducing the reactivity of limestone. The reactivity of limestone is calculated using the grain model developed by Ishida and Wen (1971). Typical profiles of limestone reactivity as a function of conversion for various particle sizes are shown in Fig. 3.

3. NO_x-Char Reaction:

Nitrogen oxides are generated during the combustion of volatiles and char, and are subsequently reduced to N_2 by reaction with nitrogeneous fragments (containing NH_3) in the volatiles and also by the heterogeneous reaction with char. Fuel nitrogen compounds in the volatiles would be in the form of NH_3. When the volatiles burn, NH_3 is oxidized to NO. When the residual char burns, nitrogeneous fragments of the char are also oxidized to NO. The released nitrogen oxides are reduced by char according to the reaction

$$C + 2\ NO \longrightarrow CO_2 + N_2 \qquad (V.27)$$

The rate expression for NO reduction is

$$r_{NO} = \pi\ d_c^2\ k_{NO}\ C_{NO} \quad \text{gmole NO/sec·particle} \qquad (V.28)$$

where $k_{NO} = 5.24 \times 10^7 \exp(-34000/RT_m)$ cm/sec (Oguma, et al. 1977, Horio, et al. 1977).

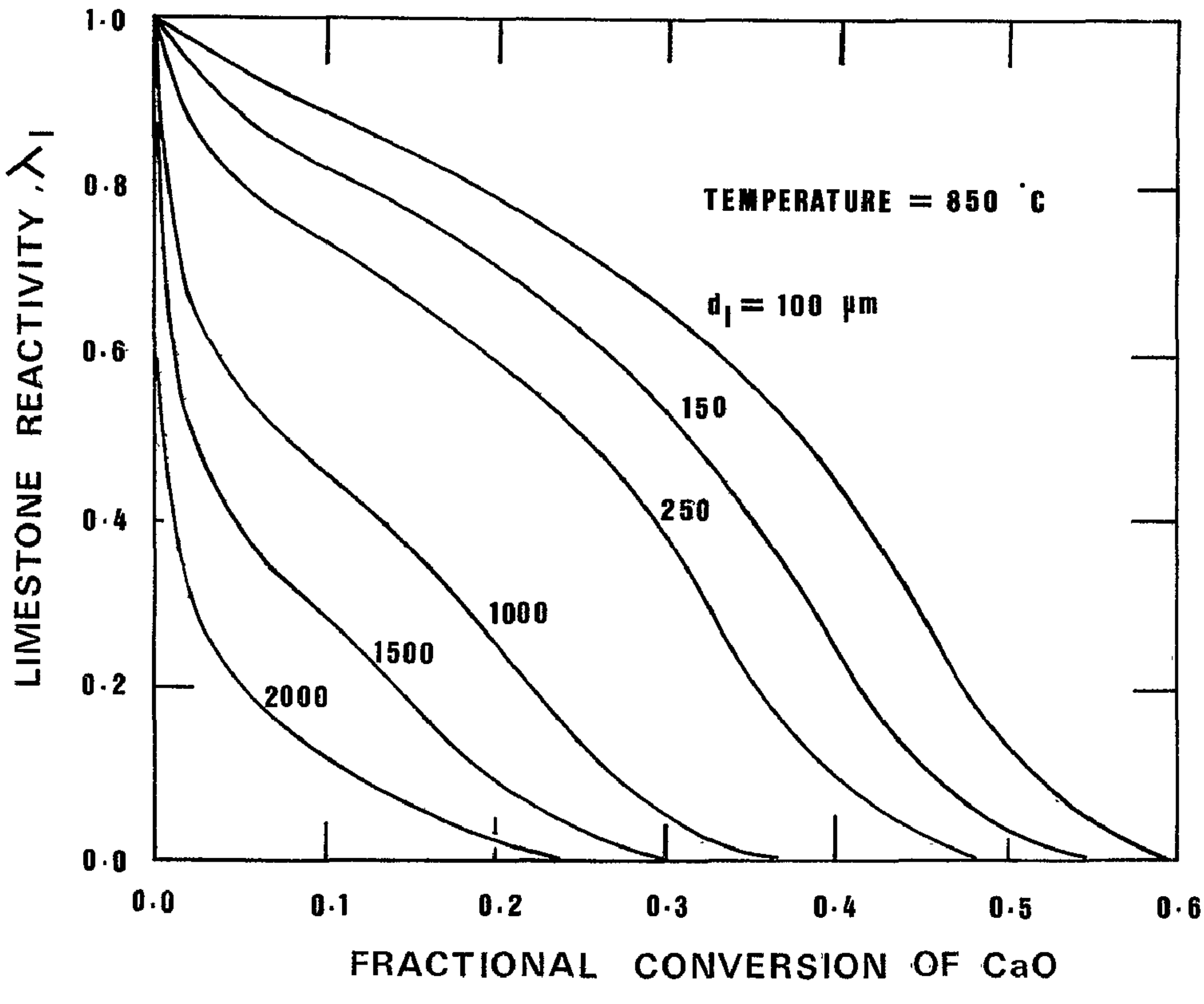


Fig.3 Limestone Reactivity Profiles

4. Attrition and Entrainment of Char and Limestone:

Limestone and char particles in the bed are subjected to erosion and attrition due to the rapid mixing of the solids. The attrition rate is proportional to the rate of energy input. The size distribution of the fines produced has been found to be approximately constant for a particular bed material and independent of the bed size distribution or operating conditions (Merrick and Highley, 1974). The rate of energy input to the particles is taken to be proportional to $(U_o - U_{mf})$ and also to the bed weight. The rate of production of fines is correlated as:

$$R_a = K(U_o - U_{mf})M_b \quad \text{gm/sec} \qquad \text{(V.29)}$$

The value of K is dependent on the friability of the material. The values of K lie in the range 9.11×10^{-8} for ash and 2.73×10^{-8} for limestone.

The rate of elutriation of char and limestone for a size fraction x, from a fluidized bed is directly proportional to their concentration in the bed, that is:

$$R_x = E_x\, b_x \quad \text{gms/sec} \qquad \text{(V.30)}$$

where R_x is the elutriation rate of the close size fraction x , for a given operating conditions, b_x is the weight fraction of the close size fraction in the bed. There are many correlations proposed to calculate the elutriation rate constant, E_x. Many of the correlations exhibit an improper qualitative behavior in the smaller particle size ranges. A recent correlation proposed by Merrick and Highley (1974) accounts properly for the boundary conditions of a maximum limiting elutriation rate constant at zero particle size and the rate constant approaching zero with increasing particle size and at $U_o = U_{mf}$. It is of the form:

$$E_x = G \exp[-10.4 \left(\frac{U_t}{U_o}\right)^{0.5} \left(\frac{U_{mf}}{U_o - U_{mf}}\right)^{0.25}] \quad \text{gm/sec} \qquad (V.31)$$

The above correlation was obtained by Merrick and Highley with data from NCB combustor in which the freeboard height was around 275 cms. When this correlation is used to simulate the performance of NCB combustor, the results agree well with data (Fig.10). This correlation does not take into account the effect of varying freeboard heights and hence cannot be used to calculate the entrainment rate along the freeboard height. In view of the fact that the entrainment below TDH is dependent on the freeboard height, the following correction is suggested to calculate the entrainment rate as a function of height above the bed surface. The rate of entrainment is given by:

$$R_x = F_{O,x} \exp[\frac{h}{275.0} \cdot \ln \left(\frac{E_x\ b_x}{F_{O,x}}\right)] \quad \text{gms/sec} \qquad (V.32)$$

where $F_{O,x}$ is the entrainment rate of particles of x th size fraction at the bed surface, h is the height above the bed surface in cms, and the constant 275.0 represents the freeboard height of the NCB combustor based on which Merrick and Highley's correlation is developed.

When the bubbles burst at the surface of the bed, solids in the wake of the bubbles are thrown into the freeboard. The amount of solids splashed into the freeboard can be calculated from the equation (Yates and Rowe, 1977).

$$F_O = A_t \cdot (U_o - U_{mf}) f_w\ (1 - \varepsilon_{mf}) \rho_s \cdot f_{sw} \quad \text{(gms/sec)} \qquad (V.33)$$

where f_w is the wake fraction and f_{sw} is the fraction of solids in the wake thrown into the freeboard. TDH represents the height (above the bed surface) above which the entrained solids density is independent of the height. There are many correlations available in literature to calculate the TDH (Zenz and Weil, 1958; Amitin, et al. 1968; Nazemi, et al. 1973; Fournol, et al. 1973). The correlation proposed by Amitin, et al. (1968) is used here because of its simplicity and accuracy in the range of fluidizing velocities encountered in the combustor.

$$TDH = 0.429\, \overline{U}_o^{\,1.2}\, (11.43 - 1.2 \ln \overline{U}_o) \text{ cms} \qquad (V.34)$$

TDH is compared with the actual height (height between the bed surface and the flue gas exit). If the TDH is smaller than the actual freeboard height, then TDH is used to calculate the solids elutriation rate. Entrainment rate of solids as a function of the height above the bed surface is calculated using Equation (V.32).

5. Bubble Hydrodynamics:

A modified version of the bubble assemblage model (Rengarajan, et al. 1977) is used to describe the bubble hydrodynamics. Fig. 4 is a schematic representation of the gas phase model. Gas flow rate in the emulsion phase is assumed to be that at minimum fluidization velocity. The minimum fluidization velocity is calculated using Wen and Yu's (1966) correlation:

$$U_{mf} = \left(\frac{\mu}{d_p\, \rho_g}\right)\left\{\left[33.7^2 + \frac{0.0408\, d_p^{\,3}\, \rho_g(\rho_s - \rho_g)}{\mu_2}\right]^{1/2} - 33.7\right\} \qquad (V.35)$$

Estimation of the bubble diameter along the bed height is one of the most critical factors in FBC modeling. For a non-cylindrical bed, the bubble size, D_B, is calculated from (Mori and Wen, 1975):

$$\frac{dD_B}{dz} = \frac{0.3}{D_t}\,(D_{BM} - D_B) \qquad (V.36)$$

I.C. $D_B = D_{BO}$ at $z = 0$, D_{BO} = initial bubble diameter where D_{BM} is the

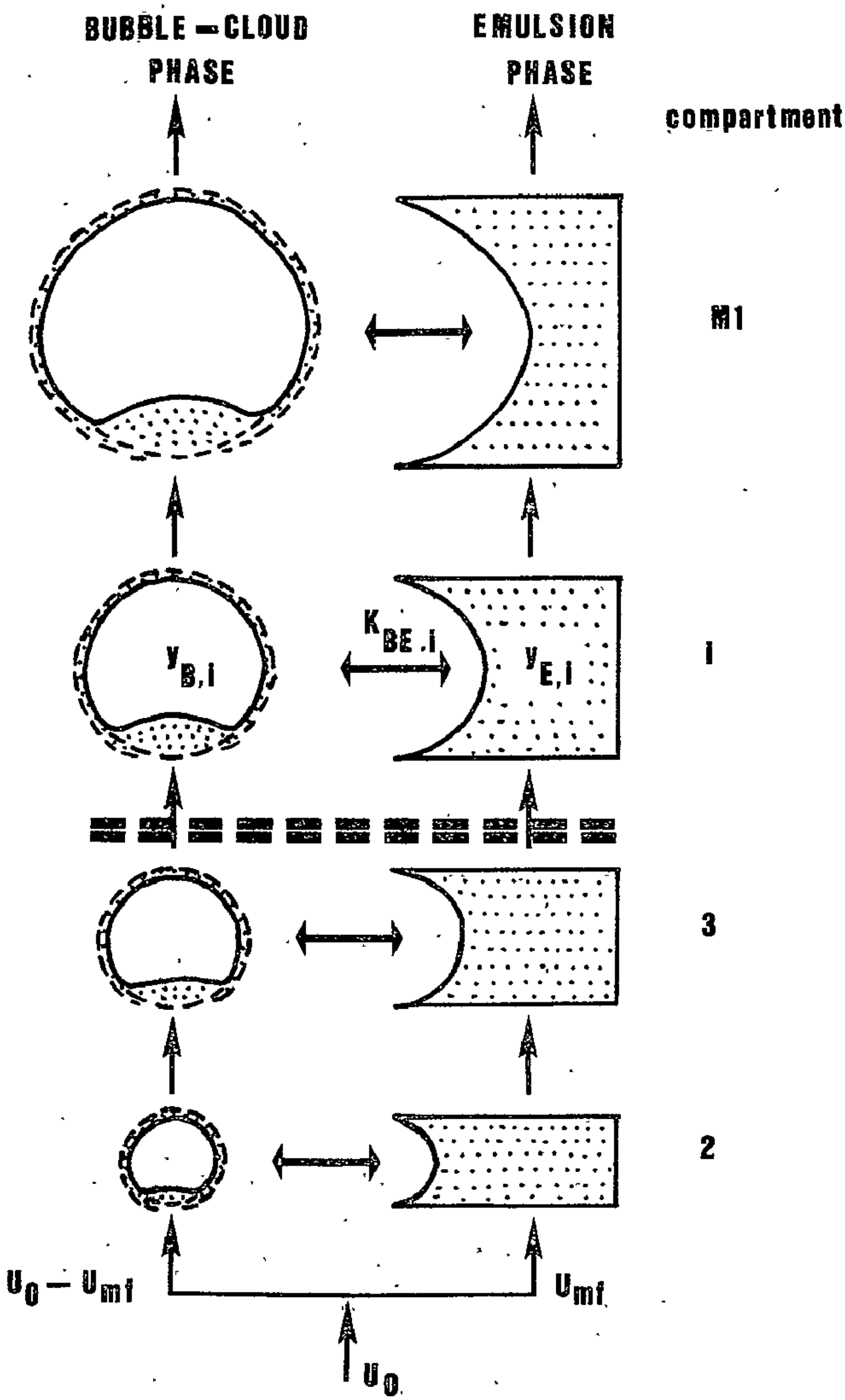


Fig.4 Schematic Illustration of the Gas Phase Model

fictitious maximum bubble diameter defined by Mori and Wen (1975) as:

$$D_{BM} = 0.652 \ [A_t \ (U_o - U_{mf})]^{0.4} \tag{V.37}$$

When cooling tubes are present, the ascending bubbles impinge on the tubes. If the tubes are packed closely, depending on the horizontal pitch distance and tube diameter, bubbles may be broken, and coalescence may not occur. For lack of experimental evidence on the bubble sizes in the presence of internals of various designs, it is assumed here that if the impinging bubbles are of smaller size than the horizontal pitch distance, the bubbles coalesce as if tubes were absent. If the approaching bubble is bigger than the horizontal pitch distance, it is assumed that coalescence does not occur and hence the bubble size in the coils section of the bed is set equal to the pitch distance.

Bubble velocity is calculated from the following relation (Davidson and Harrison, 1963):

$$U_B = U_o - U_{mf} + 0.711 \ \sqrt{gD_B} \tag{V.38}$$

The gas interchange coefficient between the bubble phase and emulsion phase is estimated from (Kobayashi, et al. 1967)

$$K_{BE} = 11.0/D_B \tag{V.39}$$

6. Solids Mixing:

The mixing of solids is caused by the motion of bubbles and their wakes. Both bulk circulation and turbulent mixing of solids are the effects of bubbling phenomena of the bed. The bulk circulation rate, W_{mix}, caused by the lifting of particles by bubble wakes is expressed as:

$$W_{mix} = (U_o - U_{mf}) \ A_t \ f_w \ (1 - \varepsilon_{mf}) \rho_s \tag{V.40}$$

where f_w is the ratio of wake volume to the bubble volume including the wake. The estimation of f_w for FBC has not been clearly established yet. Therefore, f_w is the parameter in the model which requires further investigations. A schematic representation of the solids mixing pattern and the backflow cell model used to describe the solids circulation in the bed are shown in Fig. 5 and Fig. 6. The bed is divided into compartments of size equal to bubble diameter at that height.

7. Heat Transfer:

In calculating the reaction rate for char combustion, the temperature of char particle, T_c, is calculated separately, using a heat balance around the char particle and the surrounding gas as:

$$\frac{2\lambda}{d_c}(T_c - T) + \varepsilon_m \sigma(T_c^4 - T^4) = r_c^* M_c q_{char}/(\pi d_c^2 \cdot C_{ch}) \quad (V.41)$$

where ε_m is the emissivity of the char particle (taken as 1.0 Field, et al., 1967), λ is the thermal conductivity of the surrounding gas and σ is the Stefan-Boltzman constant. The heat generated during combustion is removed by immersed cooling coils in the bed. Water is the cooling medium. Bed to cooling tubes heat transfer coefficient used in the model is selected from experimental data and is in the range of 0.0054 to 0.011 cals/sec.cm^2. ^oC (40 to 80 Btu/hr.ft^2.^oF). Correlations of bed-wall heat transfer coefficient are also available for the estimation (Wender and Cooper, 1958; Wen and Leva, 1956).

8. Freeboard Reactions:

Char combustion, SO_2 absorption and NO_x reduction reactions take place in the freeboard. Heat generated by combustion and heat carried by the flue gases are removed by the cooling coils present in the freeboard. The hydrodynamics in the freeboard is different from that in the bed. There are no bubbles present in the freeboard. Any

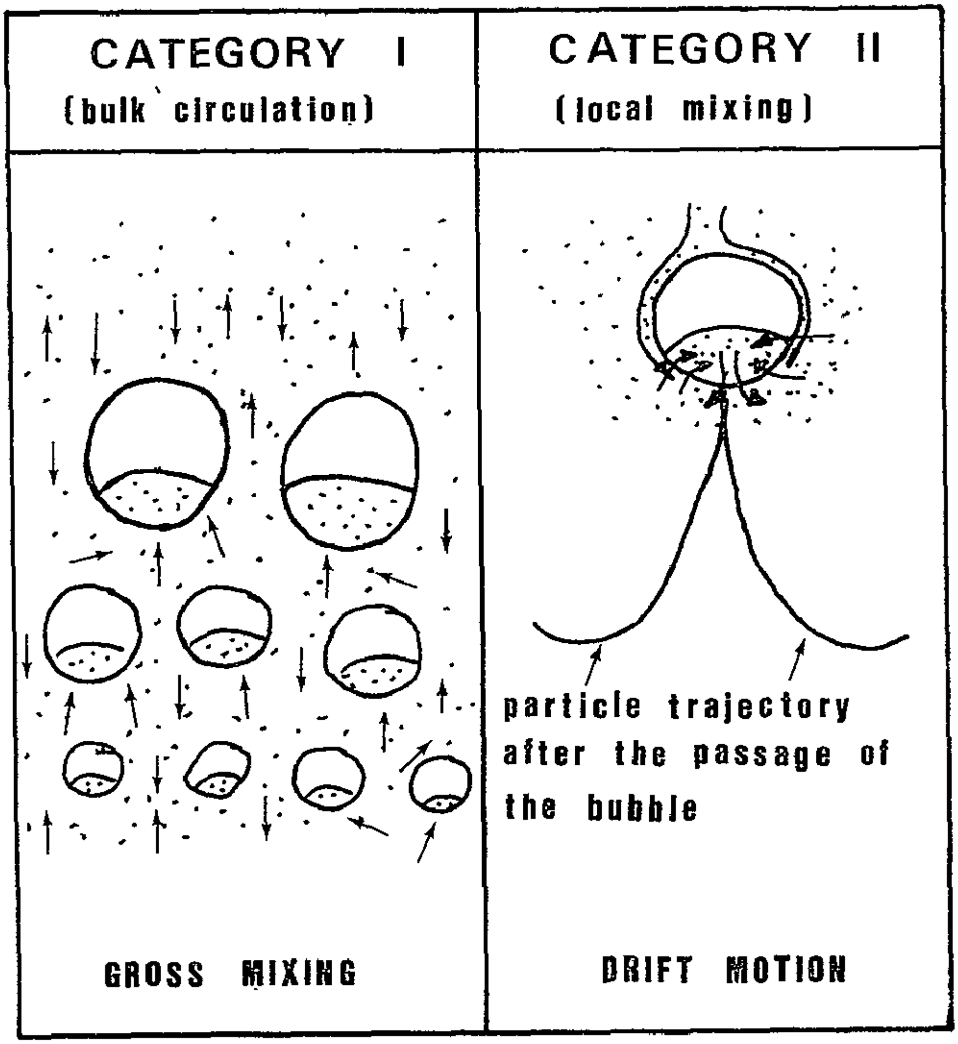
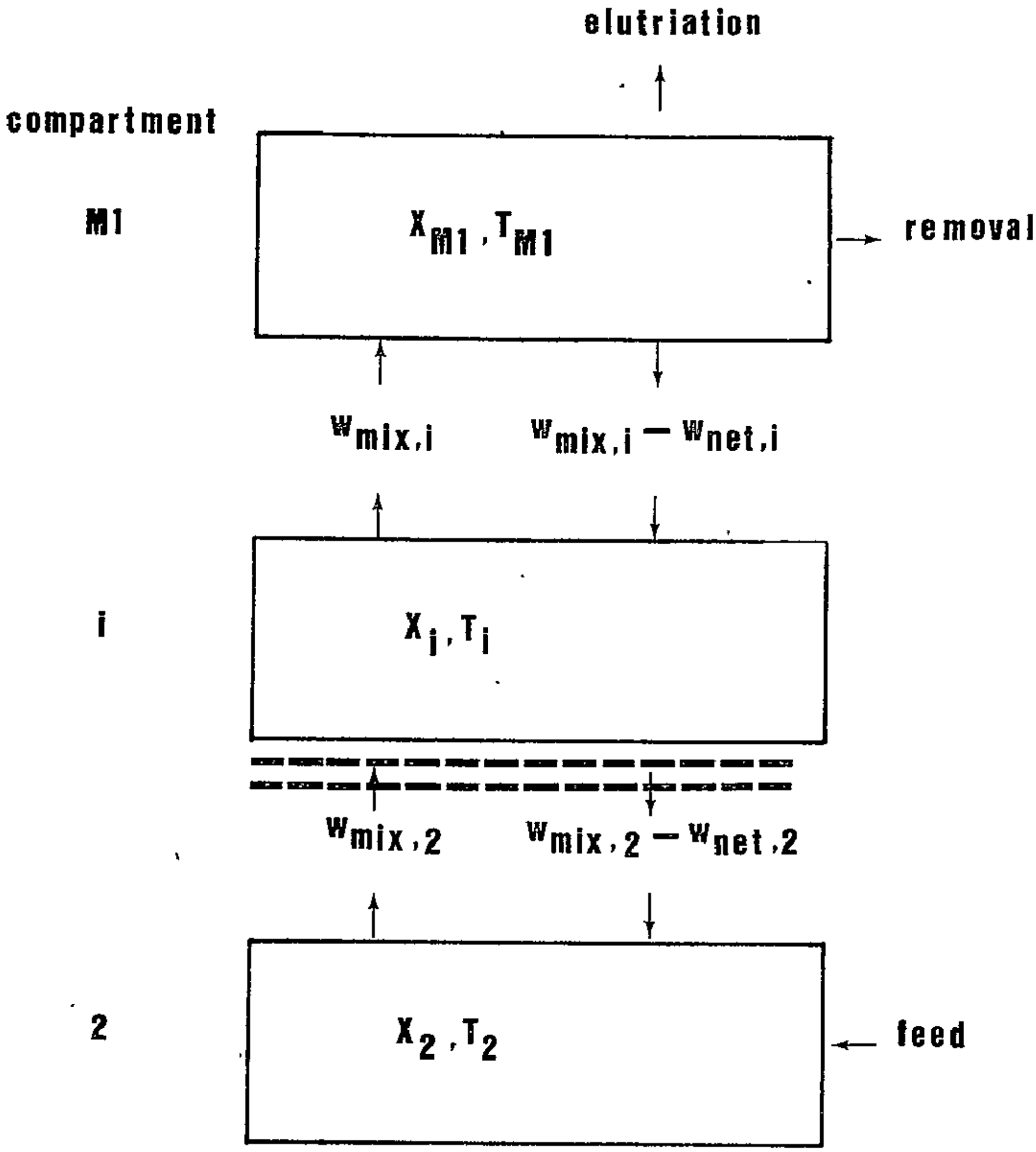


Fig.5 Two Modes of Solids Mixing



X : wt. fraction carbon

T : temperature

w_{mix} : solids mixing rate

w_{net} : net flow rate of solids

Fig. 6 Schematic Illustration of the Solid Phase Model

unburnt volatiles from the bed would be burnt in the freeboard.

The freeboard region is divided into a number of compartments of equal size. To estimate the compartment size in the freeboard region, Peclet number is calculated using the Reynolds number in the freeboard region by the following correlation (Wen and Fan, 1974)

$$N_{Re} = D_t \, \overline{U}_o \, \rho_g/\mu_g \tag{V.42}$$

$$N_{Pe} = \overline{U}_o \, D_t/E_Z \tag{V.43}$$

$$N_{Sc} = \mu_g/D \, \rho_g \tag{V.44}$$

$$\frac{1}{N_{Pe}} = \frac{1}{N_{Re} \, N_{Sc}} + \frac{N_{Re} \cdot N_{Sc}}{192} \quad \text{for } N_{Re} < 2000 \tag{V.45}$$

$$\frac{1}{N_{Pe}} = \frac{3 \times 10^7}{N_{Re}^{2.1}} + \frac{1.35}{N_{Re}^{1.8}} \quad \text{for } N_{Re} \geq 2000 \tag{V.46}$$

Knowing the axial dispersion coefficient, E_z, the average compartment size in the freeboard is calculated as:

$$\Delta Z = 2 \, E_z/\overline{U}_o \tag{V.47}$$

The concentrations of gaseous species vary with each compartment although the concentrations are uniform (completely mixed) within each compartment. Knowing the average height of each compartment above the bed surface, the solids entrainment rate at that height is calculated. Residence time of solids in each compartment is given by $\Delta Z/(U_0 - U_T)$ where ΔZ is the compartment size. Solids hold-up in each compartment is then obtained from

Solids hold-up in each compartment = (upward+downward) flow rate of solids x residence time of solids in that compartment (V.48)

Depending on the residence time of particles in the freeboard, and the char particles burning time, char particles will either be partially or completely burnt, and the partially burnt char particles are elutriated. The burning time of a char particle is estimated from the equation (Field, et al. 1967):

$$t_b = \text{burning time of a char particle} \tag{V.49}$$

$$= \rho_{c,ch} R_g T_m d_c^2 / (96 \phi D P_{O_2}) \tag{V.50}$$

VI. MODEL DESCRIPTION

1. Elutriation Calculations:

A mathematical model has been developed for elutriation in a fluid bed system with size reduction and recycle to the bed of some or all of the fines from the primary and/or secondary cyclones. The model takes into account the variation in the rates of elutriation and size reduction with particle size. If the size reduction is due to more than one process, then there will be a separate value of size reduction constant for each process. In general, the rates of size reduction by the separate processes in each size fraction are additive. A mass balance is performed for each size fraction, x, as follows:

$$W_{f,x} \quad + \quad W_{x-1} \quad + \quad a_x \, k_x \, M_x$$

(feed rate) (gain of particles from next largest size due to size reduction) (gain of fines produced by abrasion)

$$= M_x \, W_D/M_b \quad + \quad R_x \, q_{1x}(1-p_1) \quad + \quad R_x \, q_{2x}(1-q_{1x})(1-p_2)$$

(withdrawal rate from the bed) (particles captured by primary cyclone but not recycled) (particles captured by secondary cyclone but not recycled)

$$+ \quad R_x \, (1-q_{1x})(1-q_{2x}) \quad + \quad k_x \, M_x$$

(particulate emission) (loss of weight due to production of fines by abrasion or to chemical reaction)

$$+ \, W_x$$

(loss of particles to next smallest size due to size reduction) (VI.1)

The rate of loss of particles to the next smallest size, W_x, is determined by considering a mass of particles M_x, at size, d_x, and calculating the mass remaining M_{x+1} after the size has been reduced to d_{x+1}. The rate of reduction is written as:

$$\frac{dM}{d\theta} = -k_x M(U_o - U_{mf}) \tag{VI.2}$$

The rate of size reduction between d_x and d_{x+1} is:

$$\frac{dd_x}{d\theta} = \frac{-k_x}{3} d_x(U_o - U_{mf}) \tag{VI.3}$$

Dividing equation (VI.2) by equation (VI.3) gives:

$$\frac{dM}{dd_x} = \frac{3M}{d_x} \tag{VI.4}$$

and integrating between d_x and d_{x+1} gives:

$$\frac{M_{x+1}}{M_x} = \left(\frac{d_{x+1}}{d_x}\right)^3 \tag{VI.5}$$

This fraction is the proportion of the total feed to the xth size fraction which is reduced in diameter to (x+1)th size fraction.

Therefore, $W_x = [W_{f,x} + a_x K(U_o - U_{mf})M_b + W_{x-1}]\left(\frac{d_{x+1}}{d_x}\right)^3$. (VI.6)

For the coarsest size fraction, W_{x-1} is zero.

The entire calculation is iterative, starting from initial guesses of the withdrawal rate of solids from the bed and the size distribution of particles in the bed. Mass balance is performed on each successive close size fraction, starting from the coarsest. The bed weight in each size fraction and hence the total bed weight and bed size distribution is calculated. The procedure is repeated till the calculated bed weight equals the given bed weight. The elutriation rate, fines collection/recycle rates, particle emission and size distribution of elutriated particles are then calculated.

2. Material and Energy Balances:

Material balances are made for volatile gases, CO, CO_2, oxygen, SO_2 and NO in the bubble and emulsion phases within the bed and in the freeboard. Depending on the concentration of oxygen in the emulsion phase, different material balances are used as shown below.

Case A: Volatiles concentration in the emulsion phase is not zero because of insufficient oxygen in emulsion phase for complete combustion of volatiles. Char and CO combustion do not proceed in the emulsion phase.

EMULSION PHASE EQUATIONS

Oxygen:

$$Y_{E,i} = 0.0 \tag{VI.7}$$

Volatiles:

$$F_{EM,i}Y_{E,v,i} = F_{EM,i-1}Y_{E,v,i-1} - a_1Y_{E,v,i-1}$$

(Volatiles out) (Volatiles in) (Volatiles Exchanged to Bubble Phase)

$$- \frac{(F_{EM,i-1}Y_{E,i-1} + a_1Y_{B,i})}{X_{O_2}} + R_{v,i} \tag{VI.8}$$

(Volatiles Burnt) (Volatiles Released during Devolatilization)

where $$a_1 = K_{BE,i}\, A_{t,i}\Delta Z_i\, \varepsilon_{B,i}\, \frac{P}{R_gT_i}, \text{ gmole/sec} \tag{VI.9}$$

Carbon monoxide:

$$F_{EM,i}\, Y_{E,CO,i} = F_{EM,i-1}\, Y_{E,CO,i-1} - a_1\, Y_{E,CO,i}$$

(CO out) (CO in) (CO Exchanged to Bubble Phase)

$$- \frac{(F_{EM,i-1} Y_{E,i-1} + a_1 Y_{B,i})}{X_{O_2}} \cdot V_{CO} + R_{CO,i}$$

(CO Produced by Volatiles Burning) (CO Released during Devolatilization)

$$+ \quad 2 a_4 Y_{E,CO_2,i} \qquad \text{(VI.10)}$$

(CO Produced by C-CO_2 Reaction)

where

$$a_4 = a_m A_{t,i} \Delta Z_i \ (1-\varepsilon_{c,i} - \varepsilon_{tube,i})(k_{CO_2,i} \frac{P}{R_g T_{E,i}} X_i), \text{ gmole/sec} \qquad \text{(VI.11)}$$

$$a_m = \frac{6 \ \rho_b (1-\varepsilon_{mf})}{d_c \ \rho_{ch} \ C_{ch}} \qquad \text{(VI.12)}$$

Carbon dioxide:

$$F_{EM,i} Y_{E,CO_2,i} = F_{EM,i-1} Y_{E,CO_{2,i-1}} - a_1(Y_{E,CO_2,i} - Y_{B,CO_2,i})$$

(CO_2 out) (CO_2 in) (CO_2 Exchanged to Bubble Phase)

$$+ R_{CO_2,i} \quad - \quad a_4 Y_{E,CO_2,i} \qquad \text{(VI.13)}$$

(CO_2 Released during Devolatilization) (CO_2 Consumed by C-CO_2 Reaction)

BUBBLE PHASE EQUATIONS

Oxygen:

$$F_{BM,i} Y_{B,i} = F_{BM,i-1} Y_{B,i-1} - a_1 Y_{B,i}$$

(Oxygen out) (Oxygen in) (Oxygen Exhcanged to Emulsion Phase)

$$-a_2 Y_{B,i} \quad - \quad \frac{a_1 Y_{E,CO,i}}{2} \quad - \quad a_1 Y_{E,v,i} X_{O_2,c} \qquad \text{(VI.14)}$$

(Oxygen Consumed by Char) (Oxygen Consumed by CO Exchanged to Bubble Phase) (Oxygen Consumed by Volatiles Exchanged to Bubble Phase)

where

$$a_2 = a_m A_{t,i} \Delta Z_i (\varepsilon_{c,i} - \varepsilon_{B,i}) k_{cB,i} \frac{P}{R_g T_{B,i}} X_i \qquad \text{(VI.15)}$$

Carbon dioxide:

$$F_{BM,i} Y_{B,CO_2,i} = F_{BM,i-1} Y_{B,CO_2,i-1} - a_1 (Y_{B,CO_2,i} - Y_{E,CO_2,i})$$

(CO_2 out) (CO_2 in) (CO_2 Exchanged to Emulsion Phase)

$$+ a_2 Y_{B,i} \quad + \quad a_1 Y_{E,CO,i} \quad + \quad a_1 Y_{E,v,i} V_{CO_2} \qquad \text{(VI.16)}$$

(CO_2 Produced by Char Combustion) (CO_2 Produced by CO Combustion) (CO_2 Produced by Volatiles Burning)

FREEBOARD EQUATIONS

Oxygen:

$$Y_{O,i} = 0.0 \qquad \text{(VI.17)}$$

Volatiles:

$$F_{MT}\,Y_{v,i} = F_{MT}\,Y_{v,i-1} - F_{MT}\,Y_{O,i-1}/X_{O_2} \qquad \text{(VI.18)}$$

(Volatiles out) (Volatiles in) (Volatiles Burnt)

Carbon monoxide:

$$F_{MT}\,Y_{CO,i} = F_{MT}\,Y_{CO,i-1} + 2\,a_4'\,Y_{CO_2,i}$$

(CO out) (CO in) (CO Produced by $C-CO_2$ Reaction)

$$+ F_{MT}(Y_{v,i-1} - Y_{v,i})V_{CO} \qquad \text{(VI.19)}$$

(CO Produced by Volatiles Burning)

$$\text{where } a_4' = \frac{P}{R_g T_{B,i}}\, N_{c,i}\, \pi d_{ce,i}^2\, k_{CO_2,i}, \text{ gmole/sec} \qquad \text{(VI.20)}$$

Carbon dioxide:

$$F_{MT}\,Y_{CO_{2,i}} = F_{MT}\,Y_{CO_2,i-1} - a_4'\,Y_{CO_2,i} \qquad \text{(VI.21)}$$

(CO_2 out) (CO_2 in) (CO_2 Consumed by $C-CO_2$ Reaction)

Case B: Sufficient oxygen is present in the emulsion phase for the combustion of volatiles.

EMULSION PHASE EQUATIONS

Volatiles:

$$Y_{E,v,i} = 0.0 \qquad \text{(VI.22)}$$

Oxygen:

$$F_{EM,i}\,Y_{E,i} = F_{EM,i-1}\,Y_{E,i-1} - a_1(Y_{E,i} - Y_{B,i})$$

(Oxygen out) (Oxygen in) (Oxygen Exchanged to Bubble Phase)

$$- a_3 Y_{E,i}/\phi_{E,i} - (F_{EM,i-1} Y_{E,v,i-1} + R_{v,i}) X_{O_2}$$

(Oxygen consumed by Char) (Oxygen Consumed by Volatiles Burning)

$$- k Y_{E,CO,i} \left(\frac{17.5 Y_{E,i}}{1 + 24.7 Y_{E,i}}\right)/2.0 \quad \text{(VI.23)}$$

(Oxygen Consumed by CO)

where

$$k = 3 \times 10^{10} \exp(-16000/RT_i) \left(\frac{P}{R_g T_i}\right)^{1.8} Y_{H_2O}^{0.5} \times A_{t,i} \Delta Z_i (i - \varepsilon_{c,i} - \varepsilon_{tube,i}) \varepsilon_{mf}$$

gmole/sec (VI.24)

$$a_3 = a_m A_{t,i} \Delta Z_i (1 - \varepsilon_{c,i} - \varepsilon_{tube,i}) k_{cE,i} \frac{P}{R_g T_{E,i}} X_i \quad \text{(VI.25)}$$

<u>Carbon monoxide:</u>

$$F_{EM,i} Y_{E,CO,i} = F_{EM,i-1} Y_{E,CO,i-1} - k Y_{E,CO,i} \left(\frac{17.5 Y_{E,i}}{1+24.7 Y_{E,i}}\right)$$

(CO out) (CO in) (CO Burnt)

$$+ (F_{EM,i-1} Y_{v,i-1} + R_{v,i}) V_{CO} + R_{CO,i}$$

(CO Produced by Volatiles Burning) (CO Released during Devolatilization)

$$+ 2 a_4 Y_{E,CO_2,i} + a_3 \left(2 - \frac{2}{\phi_{E,i}}\right) Y_{E,i} \quad \text{(VI.26)}$$

(CO Produced by C-CO_2 Reaction) (CO Produced by Char Combustion)

<u>Carbon dioxide:</u>

$$F_{EM,i} Y_{E,CO_2,i} = F_{EM,i-1} Y_{E,CO_2,i-1} - a_1 (Y_{E,CO_2,i} - Y_{B,CO_2,i})$$

(CO_2 out) (CO_2 in) (CO_2 Exchanged to Bubble Phase)

$$+ k\, Y_{E,CO,i} \left(\frac{17.5\, Y_{E,i}}{1+24.7\, Y_{E,i}}\right) + R_{CO_2,i}$$

(CO_2 Produced by CO Combustion) (CO_2 Released during Devolatilization)

$$- a_4\, Y_{E,CO_2,i} + a_3\left(\frac{2}{\phi_{E,i}} - 1\right) Y_{E,i} \qquad \text{(VI.27)}$$

(CO_2 Consumed by C-CO_2 Reaction) (CO_2 Produced by Char Combustion)

BUBBLE PHASE EQUATIONS

Oxygen:

$$F_{BM,i}\, Y_{B,i} = F_{BM,i-1}\, Y_{B,i-1} - a_1(Y_{B,i} - Y_{E,i})$$

(Oxygen out) (Oxygen in) (Oxygen Exchanged to Emulsion Phase)

$$- a_2\, Y_{B,i} - a_1\, Y_{E,CO,i}/2 \qquad \text{(VI.28)}$$

(Oxygen Consumed by Char) (Oxygen Consumed by CO Exchanged to Bubble Phase)

Carbon dioxide:

$$F_{BM,i}\, Y_{B,CO_2,i} = F_{BM,i-1}\, Y_{B,CO_2,i-1} - a_1(Y_{B,CO_2,i} - Y_{E,CO_2,i})$$

(CO_2 out) (CO_2 in) (CO_2 Exchanged to Emulsion Phase)

$$+ a_2\, Y_{B,i} + a_1\, Y_{E,CO,i} \qquad \text{(VI.29)}$$

(CO_2 Produced by Char Combustion) (CO_2 Produced by CO Combustion)

FREEBOARD EQUATIONS

Volatiles:

$$Y_{v,i} = 0.0 \qquad \text{(VI.30)}$$

Oxygen:

$$F_{MT}\, Y_{O,i} = F_{MT}\, Y_{O,i-1} - F_{MT}\, Y_{v,i-1}\, X_{O_2}$$

(Oxygen out) (Oxygen in) (Oxygen Consumed by Volatiles)

$$- k' Y_{CO,i}\left(\frac{17.5\ Y_{O,i}}{1+24.7\ Y_{O,i}}\right)/2 \quad - \quad a_2' Y_{O,i}/\phi_{B,i} \qquad \text{(VI.31)}$$

(Oxygen Consumed by CO Combustion) (Oxygen Consumed by Char Combustion)

where

$$k' = 3 \times 10^{10} \exp(-16000/RT_i)\left(\frac{P}{R_g T_i}\right)^{1.8} Y_{H_2O}^{0.5} A_{t,i} \Delta Z_i (1-\varepsilon_{tube,i}), \text{gmole/sec} \qquad \text{(VI.32)}$$

$$a_2' = \left(\frac{P}{R_g T_{B,i}}\right) N_{c,i} \pi d_{ce,i}^2 k_{c,i}, \text{ gmole/sec} \qquad \text{(VI.33)}$$

Carbon monoxide:

$$F_{MT} Y_{CO,i} \quad = \quad F_{MT} Y_{CO,i-1} \quad + \quad 2\ a_4' Y_{CO,i}$$

(CO out) (CO in) (CO Produced by $C-CO_2$ Reaction)

$$+ F_{MT} Y_{v,i-1} V_{CO} \quad + \quad a_2' Y_{O,i}\left(2 - \frac{2}{\phi_{B,i}}\right)$$

(CO Produced by Volatiles Burning) (CO Produced by Char Combustion)

$$- k' Y_{CO,i}\left(\frac{17.5\ Y_{O,i}}{1.24.7\ Y_{O,i}}\right) \qquad \text{(VI.34)}$$

(CO Burnt)

Carbon dioxide:

$$F_{MT} Y_{CO_2,i} \quad = \quad F_{MT} Y_{CO_2,i-1} \quad - \quad a_4' Y_{CO_2,i}$$

(CO_2 out) (CO_2 in) (CO_2 Consumed by $C-CO_2$ Reaction)

$$+ a_2' Y_{O,i}\left(\frac{2}{\phi_{B,i}} - 1\right) \quad + \quad k' Y_{CO,i}\left(\frac{17.5\ Y_{O,i}}{1+24.7\ Y_{O,i}}\right) \qquad \text{(VI.35)}$$

(CO_2 Produced by Char Combustion) (CO_2 Produced by CO Combustion)

The boundary conditions are:

$$Y_{B,1} = 0.21\ F_{MF}/F_{MT} \tag{VI.36}$$

$$Y_{E,1} = Y_{B,1} \tag{VI.37}$$

$$Y_{E,v,1} = 0.0 \tag{VI.38}$$

$$Y_{E,CO,1} = 0.0 \tag{VI.39}$$

$$Y_{E,CO_2,1} = 0.0 \tag{VI.40}$$

$$Y_{B,CO_2,1} = 0.0 \tag{VI.41}$$

SULFUR DIOXIDE AND NITRIC OXIDE BALANCES

Nitrogen and sulfur content in the volatile products released during devolatilization is a function of bed temperature. Volatile nitrogen increases from 20 to 70% as temperature rises from 800 to 1300°K (Fine, et al. 1974) and is expressed as:

$$V_N = 0.001T - 0.6 \tag{VI.42}$$

Similarly the sulfur content in the volatiles is expressed as:

$$V_S = 0.001T - 0.6 \tag{VI.43}$$

Sulfur and nitrogen left in the residual char are released as SO_2 and NO when char burns. The following material balances are made for sulfur dioxide and NO in the bed and in the freeboard.

EMULSION PHASE EQUATIONS

$$\underbrace{F_{EM,i}\ Y_{E,SO_2,i}}_{(SO_2\ \text{out})} = \underbrace{F_{EM,i-1}\ Y_{E,SO_2,i-1}}_{(SO_2\ \text{in})} - \underbrace{a_1(Y_{E,SO_2,i} - Y_{B,SO_2,i})}_{(SO_2\ \text{Exchanged to Bubble Phase})}$$

$$-a_{E,SO_2,i}\, Y_{E,SO_2,i} \quad + \quad R_{E,SO_2,c,i} \quad + \quad R_{E,SO_2,V,i} \qquad \text{(VI.44)}$$

(SO_2 Absorbed by Limestone) (SO_2 Released during Char Combustion) (SO_2 Released during Volatiles Combustion)

where

$$a_{E,SO_2,i} = A_{t,i}\Delta Z_i(1-\varepsilon_{c,i} - \varepsilon_{tube,i})(1-\varepsilon_{mf})k_{v1}\left(\frac{P}{R_g T_i}\right), \text{ gmole/sec} \qquad \text{(VI.45)}$$

$$F_{EM,i}\, Y_{E,NO,i} = F_{EM,i-1}\, Y_{E,NO,i-1} - a_1(Y_{E,NO,i} - Y_{B,NO,i})$$

(NO out) (NO in) (NO Exchanged to Bubble Phase)

$$-\, a_{E,NO,i}\, Y_{E,NO,i} + R_{E,NO,c,i} + R_{E,NO,V,i} \qquad \text{(VI.46)}$$

(NO Reduced by Char) (NO Released during Char Combustion) (NO Released during Volatiles Combustion)

where

$$a_{E,NO,i} = a_m\, A_{T,i}\, \Delta Z_i\, (1-\varepsilon_{c,i} - \varepsilon_{tube,i})k_{E,NO,i} \frac{P}{R_g T_{E,i}}\, X_i, \text{ gmole/sec} \qquad \text{(VI.47)}$$

BUBBLE PHASE EQUATIONS

$$F_{BM,i}\, Y_{B,SO_2,i} = F_{BM,i-1}\, Y_{B,SO_2,i-1} - a_1(Y_{B,SO_2,i} - Y_{E,SO_2,i})$$

(SO_2 out) (SO_2 in) (SO_2 Exchanged to Emulsion Phase)

$$-\, a_{B,SO_2,i}\, Y_{B,SO_2,i} + R_{B,SO_2,c,i} + R_{B,SO_2,V,i} \qquad \text{(VI.48)}$$

(SO_2 Absorbed by Limestone) (SO_2 Released during Char Combustion) (SO_2 Released during Volatiles Combustion)

where

$$a_{B,SO_2,i} = A_{t,i}\Delta Z_i(\varepsilon_{c,i} - \varepsilon_{B,i})(1-\varepsilon_{mf})k_{v1}\left(\frac{P}{R_g T_i}\right), \text{gmole/sec} \qquad \text{(VI.49)}$$

$$F_{BM,i}\, Y_{B,NO,i} = F_{BM,i-1} Y_{B,NO,i-1} - a_1 (Y_{B,NO,i} - Y_{E,NO,i})$$

(NO out) (NO in) (NO Exchanged to Emulsion Phase)

$$- a_{B,NO,i}\, Y_{B,NO,i} + R_{B,NO,c,i} + R_{B,NO,V,i} \qquad \text{(VI.50)}$$

(NO Reduced by Char) (NO Released during Char Combustion) (NO Released during Volatiles Combustion)

where

$$a_{B,NO,i} = a_m\, A_{t,i}\, \Delta Z_i (\varepsilon_{c,i} - \varepsilon_{tube,i}) k_{B,NO,i} \frac{P}{R_g T_{B,i}} X_i \text{ , gmole/sec} \qquad \text{(VI.51)}$$

FREEBOARD EQUATIONS

$$F_{MT}\, Y_{SO_2,i} = F_{MT}\, Y_{SO_2,i-1} + R_{SO_2,i} - a_{SO_2,i}\, Y_{SO_2,i} \qquad \text{(VI.52)}$$

(SO_2 out) (SO_2 in) (SO_2 Released) (SO_2 Absorbed by Limestone)

where $$a_{SO_2,i} = \left(\frac{P}{R_g T_i}\right) N_{A,i} \frac{\pi\, d^3_{\ell e,i}}{6} k_{vi}\text{, gmole/sec} \qquad \text{(VI.53)}$$

$$F_{MT}\, Y_{NO,i} = F_{MT}\, Y_{NO,i-1} + R_{NO,i} - a_{NO,i}\, Y_{NO,i} \qquad \text{(VI.54)}$$

(NO out) (NO in) (NO Released) (NO Reduced by Char)

where $$a_{NO,i} = \left(\frac{P}{R_g T_{B,i}}\right) N_{c,i}\, \pi\, d^2_{ce,i}\, k_{NO,i}\text{, gmole/sec} \qquad \text{(VI.55)}$$

The boundary conditions are:

$$Y_{E,SO_2,1} = Y_{B,SO_2,1} = Y_{E,NO,1} = Y_{B,NO,1} = 0.0 \qquad \text{(VI.56)}$$

SOLID PHASE MATERIAL BALANCE

The overall material balance for the solids in ith compartment in terms of net solids flow, $W_{net,i}$ is given by:

$$W_{net,i} = W_{net,i-1} + W_{fc,i} R_{ch} + W_{fa,i}$$

(solids out) (solids in) (Char feed) (Additives Feed)

$$-W_{D,i} - r_i$$

(Solids Withdrawal (Char Burnt) (VI.57)

The boundary condition is $W_{net,1} = 0.0$

The material balance for the carbon in ith compartment is given as follows by introducing the backmix flow, W_{mix}.

$$(W_{mix,i} - W_{net,i})X_{i+1} - [W_{mix,i-1} - W_{net,i-1} + W_{mix,i} - W_{D,i}]X_i$$

$$+ W_{mix,i-1} = r_i - W_{fc,i} C_{ch} M_c \quad (VI.58)$$

where X_i is the weight fraction of carbon in the ith compartment.

The boundary conditions are:

$$W_{mix,1} = W_{mix,M1} = 0.0 \quad (VI.59)$$

The energy balance for the ith compartment is given as follows:

$$C_S(W_{mix,i} - W_{net,i})T_{i+1}$$

(heat in from (i+1)th cell)

$$-C_S\{(W_{mix,i-1} - W_{net,i-1} + W_{mix,i} - W_{D,i}) + C_{gm} F_{MT}\}T_i$$

(heat out from ith cell)

$$+ [C_S W_{mix,i-1} + C_{gm} F_{MT}]T_{i-1} + r_i q_{ch}$$

(heat in from (i-1)th cell) (heat generated by char combustion)

$$+ g_{E,i} q_{V,CO} + g_{B,i} q_V + g_{CO,i} q_{CO}$$

(heat generated by volatiles combustion in emulsion phase) (heat generated by volatiles combustion in bubble phase) (heat generated by CO combustion)

$$-q_{cal}\, W_{fa,i} \quad + \quad (W_{fa,i}\, C_{sf} + W_{fc,i}\, C_{cf})\, T_{sf,i}$$

(heat of calcination) (sensible heat of solids feed)

$$= A_{t,i}\, \Delta Z_i\, a_{HE,i}\, U_i\, (T_i - T_{w,i}) + A_{t,i}\, \Delta Z_i\, a_{HEW,i}\, U_{w,i}$$

(heat removed by cooling tubes) $(T_i - T_{wall,i})$ (VI.60)

(heat losses through the walls)

ENERGY BALANCE IN THE FREEBOARD

The following equations are obtained for energy balance in the freeboard in ith compartment.

$$(W_{ent,i}\, C_S + C_{gm}\, F_{MT})\, T_{i-1} \quad + r_i\, q_{ch}$$

(heat in from (i-1)th compartment) (heat generated by char combustion)

$$+ g_{E,i}\, q_{V,CO} \quad + \quad g_{CO,i}\, q_{CO}$$

(heat generated by volatiles combustion) (heat generated by CO combustion)

$$-\, (W_{ent,i}\, C_S + C_{gm}\, F_{MT})\, T_i \quad = \quad A_{t,i}\, \Delta Z_i\, a_{HE,i}\, U_i\, (T_i - T_{w,i})$$

(heat out from ith cell) (heat removed by cooling tubes)

$$+ A_{t,i}\, \Delta Z_i\, a_{HEW,i}\, U_{w,i}\, (T_i - T_{wall,i}) \qquad \text{(VI.61)}$$

(heat losses through the walls)

Some of the correlations used in simulation are listed in Table 2. Table 3 indicates the assumed values for the parameters involved in the model. If, in future, proper and accurate correlations become available, these parameters can be substituted with those correlations. The logic diagrams for the computer programs are shown in Figures 7, 8 and 9. Symbols are explained in Appendix VIII. Algebraic equations obtained are solved using IBM 360 computer available at WVU.

TABLE 2. CORRELATIONS USED IN SIMULATION

Heat capacity of solids, $C_S = 0.215$ cals/gm·°C

Heat capacity of gas, $C_{gm} = 6.8 + 0.5 \times 10^{-3}\, t(°C)$

Density of limestone = 2.4 gms/cm^3

Density of coal = 1.4 gms/cm^3

Minimum fluidization velocity,

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

Bubble diameter, $D_B = D_{BM} - (D_{BM} - D_{BO})\exp(-0.3\, Z/D_t)$, cm

where

$$D_{BM} = 0.652\, \{A_t\, (U_o - U_{mf})\}^{0.4}$$

$$D_{BO} = 0.347\, \{A_t\, (U_o - U_{mf})/n_d\}^{0.4}$$

Bubble velocity, $U_B = U_o - U_{mf} + 0.711\sqrt{gD_B}$

Bubble fraction, $\varepsilon_B = (U_o - U_{mf})/U_B$

Cloud fraction, $\varepsilon_c = \varepsilon_B\ \alpha_b/(\alpha_b - 1)$

where $\alpha_b = \varepsilon_{mf}\, U_B/U_{mf}$

Void fraction at minimum fluidization, $\varepsilon_{mf} = 0.5$

TABLE 3. PARAMETERS IN THE MODEL

Bed to tube heat transfer coefficient, $U = 0.00765$, cals/sec·cm^2°K

Freeboard heat transfer coefficient = $(1/3)U$, cals/sec·cm^2°K

Bed to wall heat transfer coefficient = 0.0021, cals/sec·cm^2°K

Solids mixing parameter, $f_w = 0.075 \sim 0.3$

Fraction of wake solids thrown into the freeboard, $f_{sw} = 0.1 \sim 0.5$

Cooling water temperature = 300°K

Wall heat transfer coefficient in the freeboard = 0.00025 cals/sec

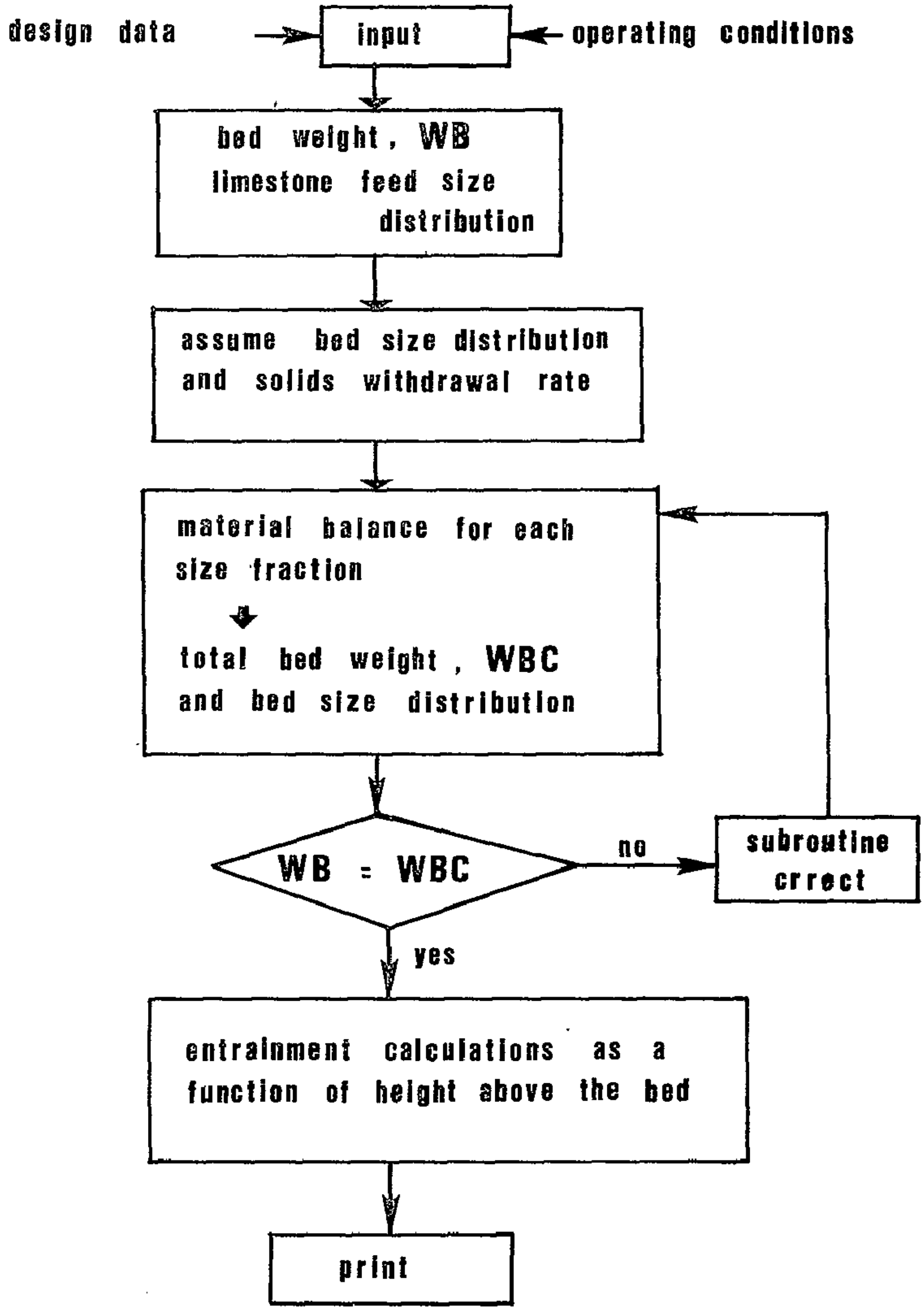


Fig.7 Logic Diagram for the Computation of Limestone Entrainment

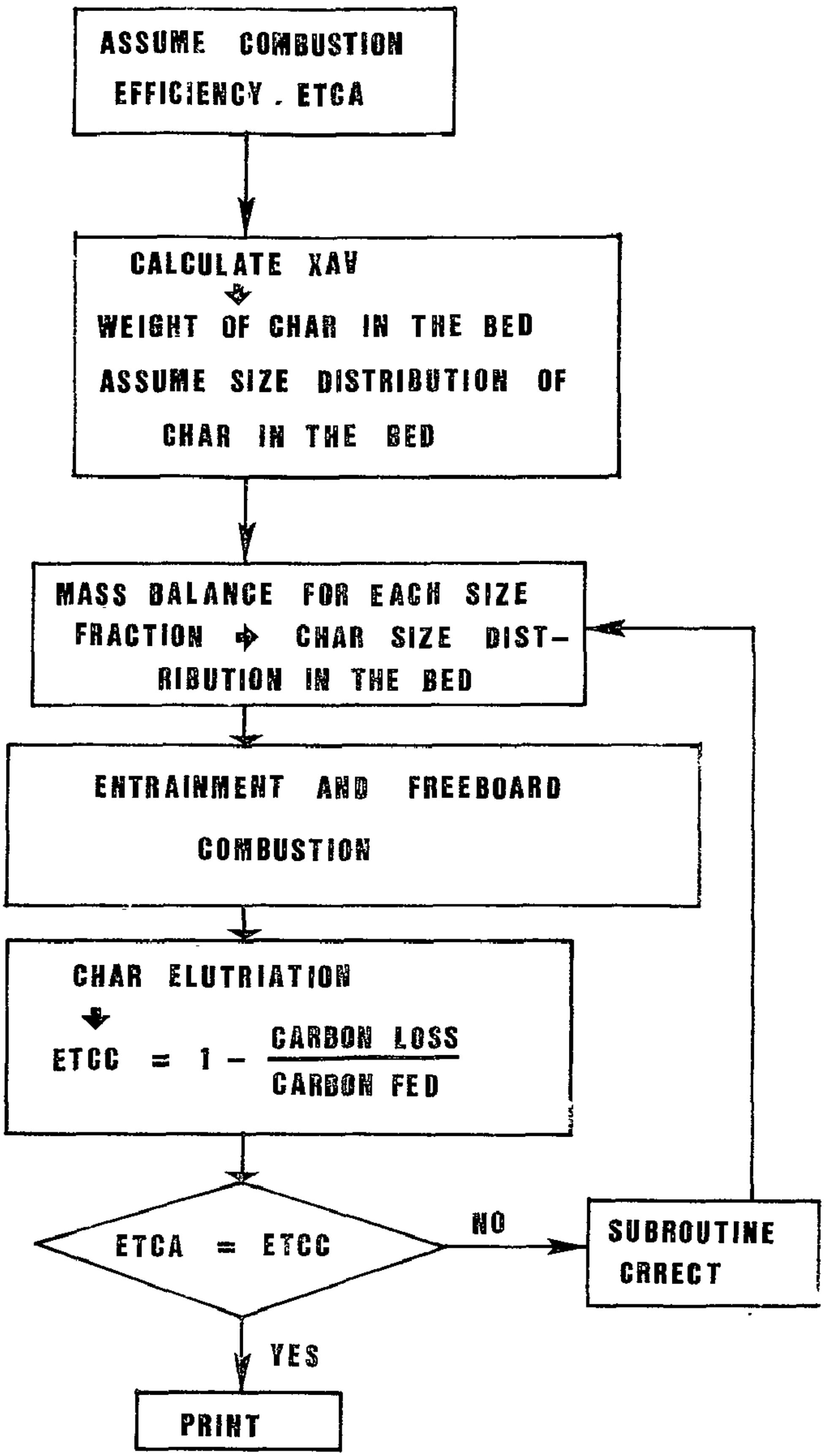


Fig.8 Logic Diagram for the Computation of Char Entrainment

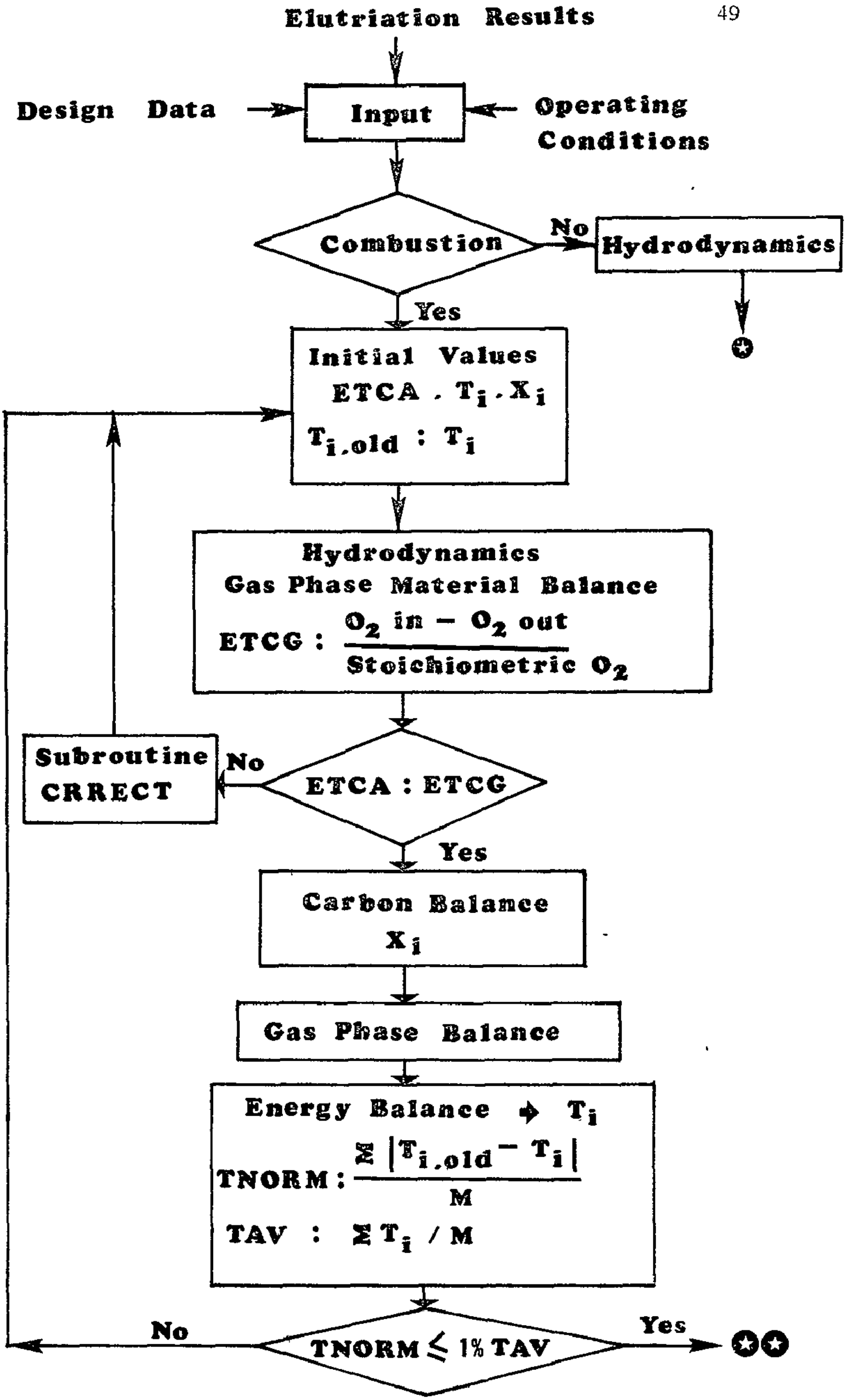


Fig.9 Logic Diagram for Combustion Calculations

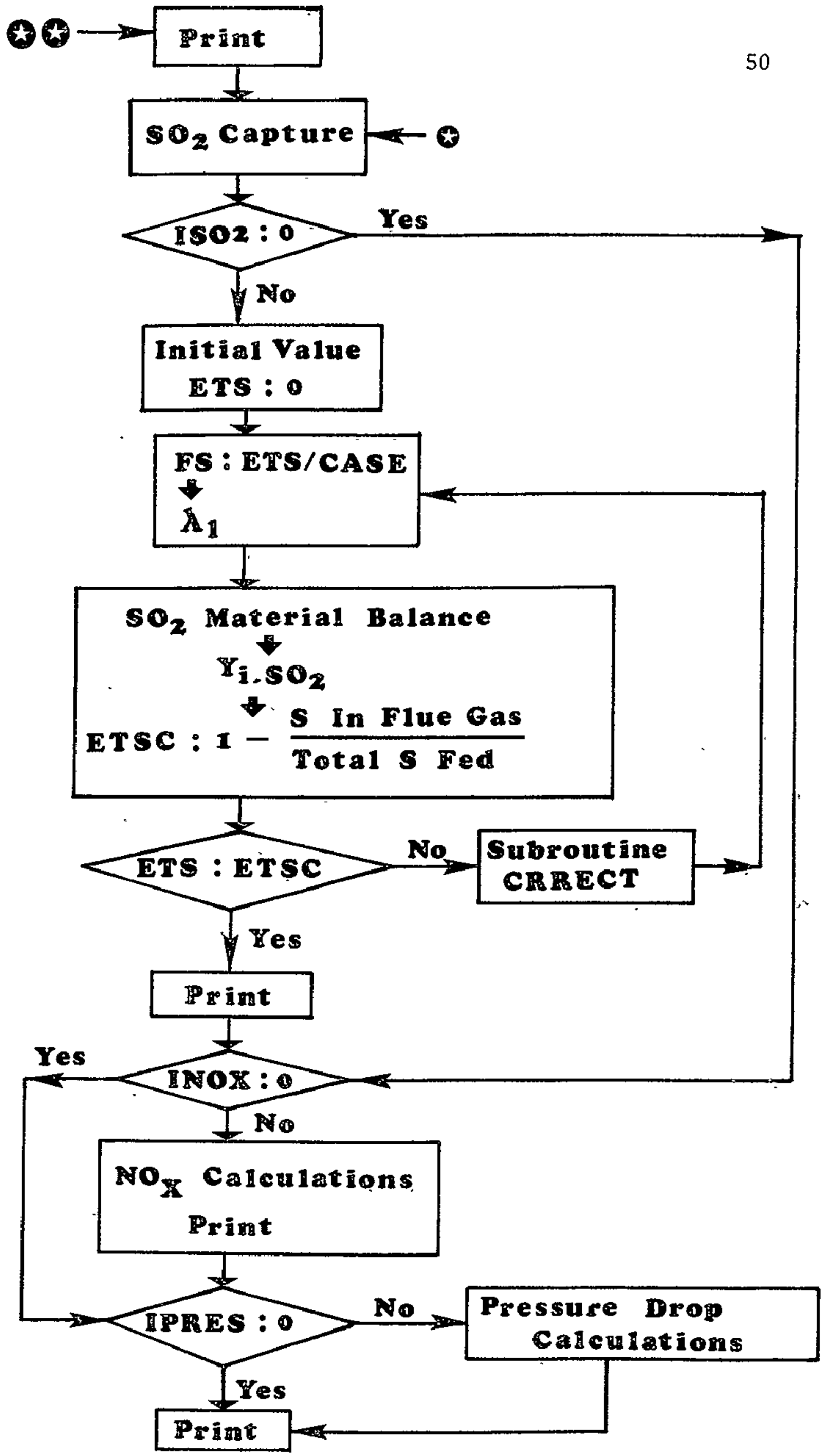


Fig.9 (Continued).

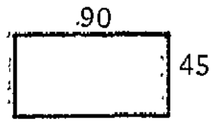
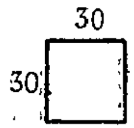
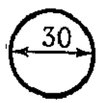
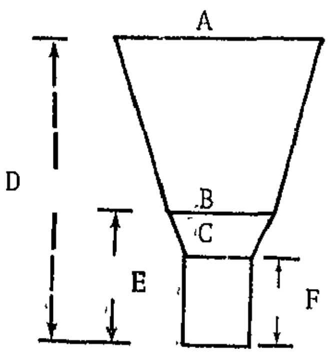
VII. RESULTS AND DISCUSSION

The validity of the proposed fluidized bed combustor model is tested under a set of operating conditions based on the experimental data reported by the National Coal Board, England (1971), Gibbs and his associates in Sheffield (1975), the Exxon Research and Engineering Company, U.S.A. (1976) and NASA Lewis Research Center, Cleveland, Ohio (1978). Table 4 gives the dimensions of the various beds simulated and the configuration of heat-exchange coils used.

Fig. 10 shows the size distributions of the particles in the bed and in the elutriated material for a given feed size distribution of particles under the set of operating conditions specified in the figure. The solid lines in Fig.10 representing the results of the model simulation indicate close agreement with experimental data. The fine particles in the feed are entrained by the gas stream leaving the bed, and hence the bed particle size is larger than that of the feed particles. The fine particles are splashed into the freeboard by the bursting bubbles at the bed surface. Bigger particles return to the bed while the smaller ones are completely elutriated.

Fig.11 shows the results of the simulation on axial bed temperature profiles for two different configurations of cooling tubes in the bed. The difference in the profiles is due to the solids mixing pattern in the bed. When horizontal tubes having closer horizontal pitch distance between the tubes are used, solids mixing is considerably hindered, resulting in steeper temperature profile in the bed. The solids mixing is promoted significantly by the action of bubbles lifting the solids in the wake while ascending. If internals are closely packed in the

TABLE 4. DIMENSIONS OF FBC EXAMINED

Type	Bed Cross-section (sizes in cms)	Specific surface area cm^2/cm^3 bed	Tube Outside Diameter cms	Vertical Pitch cms	Horizontal Pitch cms	Tube configuration
NCB		0.15	5.4	9.9	11.4	Horizontal - staggered
Gibbs, et al. (1975)		-	1.25	-	-	-
Exxon Mini Plant		0.205	1.9	-	5.5	Horizontal serpentine
		0.149	1.9	-	-	Vertical coils
NASA	 A = 52.8 E = 81.3 B = 29.2 F = 62.7 C = 22.7 D = 260	0.1744	1.25	8.0	2.86	Horizontal In line

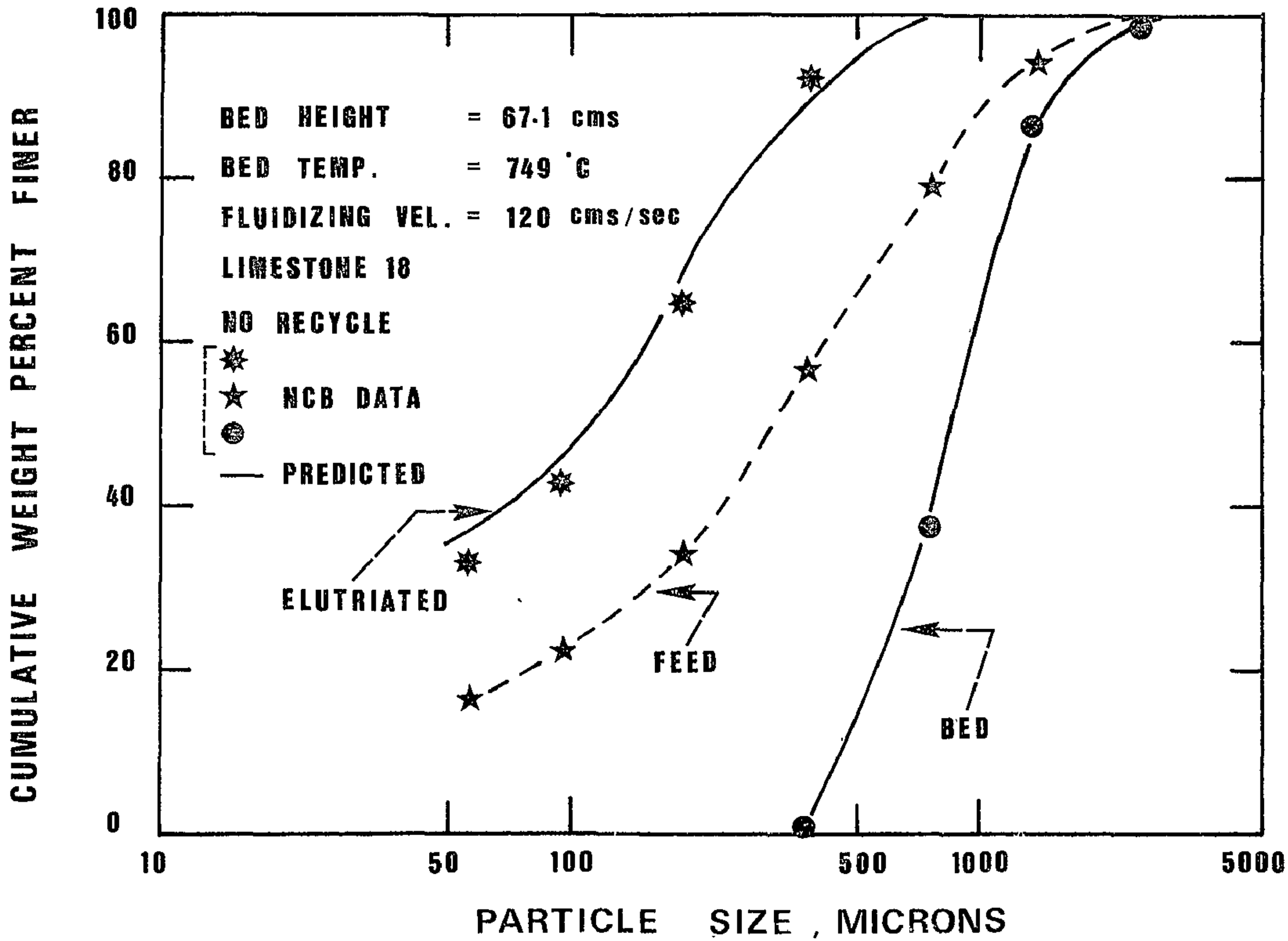


Fig.10 Size Distributions of the Particles in the FBC

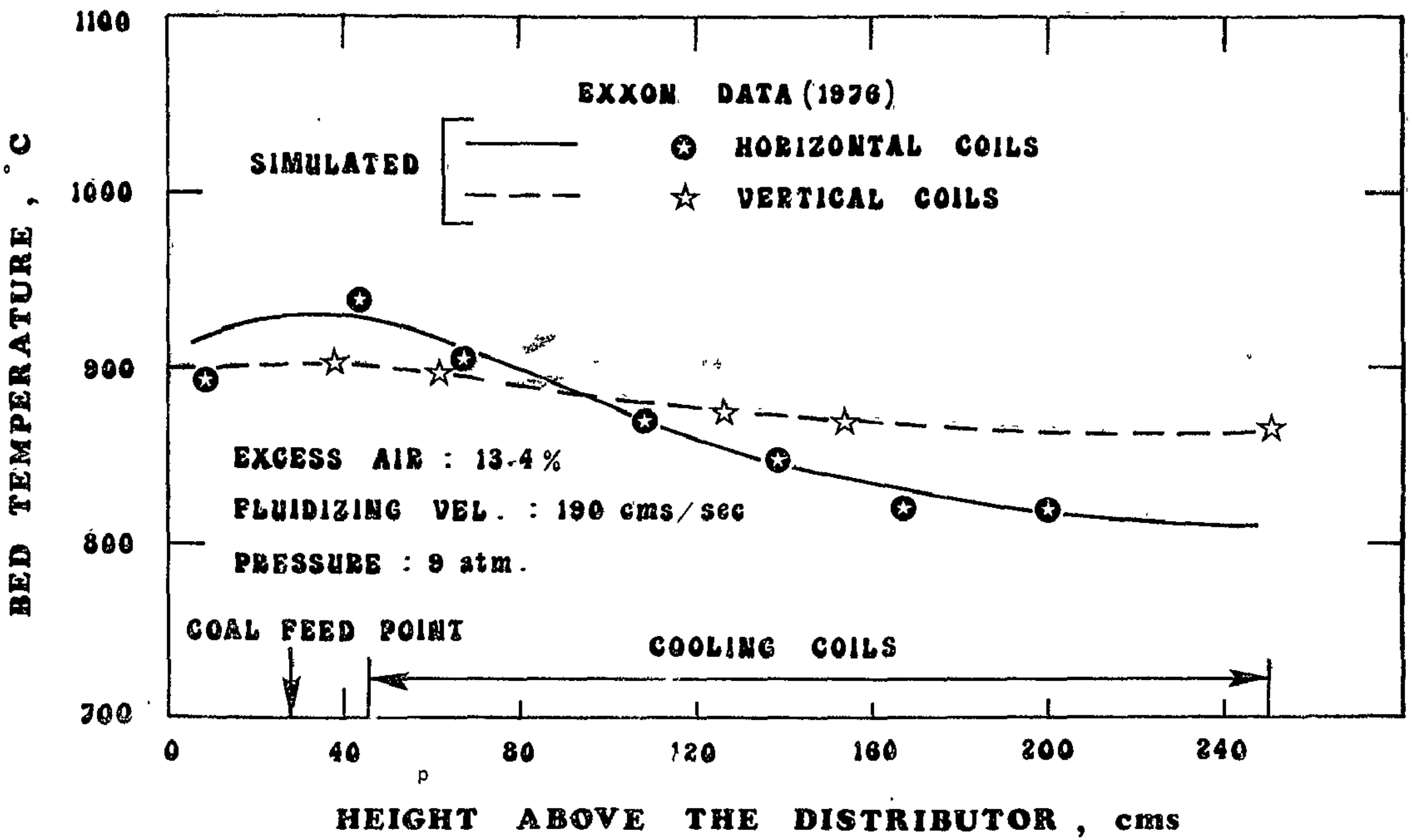


Fig.11 Simulation of Axial Bed Temperature Profile

bed, the free moving, coalescing bubbles are constrained and may be broken as they impinge on the walls of the tubes. Hence the solids movement is retarded which in turn affects the temperature profile. In the model the solids mixing in the bed is represented by the mixing coefficient, f_w. For poor solids mixing f_w takes on low values (0.05-0.2) and for vigorous mixing it takes high values (0.2-0.4). A simulation of the operation of NASA fluid bed combustor is presented in Fig. 12. Again in this combustor, closely packed horizontal tubes are employed for heat removal. As indicated earlier, the solids mixing is poor which is clearly shown by the non-uniform temperature profile and the non-uniform carbon concentration profile in the bed. Carbon concentration peaks at the coal feed point and decreases rapidly within the bed as combustion proceeds. Because of the higher concentration of carbon and oxygen near the coal feed point near the distributor, the combustion rate and the heat release rate are higher than the remaining part of the bed. This results in a high temperature zone near the coal feed point. On the other hand, in the freeboard region, though combustion takes place, due to the heat losses through the wall, the temperature drops.

The concentration profiles of oxygen in the bubble and emulsion phases together with the volatiles concentration in the bed are shown in Fig. 13. Experimental observations reported by Gibbs, et al. (1975) on the time averaged oxygen concentrations along the bed height are also shown. Time averaged concentration is neither the bubble phase nor the emulsion phase concentrations since they are obtained from gas analyzer probes. The peaks and valleys of the analyzer response which

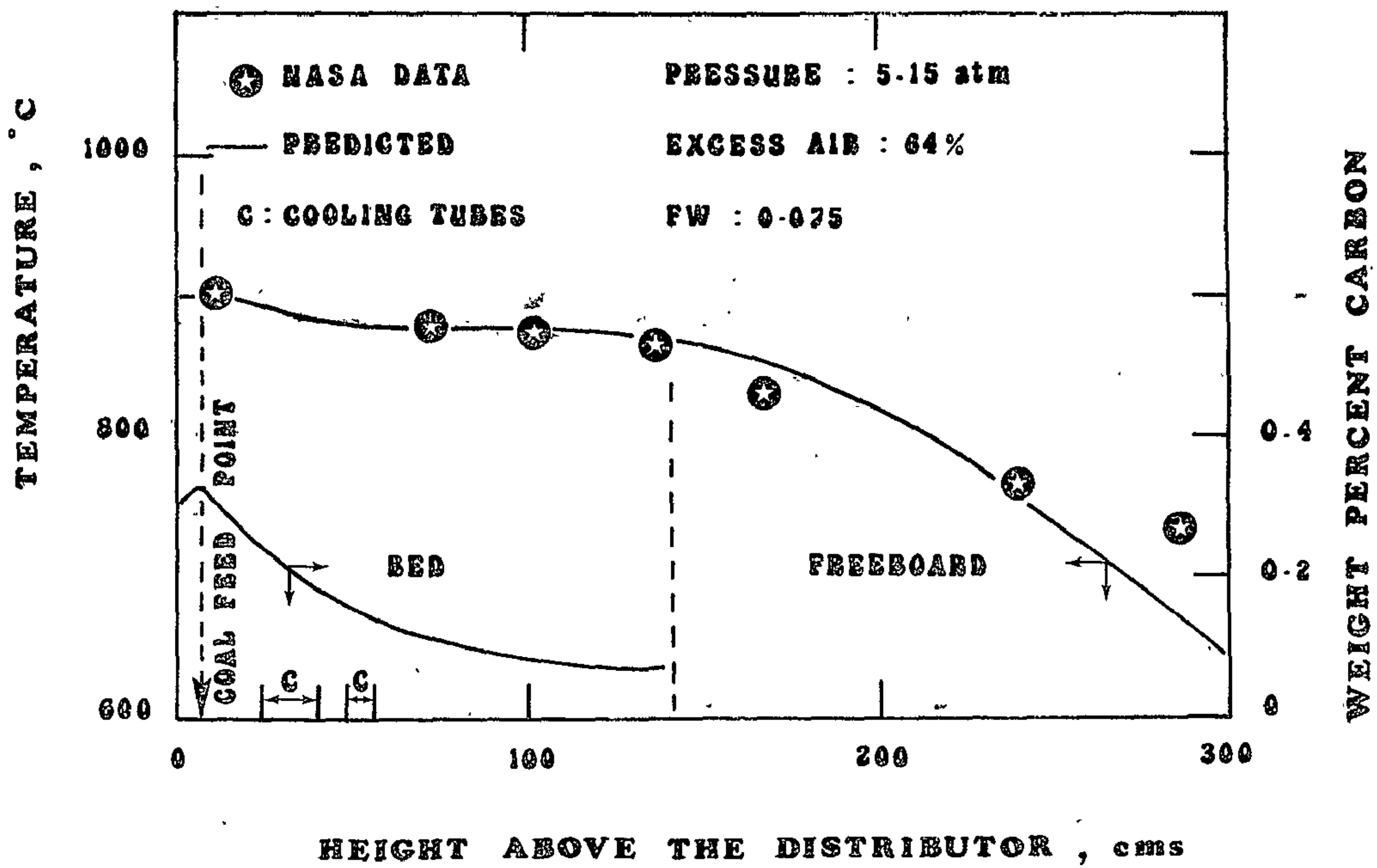


Fig.12 Temperature and Carbon Concentration Profiles in the Bed

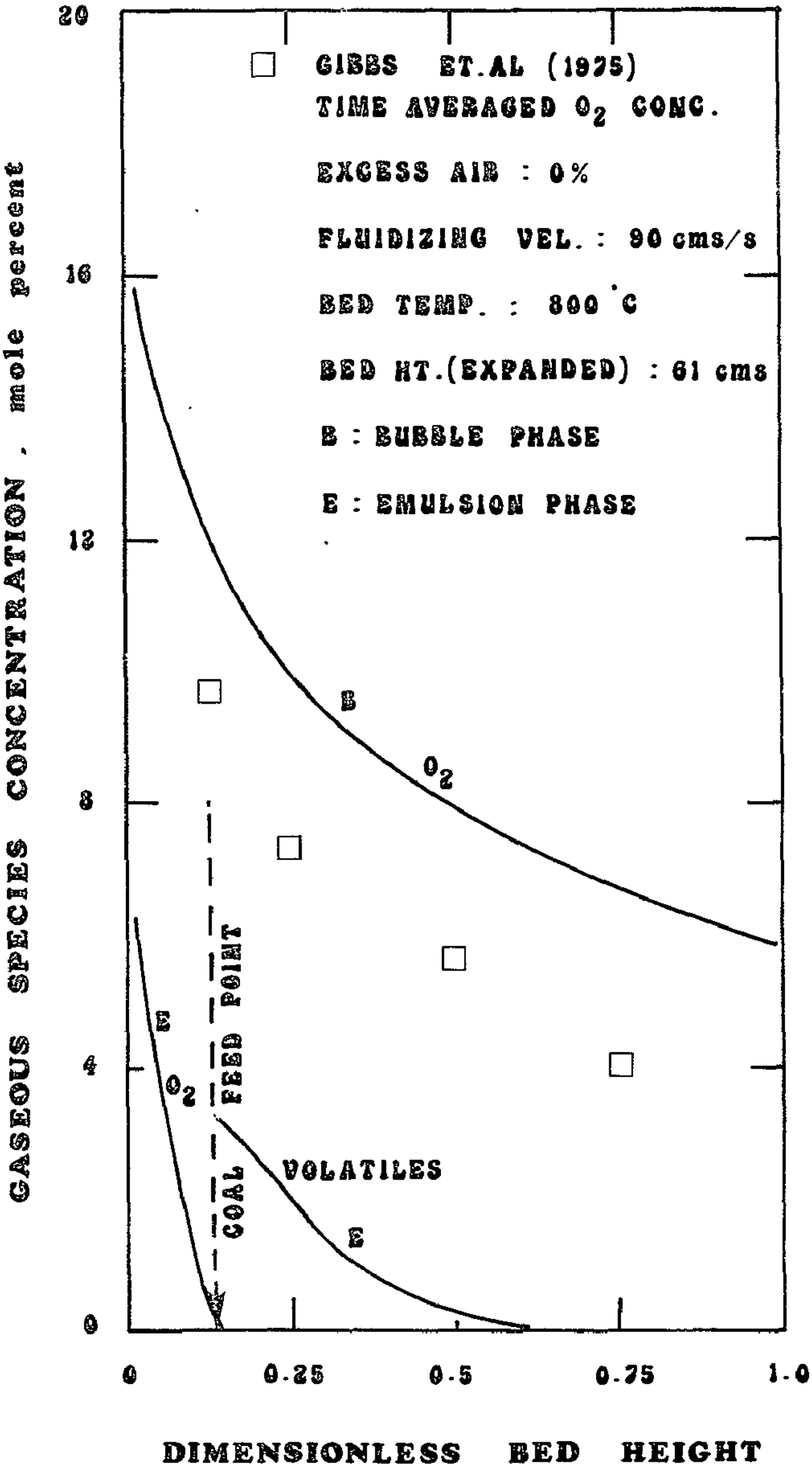


Fig.13 Oxygen Concentration Profile in the Bed

correspond to that of bubble and emulsion phase oxygen concentrations respectively are averaged to obtain the concentration profile.

Near the coal feed point, a large portion of the volatiles is released in the emulsion phase due to the rapid devolatilization of coal. These volatiles immediately burn consuming the available oxygen in the emulsion phase. The oxygen concentration in the emulsion phase is quickly reduced to zero. The volatiles in the emulsion phase are exchanged with the gas in the bubble phase where they are burnt completely. The excess volatiles move up to top compartments while they are burnt on the way. Thus, the oxygen concentration decreases gradually in the bubble phase along the bed height.

Fig. 14 shows the concentration profiles of CO_2, CO and volatiles in the bubble and emulsion phases. The concentrations of CO and volatile products in the bubble phase are zero since complete combustion of these gases is assumed in this phase. The experimental data shown are the time averaged concentrations of CO_2 and CO in the bed. Near the coal feed point, the volatiles released in the emulsion phase burn to form carbon monoxide, the concentration of which increases along the combustor height. As long as volatiles are present in the emulsion phase the combustion of char and CO does not take place. whereas the C-CO_2 reaction takes place. Hence the CO_2 concentration in the emulsion phase along the bed height decreases until all the volatiles are burnt. Once CO and char combustion start, CO_2 concentration increases in the emulsion phase. On the other hand, CO_2 concentration in the bubble phase increases gradually as a function of the bed height indicative of the progressive combustion of char and volatiles in the bubble phase.

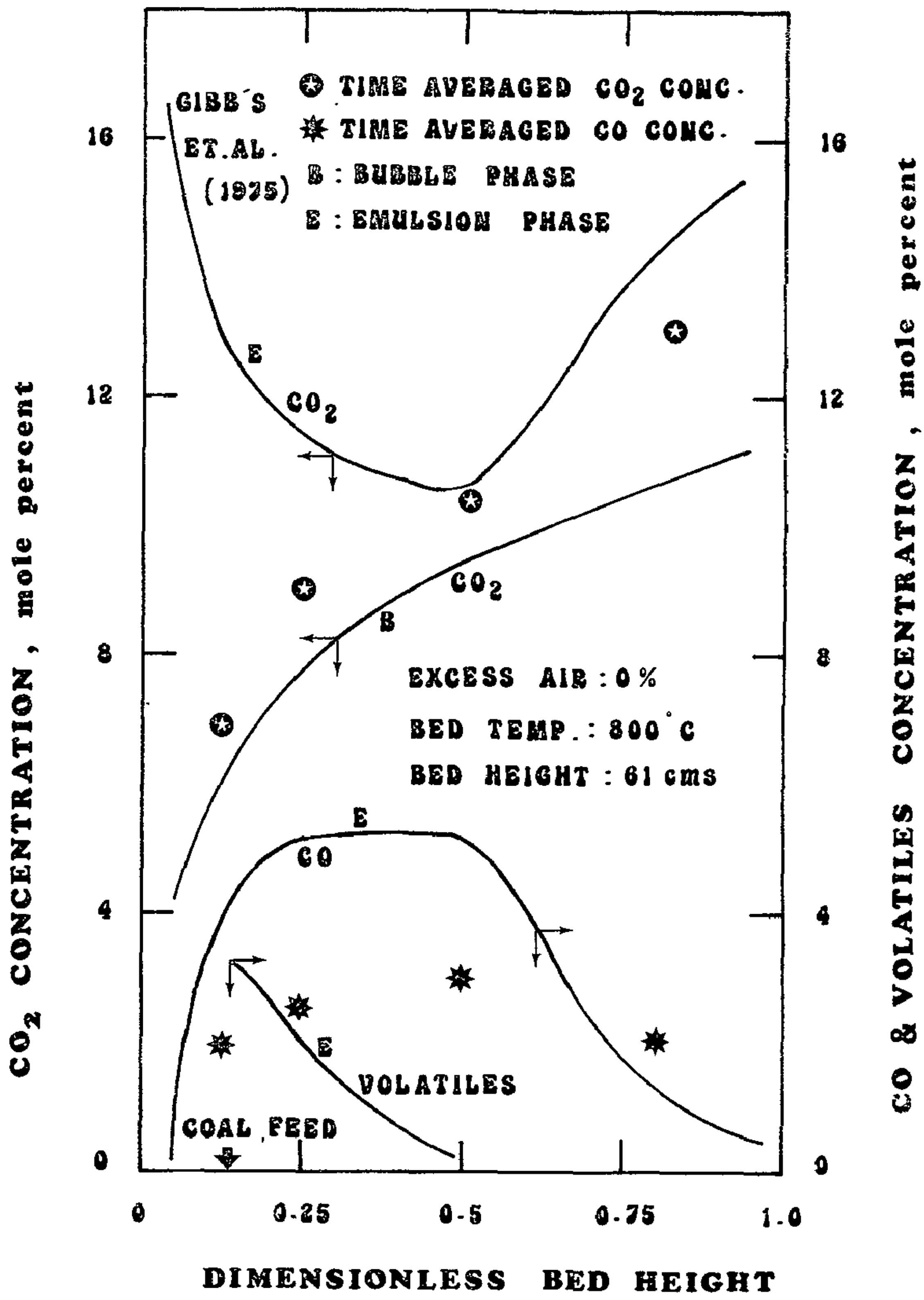


Fig.14 CO, CO_2 & Volatiles Concentration Profiles in the Bed

In regard to the absorption of SO_2 by the limestone present in fluidized bed combustors, the percentage absorption increases with an increase in the Ca/S ratio. Ca/S ratio is the most significant operating variable determing the reduction of SO_2 in the flue gas. Stoichiometrically, one mole of calcium is needed to capture one mole of sulfur. But experimental evidences indicate that even with a Ca/S ratio of 3, sulfur capture is not complete. This is due to the fact that as SO_2 reacts with fresh calcined limestone, an impervious layer of $CaSO_4$ is formed surrounding the particle and thereby rendering the particle ineffective in capturing SO_2 further. At Ca/S ratio of 1.2, SO_2 capture efficiency is about 60 percent (Fig. 15). SO_2 retention efficiency improves to 93 percent when Ca/S ratio is increased to 3.3. The experimental data and the calculated result from the proposed model are shown in the figure demonstrating good agreement between the two. The current EPA regulation on SO_2 emission (1.2 lbs. SO_2 per million Btu burnt) corresponds to a SO_2 retention efficiency of around 72 percent for 2.75 percent sulfur coal (Pittsburgh coal). From Fig. 15, a minimum Ca/S ratio of around 1.8 is needed based on the model calculation to meet the EPA requirements for the set of operating conditions specified in the figure.

The effect of operating temperature on SO_2 retention is shown in Fig. 16. An optimum temperature range of 800 to 850°C can be observed in which the SO_2 retention efficiency is maximum. At lower temperatures the rate of SO_2 capture is low, resulting in a lower sulfur retention efficiency. At higher temperatures, plugging of the pores occurs due to rapid formation of $CaSO_4$ around the outer shell

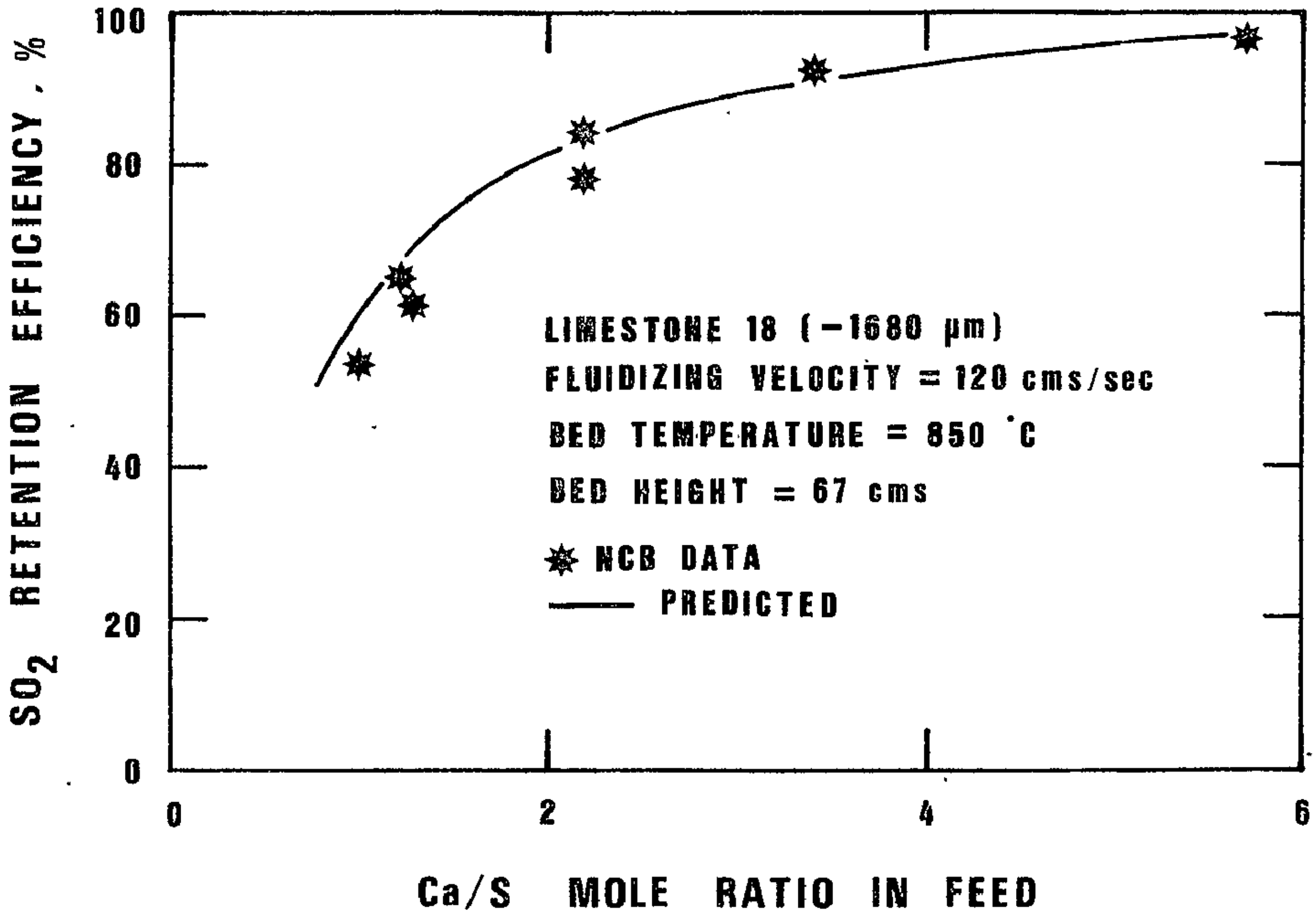


Fig.15 Effect of Ca/S Ratio on SO_2 Retention

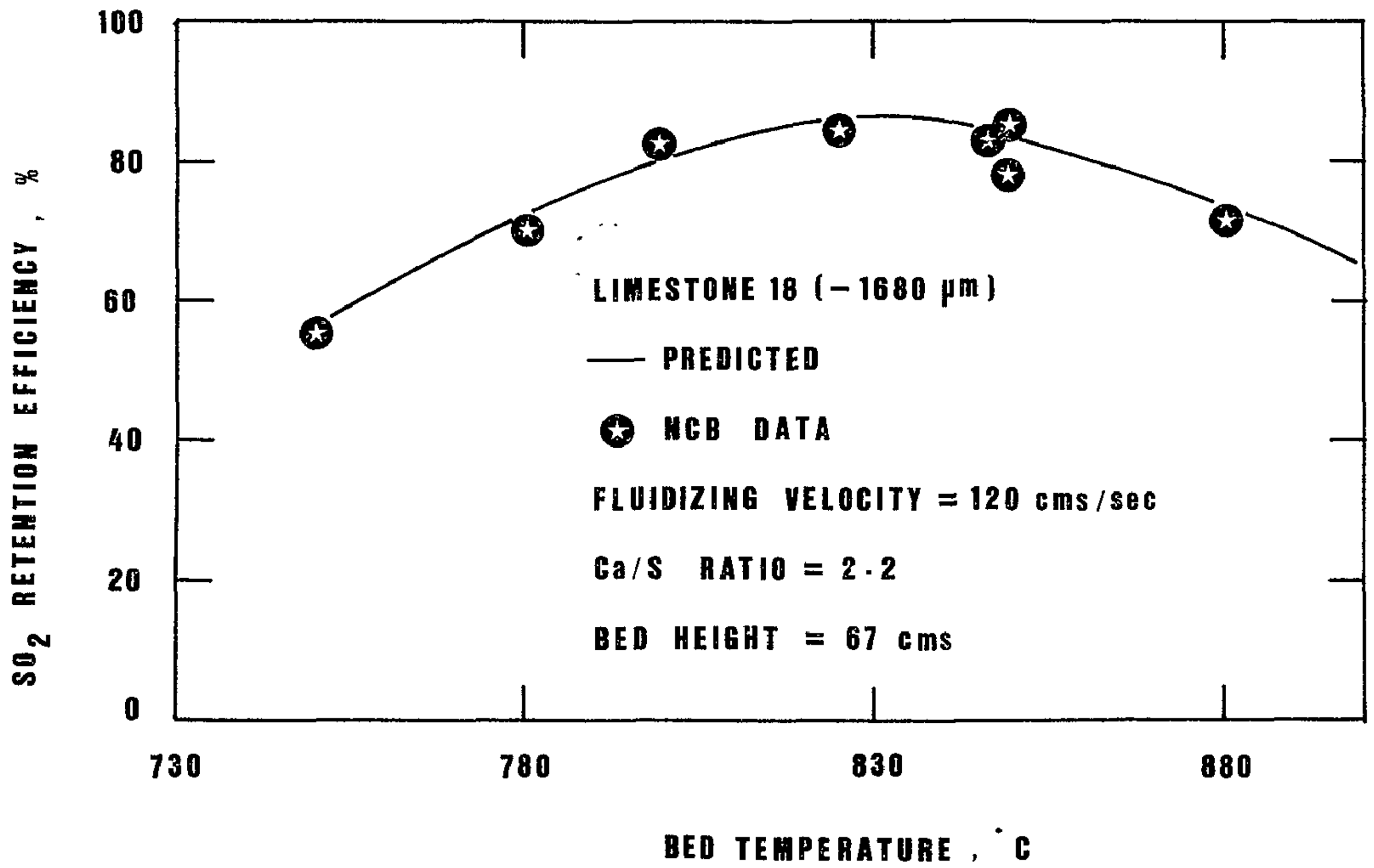


Fig.16 Effect of Temperature on SO_2 Retention

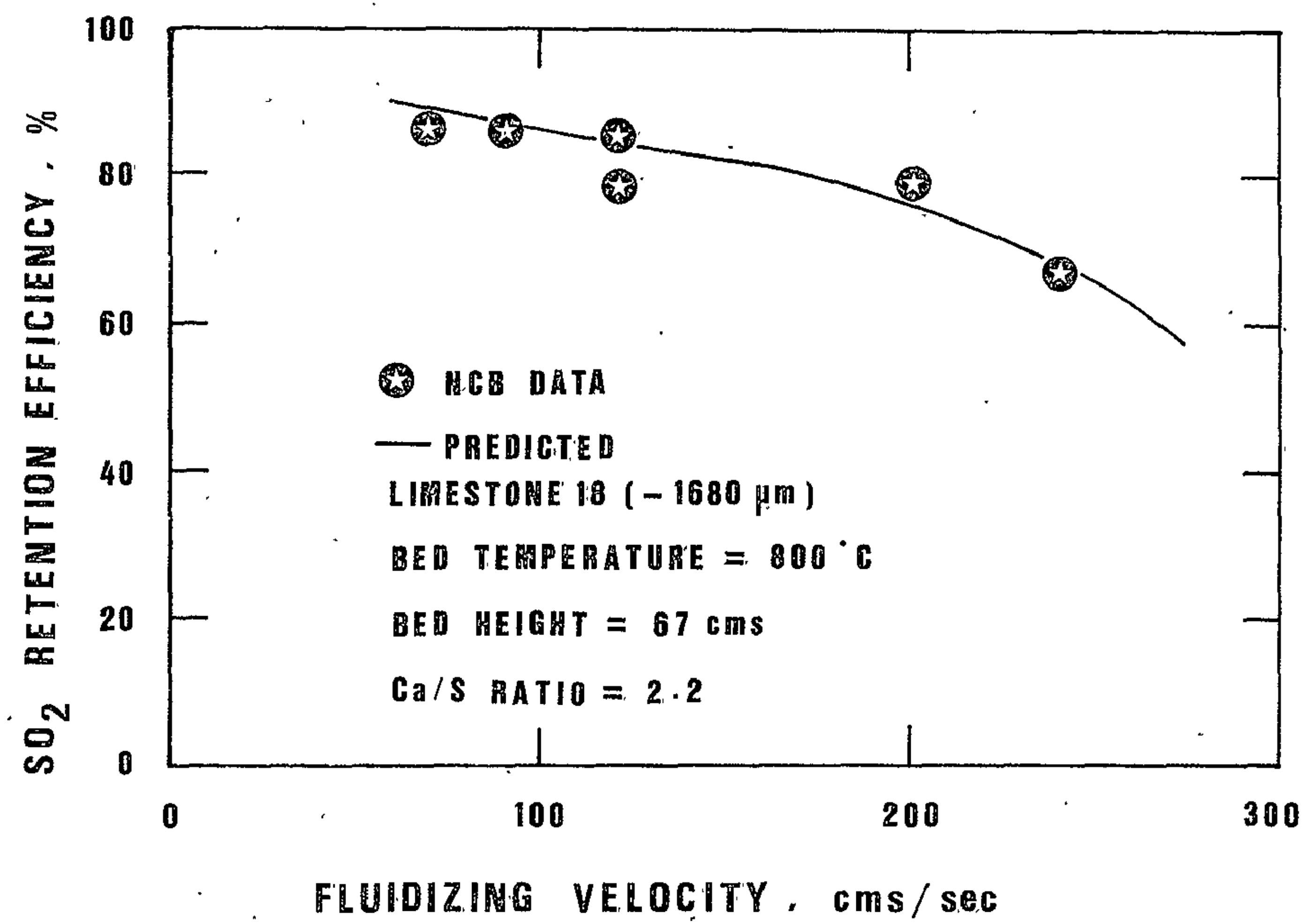


Fig.17 Effect of Fluidizing Velocity on SO_2 Retention

and reduces the effective specific surface area of the limestone particles resulting in a lower SO_2 retention efficiency. The agreement between the model predictions and the experimental data is satisfactory.

Fig. 17 shows the effect of fluidizing velocity on sulfur retention efficiency. At low velocities, elutriation is small and hence the average bed particle size is small. This implies a greater reactivity of the limestone particles. Also, the gas and solids residence times are increased. Hence a higher SO_2 retention efficiency is obtained. But, at higher fluidizing velocities, entrainment is large, and the particles entrained are also larger. Bed particle sizes are consequently larger resulting in lower reactivities. At higher superficial velocities, residence time is also short. A combination of these effects results in a lower sulfur dioxide retention efficiency. Fig. 18 shows the SO_2 concentration profiles obtained from simulation of the NASA combustor. Near the coal feed point, because of the combustion of volatiles, a large proportion of SO_2 is released into the emulsion phase. A high concentration of SO_2 is seen at this location. SO_2 is then absorbed by the calcined limestone particles in the bed and its concentration in the emulsion phase decreases as a function of height above the distributor. The gases leaving the bed surface come in contact with the fine limestone particles entrained into the freeboard, and sulfur capture is appreciable in the freeboard region. Also, in the case of NASA combustor, since the cross sectional area of the freeboard region increases as a function of bed height, the gas and solids residence time in the freeboard increases; hence the SO_2 retention is high and its concentration in the freeboard is low.

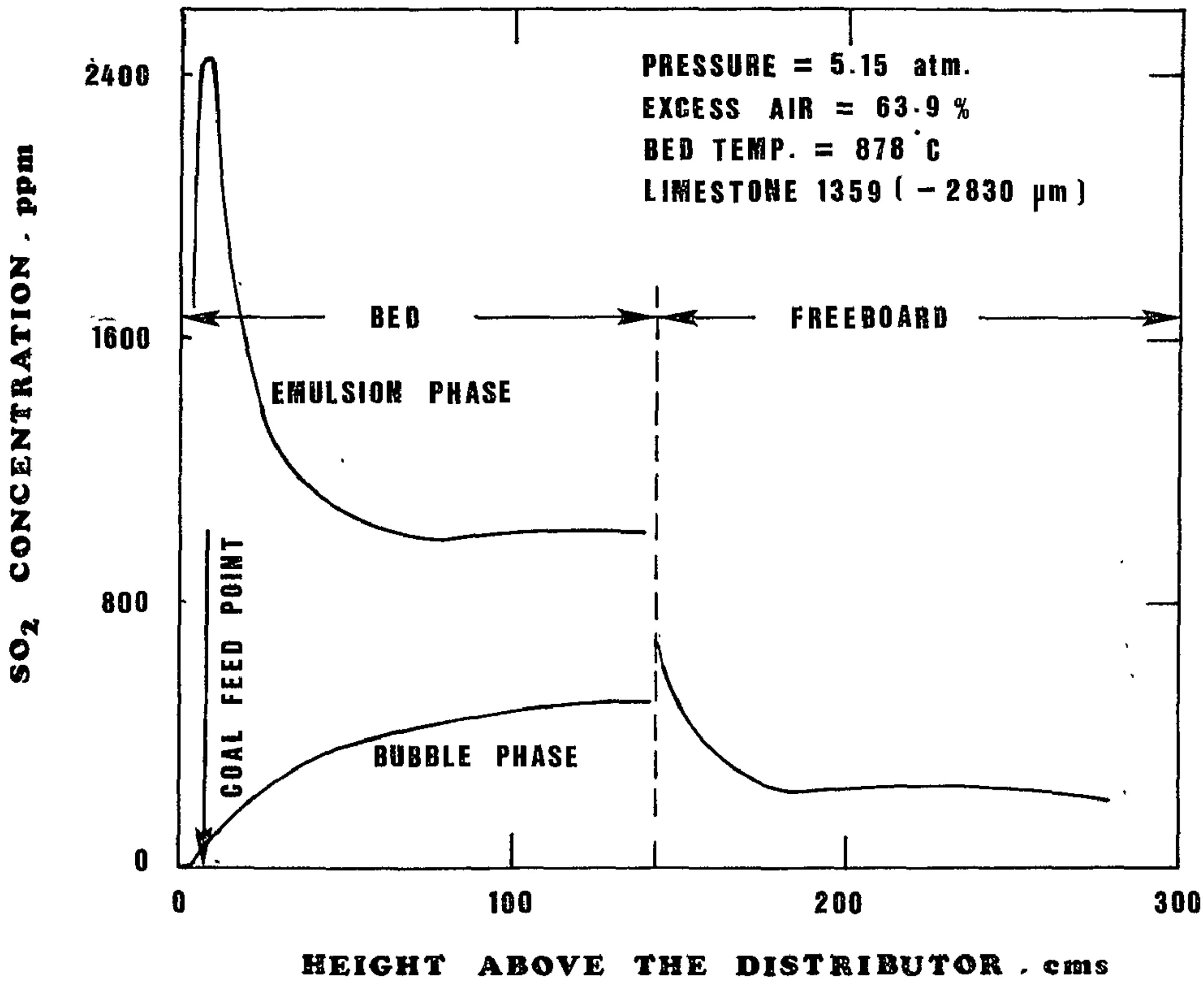


Fig.18 SO_2 Concentration Profile in the Combustor

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The effect of bed temperature on NO emission is shown in Fig. 19. The average carbon concentration in the bed which is closely related to NO reduction is also shown in the figure. NO concentration at the exit in the flue gas increases with the bed temperature while the average carbon concentration in the bed decreases. At low temperatures, NO formed is reduced by the large amount of char in the bed. At higher temperatures, the NO emission increases since the char content is low affecting the NO-char reaction rate. At temperatures above 825°C, the NO emission plateaus off. This is due to the fact that while the NO reduction rate by char above this temperature becomes fast, the char content of the bed is significantly lowered. EPA regulation limits the NO emission to 0.7 lbs per million Btu of heat released. This limit corresponds to a NO concentration of about 970 ppm in the exit gas under the conditions specified in the figure. Hence it is clearly demonstrated that fluidized bed coal combustors can meet the current EPA NO_x emission standard.

Fig. 20 is an example of the NO concentration profiles in the bubble and emulsion phases. Data points are the time averaged NO concentrations obtained experimentally (Gibbs, et al, 1975) near the wall and at the center of the bed. The NO concentration near the wall is higher than that at the center of the bed. The probability of a probe sampling the bubble is higher at the center and the emulsion near the wall since the proportion of the bubbles is small near the walls. These results indicate that NO is preferentially formed in the emulsion phase due to the release and subsequent combustion of volatiles in the emulsion phase.

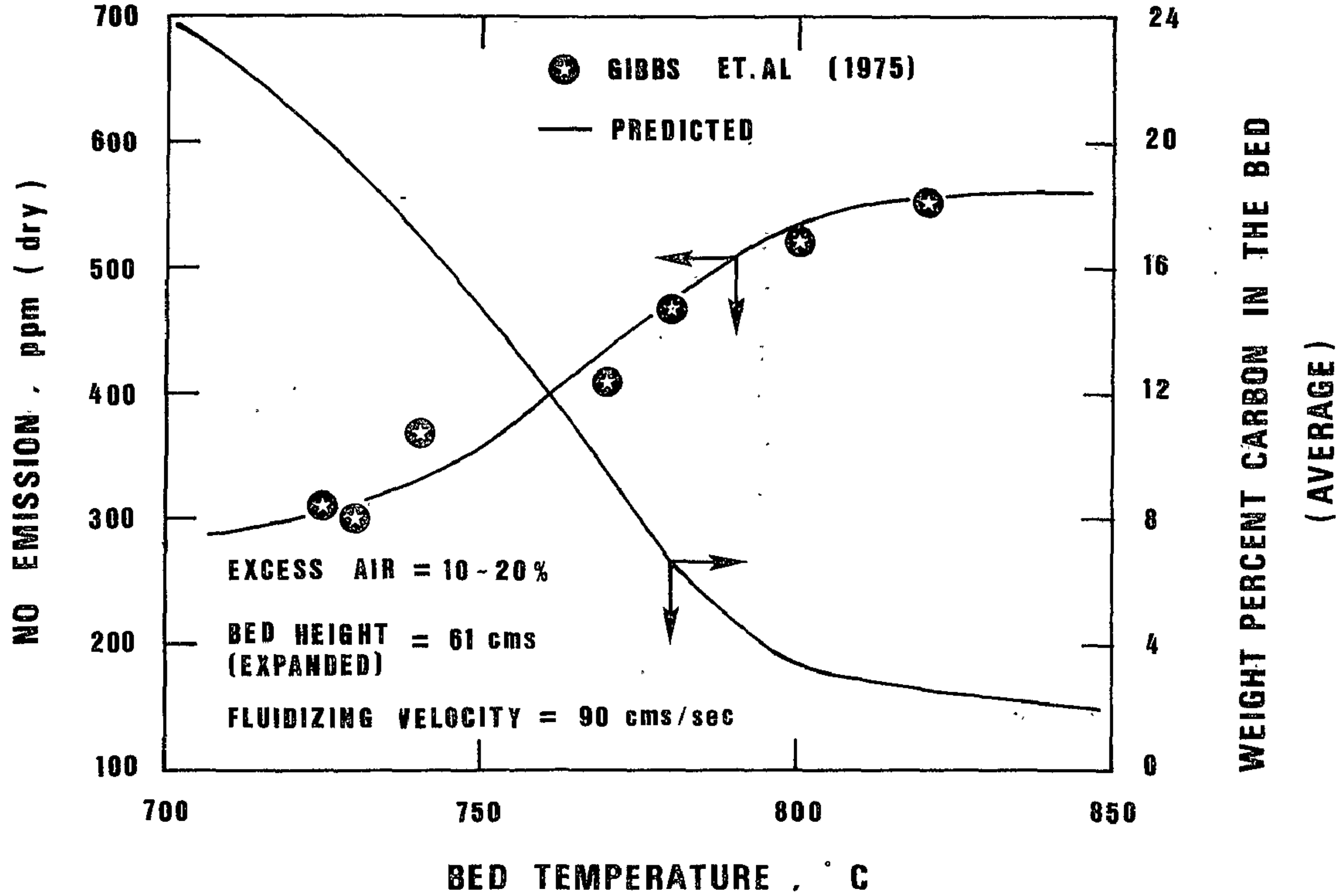

Fig. 19 Effect of Temperature on NO Emission

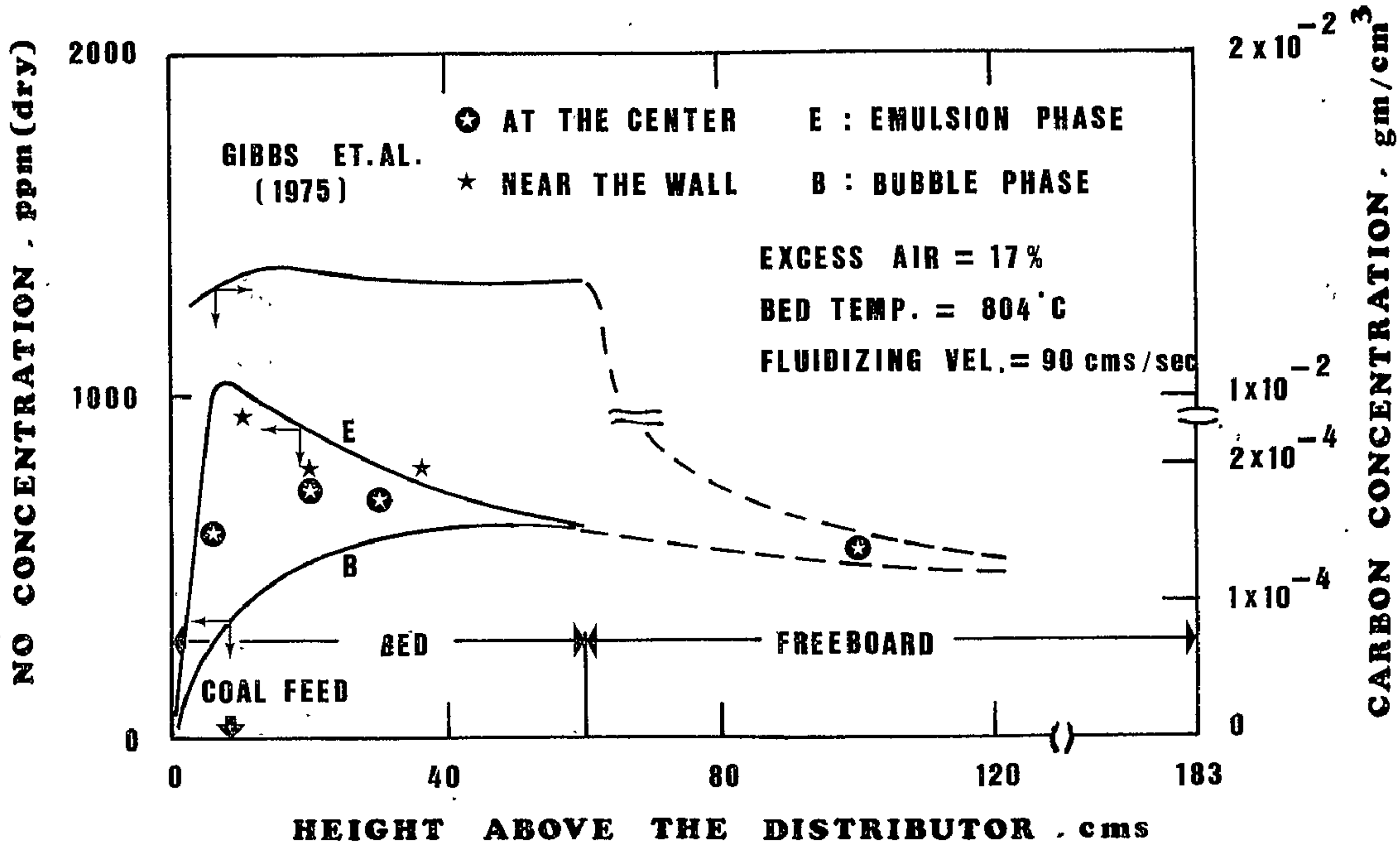

Fig.20 NO and Carbon Concentration Profiles in the Bed

Higher concentrations of NO in the emulsion phase near the coal feed point are the results of rapid evolution and combustion of volatiles from coal in this region. The NO concentration in the bubble phase increases because of char and volatiles combustion. Fig. 20 also indicates the NO concentrations in the freeboard. In the freeboard both char combustion and NO reduction take place. When the char burns NO is released from the nitrogen contained in the char. These two competing reactions determine the total NO emission at the outlet of the combustor.

VIII. SENSITIVITY OF THE MODEL PARAMETERS

The most important parameters in the model are the solids mixing parameter f_w, the fraction of wake solids thrown into the freeboard f_{sw}, and the bed to tube heat transfer coefficient U. The effects of these parameters on the temperature profile in the bed are shown in Fig. 21, 22 and 23. For this parametric study, the bed dimensions and cooling location coils are similar to the NASA fluid bed combustor (Table 4). In future when more accurate correlations are developed these new correlations should be used for estimation of these parameters in the model. Fig. 21 shows the effect of f_w on the temperature profile in the bed. Low values of f_w represent poor solids mixing. When solids mixing is poor, most of the volatiles are released near the coal feed point. Combustion of these volatiles causes a rise in the temperature of the bed in the neighborhood of the solids feed point. As f_w increases, solids mixing becomes more vigorous, and heat liberated by the combustion of volatiles near the feed point is immediately dissipated by the rapidly mixing solids. Because of improved mixing, the bed temperature profile becomes uniform.

The extent of freeboard reactions depends on the solids hold up in the freeboard. Solids hold-up in turn depends on the amount of solids thrown up into the freeboard by the bursting bubbles at the bed surface. The rate of entrainment of solids from the bed surface, F_0, may be given by (Yates and Rowe, 1977).

$$F_0 = A_t(U_o - U_{mf}) f_w (1 - \varepsilon_{mf}) \rho_s \quad f_{sw} \quad \text{gm/sec} \qquad \text{(VIII.1)}$$

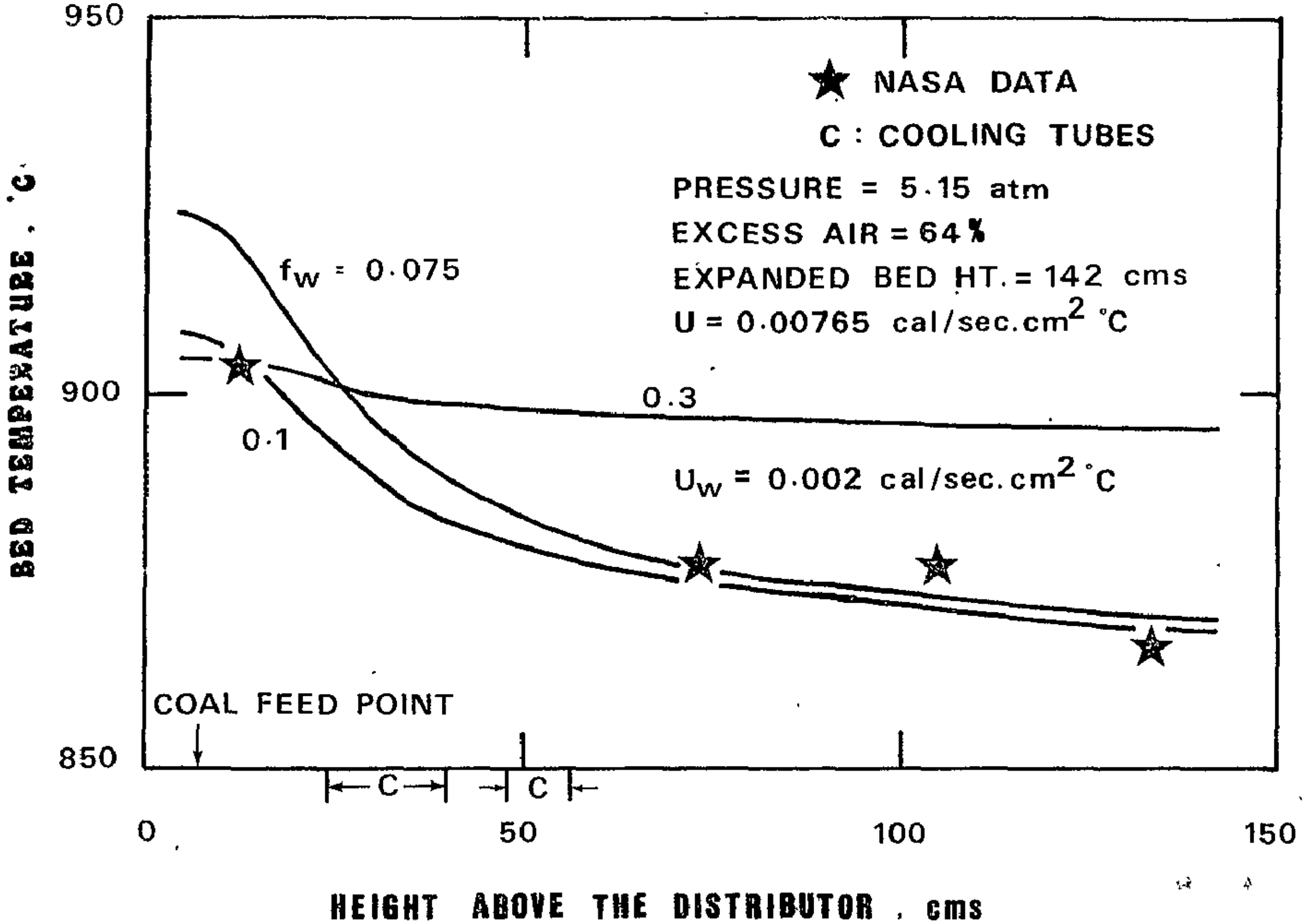

Fig. 21 Effect of Solids Mixing on the Bed Temperature Profile

for a set of operating conditions, increasing the value of f_{sw} increases the solids splashing rate at the bed surface. If a large portion of char leaves the bed, char elutriation from the combustor will also be large. This will result in lower combustion efficiency, and hence a lower temperature in the bed. The temperature drop in the freeboard decreases as f_{sw} increases because of increased combustion in the freeboard. This is clearly illustrated in the Fig. 22. It should be borne in mind that the NASA fluidized bed combustor is a small unit and heat losses from the wall in the freeboard are considerable. If the bed is bigger in size than that is used here for simulation, the heat losses through the walls will be minimal. Also, with good insulation, heat losses can be reduced. In large commercial combustors, if the entrainment is increased, combustion of char in the freeboard will also increase resulting in higher temperatures in the freeboard. Hence it is seen that the parameter f_{sw} is very critical and has to be carefully evaluated in order to properly account for the freeboard reactions.

Fig. 23 is a parametric study of the effect of bed to tube heat transfer coefficient on the temperature profile in the bed. Changes in the value of the heat transfer coefficient do not significantly affect the shape of the temperature profile but affect the level of bed temperature. As can be seen from Fig. 23, if the actual heat transfer coefficient were 0.00765 cals/sec.cm^2,°C (56 Btu/hr.ft^2.°F), assuming a lower heat transfer coefficient of 0.0063 cals/sec.cm^2,°C (46 Btu/hr.ft^2,°F) would result in a temperature difference of about 40°C above the actual temperature. So it is apparent that an accurate

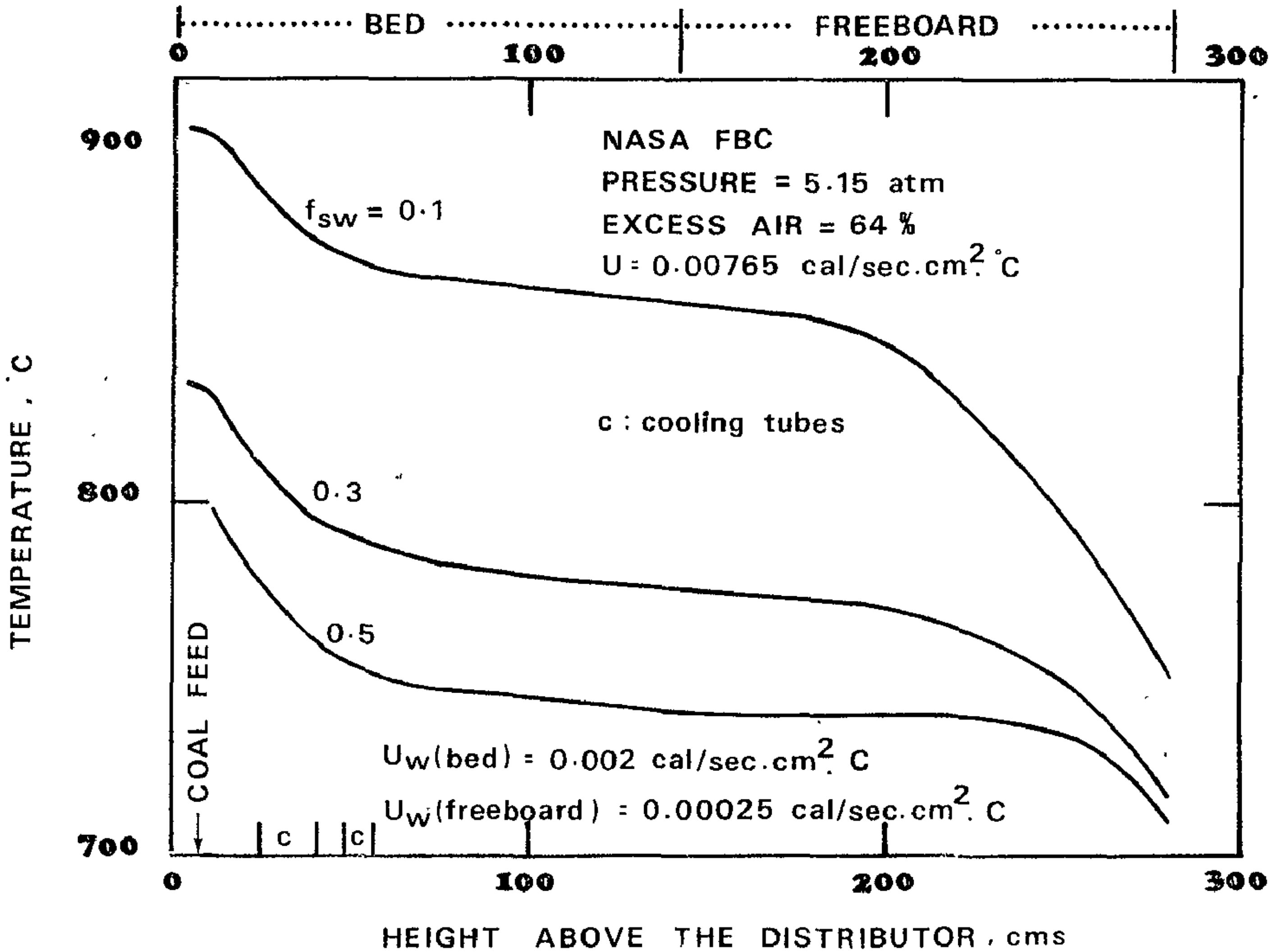

Fig. 22 Effect of Solids Entrainment on the Temperature Profile

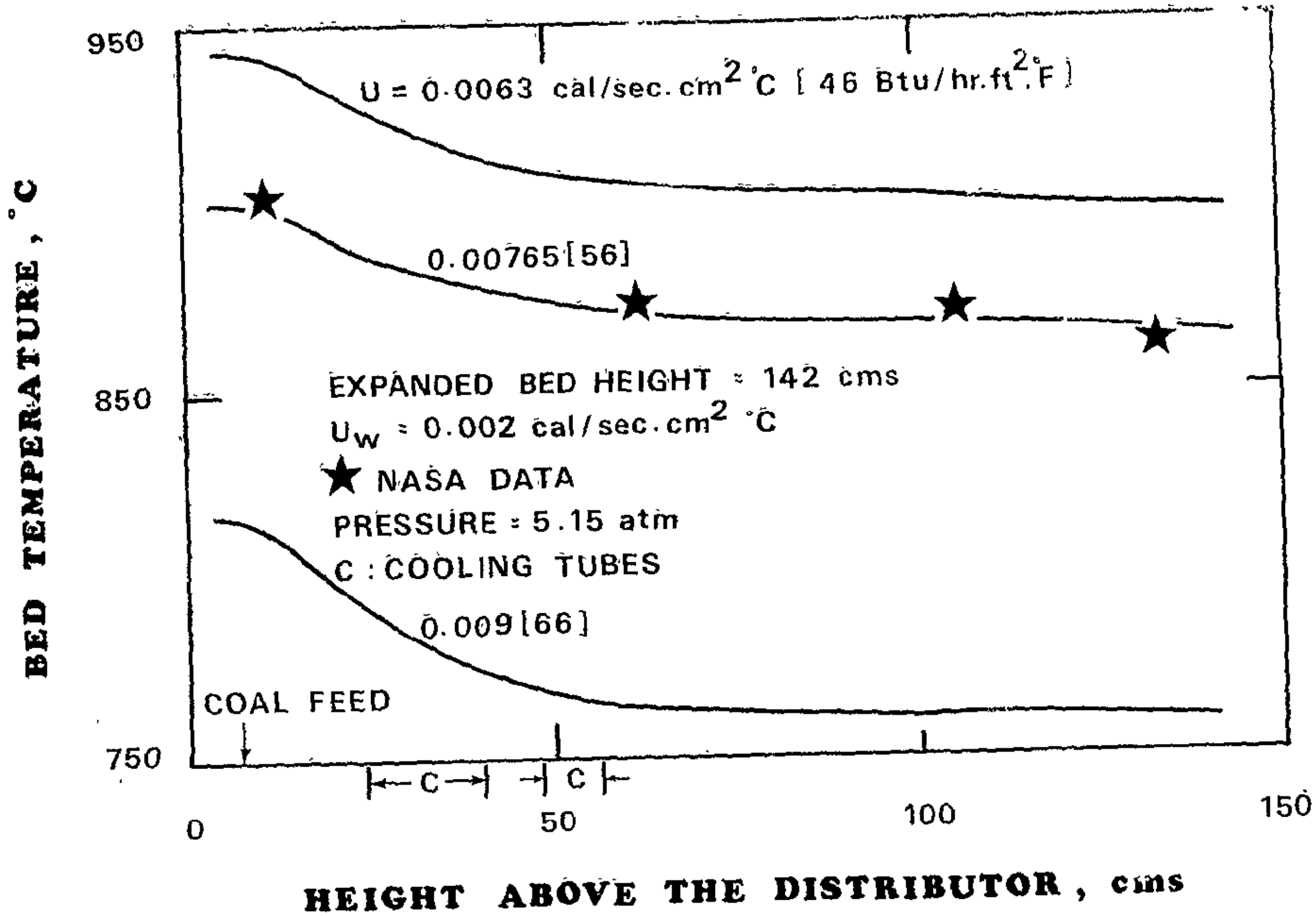

Fig. 23 Effect of Bed to Tube Heat Transfer Coefficient on the Bed Temperature

estimation of the heat transfer coefficient for a wide range of design is critical to make accurate predictions of bed temperatures.

Fig. 24 brings out the effect of bubble size (or the compartment size, since bubble size is same as compartment size) on the bed temperature profile. When a single bubble diameter is used as an adjustable parameter, a small value for the bubble diameter overestimates the combustion rate in the bed. This is because of increased mass transfer of oxygen to the emulsion phase from the bubble phase. This results in steep temperature profiles. As the bubble diameter is increased, the profile becomes less steep and also the average temperature decreases because of less combustion in the bed. Fig. 24 also indicates the predictions from the present work compared with experimental data. Clearly it is seen that bubble size cannot be assumed as an arbitrary parameter, and the coalescence of bubbles has to be incorporated in any realistic FBC model. The effect of the location of cooling tubes on the bed temperature profile is shown in Fig. 25 by moving the heat exchange zone. In this calculation, the other variables are kept constant. It appears that by properly adjusting the location of the cooling coils, the bed temperature can be maintained uniform.

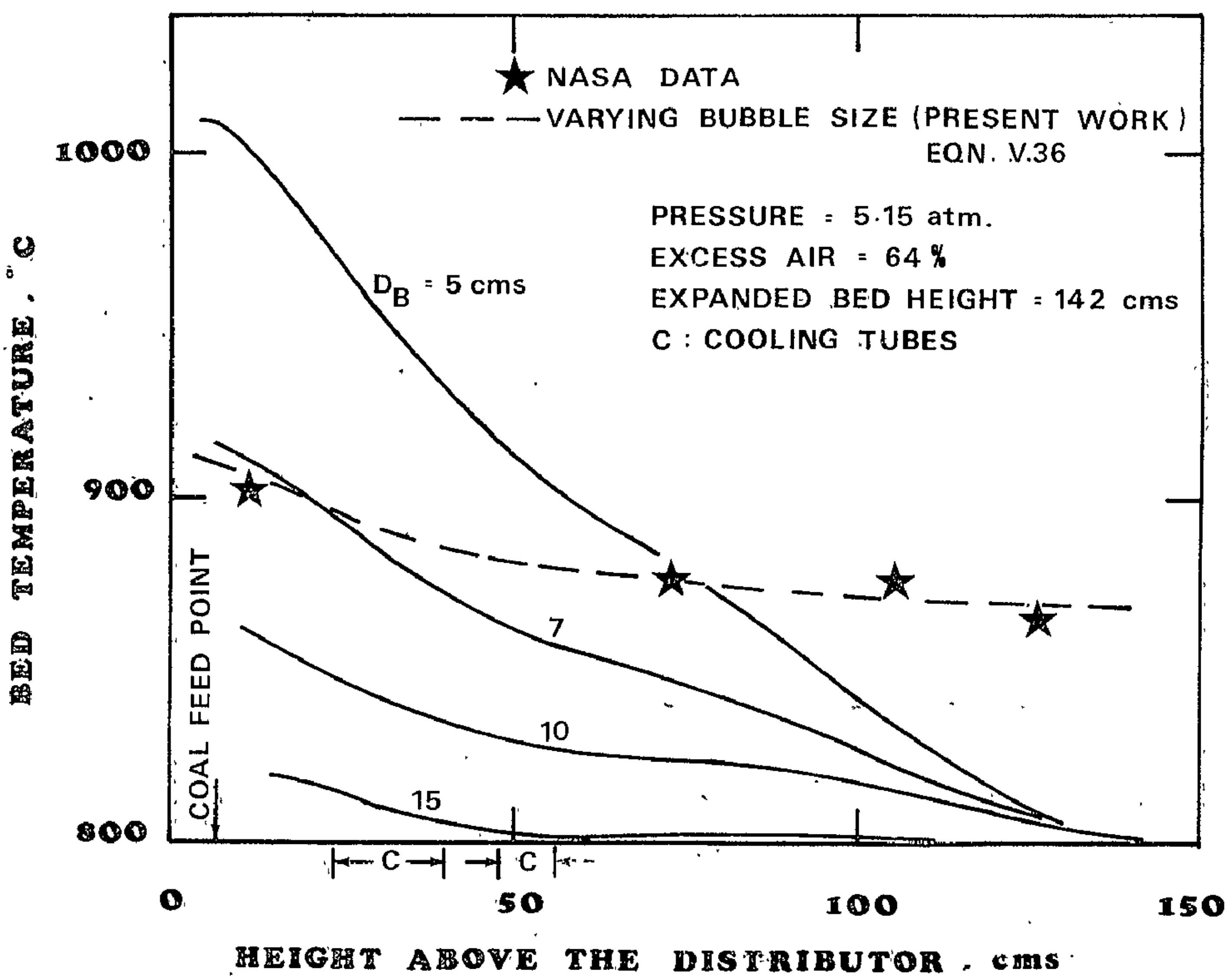

Fig. 24 Effect of Bubble Size (≡ Compartment Size) on the Bed Temperature Profile

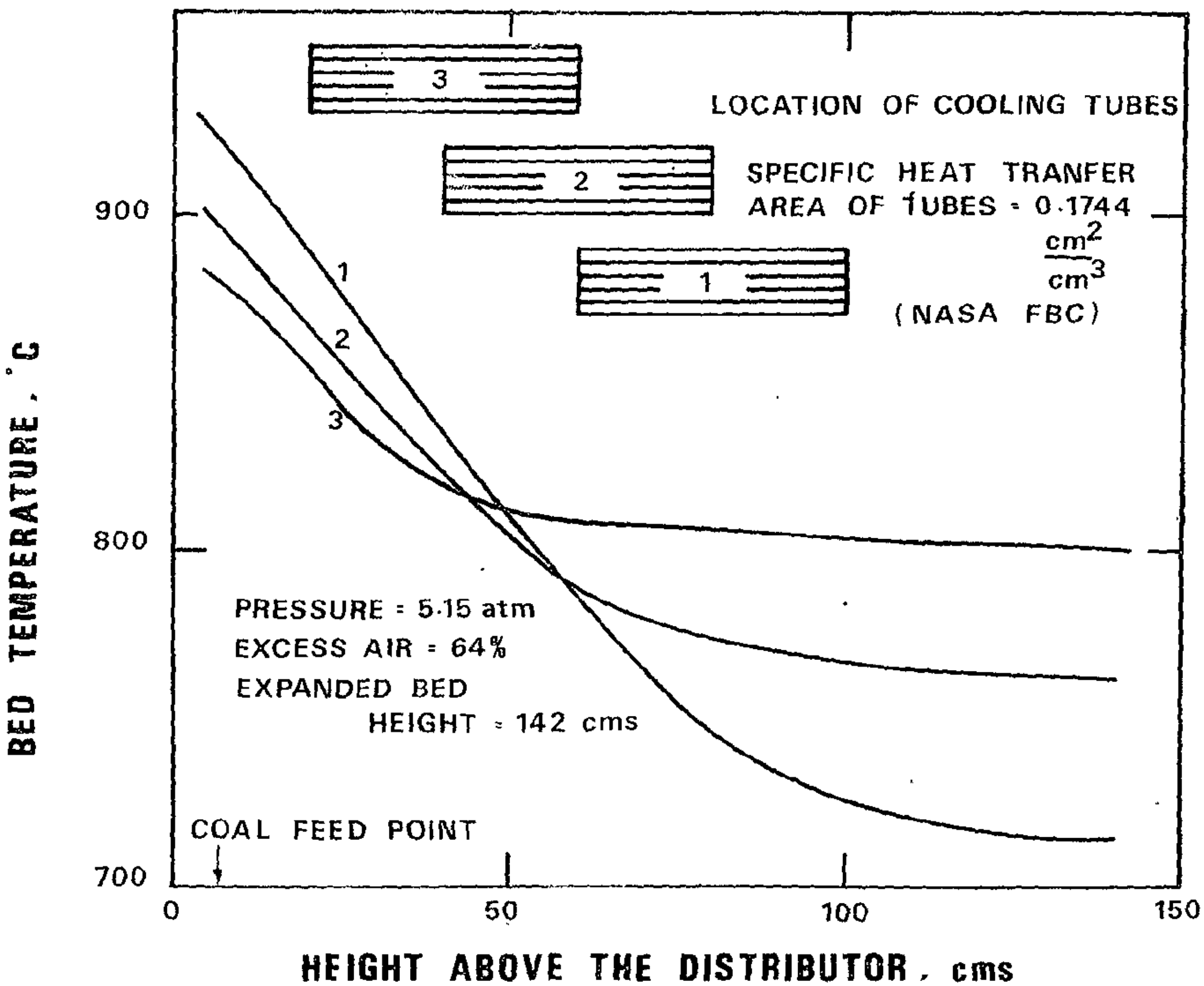

Fig. 25 Effect of Location of Cooling Tubes on the Bed Temperature Profile

IX. CONCLUSIONS

The following conclusions can be drawn from this study:

1. The agreement between the simulated results and the experimental data attest to the validity of the proposed model for the fluid bed coal combustion and of the assumptions made.

2. The elutriation phenomenon is taken into consideration in the model. The results of simulation on elutriation agree well with the experimental data.

3. The model confirms the importance of the role of solids mixing in maintaining a uniform bed temperature. Poor solids mixing results in nonuniform temperature profile and carbon concentration profile in the bed. The poor mixing is accounted for by f_w, the solids mixing parameter in the model. This important parameter in the model also accounts for the devolatilization of coal. The assumption of a major portion of the volatiles being released near the feed point is justified by the concentrations of NO, O_2 and CO observed experimentally near the coal feed point.

4. Although a simple approach is taken to calculate the bubble size through internals (and the results seem reasonable), a proper bubble size correlation in the presence of cooling tubes with different configurations needs to be developed. Bubble size cannot be assumed as an adjustable parameter, and bubble coalescence has to be considered.

5. Attention has to be focused on the evaluation of the solids mixing parameter f_w, the fraction of wake solids thrown into the freeboard f_{sw}, and the bed to tube heat transfer coefficients. A parametric study of these variables indicates the necessity of accurate estimation for properly accounting for solids mixing,

freeboard reactions and bed temperature profile.

6. Although the validity of the two phase theory has been questioned for very large particles (> 2000 μm) and very small particles (< 50 μm), the predicted results indicate that the proposed two phase model can effectively simulate the performance of the FBC.

7. The concentration profiles of O_2, CO, CO_2 and volatiles computed based on the model are in accordance with the experimental observations.

8. NO (nitrogen oxide) emission is shown to be dependent on the operating temperature. NO emission can be maintained below the EPA limits by maintaining a higher concentration of carbon in the bed and in the freeboard. NO concentrations in the bed indicate that most of the NO is formed in the vicinity of the coal feed point.

9. In operation of a FBC a balance has to be made between the combustion efficiency, the carbon loss, higher SO_2 retention and lower NO emission. Based on the analysis, the approximate optima are found to be (i) for the temperature range between 800 to 850°C, (ii) for the velocity between 90 to 100 cms/sec, (iii) for the particle sizes below 3000 μm, and for the excess air between 10 to 25%.

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APPENDIX I

ELUTRIATION PROGRAM

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C***********************************************************************
C                A GENERAL MODEL FOR FBC ELUTRIATION CALCULATIONS      *
C                                                                      *
C                             PROGRAMMED BY                            *
C                                                                      *
C                             RENGA RAJAN                              *
C                                                                      *
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C                             WEST VIRGINIA UNIVERSITY                 *
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      REAL MC,MH2,MS,MO2,MN2,MNO,MH2O,MSO2,MH2S,MCO,MCO2,MCAO,MGAS,MVGAS
     1,MAIR,NCHAR,MCASO4
      COMMON /A/ ZHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZB(30),
     1ATB(30),UMF(30),DVB(30),DVBEFF(30),UTA(30),UTC(30),
     2EMF,RG,G,PI,HLMF,HLF,PAV,TAV,FMO,RHOCH,RHOBED,DZAV,VMF,XAV,ETCC,
     3DPSVB,DPWMB,DCSVB,DCWMB,U0,MGAS,MTB
      COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),FRA(30),
     1WF(30),Q1(30),Q2(30),BB(30),RKI(30),W(30),E(30),ENTA(30),ELUA(30),
     2ENTC(30,30),FRAEN(30),FRAEL(30),CU(30),
     3PFA(30),GFLOW,WCOAL,WAD,WB,WBC,WELUA,CELU,EFF,XC,XCF,
     4XA,XW,RCHAR,CCHAR,WDIS,RHOAD,TDHC,HFB,NDP
      NAMELIST /OPCF/ HLMF,VMF,HLF,WB,WBC,RHOBED,RHOCH,RCHAR,
     1CCHAR,HCHAR,OCHAR,NCHAR,SCHAR,
     2U0,GFLOW,MGAS,FMO,FMF,EXAIR,TAV,PAV,CAS,WAD,WCOAL,TDHC,HFB
     1/RES/ WDIS,WELUA,CELU,EFF,DPSVB,DPWMB,DCSVB,DCWMB,
     2DASVF,DAWMF,DCSVF,DCWMF
      DATA MC,MH2,MS,MO2,MN2,MNO,MH2O,MSO2,MH2S,MCO,MCO2,MCAO,MCASO4
     1/12.,2.,32.,32.,28.,30.,18.,64.,34.,28.,44.,56.08,136.14/
      DATA RHOC,RHOASH/1.4,1.4/
      RHOAD = 2.4
      EMF = 0.5
      RG = 82.05
      G  =  980.1
      PI = 3.141593
C
C     FBC DESIGN DATA AND FEED PARTICLE SIZE DISTRIBUTION
C
      CALL DESIGN
      READ(5,1000) NDP,(DIA(I),I=1,NDP)
      READ(5,1001)(FRACTA(I),I=1,NDP)
      READ(5,1001) (FRACTC(I),I=1,NDP)
      DP(1) = DIA(1)
      SUMA = 0.0
      SUMB = 0.0
      SUMC = 0.0
      SUMD = 0.0
                        DO 10 I = 2,NDP
      DP(I) = (DIA(I-1)+DIA(I)) * 0.5
      SUMA = SUMA + FRACTA(I)/DP(I)
      SUMB = SUMB + FRACTA(I)*DP(I)
      SUMC = SUMC + FRACTC(I)/DP(I)
      SUMD = SUMD + FRACTC(I)*DP(I)
10    CONTINUE
      DASVF = 1./SUMA
      DAWMF = SUMB
      DCSVF = 1./SUMC
      DCWMF = SUMD
```

```
C
C     LIMESTONE COMPOSITION
C
      READ(5,1010)NAMEL1,NAMEL2,XCAO,XMGO,XSIO2,XCO2
C
C    COMPOSITION AND NET HEATING VALUE OF COAL
C
C     -----------------------------------------------------------
C     XCF  : FIXED CARBON
C     XCV  : VOLATILE CARBON
C     XH   : HYDROGEN
C     XS   : SULPHUR
C     XO   : OXYGEN
C     XN   : NITROGEN
C     XW   : MOISTURE
C     ----------------  DRY BASIS  ----------------------
C
      READ(5,1010)NAMEC1,NAMEC2,XC,XH,XN,XS,XO,XW,XA,VM
C
C      OPERATING CONDITIONS 1 (BED CONDITION)
C
      READ(5,1001)HLMF,HLF,PAV,TAV
C
C     OPERATING CONDITION 2 (SOLIDS AND GAS FEEDS)
C
      READ(5,1001)WCOAL,WAD,CAS,UO,FMF,EXAIR
C
C     CALCULATION OF VOLATILES YIELD AND THE COMPOSITION OF VOLATILES
C
      WW = 0.2*(100.*VM-10.9)
      R = EXP(26.41-3.961*ALOG((TAV-273.))+0.0115*100.*VM)
      V = (100.*VM - R - WW)*0.01
      V = V*(1.-XW-XA)
      RN = 1.6-0.001*TAV
      IF (RN .GT. 1.) RN = 1.0
      IF (RN .LT. 0.) RN = 0.0
      RS = RN
      RO = 0.0
      RH = 0.0
      CH4 = 0.201-0.469*VM+0.241*VM**2
      H2  = 0.157-0.868*VM+1.338*VM**2
      CO2 = 0.135-0.900*VM+1.906*VM**2
      CO  = 0.423-2.653*VM+4.845*VM**2
      H2O = 0.409-2.389*VM+4.554*VM**2
      TAR = -.325+7.279*VM-12.88*VM**2
      HTAR = XH*(1.-RH)*(1.-XW) - V*(CH4/16.*2.0+H2/2.+H2O/18.)*2.0
      OTAR = XO*(1.-RO) - V*(CO2/44.+CO/28.*0.5+H2O/18.0*0.5)*32.0
      MTAR = 120.0
      CH4 = V*CH4/16.0
      H2  = V*H2/2.0
      CO2 = V*CO2/44.0
      CO  = V*CO/28.0
      H2O = V*H2O/18.0
      CTAR = V*TAR - HTAR - OTAR
      TAR = (CTAR+HTAR+OTAR)/MTAR
      RVGAS = CH4+H2+TAR
      COV   = CO/RVGAS
      CO2V = CO2/RVGAS
      COVB = (CH4+CTAR/12.0)/RVGAS
      CO2VB = COVB
```

```
      XCV = CTAR + (CH4+CO2+CO)*12.0
      XCF = XC - XCV
      RC = XCF / XC
      COALC = XC / 12.0
      COALH = XH
      COALO = XO / 16.0
      COALN = XN /14.0
      COALS = XS / 32.0
      CHARC = RC * COALC
      CHARH = RH * COALH
      CHARO = RO * COALO
      CHARN = RN * COALN
      CHARS = RS * COALS
      RCHAR = 1.0 - V - XW
      CCHAR = CHARC*12.0/RCHAR
      HCHAR = CHARH*1.0/RCHAR
      OCHAR = CHARO*16.0/RCHAR
      NCHAR = CHARN*14.0/RCHAR
      SCHAR = CHARS*32.0/RCHAR
      MAIR =  0.21*MO2+(1.-0.21)*MN2
      A2 = XC/MC+XH/MH2*0.5+XS/MS+XN/MN2-XO/MO2
      FMTH = WCOAL*(1.-XW)*A2/0.21
      IF (EXAIR .GT. 0.) FMF=FMTH*(1.+EXAIR)
      IF (EXAIR .EQ. 0. .AND .FMF .EQ. 0.) FMF = ATB(1)*UO*PAV/RG/TAV
      IF (EXAIR .EQ. 0.) EXAIR = FMF/FMTH - 1.
      UO = FMF*RG*TAV/PAV/ATB(1)
      FMO = FMF*(1.-0.21)+((XC/MC+XH/MH2+XS/MS*0.2+XN/MN2*2.0)*(1.-XW)+
     1XW/MH2O)*WCOAL+FMTH*0.21*EXAIR
      GFLOW = FMF*(1.-0.21)*MN2+((XC/MC*MCO2+XH/MH2*MH2O+XS/MS*MSO2*0.2+
     1XN/MN2*2.0*MNO)*(1.-XW)+XW)*WCOAL+FMTH*0.21*EXAIR*MO2
      MGAS = GFLOW/FMO
C
C       FMO : AVERAGE FLOW RATE OF GAS IN THE BED        MOLE/SEC
C
C
C       RHOCH : DENSITY OF CHAR
      RHOCH = RCHAR*RHOC
      IF(CAS.EQ.0..AND.WAD.GT.0.)
     1CAS=WAD*XCAO/MCAO/(WCOAL*(1.-XW)*XS/MS)
      IF(CAS.GT.0..AND.WAD.EQ.0.)
     1WAD=CAS*(WCOAL*(1.-XW)*XS/MS)/(XCAO/MCAO)
C
C      SULFUR CAPTURE EFFICIENCY ASSUMED TO BE AROUND 85 PERCENT TO
C      CALCULATE THE DENSITY OF THE PARTICLES IN THE BED
C
      A1 = 0.0
      IF (CAS .GT. 0.0) A1 = 0.85/CAS
      IF (A1 .GT. 0.4) A1 = 0.4
      RHOBED = (1.-XCO2+XCAO/MCAO*A1*MCASO4)*RHOAD
      IF (CAS .EQ. 0.0) RHOBED = RHOAD
      WRITE (6,2000) NAMEL1,NAMEL2,XCAO,XMGO,XSIO2,XCO2,
     *(DIA(I),FRACTA(I),I = 1,NDP)
      WRITE(6,2010) DASVF,DAWMF
      WRITE(6,2020) NAMEC1,NAMEC2,XCF,XCV,XH,XN,XS,XO,XW,XA,VM,V
      WRITE (6,2030) ( DIA(I),FRACTC(I), I = 1 , NDP )
      WRITE (6,2040) DCSVF,DCWMF
      IF (HLF .EQ. 0.0) VMF = VOLUME(HLMF)
      IF (HLMF .GT. 0.0) WB = VMF*(1.-EMF)*RHOBED
      CALL ELUT
      WRITE (6,OPCF)
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      WRITE (6,RES)
 1000 FORMAT(I2,/,(8F10.0))
 1001 FORMAT(8F10.0)
 1010 FORMAT(2A4/(8F10.0))
 2000 FORMAT ('0',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMGO = ',F6.3,10X,
     *'XSIO2 = ',F6.3,10X,'XCO2 = ',F6.3,/,'0',
     *T41,'DIAMETER , CM',T81,'WT.FRACTION',/,'0',(T41,F8.4,T81,F8.4))
 2010 FORMAT('0',5X,'SURFACE VOL MEAN DIA OF ADDITIVES FEED = DASVF =
     *F10.4,3X,'CM',5X,'WEIGHT MEAN DIA. = DAWMF = ',F10.4,3X,'CM',/)
 2020 FORMAT ('0',1X,2A4,3X,'XCF = ',F5.3,3X,'XCV = ',F5.3,3X,'XH = ',
     *F5.3,3X,'XN = ',F5.3,3X,'XS = ',F5.3,3X,'XO = ',F5.3,3X,'XW = ',
     $F5.3,3X,'XA = ',F5.3,/,'0',12X,'VM = ',F5.3,4X,'V = ',F5.3)
 2030 FORMAT ('0',T41,'DIAMETER , CM',T81,'WT.FRACTION'/'0',(T41,F8.4,
     *T81,F8.4))
 2040 FORMAT('0',5X,'SURFACE VOL MEAN DIA OF COAL FEED = DCSVF =',
     *F10.4,3X,'CM',5X,'WT.MEAN DIAMETER = DCWMF = ',F10.4,/)
10000 STOP
      END
      SUBROUTINE AREA ( ZI, DTI, ATI )
      COMMON /A/ ZHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZB(30),
     1ATB(30),UMF(30),DVB(30),DVBEFF(30),UTA(30),UTC(30),
     2EMF,RG,G,PI,HLMF,HLF,PAV,TAV,FMO,RHOCH,RHOBED,DZAV,VMF,XAV,ETCC,
     3DPSVB,DPWMB,DCSVB,DCWMB,UO,MGAS,MTB
      COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),FRA(30),
     1WF(30),Q1(30),Q2(30),BB(30),RKI(30),W(30),E(30),ENTA(30),ELUA(30),
     2ENTC(30,30),FRAEN(30),FRAEL(30),CU(30),
     3PFA(30),GFLOW,WCOAL,WAD,WB,WBC,WELUA,CELU,EFF,XC,XCF,
     4XA,XW,RCHAR,CCHAR,WDIS,RHOAD,TDHC,HFB,NDP
C
C     CALCULATION OF THE CROSS SECTIONAL AREA GIVEN THE HEIGHT ABOVE
C     THE DISTRIBUTOR
C
                                   DO 10 J = 1 , MTB
      IF ( ZI .GT. ZB(J) ) GO TO 10
      RJM1 = SQRT ( ATB(J-1) / PI )
      A1 = ( ZI - ZB(J-1) ) / ( ZB(J) - ZB(J-1) )
      B1 = SQRT ( ATB(J) / ATB(J-1) ) - 1.0
      RI = ( 1.0 + A1 * B1 ) * RJM1
      DTI = 2.0 * RI
      ATI = PI * RI ** 2
      GO TO 20
   10                              CONTINUE
   20 CONTINUE
      RETURN
      END
      SUBROUTINE ATTR(RHOCCH,T,DC,P,YO2,RG,TB,RKI)
      REAL MC
C
C  THIS SUBROUTINE COMPUTES BURNING TIME OF A CHAR PARTICLE
C
      EM=1.0
      SIGM=1.36E-12
      INDX=0
      DTS= 100.0
      TP=T
      MC = 12.0
                                  DO 100 I=1,20
      ETSMAX=0.001*TP
      AKS=8710.0*EXP(-35700.0/1.986/TP)
      TAV = (T+TP)*.5
```

```
      D=4.26*(TAV/1800.)**1.75/P
      COND=0.632E-5*SQRT(TAV)/(1.+245./TAV*10.**(-12./TAV))
      Z = 2500. * EXP(-12400./1.986/TAV)
      IF (DC .LE. 0.005) PHI = (2.*Z+1.)/(Z+1.)
      IF (DC .GT. 0.005 .AND. DC .LE. 0.10) PHI = 1./(Z+1.)*((2.*Z+1.)
     * - Z*(DC-0.005)/0.095)
      IF (DC .GT. 0.10) PHI = 1.0
      Q = 7900.0*(2./PHI-1)+2340.0*(2.-2./PHI)
      AKF=24.*PHI*D/(DC*RG*TAV)
      AKR=(RG*TAV/MC)/(1./AKS+1./AKF)
      RHS = AKR*P*YO2*MC*Q/(RG*TAV) - EM*SIGM*(TP**4-T**4)
      ETS = TP - T - RHS*DC/(2.0*COND)
      CALL CRRECT(I,INDX,DTS,TP1,TP2,TP,E1,E2,ETS,ETSMAX)
      IF (INDX.EQ.2) GO TO 110
  100 CONTINUE
      WRITE (6, 4000)
 4000 FORMAT ('0',10X,'TP CALCULATION HAS NOT CONVERGED. S.NO.=4000',/)
  110 CONTINUE
      TB = RHOCCH*RG*TAV*DC**2 / (96.*PHI*D*P*YO2)
      RKI = 1./TB
      RETURN
      END
      SUBROUTINE CRRECT(I,INDX,DX,X1,X2,XNEW,E1,E2,E,EMAX)
C     I: NUMBER OF THIS TRIAL, 1 FOR FIRST TRIAL
C     INDX: INDEX OF THE TRIAL LEVEL
C     INDX=0: JUST PROCEEDING
C     INDX=1: THE ROOT HAS BEEN CAUGHT BETWEEN X1 AND X2
C     INDX=2: THE ITERATION HAS CONVERGED
      IF (ABS(E).GT.EMAX) GO TO 5
      INDX=2
      RETURN
    5 CONTINUE
      IF(INDX.EQ.1) GO TO 100
      X2=XNEW
      E2=E
      IF(I.EQ.1) GO TO 10
      IF(E1*E2.LE.0.)INDX=1
      IF(INDX.EQ.1)GO TO 150
   10 X1=X2
      E1=E2
      XNEW=XNEW+DX
      RETURN
  100 CONTINUE
      IF(E1*E.LT.0.) GO TO 110
      E1=E
      X1=XNEW
      GO TO 150
  110 E2=E
      X2=XNEW
  150 CONTINUE
      XNEW=(X1-X2)*E2/(E2-E1)+X2
      RETURN
      END
      SUBROUTINE DESIGN
      COMMON /A/ ZHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZB(30),
     1ATB(30),UMF(30),DVB(30),DVBEFF(30),UTA(30),UTC(30),
     2EMF,RG,G,PI,HLMF,HLF,PAV,TAV,FMO,RHOCH,RHOBED,DZAV,VMF,XAV,ETCC,
     3DPSVB,DPWMB,DCSVB,DCWMB,U0,MGAS,MTB
      COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),FRA(30),
     1WF(30),Q1(30),Q2(30),BB(30),RKI(30),W(30),E(30),ENTA(30),ELUA(30),
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          2ENTC(30,30),FRAEN(30),FRAEL(30),CU(30),
          3PFA(30),GFLOW,WCOAL,WAD,WB,WBC,WELUA,CELU,EFF,XC,XCF,
          4XA,XW,RCHAR,CCHAR,WDIS,RHOAD,TUHC,HFB,NDP
           DIMENSION IARR(30)
     C
     C     AXIAL VARIATION OF BED CROSS SECTION
     C
           READ (5,1000) A1,A2,A3,A4
           READ (5,1001) MTB,(ZB(J),ATB(J), J = 1, MTB)
     C
     C     IARRNG          1                2              3
     C     1 -----    VERTICAL INLINE ARRANGEMENT
     C     2 -----    VERTICAL STAGGERED ARRANGEMENT
     C     3 -----    HORIZONTAL INLINE ARRANGEMENT
     C     4 -----    HORIZONTAL STAGGERED ARRANGEMENT
     C
     C
     C     HEAT EXCHANGE TUBES
           READ (5,1002) MTHE (ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),
          1IARR(J), J = 1,MTHE)
                                         DO 100 J = 1, MTHE
           IF (AHE(J) .GT. 0.0) GO TO 100
           IF (DTUBE(J) .EQ. 0.0) GO TO 100
           AHE(J) = PI * DTUBE(J) / (PH(J)*PV(J))
      100                                CONTINUE
           WRITE (6,2000) A1,A2,A3,A4
           WRITE (6,2001)
           WRITE (6,2002) (ZB(J),ATB(J), J = 1,MTB)
           WRITE (6,2003)
           WRITE (6,2004) (ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),IARR(J),
          1J = 1, MTHE)
           Z1 = ZB(1)
           ABED1 = ATB(1)
           DBED1 = SQRT(4.0 * ABED1 / PI)
           DVB(1) = 0.0
           DVBEFF(1) = 0.0
           ZHE(1) = 0.0
           DZAV = 30.0
           N = IFIX(ZB(MTB)/DZAV)
                                         DO 10 I = 1,N
           Z2 = Z1 + DZAV
                                         DO 20 J = 1,MTHE
           IF ( ZHE(J) .LE. Z1 .AND. ZHE(J+1) .GE. Z2 ) GO TO 30
           IF ( ZHE(J) .LE. Z2 .AND. ZHE(J+1) .LT. Z2 ) GO TO 20
           F1 = ( Z2 - ZHE(J) ) / DZAV
           F2 = ( ZHE(J) - Z1 ) / DZAV
           AH = F1 * AHE(J) + F2 * AHE(J-1)
           DIAT = F1 * DTUBE(J) + F2 * DTUBE(J-1)
           GO TO 40
      30   AH = AHE(J)
           DIAT = DTUBE(J)
      40   CONTINUE
           GO TO 50
      20                                 CONTINUE
      50   CONTINUE
           CALL AREA ( Z2,DBED,ABED )
           DVB(I+1) = 0.5 * (ABED+ABED1) * DZAV
            DVBEFF(I+1) = DVB(I+1) * (1.0 - 0.25 * AH * DIAT)
           Z1 = Z2
           ABED1 = ABED
```

```
10                                   CONTINUE
1000  FORMAT (4A4)
1001  FORMAT (I1/(8F10.0))
1002  FORMAT (I1/(5F10.0,I10))
2000  FORMAT ('1',20X,4A4,//)
2001  FORMAT ('0',T41,'HT.ABOVE DISTRIBUTOR,CM',T81,'CROSS SECTIONAL
     1'AREA OF BED,SQ.CM.',/)
2002  FORMAT (T49,F8.4,T96,F10.3)
2003  FORMAT ('0',T6,'HEIGHT,CM',T20,'SP.HEAT TRANS.AREA,SQ.CM/CU.CM',
     1T58,'DIA.OF TUBES,CM',T78,'VER.PITCH,CM',T95,'HOR.PITCH,CM',
     2T113,'TUBES ARRNGT',/)
2004  FORMAT (T8,F6.2,T33,F8.4,T62,F6.3,T82,F6.3,T99,F6.3,T118,I2)
      RETURN
      END
      SUBROUTINE ELUT
C
C     THIS SUBROUTINE PERFORMS THE ENTRAINMENT AND ELUTRIATION CALCULATION
C     USING THE MASS BALANCE FOR EACH SIZE FRACTION OF THE PARTICLES
C
      REAL MGAS
      COMMON /A/ ZHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZB(30),
     1ATB(30),UMF(30),DVB(30),DVBEFF(30),UTA(30),UTC(30),
     2EMF,RG,G,PI,HLMF,HLF,PAV,TAV,FMO,RHOCH,RHOBED,DZAV,VMF,XAV,ETCC,
     3DPSVB,DPWMB,DCSVB,DCWMB,UO,MGAS,MTB
      COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),FRA(30),
     1WF(30),Q1(30),Q2(30),BB(30),RKI(30),W(30),E(30),ENTA(30),ELUA(30),
     2ENTC(30,30),FRAEN(30),FRAEL(30),CU(30),
     3PFA(30),GFLOW,WCOAL,WAD,WB,WBC,WELUA,CELU,EFF,XC,XCF,
     4XA,XW,RCHAR,CCHAR,WDIS,RHOAD,TDHC,HFB,NDP
      DIMENSION FFI(30),R(30),FO(30),HB(30),DPSE(30),DPWE(30),DCSE(30),
     1DCWE(30),DCE(30,30),FCE(30,30),WEA(30),WEC(30)
      IF (HLMF .GT. 0.0) GO TO 1
      HLMF = 0.5*HLF
      VMF = VOLUME(HLMF)
      WB = VMF*(1.-EMF)*RHOBED
1     CONTINUE
      WTF = WCOAL*XA + WAD*RHOBED/RHOAD
      BB(1) = 0.0
      BB(NDP) = 0.0
      DO 25 I = 2,NDP
      FFI(I) = 0.0
      IF (DP(I) .LT. 0.0125 .AND. DP(I) .GE. 0.0063) FFI(I) = 0.2
      IF (DP(I) .LT. 0.0063 .AND. DP(I) .GE. 0.0031) FFI(I) = 0.2
      IF (DP(I) .LT. 0.0031) FFI(I) = 0.6
25    CONTINUE
      FW = 0.075
      FSW = 0.1
      P1 = 0.0
      P2 = 0.0
      IF (HLF .EQ. 0.0) HLF = 2.0*HLMF
      HT = HLF
      CALL AREA(HT,DT,CSAREA)
      RHOGAS = PAV*MGAS/RG/TAV
      VISC = 3.72E-6*TAV**0.676
      UO = GFLOW/CSAREA/RHOGAS
      TDH = 0.429*UO**1.2*(11.43-1.2*ALOG(UO))
      TDHC = TDH
      HFB = ZB(MTB)-HLF
      IF (TDH .GT. HFB) TDH = HFB
      DO 10 I = 1,NDP
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              CALL VEL(VISC,RHOGAS,G,RHOBED,DP(I),UMF(I),UTA(I))
              WF(I) = FRACTA(I)*WAD*RHOBED/RHOAD + FRACTC(I)*WCOAL*XA
              FRA(I)= WF(I)/WTF
              Q1(I) = 0.0
              Q2(I) = 0.0
      10      CONTINUE
      C       WRITE(6,11) (I,UTA(I),UMF(I),I=1,NDP)
      C 11    FORMAT ('0',5X,'I,UTA,UMF = ',I5,1P2E12.3)
              WDIS = 0.01
      C
      C       RK REPRESENTS THE ATTRITION RATE CONSTANT AND IS ASSUMED TO BE THE
      C       FOR LIMESTONE,ASH, AND  CHAR PARTICLES
      C
              RK = 0.003/3600./30.48
              EWB = 0.02*WB
              DWDIS = 0.3*WTF
              INDEX = 0
              W(1) = 0.0
              DO 30 L = 1,100
      12      CONTINUE
              SUMA = 0.0
              DO 5 I = 2,NDP
              IF ((UTA(I)-UO) .LT. 0.2*UO) FRA(I) = 0.0
              SUMA = SUMA + FRA(I)
      5       CONTINUE
              DO 15 I = 1,NDP
              FRA(I) = FRA(I)/SUMA
      15      CONTINUE
              WBC = 0.0
              DO 40 I = 2,NDP
              BB(I) = FRA(I)*WB
              R(I) = 0.0
              DIFF = UO-UMF(I)
              PFA(I) = FFI(I)*RK*DIFF*WB
              IF (FRA(I) .EQ. 0.0) GO TO 55
              CU(1) = 1.0
              DO 45 K = 2,NDP
              CU(K) = CU(K-1) - FRA(K)
      45      CONTINUE
              IF (UMF(I) .GE. UO) DIFF = 0.0
              W(I) = (WF(I)+PFA(I)+W(I-1))*(DP(I+1)/DP(I))**3
              DR = Q1(I)*(1.-P1)+Q2(I)*(1.-Q1(I))*(1.-P2)+(1.-Q1(I))*(1.-Q2(I))
              IF (UMF(I) .GE. UO) GO TO 56
              ARG = -10.4*SQRT(UTA(I)/UO)*(UMF(I)/DIFF)**0.25
              E(I) = (18.0*EXP(ARG))*GFLOW
              FO(I) = DIFF*CSAREA*FW*FSW*(1.-EMF)*RHOBED*FRA(I)
              R(I) = FO(I)*EXP(TDHC/275.0*ALOG(E(I)*FRA(I)/FO(I)))
      56      CONTINUE
              ANR = WF(I)+PFA(I)+W(I-1)
             1-W(I)-RK*DIFF*WB*FRA(I)*CU(I-1)-R(I)*DR
              IF (ANR .GT. 0.0) GO TO 57
              FRA(I) = FRA(I)*0.5
              GO TO 12
      57      CONTINUE
              BB(I) = WB*ANR/WDIS
      55      CONTINUE
              WBC = WBC + BB(I)
      C       WRITE(6,110)I,FRA(I),ANR,E(I),BB(I),WF(I),W(I),CU(I)
      C110    FORMAT (2X,'I,FRA,ANR,E,BB,WF,W,CU =  ',I2,1P7E11.3)
      40      CONTINUE
```

```
C        WRITE (6,111) L,WB,WBC,WDIS
C111     FORMAT ('0',5X,'L,WB,WBC,WDIS = ',I2,1P3E12.3)
         ERR = WBC-WB
         CALL CRRECT (L,INDEX,DWDIS,X1,X2,WDIS,E1,E2,ERR,EWB)
         IF (WDIS .LT. 0.0) WDIS = 0.0
         IF (INDEX .EQ. 2) GO TO 70
         DO 60 I = 1,NDP
         FRA(I)= BB(I)/WBC
 60      CONTINUE
 30      CONTINUE
 70      CONTINUE
C        USING THE GAS REYNOLDS NUMBER,PECLET NUMBER IS CALCULATED
C        AND HENCE THE GAS DISPERSION COEFFICIENT AND THE NO. OF
C        COMPARTMENTS IN THE FREEBOARD AND THE AVERAGE COMPARTMENT SIZE
C
         REY = DT*UO*RHOGAS/VISC
         IF (REY .LT. 2000.0) GO TO 300
         PECI = 3.E7/REY**2.1 + 1.35/REY**0.125
         GO TO 310
 300     D = 4.26*(TAV/1800.0)**1.75/PAV
         SC = VISC/RHOGAS/D
         PECI = 1./REY/SC + REY*SC/192.
 310     EZ = UO*DT*PECI
         DZ = 2.0*EZ/UO
C
C        SOLIDS ENTRAINMENT RATE ALONG THE FREEBOARD IS CALCULATED
C
         HB(1) = 0.0
         DO 320 K = 1,30
         IF (K.GT.1) HB(K) = HB(K-1) + DZ
         IF (HB(K) .GE. TDH) HB(K) = TDH
         DO 340 I = 2,NDP
         R(I) = 0.0
         DIFF = UO - UMF(I)
         IF (FRA(I) .EQ. 0.0) GO TO 340
         IF (UMF(I) .GE. UO) GO TO 340
         ARG = -10.4*SQRT(UTA(I)/UO)*(UMF(I)/DIFF)**0.25
         E(I) = 18.0*EXP(ARG)*GFLOW
         FO(I) = DIFF*CSAREA*FW*FSW*(1.-EMF)*RHOBED*FRA(I)
         R(I) = FO(I)*EXP(HB(K)/275.0*ALOG(E(I)*FRA(I)/FO(I)))
 340     CONTINUE
         WENTA = 0.0
         DO 350 I = 2,NDP
         ENTA(I) = R(I)
         IF (FRA(I) .EQ. 0.0 .AND. UO .GT. 0.833*UTA(I))
        1 ENTA(I) = WF(I) + PFA(I)
         WENTA = WENTA + ENTA(I)
 350     CONTINUE
         WEA(K) = WENTA
         DO 360 I = 2,NDP
         FRAEN(I) = ENTA(I)/WENTA
         IF (FRAEN(I) .LT. 1.E-3) FRAEN(I) = 0.0
 360     CONTINUE
         SUMA = 0.0
         SUMB = 0.0
         DO 370 I = 2,NDP
         SUMA = SUMA + FRAEN(I)/DP(I)
         SUMB = SUMB + FRAEN(I)*DP(I)
 370     CONTINUE
         DPSE(K) = 1./SUMA
```

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            DPWE(K) = SUMB
            IF (HB(K) .EQ. TDH) GO TO 380
  320       CONTINUE
  380       KT = K
            WELUA = 0.0
            DO 80 I = 2,NDP
            ELUA(I) = (1.-Q1(I))*(1.-Q2(I))*ENTA(I)
            WELUA = WELUA + ELUA(I)
   80       CONTINUE
            DO 90 I = 2,NDP
            FRAEL(I) = ELUA(I)/WELUA
            IF (FRAEL(I) .LT. 1.E-3) FRAEL(I) = 0.0
   90       CONTINUE
            SUMA = 0.0
            SUMB = 0.0
            SUMC = 0.0
            SUMD = 0.0
            DO 100 I = 2,NDP
            SUMA = DP(I)*FRA(I)+SUMA
            SUMB = FRA(I)/DP(I)+SUMB
            SUMC = DP(I)*FRAEN(I)+SUMC
            SUMD = FRAEN(I)/DP(I)+SUMD
  100       CONTINUE
            DPSVB = 1/SUMB
            DPWMB = SUMA
            DPSVE = 1./SUMD
            DPWME = SUMC
            WRITE (6,101) WDIS,WTF,WELUA,DPSVB,DPWMB,
           1(DP(I),FRA(I),FRAEL(I),I=2,NDP)
  101       FORMAT ('0',T10,'WDIS,WTF,WELUA,DPSVB,DPWMB = ',
           15F9.5,/,'0',T10,'PAR.DIA.,CM',T30,'BED SIZE FRACTION',T60,' ELUT.
           2SIZE FRACTION',/,'0',(T10,1PE10.3,T33,1PE10.3,T63,1PE10.3,/))
C
C
C           SIMILAR ENTRAINMENT CALCULATIONS ARE PERFORMED FOR CHAR
C
            DO 210 I = 1,NDP
            WF(I) = FRACTC(I)*WCOAL
            FRC(I) = FRACTC(I)
            CALL VEL(VISC,RHOGAS,G,RHOCH,DP(I),UMF(I),UTC(I))
  210       CONTINUE
            ETCA = 0.9995
            IND = 0
            DETC = -0.001
            EETC = 0.001
            CENT = 0.0
            DO 200 L = 1,30
  211       CONTINUE
            SUMA = 0.0
            DO 150 I = 2,NDP
            IF ((UTC(I)-U0) .LT. 0.2*U0) FRC(I) = 0.0
            SUMA = SUMA + FRC(I)
  150       CONTINUE
            DO 160 I = 1,NDP
            FRC(I) = FRC(I)/SUMA
  160       CONTINUE
            XAV = ((WCOAL*RCHAR-CENT)*CCHAR*(1.-ETCA))/WDIS
            CBED = XAV*WBC/CCHAR
            CELU = 0.0
            CENT = 0.0
```

```
        CBEDC = 0.0
        DO 220 I = 2,NDP
        BB(I) = FRC(I)*CBED
        R(I) = 0.0
        DIFF = UO-UMF(I)
        PFA(I) = FFI(I)*RK*DIFF*CBED/CCHAR
        FSC = 0.01
        IF (FRC(I) .EQ. 0.0) GO TO 256
        DO 252 K = 2,NDP
  252   CU(K) = CU(K-1)-FRC(K)
        IF (UMF(I) .GE. UO) DIFF = 0.0
        W(I) = (WF(I)+PFA(I)+W(I-1))*(DP(I+1)/DP(I))**3
        DR = Q1(I)*(1.-P1)+Q2(I)*(1.-Q1(I))*(1.-P2)+(1.-Q1(I))*(1.-Q2(I))
  250   IF (UMF(I) .GE. UO) GO TO 255
        ARG = -10.4*SQRT(UTC(I)/UO)*(UMF(I)/DIFF)**0.25
        E(I) = (18.0*EXP(ARG))*GFLOW
        FO(I) = DIFF*CSAREA*FW*FSW*(1.-EMF)*RHOBED*XAV*FRC(I)
        R(I) = FO(I)*EXP(TDHC/275.0*ALOG(E(I)*FRC(I)/FO(I)))
  255   CONTINUE
        YO2 = 0.15
        RHOCCH = RHOCH*CCHAR
        CALL ATTR(RHOCCH,TAV,DP(I),PAV,YO2,RG,TB,RKI(I))
        ANR = WF(I)+PFA(I)+W(I-1)-W(I)
       1-RK*DIFF*CBED*FRC(I)*CU(I-1)-RKI(I)*CBED*FRC(I)*FSC-R(I)*DR
        IF (ANR .GT. 0.0) GO TO 175
        FRC(I) = FRC(I)*0.5
        GO TO 211
  175   CONTINUE
        BB(I) = WB*ANR/WDIS
  256   CONTINUE
        CBEDC = CBEDC + BB(I)
C       WRITE(6,170)I,FRC(I),ANR,E(I),BB(I),W(I),WF(I),RKI(I)
C170    FORMAT (2X,'I,FRA,ANR,E,BB,W,WF,RKI  =  ',I2,1P7E11.3)
  220   CONTINUE
        DO 400 I = 2,NDP
        DIFF = UO - UMF(I)
        IF (FRC(I) .EQ. 0.0) GO TO 410
        IF (UMF(I) .GE. UO)  GO TO 410
        ARG = -10.4*SQRT(UTC(I)/UO)*(UMF(I)/DIFF)**0.25
        E(I) = 18.0*EXP(ARG)*GFLOW
        FO(I) = CSAREA*DIFF*FW*FSW*(1.-EMF)*RHOBED*XAV*FRC(I)
        GO TO 415
  410   FO(I) = 0.0
  415   ENTC(1,I) = FO(I)
        IF (FRC(I) .EQ. 0.0 .AND. UO .GT. 0.833*UTC(I)) ENTC(1,I) = WF(I)*
       1RCHAR + PFA(I)
        CENT = CENT + ENTC(1,I)
  400   CONTINUE
C
C       CHAR ENTRAINMENT RATE AS A FUNCTION OF THE FREEBOARD HEIGHT IS
C       CALCULATED TAKING INTO ACCOUNT THE DECREASING PARTICLE SIZE DUE TO
C       CHAR COMBUSTION
C
        WEC(1) = CENT
        DO 430 I = 2,NDP
        DCE(1,I) = DP(I)
        FCE(1,I) = ENTC(1,I)/CENT
  430   CONTINUE
        DO 420 J = 2,KT
        CENT = 0.0
```

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          DO 440 I = 2,NDP
          IF (DCE(J-1,I) .GT. 0.0) GO TO 435
          RT = 1.E6
          TB = 0.0
          GO TO 436
    435   CONTINUE
          CALL VEL(VISC,RHOGAS,G,RHOCH,DCE(J-1,I),UMF(I),UTC(I))
          HT = HLF + HB(J)
          CALL AREA (HT,DT,CSAREA)
          UAV = GFLOW/CSAREA/RHOGAS
          RT = (HB(J)-HB(J-1))/ABS(UAV-UTC(I))
          YO2 = 0.09
          CALL ATTR (RHOCCH,TAV,DCE(J-1,I),PAV,YO2,RG,TB,RKI(I))
          IF (TB.GT.RT) DCE(J,I) = (1.-RT/TB)**0.5*DCE(J-1,I)
    436   CONTINUE
          IF (TB .LE. RT) DCE(J,I) = 0.0
          IF (DCE(J,I) .GT. 0.0) GO TO 437
          ENTC(J,I) = 0.0
          GO TO 438
    437   CONTINUE
          CALL VEL(VISC,RHOGAS,G,RHOCH,DCE(J,I),UMF(I),UTC(I))
          IF (FRC(I) .GT. 0.0 .AND. UTC(I) .GT. UO) GO TO 439
          CONV = 1.
          IF (TB .GT. RT) CONV = 1.- (1.-RT/TB)**1.5
          ENTC(J,I) = ENTC(J-1,I)*(1.-CONV)
          GO TO 438
    439   CONTINUE
          CALL VEL(VISC,RHOGAS,G,RHOCH,DP(I),UMF(I),UTC(I))
          RT = HB(J)/ABS(UO-UTC(I))
          DIFF = UO-UMF(I)
          IF (UMF(I) .GE. UO) GO TO 431
          ARG = -10.4*SQRT(UTC(I)/UO)*(UMF(I)/DIFF)**0.25
          E(I) = 18.0*EXP(ARG)*GFLOW
          IF (FO(I) .GT. 0.0) R(I) = FO(I)*EXP(HB(J)/275.0*ALOG(E(I)*
         1FRC(I)/FO(I)))
          CONV = 1.0
          IF (TB .GT. RT) CONV = 1.-(1.-RT/TB)**1.5
          R(I)=R(I)*(1.-CONV)
          GO TO 432
    431   R(I) = 0.0
    432   ENTC(J,I) = R(I)
    438   CONTINUE
          CENT = CENT + ENTC(J,I)
    440   CONTINUE
          WEC(J) = CENT
          DO 450 I = 2,NDP
          IF (CENT .GT. 0.0) FCE(J,I) = ENTC(J,I)/CENT
          IF (CENT .EQ. 0.0) FCE(J,I) = 0.0
    450   CONTINUE
C         WRITE(6,190)CELU,CENT,DCSVB,DCWMB,(DP(I),FRC(I),DCE(J,I),FCE(J,I),
C        1I=2,NDP)
    420   CONTINUE
          DO 460 K = 1,KT
          SUMA = 0.0
          SUMB = 0.0
          DO 470 I = 2,NDP
          IF (DCE(K,I) .GT. 0.0) SUMA = SUMA + FCE(K,I)/DCE(K,I)
          SUMB = SUMB + FCE(K,I)*DCE(K,I)
    470   CONTINUE
          DCSE(K) = 0.0
```

```
      IF (SUMA .GT. 0.0) DCSE(K) = 1./SUMA
      DCWE(K) = SUMB
  460 CONTINUE
      CELU = WEC(KT)
      ETCC = 1.- WDIS*XAV/((WCOAL*RCHAR-CENT)*CCHAR)
      XAV = ((WCOAL*RCHAR-CENT)*CCHAR*(1.-ETCC))/WDIS
C     WRITE (6,180) L,CBED,CBEDC,XAV,ETCA,ETCC,CELU,CENT
C180  FORMAT ('0',2X,'L,CBED,CBEDC,XAV,ETCA,ETCC,CELU,CENT = ',I2,
C    11P7E12.3)
      ERR = ETCA - ETCC
      CALL CRRECT(L,IND,DETC,X1,X2,ETCA,E1,E2,ERR,EETC)
      IF (IND .EQ. 2) GO TO 230
      DO 240 I = 2,NDP
      FRC(I) = BB(I)/CBEDC
  240 CONTINUE
  200 CONTINUE
  230 CONTINUE
      SUMA = 0.0
      SUMB = 0.0
      DO 270 I = 2,NDP
      SUMA = DP(I)*FRC(I) + SUMA
      SUMB = FRC(I)/DP(I) + SUMB
  270 CONTINUE
      DCSVB = 1./SUMB
      DCWMB = SUMA
      EFF = 1.-(WDIS*XAV+CELU*CCHAR)/(WCOAL*(1.-XW)*XC)
      WRITE (6,190) CELU,CENT,DCSVB,DCWMB,(DP(I),FRC(I),DCE(KT,I),
     1FCE(KT,I),I=2,NDP)
      WRITE (6,390) (K,HB(K),DPSE(K),DPWE(K),WEA(K),K=1,KT)
      WRITE (6,490) (K,HB(K),DCSE(K),DCWE(K),WEC(K),K=1,KT)
  490 FORMAT ('0',9X,'K',9X,'FREEBOARD HT.',9X,'DCSE',12X,'DCWE',12X,'EN
     1T.RATE',//,(9X,I2,8X,1PE11.3,8X,1PE11.3,6X,1PE11.3,6X,1PE11.3))
  390 FORMAT ('0',9X,'K',9X,'FREEBOARD HT.',9X,'DPSE',12X,'DPWE',12X,'EN
     1T.RATE',//,(9X,I2,8X,1PE11.3,8X,1PE11.3,6X,1PE11.3,6X,1PE11.3))
  190 FORMAT ('0',9X,'CELU,CENT,DCSVB,DCWMB = ',1P4E12.3,/,
     1'0',9X,'BED PAR.DIA.,CM',5X,'BED SIZE FRACTION',5X,'ENT.PAR.DIA.,
     2CM',5X,'ENT.SIZE FRACTION',/,'0',(T10,1PE11.3,T31,1PE11.3,T54,
     31PE11.3,T74,1PE11.3,/))
      RETURN
      END
      SUBROUTINE VEL(VISC,RHOGAS,G,RHOS,DPAR,UM,UT)
C
C     THIS SUBROUTINE CALCULATES THE MINIMUM FLUIDIZATION VELOCITY AND
C     THE TERMINAL VELOCITY OF THE PARTICLE
C
      A1 = 33.7**2+0.0408*DPAR**3*G*(RHOS-RHOGAS)*RHOGAS/VISC**2
      UM = VISC/(DPAR*RHOGAS)*(SQRT(A1)-33.7)
      UT = (4.0*(RHOS-RHOGAS)**2*G**2/225.0/RHOGAS/VISC)**(1./3.)*DPAR
      REP = DPAR*RHOGAS*UT/VISC
      IF (REP .GT. 0.4 .AND. REP .LE. 500.0) GO TO 210
      UT = G*(RHOS-RHOGAS)*DPAR**2/18./VISC
      REP = DPAR*RHOGAS*UT/VISC
      IF(REP.LE.0.4) GO TO 210
      UT = SQRT(3.1*G*(RHOS-RHOGAS)*DPAR/RHOGAS)
  210 RETURN
      END
      FUNCTION VOLUME (ZZ)
      COMMON /A/ ZHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZB(30),
     1ATB(30),UMF(30),DVB(30),DVBEFF(30),UTA(30),UTC(30),
     2EMF,RG,G,PI,HLMF,HLF,PAV,TAV,FMO,RHOCH,RHOBED,DZAV,VMF,XAV,ETCC,
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     3DPSVB,DPWMB,DCSVB,DCWMB,U0,MGAS,MTB
      COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),FRA(30,
     1WF(30),Q1(30),Q2(30),BB(30),RKI(30),W(30),E(30),ENTA(30),ELUA(30
     2ENTC(30,30),FRAEN(30),FRAEL(30),CU(30),
     3PFA(30),GFLOW,WCOAL,WAD,WB,WBC,WELUA,CELU,EFF,XC,XCF,
     4XA,XW,RCHAR,CCHAR,WDIS,RHOAD,TDHC,HFB,NDP
C
C     CALCULATON OF THE EFFECTIVE VOLUME OF THE BED GIVEN THE HEIGHT
C
      N = IFIX (ZZ/DZAV)+1
      IF (N.EQ.1) N = 2
      SUM = 0.0
      ZN = FLOAT(N-1)*DZAV
                                DO 100 I = 2 , N
      SUM = SUM + DVBEFF(I)
      IF ( I .LT. N ) GO TO 100
      A1 = ( ZZ - ZN ) / DZAV
      SUM = SUM + DVBEFF(I) * A1
100                             CONTINUE
      VOLUME = SUM
      RETURN
      END
```

APPENDIX II

INPUT TO ELUTRIATION PROGRAM

```
12345678901234567890123456789012345678901234567890123456789012345678901234567890

A1  A2  A3  A4
NASA LEWIS 1A
MTB
4
 ZB(1)     ATR(1)    ZB(2)     ATB(2)    ZB(3)     ATB(3)    ZB(4)     ATB(4)
 0.0       405.0     62.7      405.0     81.3      670.0     280.0     2193.0
MTHE
5
 ZHE(2)    AHE(1)    DTUBE(1)  PV(1)     PH(1)        IARR(1)
 24.0      0.0       0.0       0.0       0.0                0
 ZHE(3)    AHE(2)    DTUBE(2)  PV(2)     PH(2)        IARR(2)
 40.0      0.1744    1.27      8.0       2.86               3
 ZHE(4)    AHE(3)    DTUBE(3)  PV(3)     PH(3)        IARR(3)
 48.0      0.0       0.0       0.0       0.0                0
 ZHE(5)    AHE(4)    DTUBE(4)  PV(4)     PH(4)        IARR(4)
 56.0      0.1744    1.27      8.0       2.86               3
 ZHE(6)    AHE(5)    DTUBE(5)  PV(5)     PH(5)        IARR(5)
 280.0     0.0       0.0       0.0       0.0                0
NDP
21
 DIA(1)    DIA(2)    DIA(3)    DIA(4)    DIA(5)    DIA(6)    DIA(7)    DIA(8)
 0.283     0.238     0.2       0.168     0.141     0.119     0.1       0.0841
 DIA(9)    DIA(10)   DIA(11)   DIA(12)   DIA(13)   DIA(14)   DIA(15)   DIA(16)
 0.0707    0.059     0.05      0.042     0.035     0.0297    0.0212    0.0177
 DIA(17)   DIA(18)   DIA(19)   DIA(20)   DIA(21)
 0.015     0.010     0.0074    0.0045    0.001
FRACTA(1) FRACTA(2) FRACTA(3) FRACTA(4) FRACTA(5) FRACTA(6) FRACTA(7) FRACTA(8)
 0.0       0.0038    0.0854    0.1433    0.1856    0.1406    0.1259    0.1424
FRACTA(9) FRACTA(10)FRACTA(11)FRACTA(12)FRACTA(13)FRACTA(14)FRACTA(15)FRACTA(16)
 0.0622    0.0255    0.0123    0.0114    0.0091    0.0053    0.0088    0.0032
FRACTA(17)FRACTA(18)FRACTA(19)FRACTA(20)FRACTA(21)
 0.0026    0.0135    0.0068    0.0123    0.001
FRACTC(1) FRACTC(2) FRACTC(3) FRACTC(4) FRACTC(5) FRACTC(6) FRACTC(7) FRACTC(8)
 0.0       0.0138    0.0194    0.0747    0.15      0.096     0.0963    0.1172
FRACTC(9) FRACTC(10)FRACTC(11)FRACTC(12)FRACTC(13)FRACTC(14)FRACTC(15)FRACTC(16)
 0.0766    0.0825    0.0594    0.0553    0.0538    0.0425    0.0356    0.0163
FRACTC(17)FRACTC(18)FRACTC(19)FRACTC(20)FRACTC(21)
 0.0025    0.0069    0.0009    0.0003    0.0
NAMEL1  NAMEL2
LIMEST13
 XCAO      XMGO      XSIO2     XCO2
 0.557     0.003     0.006     0.434
NAMEC1  NAMEC2
PTGHCOAL
 XC        XH        XN        XS        XO        XW        XA        VM
 0.754     0.051     0.015     0.02      0.076     0.022     0.084     0.412
 HLMF      HLF       PAV       TAV
 0.0       141.9     5.15      1151.0
 WCOAL     WAD       CAS       UO        FMF       EXAIR
 4.51      0.4638    0.0       0.0       0.0       0.639

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APPENDIX III

OUTPUT OF ELUTRIATION PROGRAM

NASA LEWIS 1A

HT.ABOVE DISTRIBUTOR,CM	CROSS SECTIONAL AREA OF BED,SQ.CM.
0.0000	405.000
62.7000	405.000
81.3000	570.000
280.0000	2193.000

HEIGHT,CM	SP.HEAT TRANS.AREA,SQ.CM/CU.CM	DIA.OF TUBES,CM	VER.PITCH,CM	HOR.PITCH,CM	TUBES ARRNGT
24.00	0.0000	0.000	0.000	0.000	0
40.00	0.1744	1.270	8.000	2.860	3
48.00	0.0000	0.000	0.000	0.000	0
50.00	0.1744	1.270	8.000	2.860	3
280.00	0.0000	0.000	0.000	0.000	0

LIMESTONE   XCAO = 0.557   XMGO = 0.003   XSIO2 = 0.006   XCO2 = 0.434

DIAMETER , CM	WT.FRACTION
0.2830	0.0000
0.2380	0.0038
0.2000	0.0854
0.1680	0.1433
0.1410	0.1856
0.1190	0.1406
0.1000	0.1259
0.0841	0.1424
0.0707	0.0622
0.0590	0.0255
0.0500	0.0123
0.0420	0.0114
0.0350	0.0091
0.0297	0.0053
0.0212	0.0088
0.0177	0.0032
0.0150	0.0026
0.0100	0.0135
0.0074	0.0068
0.0045	0.0123
0.0010	0.0010

SURFACE VOL MEAN DIA OF ADDITIVES FEED = DASVF = 0.0758 CM   WEIGHT MEAN DIA. = DAWMF = 0.1287 CM

[illegible]   XCF = 0.575   XCV = 0.179   XH = 0.051   XN = 0.015   XS = 0.020   XO = 0.076   XW = 0.022   XA = 0.084

VM = 0.412   V = 0.305

DIAMETER , CM	WT.FRACTION
0.2830	0.0000
0.2380	0.0138
0.2000	0.0194
0.1680	0.0747
0.1410	0.1500
0.1190	0.0960
0.1000	0.0963
0.0841	0.1172
0.0707	0.0766
0.0590	0.0825
0.0500	0.0594
0.0420	0.0553
0.0350	0.0530
0.0297	0.0425
0.0212	0.0356
0.0177	0.0163
0.0150	0.0025
0.0100	0.0069
0.0074	0.0009
0.0045	0.0003
0.0010	0.0000

SURFACE VOL MEAN DIA OF COAL FEED = DCSVF = 0.0677 CM   WT.MEAN DIAMETER = DCWMF = 0.1004

NOIS,WTF,WELUA,DPSVD,DPWMD = 0.05172 0.09221 0.72600 0.07498 0.10011

PAR.DIA.,CM	BED SIZE FRACTION	ELUT. SIZE FRACTION
2.605E-01	3.501E-03	0.000E-01
2.190E-01	2.711E-02	0.000E-01
1.840E-01	6.606E-02	0.000E-01
1.545E-01	1.126E-01	0.000E-01
1.300E-01	1.192E-01	0.000E-01
1.095E-01	1.202E-01	0.000E-01
9.205E-02	1.275E-01	0.000E-01
7.740E-02	1.067E-01	0.000E-01
6.485E-02	8.341E-02	0.000E-01
5.450E-02	6.233E-02	3.502E-03
4.600E-02	5.218E-02	1.604E-02
3.850E-02	5.226E-02	5.442E-02
3.235E-02	4.274E-02	1.716E-01
2.545E-02	2.978E-02	4.131E-01
1.945E-02	2.638E-03	1.058E-01
1.635E-02	1.417E-03	6.759E-02
1.290E-02	4.308E-04	5.775E-02
8.700E-03	0.000E-01	1.819E-02
5.950E-03	0.000E-01	2.181E-02
2.750E-03	0.000E-01	3.966E-02

CELU.CENT.DCSVD.DCWMD = 2.605E-02 2.605E-02 7.871E-02 1.049E-01

BED PAR.DIA.,CM	BED SIZE FRACTION	ENT.PAR.DIA., CM	ENT.SIZE FRACTION
2.605E-01	1.458E-02	2.604E-01	0.000E-01
2.190E-01	2.050E-02	2.189E-01	1.537E-13
1.840E-01	7.893E-02	1.838E-01	2.341E-08
1.545E-01	1.585E-01	1.542E-01	8.009E-06
1.300E-01	1.014E-01	1.296E-01	1.631E-04
1.095E-01	1.018E-01	1.090E-01	1.882E-03
9.205E-02	1.238E-01	9.119E-02	1.629E-02
7.740E-02	6.094E-02	7.597E-02	4.968E-02
6.485E-02	8.717E-02	6.250E-02	1.023E-01
5.450E-02	6.276E-02	5.064E-02	3.163E-01
4.600E-02	5.843E-02	3.956E-02	4.334E-01
3.850E-02	5.685E-02	2.815E-02	0.000E-01
3.235E-02	4.491E-02	0.000E-01	0.000E-01
2.545E-02	9.408E-03	0.000E-01	0.000E-01
1.945E-02	0.000E-01	0.000E-01	0.000E-01

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1.635E-02	0.000E-01	0.000E-01	0.000E-01
1.250E-02	0.000E-01	0.000E-01	0.000E-01
8.700E-03	0.000E-01	0.000E-01	0.000E-01
5.950E-03	0.000E-01	0.000E-01	0.000E-01
2.750E-03	0.000E-01	0.000E-01	0.000E-01

K	FREEBOARD HT.	DPSE	DPWE	ENT.RATE
1	0.000E-01	9.090E-02	6.139E-02	1.933E 02
2	5.643E 01	2.950E-02	3.409E-02	9.527E 00
3	1.129E 02	2.007E-02	2.651E-02	1.446E 00
4	1.381E 02	1.675E-02	2.386E-02	7.261E-01

K	FREEBOARD HT.	DCSE	DCWE	ENT.RATE
1	0.000E-01	4.610E-02	7.720E-02	5.870E-01
2	5.643E 01	4.491E-02	5.237E-02	1.387E-01
3	1.129E 02	4.065E-02	4.673E-02	5.128E-02
4	1.381E 02	4.765E-02	5.004E-02	2.685E-02

```
&OPER
PLMF=   0.7095000E 02,VMF=   0.2801805E 05,HLF=   0.1419000E 03,WR=   0.3721474E 05,WBC=   0.3708662E 05,RHOBED=   0.2656481E 01,
RHOCH=   0.9123025E 00,RCHAR=   0.6731305E 00,CCHAR=   0.8539222E 00,HCHAR=   0.0000000F 00,OCHAR=   0.0000000E 00,NCHAR=
   0.1000551E-01,SCHAR=   0.1334068E-01,U0=   0.4635152E 02,CFLCW=   0.7783318E 02,MGAS=   0.2956806E 02,FMD=   0.2632535E 01,FMF=
   0.2560154E 01,EXAIR=   0.6390000E 00,TAV=   0.1151000E 01,PAV=   0.5150000E 01,CAS=   0.1671022E 01,WAD=   0.4638000E 00,WCOAL=
   0.4510000E 01,TBHC=   0.2923691E 03,HFP=   0.1381000E 03,&END
&RES
WDIS=   0.8517234E 00,WELUA=   0.7260781E 00,CELU=   0.2684845E-01,EFF=   0.9927166E 00,DPSVB=   0.7457513E-01,DPWMB=
   0.1001132F 00,DCSVB=   0.7870710F-01,DCWMB=   0.1049331E 00,DASVF=   0.7578474E-01,DAWMF=   0.1287234E 00,DCSVF=   0.6770360E-01,
DCWMF=   0.1004419F 00,&END

STATEMENTS EXECUTED=   60272

CORE USAGE        OBJECT CODE=   39704 BYTES,ARRAY AREA=   16012 BYTES,TOTAL AREA AVAILABLE=  126976  BYTES

DIAGNOSTICS         NUMBER OF ERRORS=        0, NUMBER OF WARNINGS=        0, NUMBER OF EXTENSIONS=        0

COMPILE TIME=     2.02 SEC,EXECUTION TIME=      4.78 SEC,      17.03.53    WEDNESDAY      1 NOV 78    WATFIV - JUN 1977 V1L6

        $IBSYS                                                                          828.
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APPENDIX IV

COMBUSTION PROGRAM

```
C***********************************************************************
C              A GENERAL MODEL OF FLUIDIZED BED COAL COMBUSTOR          *
C                                                                       *
C                             PROGRAMMED BY                             *
C                                                                       *
C                             RENGA RAJAN                               *
C                                                                       *
C                             AT                                        *
C                                                                       *
C                             WEST VIRGINIA UNIVERSITY                  *
C                                                                       *
C***********************************************************************
      REAL MC,MH2,MS,MO2,MN2,MH2O,MSO2,MH2S,MCO,MCO2,MCACO3,MCAO,MCASO4
     1,MMGCO3,MMGO,MAIR,MGAS,MVGAS,MN,NC,NA,MNO,NCHAR,MTAR
      COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
     2UO(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKBE(60),YB(60),
     3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
     4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
      COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
     1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
     2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
     3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFBC,NTC
      COMMON /C/ DPSE(30),DPWE(30),DCSE(30),DCWE(30),WEA(30),WEC(30),
     1HB(30),WCHOLD(30),WAHOLD(30),KT
      DIMENSION ALFA(60),BETA(60),GAMA(60),DELT(60),UHE(60),GB(60),
     1GE(60),COB(60),WMIX(60),WNET(60),WFC(60),WFAD(60),WD(60),YCO2(60),
     2TW(60),YGO(5),YO(60),YCO(60),YV(60),YSO2(60),YNOX(60),
     3VPROD(60),RELB(60),RELE(60),TPB(60),TPE(60),CARCON(60),
     4RR(60),RRB(60),RRE(60),TOLD(60),AAA(3600),BBB(60),FEM(60),FBM(60),
     5YCO2B(60),YCO2E(60),UHEW(60),AHEW(60),TWALL(60)
      NAMELIST /OPCF/ HLMF,HLF,PAV,TAV,TSTA,TWIN,TWOUT,TWALLA,UHEAV1,
     *UHEAV2,UWALL1,UWALL2,TF,TSF,WCOAL,WAD,CAS,EXAIR,MGAS,FMTH,FMF,FMO,
     $H2SV,ANH3V,RHOCH,RHOBED,RVGAS,RCHAR,QVGAS,QVCO,QCLCN
     */OPCF1/ ICR,IFBC,NTC,HCR,HLF,HLMF,VMF,BEDVOL,EFFVOL,SOLVOL,TETUBE,
     *HAREA,QTRANS,QVOL,QAREA,HFB,BEDCOM,FBCOM,TCRATE,XO2,XO2C
      NAMELIST /OC/ WDIS,WELUA,CELU,EFF,DPSVB,DPWMB,DCSVB,DCWMB,GFLOW,
     1UO,CLOSS,CCHAR,HCHAR,OCHAR,NCHAR,SCHAR,TARC
      DATA MC,MH2,MS,MO2,MN2,MH2O,MSO2,MH2S,MCO,MCO2,MCACO3,MCAO,MCASO4
     1,MMGCO3,MMGO,MNO,MN
     1/12.,2.,32.,32.,28.,18.,64.,34.,28.,44.,100.1,56.08,136.14,84.32
     2,40.31,30.0,14.0/
      DATA AAA,BBB/3660*0./,RHOC,RHOASH,RHOAD/1.4,1.4,2.4/,HAREA,QTRANS,
     *QVOL,QAREA,RR(1),RRB(1),RRE(1)/7*0.0/,
     *CADF,CCF,CGMF/0.198,0.193,6.79/
      M1 = 100
      M1OLD = M1
      EMF = 0.5
      RG = 82.05
      G  =  980.1
      PI = 3.141593
      ETUBE(1)=0.
      EPB(1)=0.
      EPC(1)=0.
      DBAV(1)=0.
      UB(1)=0.
      DVBB(1)=0.
      AHEAV(1)=0.
C
```

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```
C     FBC DESIGN DATA
C
C     INPUT DATA FROM ENTRAINMENT CALCULATIONS
C
      READ(5,1000) KT
      READ (5,1001) (HB(K),DPSE(K),DPWE(K),WEA(K),K=1,KT),
     1(DCSE(K),DCWE(K),WEC(K),K=1,KT)
      READ(5,1001) WDIS,WELUA,CELU,EFF,DPSVB,DPWMB,DCSVB,DCWMB,
     1DASVF,DAWMF,DCSVF,DCWMF
      CALL DESIGN
C
C     COMPOSITION OF LIMESTONE
C
      READ(5,1010)NAMEL1,NAMEL2,XCAO,XMGO,XSIO2,XCO2
C
C    COMPOSITION AND NET HEATING VALUE OF COAL
C
      READ(5,1010)NAMEC1,NAMEC2,XC,XH,XN,XS,XO,XW,XA,VM,HCOAL,XACAO
C
C     OPERATING CONDITIONS
C
      READ(5,1001)HLMF,HLF,PAV,TAV,TSTA,TWIN,TWOUT,TWALLA,UHEAV1,UHEAV2,
     1UWALL1,UWALL2,TF,TSF,PF
      READ (5,1001) WCOAL,WAD,CAS,U0,FMF,EXAIR
      READ(5,1000)IGNITE,ISO2,INOX,ITEMP,IPRES
C
C     CALCULATION OF VOLATILES YIELD AND THE COMPOSITION OF VOLATILES
C
      WW = 0.2*(100.*VM-10.9)
      R = EXP(26.41-3.961*ALOG((TAV-273.))+0.0115*100.*VM)
      V = (100.*VM - R - WW)*0.01
      V = V*(1.-XW-XA)
      RN = 1.6-0.001*TAV
      IF (RN .GT. 1.) RN = 1.0
      IF (RN .LT. 0.) RN = 0.0
      RS = RN
      VGASS = XS*(1.-XW)*(1.-RS)/32.0
      VGASN = XN*(1.-XW)*(1.-RN)/14.0
      RO = 0.0
      RH = 0.0
      QCHAR = 7000.0
      QCO = 26350.0
      CH4 = 0.201-0.469*VM+0.241*VM**2
      H2  = 0.157-0.868*VM+1.338*VM**2
      CO2 = 0.135-0.900*VM+1.906*VM**2
      CO  = 0.423-2.653*VM+4.845*VM**2
      H2O = 0.409-2.389*VM+4.554*VM**2
      TAR = -.325+7.279*VM-12.88*VM**2
      HTAR = XH*(1.-RH)*(1.-XW) - V*(CH4/16.*2.0+H2/2.+H2O/18.)*2.0
      OTAR = XO*(1.-RO) - V*(CO2/44.+CO/28.*0.5+H2O/18.0*0.5)*32.0
      MTAR = 120.0
      CH4 = V*CH4/16.0
      H2  = V*H2/2.0
      CO2 = V*CO2/44.0
      CO  = V*CO/28.0
      H2O = V*H2O/18.0
      CTAR = V*TAR - HTAR - OTAR
      TAR = (CTAR+HTAR+OTAR)/MTAR
      RVGAS = CH4+H2+TAR
      COV  = CO/RVGAS
```

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```
      CO2V = CO2/RVGAS
      COVB = (CH4+CTAR/12.0)/RVGAS
      CO2VB = COVB
      XO2 = (CTAR/12.0*0.5+HTAR/2.0*0.5-OTAR/32.0+VGASS+VGASN*0.5+
     1CH4*1.5+H2*0.5)/RVGAS
      XO2C = (CTAR/12.0+HTAR/2.0*0.5-OTAR/32.0+VGASS+VGASN*0.5+
     1CH4*2.0+H2*0.5)/RVGAS
      XCV = CTAR + (CH4+CO2+CO)*12.0
      XCF = XC - XCV
      RC = XCF / XC
      H2SV = VGASS/RVGAS
      ANH3V = VGASN/RVGAS
      COALC = XC / 12.0
      COALH = XH
      COALO = XO / 16.0
      COALN = XN /14.0
      COALS = XS / 32.0
      CHARC = RC * COALC
      CHARH = RH * COALH
      CHARO = RO * COALO
      CHARN = RN * COALN
      CHARS = RS * COALS
      RCHAR = 1.0 - V - XW
      CCHAR = CHARC*12.0/RCHAR
      HCHAR = CHARH*1.0/RCHAR
      OCHAR = CHARO*16.0/RCHAR
      NCHAR = CHARN*14.0/RCHAR
      SCHAR = CHARS*32.0/RCHAR
      TARC = (CHARC+CHARH*0.5+CHARS+CHARN*0.5-CHARO*0.5)/(RCHAR*0.21)
      QVGAS = ( HCOAL - RCHAR * QCHAR - CO*QCO) / RVGAS
      QVCO = QVGAS - QCO*COVB
      T(1) = TF
      IF(WCOAL.EQ.0.)IGNITE=0
C-----------------------------------------------------
C     IGNITE       0            1
C              NO COMBUSTION   COMBUSTION
C-----------------------------------------------------
      MAIR =  0.21*MO2+(1.-0.21)*MN2
      A2 = XC/MC+XH/MH2*0.5+XS/MS+XN/MN2-XO/MO2
      FMTH = WCOAL*(1.-XW)*A2/0.21
      IF (EXAIR .GT. 0.) FMF=FMTH*(1.+EXAIR)
      IF (EXAIR .EQ. 0. .AND .FMF .EQ. 0.) FMF = ATB(1)*UO*PAV/RG/TAV
      IF (EXAIR .EQ. 0.) EXAIR = FMF/FMTH - 1.
      UO = FMF*RG*TAV/PAV/ATB(1)
      FMO = FMF*(1.-0.21)+((XC/MC+XH/MH2+XS/MS*0.2+XN/MN2*2.0)*(1.-XW)+
     1XW/MH2O)*WCOAL*EFF+FMTH*0.21*EXAIR
      GFLOW = FMF*(1.-0.21)*MN2+((XC/MC*MCO2+XH/MH2*MH2O+XS/MS*MSO2*0.2+
     1XN/MN2*2.0*MNO)*(1.-XW)+XW)*WCOAL+FMTH*0.21*EXAIR*MO2
      MGAS = GFLOW/FMO
C
C      FMO : AVERAGE FLOW RATE OF GAS IN THE BED          MOLE/SEC
C     AVERAGE H2O CONCENTRATION IN FBC
      YH2O =(WCOAL*(XW/MH2O+XH*(1.-XW)/MH2))/FMO
C
      RHOCH = RCHAR*RHOC
      IF(IGNITE.EQ.0)RHOCH=RHOC
      IF(IGNITE.EQ.0)RHOBED=RHOAD
      IF(CAS.EQ.0..AND.WAD.GT.0.)
     1CAS=WAD*XCAO/MCAO/(WCOAL*(1.-XW)*XS/MS)
      IF(CAS.GT.0..AND.WAD.EQ.0.)
```

```
     1WAD=CAS*(WCOAL*(1.-XW)*XS/MS)/(XCAO/MCAO)
      A1 = 0.0
      IF(CAS .GT. 0.0) A1 = 0.85/CAS
      IF (A1 .GT. 0.4) A1 = 0.4
      RHOBED=(1.-XCO2+XCAO/MCAO*A1*MCASO4)*RHOAD
      IF (CAS .EQ.0.0) RHOBED = RHOAD
      RHOGAS=PAV*MGAS/(RG*TAV)
      VISC=3.72E-6*(TAV**0.676)
C
C    QCLCN   : HEAT OF CALCINATION PER GRAM ADDITIVE
C
      QCLCN=(42500.0*XCAO/MCAO + 23810.0*XMGO/MMGO)
      CS=0.215
C      =============
C     MAIN OUTPUT 2
C      =============
      WRITE (6,2000) NAMEL1,NAMEL2,XCAO,XMGO,XSIO2,XCO2
      WRITE(6,2010) DASVF,DAWMF
      WRITE(6,2020) NAMEC1,NAMEC2,XCF,XCV,XH,XN,XS,XO,XW,XA,VM,V,HCOAL
     1,XACAO
      WRITE (6,2040) DCSVF,DCWMF
      WRITE (6,2030) (K,HB(K),DPSE(K),DPWE(K),WEA(K),DCSE(K),DCWE(K),
     1WEC(K),K=1,KT)
      WRITE (6,OPCF)
      ZAVG(1) = 0.0
      X(1) = 0.0
      IF (ITEMP .GT. 0) TAV = TSTA
                              DO 20 I=2,60
      T(I)=TAV
   20                         CONTINUE
C     ***************************************
C     INITIAL BUBBLE HYDRODYNAMIC CALCULATION
      IF (HLF .EQ. 0.0) VMF = VOLUME(HLMF)
      IF (HLMF .GT. 0.0) WB = VMF*(1.-EMF)*RHOBED
C     ***************************************
      IF(IGNITE.EQ.1)GO TO 41
      CALL HYDRO
                              DO 35 I=2,M1
      ZAVG(I) = ( H(I) + H(I-1) ) * .5
35                            CONTINUE
      ETC=0.
      YAV=0.21
      XAV=WCOAL*XC/(WCOAL+WAD)*(1.-XW)
      FMO=FMF
      IF (WAD.EQ.0.0 .AND. IGNITE .EQ. 0) GO TO 900
C     *******************************************************************
C     FOR CONDITIONS  OF NO COAL COMBUSTION. IGNITION IS ZERO AND
C     MATERIAL AND ENERGY BALANCES CALCULATIONS ARE SKIPPED
C     *******************************************************************
      YB(1) = YAV
      YE(1) = YB(1)
      FEM(1) = UMF(1) * AT(1) * PAV / (RG*T(2))
      FBM(1) = FMO - FEM(1)
                              DO 115 I = 2,60
      RRB(I) =0.0
      RRE(I) = 0.0
      YB(I)=YAV
      YE(I)=YAV
      X(I)=XAV
      IF (I .GT. M1) GO TO 115
```

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```
            FEM(I) = UMF(I)*AT(I)*(1.0-ETUBE(I))*PAV / (RG*T(I))
            FBM(I) = FMO - FEM(I)
            IF (UO(I) .LE. UMF(I)) FEM(I) = 0.0
      115                            CONTINUE
            IF (IGNITE .EQ. 0) GO TO 630
         41 CONTINUE
      C      BOUDARY CONDITIONS FOR GAS CONCENTRATIONS
      C
            YO(1) = 0.21
            YV(1) = 0.0
            YCO(1) = 0.0
            YSO2(1) = 0.0
            YNOX(1) = 0.0
            YB(1)=FMF*0.21/FMO
            YE(1)=YB(1)
            YVE(1) = 0.0
            YCOE(1) = 0.0
            YCO2B(1) = 0.0
            YCO2E(1) = 0.0
            YCO2(1) = 0.0
      C
      C      FROM HERE TO THE STATEMENT NO.600 : TEMPERATURE ITERATION LOOP
      C
                                     DO 600  ITRIAL = 1,30
      C
      C     CALCULATION OF LOG MEAN TEMPERATURE OF THE COOLING WATER
      C
            A1 = TWOUT - TWIN
            A2 = ALOG((TAV-TWIN)/(TAV-TWOUT))
            TWAV = TAV - A1/A2
            CALL HYDRO
            DO 25 I = 1,MT
            TW(I) = TWAV
            IF (I .LE. M1) UHE(I) = UHEAV1
            IF (I .GT. M1) UHE(I) = UHEAV2
            IF (I .LE. M1) UHEW(I) = UWALL1
            IF (I .GT. M1) UHEW(I) = UWALL2
            AHEW(I) = 4.0/DT(I)
            TWALL(I) = TWALLA
      25    CONTINUE
            MP1 = M1 + 1
            IF(ITRIAL .GT. 1 .AND. M1.EQ.M1OLD)GO TO 170
            J1=1
                                     DO 56 I=2,M1
            WFC(I)=0.
            WFAD(I)=0.
            J2=J1
            IF(J1.GT.MFEED)GO TO 56
                                     DO 55 J=J1,MFEED
            IF(ZF(J).GT.H(I))GO TO 55
            WFC(I)=WCOAL*FFC(J)
            WFAD(I)=WFAD(I)+WAD*FFAD(J)
            J2=J+1
         55                          CONTINUE
            J1=J2
         56                          CONTINUE
            IF(J1.GT.MFEED)GO TO 58
                                     DO 57 J=J1,MFEED
            WFC(M1)=WCOAL*FFC(J)
            WFAD(M1)=WFAD(M1)+WAD*FFAD(J)
```

```
   57                                 CONTINUE
   58 CONTINUE
  170 CONTINUE
      FEM(1) = UMF(1)*AT(1)*(1.0-ETUBE(1))*PAV/(RG*T(2))
      FBM(1) = FMF - FEM(1)
                                    DO 133 I=2,M1
      TOLD(I)=T(I)
C
C     DISTRIBUTION OF THE VOLATILES EVOLVED
C
      VPROD(I) = WCOAL * RVGAS * (H(I)-H(I-1))/H(M1)*FW
      VPROD(I) = VPROD(I)+WFC(I)*RVGAS*(1.-FW)
      FEM(I) = FEM(I-1)+VPROD(I)
      IF(UO(I).LE.UMF(I)) FEM(I) = FMO
      FBM(I)=FMO-FEM(I)
133                                   CONTINUE
C
C      FROM THE STATEMENT NO. 200 TO 300 : ITERATION OF MATERIAL BALANCE
C     BASED ON THE GIVEN TEMPERATURE PROFILE. GAUSS SEIDEL METHOD
C
  200 CONTINUE
      INDEX = 0
      DETC = -0.0001
      IF (TAV .GE.1100.0 .AND. TAV .LT. 1150.0) DETC = -0.0002
      IF (TAV .GE. 1050.0 .AND. TAV.LT.1100.0) DETC = -0.002
      IF (TAV .LT. 1050.0 .AND. TAV .GE. 1000.0) DETC = -0.005
      IF (TAV .LT. 1000.0) DETC = -0.01
      EETCM = 0.01
      ETCA = 0.99999
      IF (ITRIAL .GT. 1) GO TO 175
      AMODF = 6.0*RHOBED*(1.-EMF)/(DCSVB*RHOCH*CCHAR)
C
C      PREPARATORY STATEMENTS FOR THE WHOLE ITERATION.
C
                                      DO 130 I = 2,60
      YAV = 0.16
      IF (I .GT. M1) YAV = 0.09
      YB(I) = YAV
      YE(I) = YAV
      YO(I) = YAV
130                                   CONTINUE
175   CONTINUE
C
C     ASSUMING THE CARBON COMBUSTION EFFICIENCY,CARBON CONC. IN THE
C     BED IS CALCULATED. KNOWING THE CARBON CONCENTRATION IN THE BED,GAS
C     PHASE MATERIAL BALANCE IS PERFORMED AND THE COMBUSTION EFFICIENCY
C     IS CALCULATED. ITERATION IS CONTINUED TILL THE ASSUMED COMBUSTION
C     EFFCIENCY EQUALS THE CALCULATED EFFICIENCY FROM OXYGEN BALANCE.
C
                                      DO 201 NT = 1,30
      XAV = ((WCOAL*RCHAR-CELU)*CCHAR*(1.-ETCA))/WDIS
                                      DO 1 I = 1,M1
1     X(I) = XAV
      TCRATE = 0.0
C
C     GAS PHASE MATERIAL BALANCE IN THE BED
C
                                      DO 233 I=2,M1
      CALL AKK(AKB,T(I),PAV,DCSVB,TPB(I),YB(I),RG,MC,AKCO2,PHIB)
      TAVB=(T(I)+TPB(I))/2.
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```
            CALL AKK(AKE,T(I),PAV,DCSVB,TPE(I),YE(I),RG,MC,AKCO2,PHIE)
            TAVE=(T(I)+TPE(I))/2.
            I1=I-1
            CALL GPB (YH2O,AKB,AKE,AKBE(I),AMODF,DVBB(I),EMF,EPB(I),EPC(I),
           1ETUBE(I),FBM(I1),FBM(I),FEM(I1),FEM(I),GB(I),COB(I),GE(I),PAV,
           2PHIE,RG,RVGAS,T(I),TAVB,TAVE,VPROD(I),X(I),XO2,XO2C,YB(I1),YB(I),
           3YCOE(I1),YCOE(I),YE(I1),YE(I),YVE(I1),YVE(I),AKCO2,COV,CO2V,COVB,
           4CO2VB,YCO2B(I1),YCO2B(I),YCO2E(I1),YCO2E(I))
            AM = DVBB(I)*AMODF*X(I)*MC
            RRB(I) = AM*(PAV/RG)*(EPC(I)-EPB(I))*YB(I)*AKB/TAVB/CCHAR
            RRE(I) = AM*(PAV/RG/TAVE)*(1.-EPC(I)-ETUBE(I))/CCHAR*(YE(I)*AKE+
           1YCO2E(I)*AKCO2)
            RR(I) = ( RRB(I)+RRE(I))/X(I)
            TCRATE = TCRATE + RR(I)*X(I)
            YO(I) = (FEM(I)*YE(I)+FBM(I)*YB(I))/FMO
            YCO2(I) = (FEM(I)*YCO2E(I)+FBM(I)*YCO2B(I))/FMO
            YV(I) = FEM(I)*YVE(I)/FMO
            YCO(I) = FEM(I)*YCOE(I)/FMO
      233                          CONTINUE
      C
      C     GAS PHASE MATERIAL BALANCE IN THE FREEBOARD
      C
                                   DO 234 I = MP1,MT
            J = I-M1
            K = J+1
            HAV = (H(I-1)+H(I))/2.0
            CALL AREA(HAV,DTAV,ATAV)
            RHOGAS = PAV*MGAS/RG/T(I)
            VISC = 3.72E-6*T(I)**0.676
            DCSVE = 0.5*(DCSE(J)+DCSE(K))
            DCWME = 0.5*(DCWE(J)+DCWE(K))
            CALL VEL(VISC,RHOGAS,G,RHOCH,DCSVE,UMFAV,UTAV)
            UO(I) = FMO*MGAS/RHOGAS/ATAV/(1.-ETUBE(I))
            RT = (HB(K)-HB(J))/ABS(UO(I)-UTAV)
            WCHOLD(I) = (2.0*WEC(J)-WEC(K))*RT
            VCHOLD = WCHOLD(I)/RHOCH
            NC = VCHOLD*6.0/(PI*DCSVE**3)
            CALL AKK(AKC,T(I),PAV,DCSVE,TPB(I),YO(I),RG,MC,AKCO2,PHIB)
            TPE(I) = TPB(I)
            TAVB = (T(I)+TPB(I))/2.0
            I1 = I-1
            CALL FBC(YH2O,AKC,DCSVE,DVBB(I),ETUBE(I),FMO,GB(I),COB(I),
           1GE(I),NC,PAV,PHIB,PI,RG,RVGAS,T(I),TAVB,XO2,YCO(I1),YCO(I),YO(I1),
           2YO(I),YV(I1),YV(I),AKCO2,COVB,CO2VB,YCO2(I1),YCO2(I))
            RRB(I) = MC*NC*PI*DCSVE**2*PAV/RG/TAVB/CCHAR*(YO(I)*AKC+
           1AKCO2*YCO2(I))
            RRE(I) = 0.0
            TCRATE = TCRATE + RRB(I)
      234                          CONTINUE
      C     WRITE(6,205) (I,YB(I),YE(I),YCOE(I),YVE(I),H(I),YCO2E(I),YCO2B(I)
      C    1UO(I),UMF(I),I=1,M1)
      C205  FORMAT ('0',T5,'I',T12,'YB',T24,'YE',T35,'YCOE',T46,'YVE',T58,
      C    1'H',T70,'YCO2E',T82,'YCO2B',T94,'UO',T106,'UMF',//,(I5,1P9E12.3))
            A1 = FMF*0.21+WCOAL*(1.-XW)*XO/MO2-FMO*YO(MT)
            ETCG = A1/(FMTH*0.21 - CELU*TARC*0.21)
      C     WRITE(6,209) NT,ETCA,ETCG,XAV
      C209  FORMAT('0',10X,'NT,ETCA,ETCG,XAV = ',I4,1P3E12.3/)
            ER=ETCG-ETCA
            CALL CRRECT(NT,INDEX,DETC,ETC1,ETC2,ETCA,E1,E2,ER,EETCM)
            IF (INDEX .EQ. 2) GO TO 236
```

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  201   CONTINUE
  236   CONTINUE
  C
  C     FROM THE GAS PHASE MATERIAL BALANCE,CHAR COMBUSTION RATE HAS BEEN
  C     ESTIMATED. KNOWING THIS AND THE SOLIDS MIXING RATE,CARBON BALANCE
  C     IS PERFORMED. THE EQUATIONS ARE SOLVED BY THE SSP SUBROUTINE SIMQ
  C     (SIMULTANEOUS SOLUTION OF ALGEBRAIC EQUATIONS). THE SOLUTION GIVES
  C     THE CARBON CONCENTRATION PROFILE IN THE BED.
  C
        WMIX(1)=0.
        WNET(1)=0.
        J1=1
                                    DO 61 I=2,M1
        WD(I)=0.
        J2=J1
        IF(J1.GT.MDIS)GO TO 61
                                    DO 60 J=J1,MDIS
        IF(ZDIS(J).GT.H(I))GO TO 60
        WD(I)=WD(I)+WDIS*FD(J)
        J2=J+1
     60                             CONTINUE
        J1=J2
     61                             CONTINUE
        IF(J1.GT.MDIS)GO TO 63
                                    DO 62 J=J1,MDIS
        WD(M1)=WD(M1)+WDIS*FD(J)
     62                             CONTINUE
     63 CONTINUE
  C
  C      WMIX : UP- AND DOWN-WARD SOLID MIXING FLOW WHICH IS SUPERPOSED ON
  C             FLOW OF SOLIDS.    G/SEC
  C     WNET(I) : NET FLOW RATE OF SOLID FROM THE TOP OF I-TH COMPARTMENT.
  C             POSITIVE VALUE MEANS THE UPWARD FLOW.
        TFC = WCOAL*RCHAR - CELU
                                    DO 255 I=2,M1
        RR(I) = RR(I)*TFC/TCRATE
        WNET(I)=WNET(I-1)+WFC(I)*RCHAR+WFAD(I)-WD(I)-RR(I)*X(I)
        WMIX(I)=AT(I)*(1.-ETUBE(I))*(UO(I)-UMF(I))*FW*(1.-EMF)*RHOBED
        IF(WMIX(I).LT.0.)WMIX(I)=0.
    255 CONTINUE
        WMIX(M1)=0.
  C
  C     CARBON CONCENTRATION CALCULATION.
  C
        MM=M*M
                                    DO 411 I=1,MM
    411 AAA(I)=0.
                                    DO 412 I=1,M
    412 BBB(I)=0.
        AAA(1) = -WMIX(2)-WD(2)-RR(2)
        AAA(M1)=WMIX(2)-WNET(2)
        AAA(MM) = -WMIX(M)+WNET(M)-WD(M1)-RR(M1)
        AAA(MM-M)=WMIX(M)
                                    DO 413 I=1,M
        I1=I+1
        BBB(I) =  - MC*CHARC*WFC(I1)
    413                             CONTINUE
        MO=M-1
                                    DO 270 I=2,MO
        II=(I-1)*M+I
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            I1=I+1
            AAA(II) = -WMIX(I1)-WMIX(I)+WNET(I)
           1-WD(I1)-RR(I1)
            AAA(II-M)=WMIX(I)
            AAA(II+M)=-WNET(I1)+WMIX(I1)
        270 CONTINUE
            CALL SIMQ(AAA,BBB,M,MM,KS)
            SUM=0.
                                      DO 280 I=1,M
            X(I+1) = BBB(I)
            SUM = SUM+X(I+1)
        280 CONTINUE
            XAV=SUM/FLOAT(M)
      C     WRITE (6,286) XAV,(I,X(I),H(I),I=1,M1)
      C286  FORMAT ('0','   XAV = ',1PE12.3,/,('     I,X,H = ',I5,1P2E12.3))
            SUM=0.
                                      DO 285 I=2,M1
            SUM=WD(I)*X(I)+SUM
            CARCON(I)=X(I)*RHOBED*(1.-EMF)*(1.-ETUBE(I)-EPB(I))/(1.-ETUBE(I))
        285                           CONTINUE
            CLOSS = SUM + CELU*CCHAR
            ETCC = 1.0 - SUM / ( (WCOAL * RCHAR - CELU)*CCHAR )
            ETC = 1. - CLOSS / ( WCOAL * XC * (1.-XW))
      C
      C     HAVING OBTAINED THE CORRECT  CARBON CONCENTRATIONS IN THE BED,
      C     GAS PHASE MATERIAL BALANCE IS REPERFORMED TO ARRIVE AT THE CORRECT
      C     CONCENTRATION PROFILES FOR THE VARIOUS GASEOUS SPECIES
      C
      C     GAS PHASE MATERIAL BALANCE IN BED
      C
            TCRATE = 0.0
                                      DO 235 I=2,M1
            CALL AKK(AKB,T(I),PAV,DCSVB,TPB(I),YB(I),RG,MC,AKCO2,PHIB)
            TAVB=(T(I)+TPB(I))/2.
            CALL AKK(AKE,T(I),PAV,DCSVB,TPE(I),YE(I),RG,MC,AKCO2,PHIE)
            TAVE=(T(I)+TPE(I))/2.
            I1=I-1
            CALL GPB (YH2O,AKB,AKE,AKBE(I),AMODF,DVBB(I),EMF,EPB(I),EPC(I),
           1ETUBE(I),FBM(I1),FBM(I),FEM(I1),FEM(I),GB(I),COB(I),GE(I),PAV,
           2PHIE,RG,RVGAS,T(I),TAVB,TAVE,VPROD(I),X(I),XO2,XO2C,YB(I1),YB(I),
           3YCOE(I1),YCOE(I),YE(I1),YE(I),YVE(I1),YVE(I),AKCO2,COV,CO2V,COVB,
           4CO2VB,YCO2B(I1),YCO2B(I),YCO2E(I1),YCO2E(I))
            AM = DVBB(I)*AMODF*X(I)*MC
            RRB(I) = AM*(PAV/RG)*(EPC(I)-EPB(I))*YB(I)*AKB/TAVB/CCHAR
            RRE(I) = AM*(PAV/RG/TAVE)*(1.-EPC(I)-ETUBE(I))/CCHAR*(YE(I)*AKE+
           1YCO2E(I)*AKCO2)
            RR(I) = ( RRB(I)+RRE(I))/X(I)
            TCRATE = TCRATE + RR(I)*X(I)
            YO(I) = (FEM(I)*YE(I)+FBM(I)*YB(I))/FMO
            YCO2(I) = (FEM(I)*YCO2E(I)+FBM(I)*YCO2B(I))/FMO
            YV(I) = FEM(I)*YVE(I)/FMO
            YCO(I) = FEM(I)*YCOE(I)/FMO
      235                             CONTINUE
            BEDCOM = TCRATE
      C
      C     GAS PHASE MATERIAL BALANCE IN THE FREEBOARD
      C
                                      DO 237 I = MP1,MT
            J = I-M1
            K = J+1
```

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      DCSVE = 0.5*(DCSE(J)+DCSE(K))
      VCHOLD =WCHOLD(I)/RHOCH
      NC = VCHOLD*6.0/(PI*DCSVE**3)
      CALL AKK(AKC,T(I),PAV,DCSVE,TPB(I),YO(I),RG,MC,AKCO2,PHIB)
      TPE(I) = TPB(I)
      TAVB = (T(I)+TPB(I))/2.0
      I1 = I-1
      CALL FBC(YH2O,AKC,DCSVE,DVBB(I),ETUBE(I),FMO,GB(I),COB(I),
     1GE(I),NC,PAV,PHIB,PI,RG,RVGAS,T(I),TAVB,XO2,YCO(I1),YCO(I),YO(I1),
     2YO(I),YV(I1),YV(I),AKCO2,COVB,CO2VB,YCO2(I1),YCO2(I))
      RRB(I) = MC*NC*PI*DCSVE**2*PAV/RG/TAVB/CCHAR*(YO(I)*AKC+
     1AKCO2*YCO2(I))
      RRE(I) = 0.0
      TCRATE = TCRATE + RRB(I)
  237                       CONTINUE
      FBCOM = TCRATE - BEDCOM
C
C  THE DEFINITION OF RR(I) IS CHANGED FOR TEMPERATURE CALCULATIONS.
C  RR(I)=(HEAT GENERATION RATE- HEAT CONSUMPTION RATE) IN THE
C  ITH COMPARTMENT.
C
                            DO 295 I=2,M1
      RR(I)=RR(I)*X(I)/TCRATE*QCHAR*(WCOAL*RCHAR-CELU)*ETCC+
     1GE(I)*QVCO+GB(I)*QVGAS+COB(I)*QCO-QCLCN*WFAD(I)*RHOAD
  295 CONTINUE
                            DO 300 I = MP1,MT
      RR(I) = RRB(I)/TCRATE*QCHAR*(WCOAL*RCHAR-CELU)*ETCC+
     1GE(I)*QVCO+GB(I)*QVGAS+COB(I)*QCO
  300 CONTINUE
      IF (ITEMP .EQ. 0) GO TO 610
C
C       CALCULATION OF TEMPERATURE
C
      A1= CADF
      A2= CCF
      CGM = 6.8+0.5E-3*(TAV-273)
      A3=CGM*FMO
      ALFA(2)=(WMIX(2)+WD(2))*CS+A3+UHE(2)*AHEAV(2)*DVBB(2)
     1+UHEW(2)*AHEW(2)*DVBB(2)
      BETA(2)=(-WNET(2)+WMIX(2))*CS
      GAMA(2)=0.
      DELT(2)=RR(2)+CGMF*FMF*(T(2)-273.)+(A1*WFAD(2)+A2*WFC(2))*(TSF-273
     1.)+UHE(2)*AHEAV(2)*DVBB(2)*(TW(2)-273.)+UHEW(2)*AHEW(2)*DVBB(2)*
     2(TWALL(2)-273.)
C
C       HEAT BALANCE IN THE BED
C
                            DO 310 I=3,M
      I1=I-1
      ALFA(I)=(-WNET(I1)+WMIX(I)+WMIX(I1)+WD(I))
     1*CS+A3+UHE(I)*AHEAV(I)*DVBB(I)+UHEW(I)*AHEW(I)*DVBB(I)
      BETA(I)=(-WNET(I)+WMIX(I))*CS
      GAMA(I)=(WMIX(I1))*CS+A3
      DELT(I)=RR(I)+(A1*WFAD(I)+A2*WFC(I))*(TSF-273.)+UHE(I)*AHEAV(I)*
     1DVBB(I)*(TW(I)-273.)+UHEW(I)*AHEW(I)*DVBB(I)*(TWALL(I)-273.)
  310                       CONTINUE
      ALFA(M1)=(-WNET(M)+WMIX(M)+WD(M1))*CS+A3
     1+UHE(M1)*AHEAV(M1)*DVBB(M1)+UHEW(M1)*AHEW(M1)*DVBB(M1)
      BETA(M1)=0.
      GAMA(M1)=(WMIX(M))*CS+A3
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      DELT(M1)=RR(M1)+(A1*WFAD(M1)+A2*WFC(M1))*(TSF-273.)
     1+UHE(M1)*AHEAV(M1)*DVBB(M1)*(TW(M1)-273.)
     2+UHEW(M1)*AHEW(M1)*DVBB(M1)*(TWALL(M1)-273.)
C
C  TEMPERATURE SOLUTION BY SIMQ
C
                                    DO 501 I=1,MM
  501 AAA(I)=0.
                                    DO 502 I=1,M
  502 BBB(I)=DELT(I+1)
      AAA(1)=ALFA(2)
      AAA(M1)= -BETA(2)
      AAA(MM)= ALFA(M1)
      AAA(MM-M)=-GAMA(M1)
                                    DO 503 I=2,M0
      II=(I-1)*M+I
      AAA(II)=ALFA(I+1)
      AAA(II-M)=-GAMA(I+1)
      AAA(II+M)=-BETA(I+1)
  503 CONTINUE
      CALL SIMQ(AAA,BBB,M,MM,KS)
      TNORM=0.
      TAV=0.
                                    DO 504 I=2,M1
      T(I)=BBB(I-1)+273.
      TAV=TAV+T(I)
      TNORM=TNORM+ABS(T(I)-TOLD(I))
  504 CONTINUE
      TAV=TAV/FLOAT(M)
      TNORM=TNORM/FLOAT(M)
C     WRITE (6,208) TNORM,TAV,BEDCOM,FBCOM
C 208 FORMAT ('0', 10X,'TNORM,TAV,BEDCOM,FBCOM = ',1P4E12.3)
C
C     HEAT BALANCE IN THE FREEBOARD
C
                                      DO 320 I = MP1,MT
      J = I-M1
      WENTI = WEA(J)+WEC(J)
      ANR = (WENTI*CS+A3)*(T(I-1)-273.)+RR(I)+DVBB(I)*UHE(I)*AHEAV(I)*
     1(TW(I)-273.)+DVBB(I)*UHEW(I)*AHEW(I)*(TWALL(I)-273.)
      DR = WENTI*CS+A3+DVBB(I)*UHE(I)*AHEAV(I)+DVBB(I)*UHEW(I)*AHEW(I)
      T(I) = ANR/DR + 273.0
320                                   CONTINUE
C
C     CONVERGENCY CRITERION FOR TEMPERATURE CALCULATION
C
      IF(TNORM.LT.0.01*TAV) GO TO 610
      M1OLD = M1
  600                               CONTINUE
      WRITE (6, 3003)
 3003 FORMAT('0',10X,'GAUSS SEIDEL TEMPERATURE TRIAL HAS NOT CONVERGED.
     1 S.NO. = 3003',/)
610   CONTINUE
                                      DO 620 I = 2,MT
      A1 = AHEAV(I) * DVBB(I)
      HAREA = HAREA + A1
      QTRANS = UHE(I) * A1 * ( T(I)-TW(I) ) + QTRANS
      RR(I) = RR(I) / DVBBEF(I)
      ZAVG(I) = ( H(I-1) + H(I) ) * 0.5
620                                   CONTINUE
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      QVOL = QTRANS/BEDVOL
      HFB = H(MT) - H(M1)
      IF (HAREA .NE. 0.0) QAREA = QTRANS/HAREA
      TPB(1)=T(1)
      TPE(1)=T(1)
      TAV=TAV-273.
                                  DO 612 I=1,MT
      T(I)=T(I)-273.
      TPB(I)=TPB(I)-273.
      TPE(I)=TPE(I)-273.
  612 CONTINUE
C      ============
C     MAIN OUTPUT 3
C      ============
      WRITE (6,2001) ETC,XAV,TAV,ITRIAL,(I,H(I),YB(I),YE(I),YVE(I),
     1YCOE(I),YCO2E(I),YCO2B(I),X(I),ZAVG(I),I=2,M1)
      WRITE (6,2002) (I,H(I),YO(I),YV(I),YCO(I),YCO2(I),T(I),TPB(I),
     1TPE(I),ZAVG(I),I=2,MT)
                                 DO 613 I = 1,MT
      TPB(I) = TPB(I)+273.0
      TPE(I) = TPE(I)+273.0
      T(I) = T(I)+273.0
  613                            CONTINUE
      YGO(1)=YO(MT)
C
C
C          CALCULATION OF SO2 REDUCTION
C
      IF (IGNITE.EQ.0) TCRATE = 0.0
                                 DO 710 I=1,MT
      IF (I .GT. M1) GO TO 709
      YEO(I) = YE(I)
      YBO(I) = YB(I)
  709 YB(I)=0.
      YE(I)=0.
  710                            CONTINUE
      IF (ISO2 .EQ. 0) GO TO 811
  630 CONTINUE
      FRS = WCOAL*XS/MS*FLOAT(IGNITE)*(1.-XW)
      IF (FRS . LE. 1.E-6) GO TO 810
C
C      CASE : EFFECTIVE RATIO OF CA TO S(ACTIVE) IN THE FEEDS
C
      CASE=(WAD*XCAO+WCOAL*XA*XACAO)/MCAO/FRS
      IF(CASE.EQ.0.) GO TO 811
      SULFUR = WCOAL*(1.-XW)*XS*RS/MS - CLOSS*SCHAR/CCHAR/MS
      RELB(1)=0.
      RELE(1)=0.
      YB(1)=0.0
      YE(1)=YB(1)
      ETS=0.0
      DETS=0.1
      EETSM=0.005
      INDX=0.
                                 DO 711 I=2,MT
      RELB(I)=0.
      RELE(I)=0.
      IF (TCRATE .LE. 0.) GO TO 711
      GENB = GB(I)*VGASS/RVGAS
      GENE = GE(I)*VGASS/RVGAS
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      RELB(I) = RRB(I)/TCRATE*SULFUR.+GENB
      RELE(I) = RRE(I)/TCRATE*SULFUR+GENE
  711                          CONTINUE
                               DO 800 ITRY=1,20
      FS=ETS/CASE
C
C      FS : FRACTIONAL CONVERSION OF ADDITIVE
C     ASSUMING THE SULFUR CAPTURE EFFICIENCY,FS IS CALCULATED AND HENCE
C     THE LIMESTONE REACTIVITY. THEN,SO2 MATERIAL BALANCE IS PERFORMED.
C     FROM THE EXIT SO2 CONC. IN THE FLUE, SO2 CAPTURE EFFICIENCY IS
C     CALCULATED. ITERATION IS CONTINUED TILL THE ASSUMED AND THE
C     CALCULATED SULFUR DIOXIDE RETENTION EFFICIENCIES AGREE.
C
      AK=AKAD(FS,DPSVB,T(I))
C
C     SO2 BALANCE IN THE BED
C
                               DO 740 I=2,M1
      I1=I-1
      AM=(1.-EMF)
      CALL GPHASE(AK,AK,AM,PAV,RG,ETUBE(I),EPB(I),EPC(I),
     1AKBE(I),DVBB(I),FBM(I1),FEM(I1),FBM(I),FEM(I),T(I),T(I),T(I),
     2YB(I1),YE(I1),YB(I),YE(I),RELB(I),RELE(I))
      YSO2(I) = (FEM(I)*YE(I)+FBM(I)*YB(I))/FMO
  740                          CONTINUE
C
C     SO2 BALANCE IN THE FREEBOARD
C
                               DO 741 I = MP1,MT
      J = I-M1
      K = J+1
      RHOGAS = PAV*MGAS/RG/T(I)
      VISC = 3.72E-6*T(I)**0.676
      DPSVE = 0.5*(DPSE(J)+DPSE(K))
      DPWME = 0.5*(DPWE(J)+DPWE(K))
      CALL VEL(VISC,RHOGAS,G,RHOBED,DPSVE,UMFAV,UTAV)
      RT = (HB(K)-HB(J))/ABS(UO(I)-UTAV)
      WAHOLD(I) = (2.0*WEA(J)-WEA(K))*RT
      VAHOLD = WAHOLD(I)/RHOBED
      NA = VAHOLD*6.0/(PI*DPSVE**3)
      AK = AKAD(FS,DPSVE,T(I))
      ANR = FMO*YSO2(I-1)+RELB(I)+RELE(I)
      DR = FMO + NA*PI*DPSVE**3/6.0 *AK*PAV/RG/T(I)
      YSO2(I) = ANR/DR
 741                          CONTINUE
      ETSC=1.-FMO*YSO2(MT)/FRS
      EE=ETS-ETSC
      CALL CRRECT(ITRY,INDX,DETS,ETS1,ETS2,ETS,E1,E2,EE,EETSM)
      IF(INDX.EQ.2)GO TO 810
  800                          CONTINUE
      WRITE(6,3600)
 3600 FORMAT('0',10X,'   ETS HAS NOT CONVERGED. S.NO.  =  3600',/)
  810 CONTINUE
      YGO(3)=YSO2(MT)
      WRITE(6,2005)ETS,FS,CAS,CASE
     1,(H(I),YB(I),YE(I),ZAVG(I),YSO2(I),RELB(I),RELE(I),I=2,MT)
C
C     NOX CALCULATIONS
C
 811  IF (INOX .EQ. 0) GO TO 814
```

```
      FRN = WCOAL * (1.-XW) * XN/MN * FLOAT(IGNITE)
      ANITRO = WCOAL * (1.-XW) * XN * RN / MN - CLOSS*NCHAR/CCHAR/MN
                                   DO 750 I = 2,MT
      GENB = GB(I)*VGASN/RVGAS
      GENE = GE(I)*VGASN/RVGAS
      RELB(I) = RRB(I)/TCRATE * ANITRO +GENB
      RELE(I) = RRE(I)/TCRATE * ANITRO  + GENE
  750                              CONTINUE
      YB(1) = 0.0
      YE(1) = 0.0
      FR = 5.24E7
      AE = 34000.0
C
C     NOX BALANCE IN THE BED
C
                                   DO 760 I = 2,M1
      I1 = I-1
      TAVB = (T(I)+TPB(I))/2.0
      TAVE = (T(I)+TPE(I))/2.0
      AKB = FR*EXP( -AE/1.986/TAVB )
      AKE = FR * EXP( -AE/1.986/TAVE )
      AMODF = 6.0*RHOBED*(1.-EMF)/(DCSVB*RHOCH*CCHAR)
      AM = AMODF*X(I)
      CALL GPHASE ( AKB,AKE,AM,PAV,RG,ETUBE(I),EPB(I),EPC(I),AKBE(I),
     1DVBB(I),FBM(I1),FEM(I1),FBM(I),FEM(I),T(I),TAVB,TAVE,YB(I1),
     2YE(I1),YB(I),YE(I),RELB(I),RELE(I) )
      YNOX(I) = ( FBM(I)*YB(I)+FEM(I)*YE(I) )/FMO
  760                              CONTINUE
C
C     NOX BALANCE IN THE FREEBOARD
C
                                   DO 770 I = MP1,MT
      TAVB = (T(I)+TPB(I))/2.0
      J = I-M1
      K = J+1
      DCSVE = 0.5*(DCSE(J)+DCSE(K))
      X(I) = WCHOLD(I)*CCHAR/(WCHOLD(I)+WAHOLD(I))
      CARCON(I) = WCHOLD(I)*CCHAR/DVBBEF(I)
      VCHOLD = WCHOLD(I)/RHOCH
      NC = VCHOLD*6.0/(PI*DCSVE**3)
      AKNO =  FR*EXP(-AE/1.986/TAVB)
      ANR = FMO*YNOX(I-1) + RELB(I) + RELE(I)
      DR = FMO + NC*PI*DCSVE**2 *AKNO*PAV/RG/TAVB
      YNOX(I) = ANR/DR
  770                              CONTINUE
      ENOX = FMO*YNOX(MT)
      EINDEX = ENOX/WCOAL
      ETN = 1.0 - ENOX /FRN
      ENOX = ENOX/FMO
      WRITE (6,2007)EXAIR,TAV,ETN,ENOX,EINDEX,(H(I),YB(I),YE(I),X(I),
     1CARCON(I),ZAVG(I),YNOX(I),RELB(I),RELE(I),I=2,MT)
  751 CONTINUE
C      ============
C     MAIN OUTPUT 4
C      ============
  814 CONTINUE
      YGO(2)=YCO2(MT)
      YGO(4)=YH2O
      YGO(5)=YCO(MT)
      WRITE(6,2006) (YGO(I),I=1,5)
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        IF (HLMF.EQ.0.0) VMF = SOLVOL
        IF (HLMF .EQ. 0.0) HLMF = HEIGHT(VMF)
        IF (HLF .EQ. 0.0) HLF = H(M1)
        IF (IPRES .EQ. 0) GO TO 950
  900   CONTINUE
  C
  C     PRESSURE DROP CALCULATION
  C
  C     ******************************************
  C     ALL THE PRESSURE DROP GIVEN IN CM OF WATER
  C     ******************************************
  C
  C     PRESSURE DROP CALCULATIONS ACROSS THE DISTRIBUTOR
  C
        TEMP = T(2)
        RHOFG = PF * MGAS / (RG*TEMP)
        UOR = FMF * RG * TEMP/ PF /(AND*0.25*PI*DNZL**2)
        DPDIS = ( UOR/0.6 ) **2 * RHOFG / (2.0*G)
        WRITE (6,2050) DPDIS
  C
  C     PRESSURE DROP CALCULATIONS IN THE FLUDIZIED BED SECTION
  C
        WRITE (6,2051)
        N1 = M1
        IF (IFBC .GT. 0) N1 = M1 - 1
                                DO 920 I = 2,N1
        DPFLU    = (1.0-EMF)*(1.0-EPB(I))*(H(I)-H(I-1)) * RHOBED
        WRITE (6,2052) I, DPFLU
  920   CONTINUE
        IF (IFBC .EQ.0) GO TO 930
  C
  C     PRESSURE DROP CALCULATIONS IN THE FIXED BED SECTION
  C
        E1 = ( H(M1) - H(M1-1) ) / G
        E2 = ( 1.0 - EMF )  / EMF ** 3
        DPFIX = E1 * ( 150.0 * ( 1.0 - EMF ) * E2 * VISC * UO(M1)
       1 / DPSVB ** 2 + 1.75 * E2 * RHOGAS * UO(M1)**2/DPSVB)
  930   CONTINUE
        IF ( IFBC .EQ. 0 ) DPFIX = 0.0
        WRITE (6,2053) DPFIX
  950   CONTINUE
        WRITE (6,OC)
        WRITE (6,OPCF1)
        WRITE(6,2060)
                                DO 910 I = 2,M1
        WRITE(6,2070) I,H(I),ZAVG(I),DBAV(I),UB(I),EPB(I),EPC(I),UO(I),
       1UMF(I)
  910                           CONTINUE
        WRITE (6,2075)
                                 DO 940 I = 1,MT
        WRITE (6,2080) I,H(I),DT(I),AT(I)
  940                            CONTINUE
   1000 FORMAT(5I1)
   1001 FORMAT(8F10.0)
   1010 FORMAT(2A4/(8F10.0))
  2000  FORMAT ('0',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMGO = ',F6.3,10X,
       *'XSIO2 = ',F6.3,10X,'XCO2 = ',F6.3,/)
   2001 FORMAT(//10X,'RESULTS ,ALL TEMPERATURES IN CENTIGRADE'//
       *' ETC,XAV,TAV,ITRIAL,=',3E12.4,I4//
       12X,'I',6X,'HT',10X,'YB',10X,'YE',10X,'YVE',8X,'YCOE',7X,'YCO2E',
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      27X,'YCO2B',9X,'X',9X,'ZAVG',/(I3,1P9E12.4))
 2002 FORMAT (//2X,'I',6X,'HT',10X,'YO',10X,'YV',10X,'YCO',9X,'YCO2',
     *9X,'T',10X,'TPB',9X,'TPE',9X,'ZAVG',/,(I3,1P9E12.3))
 2005 FORMAT('0',' (ETS,FS,CAS,CASE)='/10X,4E13.4,/,'0',7X,'HT.',8X,
     1'YSO2B',8X,'YSO2E',9X,'ZAVG',10X,'YSO2',10X,'RELB',9X,'RELE',/,
     2(1P7E13.4))
 2006 FORMAT(/' OUTLET GAS CONCENTRATION' ,//5X,'O2',10X,'CO2',9X,'SO2',
     19X,'H2O',9X,'CO',/5E12.4//)
 2007 FORMAT('0',7X,'EXAIR,TAV,ETN,ENOX,EINDEX =',/,10X,5E12.4,/,'0',
     17X,'HT',8X,'YNOXB',8X,'YNOXE',9X,'X',11X,'CARCON',8X,'ZAVG',8X,
     2'YNOX',10X,'RELB',9X,'RELE',/,(1P9E13.4))
 2010 FORMAT ('0',5X,'SURFACE VOL MEAN DIA.OF ADDITIVES FEED = DASVF =
     *',F10.4,3X,'CM',5X,'WEIGHT MEAN DIA. = DAWMF = ',F10.4,3X,'CM',/)
 2020 FORMAT ('0',1X,2A4,3X,'XCF = ',F5.3,3X,'XCV = ',F5.3,3X,'XH = ',
     *F5.3,3X,'XN = ',F5.3,3X,'XS = ',F5.3,3X,'XO = ',F5.3,3X,'XW = ',
     $F5.3,3X,'XW = ',F5.3,/,'0',12X,'VM = ',F5.3,4X,'V = ',F5.3,3X,
     $'HCOAL = ',F8.2,3X,'CALS/GM',3X,'XACAO = ',F5.3,/)
 2030 FORMAT ('0',T5,'K',T10,'FREEBOARD HT.',T29,'DPSE',T43,'DPWE',
     1T55,'WEA',T70,'DCSE',T85,'DCWE',T100,'WEC',/,'0',(T4,I2,T10,
     21PE11.3,T26,1PE11.3,T39,1PE11.3,T52,1PE11.3,T67,1PE11.3,T81,
     31PE11.3,T96,1PE11.3))
 2040 FORMAT('0',T21,'SURFACE VOL MEAN DIA OF COAL FEED = DCSVF = ',
     *F10.4,3X,'CM',5X,'WT.MEAN DIA. = DCWMF = ',F10.4,3X,'CM',/)
 2050 FORMAT ('0',40X,'PRESSURE DROP ACROSS THE DISTRIBUTOR = ',1PE11.4)
 2051 FORMAT ('0',20X,'COMP.NO',13X,'PRESSURE DROP IN THE BED',/)
 2052 FORMAT (20X,I5,20X,1PE11.4)
 2053 FORMAT ('0',40X,'PRESSURE DROP IN THE FIXED BED SECTION = ',1PE11.
     *4)
 2060 FORMAT ('0',3X,'I',3X,'HEIGHT',6X,'ZAVG',3X,'AV.BUBBLE DIA',6X,
     1'BUBBLE VEL.',4X,'BUBBLE FRAC.',5X,'CLOUD FRAC.',6X,'SUP.VELOCITY'
     2,5X,'MIN.FLU.VEL.',/)
 2070 FORMAT (I5,F8.3,2X,F8.3,6(3X,1PE12.4,2X))
 2075 FORMAT ('0',T10,'COMPT.NO.',T25,'HEIGHT',T42,'BED DIA.',T55,
     1'BED C/S AREA',/)
 2080 FORMAT (T12,I3,T25,F6.2,T40,1PE10.3,T55,1PE10.3)
10000 STOP
      END
      FUNCTION AKAD(FS,DP,T)
C
C     THIS SUBROUTINE CALCULATES  LIMESTONE-SO2  REACTION RATE CONSTANT
C
      DIMENSION FB(15),RR(15),RB(15),RC(15)
      DATA FB/0.0,0.05,0.1,0.2,0.25,0.3,0.35,0.4,0.425,0.45,0.475,0.5,
     *0.525,0.55,0.6 /
      DATA RR/1.0,0.231,0.16,0.038,0.001,0.0004,0.0003,0.00022,0.0002,
     10.00018,0.00016,0.00015,0.00014,0.00013,0.00011 /
      DATA RB/1.0,0.584,0.515,0.337,0.213,0.095,0.022,0.0071,0.006,
     1 0.005,0.004,0.0036,0.003,0.00275,0.00225 /
      DATA RC/1.0,0.938,0.894,0.802,0.749,0.687,0.609,0.51,0.445,0.367,
     1 0.272,0.18,0.121,0.076,0.022 /
      DP1=0.2
      DP2=0.1
      DP3=0.01
      IF(DP .GE. DP2 ) XXX=ALOG(DP/DP2)/ALOG(DP1/DP2)
      IF( DP .LT. DP2) XXX=ALOG(DP/DP3)/ALOG(DP2/DP3)
      ALIME=0.0
      AKAD = 0.0
      IF( FS .GE. 1.0) RETURN
                                  DO 10 I=2,13
      N=I
```

```
      IF( FS .LE. FB(I) ) GO TO 11
   10 CONTINUE
   11 CONTINUE
      N1=N-1
      A=(FS-FB(N1))/(FB(N)-FB(N1))
      IF( DP .LT. DP2) GO TO 12
      R1=(RR(N)/RR(N1))**A*RR(N1)
      R2=(RB(N)/RB(N1))**A*RB(N1)
      GO TO 13
   12 CONTINUE
      R1=(RB(N)/RB(N1))**A*RB(N1)
      R2=(RC(N)/RC(N1))**A*RC(N1)
   13 CONTINUE
      ALIME=(R1/R2)**XXX*R2
      IF( ALIME .GT. 1.0) ALIME=1.0
      IF (T .LT.1253.0) SG = 35.9*T - 3.67E04
      IF (T .GE. 1253.0) SG = -38.43*T + 5.64E04
      IF ( SG .LT. 100.0 ) SG = 100.0
      AKAD = 490.0*EXP(-17500.0/1.987/T)* SG * ALIME
      RETURN
      END
      SUBROUTINE AKK(AKR,T,P,DC,TP,YO2,RG,MC,AKCO2,PHI)
      REAL MC
C
C     THIS COMPUTES REACTION RATE CONSTANT FOR CHAR COMBUSTION AKR,
C     RATE CONSTANT FOR C-CO2 REACTION AND THE CHAR PARTICLE TEMPERATURE
C
      EM=1.0
      SIGM=1.36E-12
      INDX=0
      DTS= 200.0
      TP=300.0
                                DO 100 I=1,20
      ETSMAX=0.005*TP
      AKS=8710.0*EXP(-35700.0/1.986/TP)
      TAV = (T+TP)*.5
      D=4.26*(TAV/1800.)**1.75/P
      COND=0.632E-5*SQRT(TAV)/(1.+245./TAV*10.**(-12./TAV))
      Z = 2500. * EXP(-12400./1.986/TAV)
      IF (DC .LE. 0.005) PHI = (2.*Z+2.)/(Z+2.)
      IF (DC .GT. 0.005 .AND. DC .LE. 0.10) PHI = 1./(Z+2.)*((2.*Z+2.)
     * - Z*(DC-0.005)/0.095)
      IF (DC .GT. 0.10) PHI = 1.0
      Q = 7900.0*(2./PHI-1)+2340.0*(2.-2./PHI)
      AKF=24.*PHI*D/(DC*RG*TAV)
      AKR=(RG*TAV/MC)/(1./AKS+1./AKF)
      RHS = AKR*P*YO2*MC*Q/(RG*TAV) - EM*SIGM*(TP**4-T**4)
      ETS = TP - T - RHS*DC/(2.0*COND)
      CALL CRRECT(I,INDX,DTS,TP1,TP2,TP,E1,E2,ETS,ETSMAX)
      IF (INDX.EQ.2) GO TO 110
  100 CONTINUE
      WRITE (6, 4000) TP,ETS
 4000 FORMAT ('0',10X,'TP CALCULATION HAS NOT CONVERGED',/,10X,'TP,ETS -
     1 ',1P2E12.3)
  110 CONTINUE
      AKRCO2 = 4.1E08*EXP(-59200./1.987/TAV)
      D = 3.26*(TAV/1800.)**1.75/P
      AKFCO2 = 2.*PHI*D/DC
      AKCO2 = 1./(1./AKRCO2+1./AKFCO2)
      RETURN
```

```
      END
      SUBROUTINE AREA ( ZI, DTI, ATI )
      COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
     2UO(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKBE(60),YB(60),
     3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
     4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
      COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
     1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
     2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
     3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFBC,NTC
C
C     CALCULATION OF THE CROSS SECTIONAL AREA GIVEN THE HEIGHT ABOVE
C     THE DISTRIBUTOR
C
                                DO 10 J = 1 , MTP
      IF ( ZI .GT. ZB(J) ) GO TO 10
      RJM1 = SQRT ( ATB(J-1) / PI )
      A1 = ( ZI - ZB(J-1) ) / ( ZB(J) - ZB(J-1) )
      B1 = SQRT ( ATB(J) / ATB(J-1) ) - 1.0
      RI = ( 1.0 + A1 * B1 ) * RJM1
      DTI = 2.0 * RI
      ATI = PI * RI ** 2
      GO TO 20
10                              CONTINUE
20    CONTINUE
      RETURN
      END
      SUBROUTINE CRRECT(I,INDX,DX,X1,X2,XNEW,E1,E2,E,EMAX)
C     I: NUMBER OF THIS TRIAL, 1 FOR FIRST TRIAL
C     INDX: INDEX OF THE TRIAL LEVEL
C     INDX=0: JUST PROCEEDING
C     INDX=1: THE ROOT HAS BEEN CAUGHT BETWEEN X1 AND X2
C     INDX=2: THE ITERATION HAS CONVERGED
      IF (ABS(E).GT.EMAX) GO TO 5
      INDX=2
      RETURN
    5 CONTINUE
      IF(INDX.EQ.1) GO TO 100
      X2=XNEW
      E2=E
      IF(I.EQ.1) GO TO 10
      IF(E1*E2.LE.0.)INDX=1
      IF(INDX.EQ.1)GO TO 150
   10 X1=X2
      E1=E2
      XNEW=XNEW+DX
      RETURN
  100 CONTINUE
      IF(E1*E.LT.0.) GO TO 110
      E1=E
      X1=XNEW
      GO TO 150
  110 E2=E
      X2=XNEW
  150 CONTINUE
      XNEW=(X1-X2)*E2/(E2-E1)+X2
      RETURN
      END
      SUBROUTINE DESIGN
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      COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
     2UD(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKBE(60),YB(60),
     3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
     4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
      COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
     1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
     2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
     3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFRC,NTC
C
C     AXIAL VARIATION OF BED CROSS SECTION
C
      READ (5,1000) A1,A2,A3,A4
      READ (5,1001) MTB,(ZB(J),ATB(J), J = 1, MTB)
C
C     IARRNG        1            2            3
C     1 -----    VERTICAL INLINE ARRANGEMENT
C     2 -----    VERTICAL STAGGERED ARRANGEMENT
C     3 -----    HORIZONTAL INLINE ARRANGEMENT
C     4 -----    HORIZONTAL STAGGERED ARRANGEMENT
C
C
C     HEAT EXCHANGE TUBES
      READ (5,1002) MTHE,(ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),
     1IARR(J), J = 1,MTHE)
C
C     LOCATION OF FEED AND DISCHARGE
      READ (5,1001) MFEED,(ZF(J),FFC(J),FFAD(J), J = 1,MFEED)
C
      READ (5,1001) MDIS,(ZDIS(J),FD(J), J = 1,MDIS)
C
C     DISTRIBUTOR
C
      READ (5,1003) AND , DNZL , FW , FSW
                              DO 100 J = 1, MTHE
      IF (AHE(J) .GT. 0.0) GO TO 100
      IF (DTUBE(J) .EQ. 0.0) GO TO 100
      AHE(J) = PI * DTUBE(J) / (PH(J)*PV(J))
100                           CONTINUE
C
C     CONDITION FOR COMPUTING AVERAGE CELL SIZE
C
      WRITE (6,2000) A1,A2,A3,A4
      WRITE (6,2001)
      WRITE (6,2002) (ZB(J),ATB(J), J = 1,MTB)
      WRITE (6,2003)
      WRITE (6,2004) (ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),IARR(J),
     1J = 1,MTHE)
      WRITE (6,2005)
      WRITE (6,2006) (ZF(J),FFC(J),FFAD(J), J = 1,MFEED)
      WRITE (6,2007)
      WRITE (6,2008) (ZDIS(J),FD(J), J = 1,MDIS)
      WRITE (6,2009) AND,DNZL,FW,FSW
      Z1 = ZB(1)
      ABED1 = ATB(1)
      DBED1 = SQRT(4.0 * ABED1 / PI)
      DVB(1) = 0.0
      DVBEFF(1) = 0.0
      ZHE(1) = 0.0
      DZAV = 30.0
```

```
      NTC = IFIX(ZB(MTB)/DZAV)+1
                                  DO 10 I = 1,NTC
      Z2 = Z1 + DZAV
      IF (I.EQ.NTC) Z2 = ZB(MTB)
                                  DO 20 J = 1,MTHE
      IF ( ZHE(J) .LE. Z1 .AND. ZHE(J+1) .GE. Z2 ) GO TO 30
      IF ( ZHE(J) .LE. Z2 .AND. ZHE(J+1) .LT. Z2 ) GO TO 20
      F1 = ( Z2 - ZHE(J) ) / DZAV
      F2 = ( ZHE(J) - Z1 ) / DZAV
      AH = F1 * AHE(J) + F2 * AHE(J-1)
      DIAT = F1 * DTUBE(J) + F2 * DTUBE(J-1)
      GO TO 40
30    AH = AHE(J)
      DIAT = DTUBE(J)
40    CONTINUE
      GO TO 50
20                                CONTINUE
50    CONTINUE
      CALL AREA ( Z2,DBED,ABED )
      DVB(I+1) = 0.5 * (ABED+ABED1) * DZAV
       DVBEFF(I+1) = DVB(I+1) * (1.0 - 0.25 * AH * DIAT)
      Z1 = Z2
      ABED1 = ABED
10                                CONTINUE
1000  FORMAT (4A4)
1001  FORMAT (I1/(8F10.0))
1002  FORMAT (I1/(5F10.0,I10))
1003  FORMAT (8F10.0)
2000  FORMAT ('1',20X,4A4,//)
2001  FORMAT ('0',T41,'HT.ABOVE DISTRIBUTOR,CM',T91,'CROSS SECTIONAL ',
     1'AREA OF BED,SQ.CM.',/)
2002  FORMAT (T49,F8.4,T96,F10.3)
2003  FORMAT ('0',T6,'HEIGHT,CM',T20,'SP.HEAT TRANS.AREA,SQ.CM/CU.CM',
     1T58,'DIA.OF TUBES,CM',T78,'VER.PITCH,CM',T95,'HOR.PITCH,CM',
     2T113,'TUBES ARRNGT',/)
2004  FORMAT (T8,F6.2,T33,F8.4,T62,F6.3,T82,F6.3,T99,F6.3,T118,I2)
2005  FORMAT ('0',T21,'SOLIDS FEED LEVEL',T51,'FRACTION COAL FED',
     1T81,'FRACTION LIMESTONE FED',/)
2006  FORMAT (T27,F6.2,T58,F6.4,T88,F6.4)
2007  FORMAT ('0',T21,'SOLIDS DISCHARGE LEVEL',T51,'FRACTION DISCHARGED'
     1,/)
2008  FORMAT (T29,F6.2,T58,F6.4)
2009  FORMAT ('0', T12,'NO.OF DISTRIBUTOR HOLES ',T40,'=',T45,F5.1,/,
     1'0',T12,'NOZZLE DIAMETER ',T40,'=',T45,F7.4,3X,'CM'/'0',T12,
     4'FW',T40,'=',T45,F6.3,/,'0',T12,'FSW',T40,'=',T45,F6.3)
      RETURN
      END
      SUBROUTINE FBC(YH2O,ANC,DCSVE,DVBB,ETUBE,FMO,GB,COB,GE,NC,
     1PAV,PHIB,PI,RG,RVGAS,T,TAVB,XO2,YCO0,YCO,YO0,YO,YVO,YV,[illegible]O2,
     2COVB,CO2VB,YCO20,YCO2)
      REAL NC
C
C     THIS SUBPROGRAM PERFORMS THE GAS PHASE MATERIAL PALANCE FOR
C     O2,CO,CO2 IN THE FREEBOARD
C
      A2 = PAV/RG/TAVB*NC*PI*DCSVE**2*ANC
      A4 = PAV/RG/TAVB*NC*PI*DCSVE**2*ANCO2
      YV = YVO-YO0/XO2
      IF (YV .LT. 0.0) GO TO 100
      YO = 0.0
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      C
      C      OXYGEN S[illegible]
      C
             YCO2 = FMO*YCO20/(FMO+A4)
             YCO = YCO0+2.0*A4*YCO2/FMO+(YVO-YV)*COVB
             GB = 0.0
             GE = FMO*(YVO-YV)
             COB = 0.0
             RETURN
      100    CONTINUE
      C
      C      OXYGEN RICH CONDITION
      C
             YV = 0.0
             AKP = 3.E10*EXP(-16000./1.987/T)*(PAV/RG/T)**1.8*YH2O**0.5*DVBB*
            1(1.-ETUBE)
             INDEX = 0
             YO = 0.0
             DYO = 0.01
             EYO = 0.001
                                        DO 110 I = 1,20
             ANR = FMO*YCO0+2.0*A4/(FMO+A4)*(FMO*YCO20+A2*YO*(2./PHIB-1.))+
            1FMO*YVO*COVB+A2*YO*(2.-2./PHIB)
             DR = FMO+AKP*(17.5*YO/(1.+24.7*YO))
            1-2.0*A4*AKP*(17.5*YO/(1.+24.7*YO))/(FMO+A4)
             YCO = ANR/DR
             IF (YCO .LT. 1.E-6) GO TO 130
             YCO2 = (FMO*YCO20+A2*YO*(2./PHIB-1.)
            1+AKP*YCO*(17.5*YO/(1.+24.7*YO)))/(FMO+A4)
             YOC = YO0-YVO*XO2-AKP*YCO*(17.5*YO/(1.+24.7*YO))/2.0/FMO
            1-A2*YO/PHIB/FMO
             GO TO 140
      130    CONTINUE
             YCO = 0.0
             YCO2 = (FMO*YCO20+A2*YO+FMO*YCO0)/(FMO)
             YOC = YO0-YVO*XO2-YCO0/2.0-A2*YO/FMO
      140    CONTINUE
      C      WRITE(6,190) I,YCO,YCO2,YO,YOC
      C190   FORMAT(5X,'I,YCO,YCO2,YO,YOC - ',I4,1P4E12.3)
             IF (YOC. LT. 0.0) YOC = 0.0
             IF (YCO2 .LT. 0.0) YCO2 = 0.0
             ER = YO - YOC
             CALL CRRECT (I,INDEX,DYO,X1,X2,YO,E1,E2,ER,EYO)
             IF (INDEX .EQ. 2) GO TO 120
      110                                   CONTINUE
             WRITE (6,1000) YO,YOC,YO0
      1000   FORMAT ('0',10X,'YO HAS NOT CONVERGED. SUBROUTINE FBC',/,10X,'YO,
            1YOC,YO0 = ',1P3E12.3)
             YE = YEO
      120    GB = 0.0
             GE = FMO*YVO
             COB = AKP*YCO*(17.5*YO/(1.+24.7*YO))
             IF (YCO .EQ. 0.0) COB = FMO*YCO0
             IF (YO .GT. YOC) YO = YOC
             RETURN
             END
             SUBROUTINE GPB (YH2O,AKB,AKE,AKBE,AMODF,DVBB,EMF,EPB,EPC,ETUBE,
            1FBMO,FBM,FEMO,FEM,GB,COB,GE,PAV,PHIE,RG,RVGAS,T,TAVB,TAVE,
            2VPROD,X,XO2,XO2C,YBO,YB,YCOEO,YCOE,YEO,YE,YVEO,YVE,AKCO2,COV,CO2V,
            3COVB,CO2VB,YCO2BO,YCO2B,YCO2EO,YCO2E)
```

```
      DIMENSION A(25),B(5),AA(16),BB(4)
C
C     THIS SUBPROGRAM FORMS THE HEART OF THE CALCULATIONS FOR THE
C     GAS PHASE BALANCES IN THE BED
C
      A1 = AKBE*DVBB*EPB*PAV/(RG*T)
      A2 = AMODF*DVBB*(EPC-EPB)*AKB*PAV / (RG*TAVB) * X
      A3 = AMODF*DVBB*(1.-EPC-ETUBE)*AKE*PAV/(RG*TAVE)*X
      A4 = AMODF*DVBB*(1.-EPC-ETUBE)*AKCO2*PAV/(RG*TAVE)*X
      DO 150 I = 1,25
C
C     OXYGEN CONCENTRATION IN EMULSION PHASE IS ZERO.
C
150   A(I) = 0.0
      A(1) = FEM + A1
      A(4) = -A1*CO2VB
      A(5) = A1*XO2C
      A(7) = A(1)
      A(9) = -A1
      A(10) = A1/2.0
      A(12) = -2.0*A4
      A(13) = FEM + A1 + A4
      A(14) = -A1
      A(18) = -A1
      A(19) = FBM + A1
      A(21) = A1/XO2
      A(22) = -A1*COVB/XO2
      A(24) = -A2
      A(25) = FBM + A1 + A2
      B(1) = FEMO*YVEO-FEMO*YEO/XO2+VPROD
      B(2) = FEMO*YCOEO+FEMO*YEO*COVB/XO2+VPROD*COV
      B(3) = FEMO*YCO2EO+VPROD*CO2V
      B(4) = FBMO*YCO2BO
      B(5) = FBMO*YBO
      CALL SIMQ(A,B,5,25,KS)
      YVE = B(1)
      IF (YVE .LE. 0.0) GO TO 10
      YE = 0.0
      YCOE = B(2)
      YCO2E = B(3)
      YCO2B = B(4)
      YB = B(5)
      GE = (FEMO*YEO+A1*YB)/XO2
      GB = A1*YVE
      COB = A1*YCOE
      GO TO 60
10    CONTINUE
C
C     OXYGEN CONCENTRATION IN EMULSION PHASE IS LARGE ENOUGH TO BURN
C     THE VOLATILES RELEASED IN THAT COMPARTMENT
C
      YVE = 0.0
      AKP = 3.E10*EXP(-16000./1.987/T)*(PAV/RG/T)**1.8*YH2O**0.5*DVBB*
     1(1.-EPC-ETUBE)*EMF
      INDX = 0
      YE = 0.0
      DYE = 0.01
      IF (YEO .LE. 0.05) DYE = 0.002
      IF (YEO .LE. 0.025) DYE = 0.001
      EMAX = 0.01
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      DO 160 I = 1,16
  160 AA(I) = 0.0
      DO 50 I = 1,50
      AA(1) = FEM + A1 + AKP*(17.5*YE/(1.+24.7*YE))
      AA(2) = -AKP*(17.5*YE/(1.+24.7*YE))
      AA(3) = -A1
      AA(4) = A1/2.0
      AA(5) = -2.0*A4
      AA(6) = FEM+A1+A4
      AA(7) = -A1
      AA(10) = -A1
      AA(11) = FBM+A1
      AA(15) = -A2
      AA(16) = FBM + A1 + A2
      BB(1) = FEMO*YCOEO+(FEMO*YVEO+VPROD)*COVB+VPROD*COV+A3*
     1(2.-2./PHIE)*YE
      BB(2) = FEMO*YCO2EO+VPROD*CO2V+A3*(2./PHIE-1.)*YE
      BB(3) = FBMO*YCO2BO
      BB(4) = FBMO*YBO+A1*YE
      CALL SIMQ(AA,BB,4,16,KS)
      YCOE = BB(1)
      YCO2E = BB(2)
      YCO2B = BB(3)
      YB = BB(4)
      ANR = FEMO*YEO-A1*(YE-YB)-A3*YE/PHIE-(FEMO*YVEO+VPROD)*XO2-
     1AKP*YCOE*(17.5*YE/(1.+24.7*YE))/2.0
      YEC = ANR/FEM
      IF (YEC .LT. 0.0) YEC = 0.0
      IF (YEC .EQ. 0.0 .AND. YEO .LT. 0.005) YE = 0.0
      ER = YE-YEC
      CALL CRRECT(I,INDX,DYE,X1,X2,YE,E1,E2,ER,EMAX)
      IF (INDX .EQ. 2) GO TO 60
   50 CONTINUE
      WRITE (6,1000) YE,YEC,YB,YBO,YEO
 1000 FORMAT ('0',10X,'YE HAS NOT CONVERGED. SUBROUTINE GPB',/,10X,'YE,
     1YEC,YB,YBO,YEO = ',1P5E12.3)
      YE = YEO
   60 CONTINUE
      IF (YE .LT. 0.0) YE = 0.0
      IF (YE .GT. YEC) YE = YEC
      IF (YB .LT. 0.0) YB = 0.0
      IF (YCO2B .LT. 0.0) YCO2B = 0.0
      IF (YCO2E  .LT. 0.0) YCO2E = 0.0
      GE = FEMO*YVEO + VPROD
      GB = 0.0
      COB = AKP*YCOE*(17.5*YE/(1.+24.7*YE))+A1*YCOE
      RETURN
      END
      SUBROUTINE GPHASE(AKB,AKE,AM,PAV,RG,ETUBE,EPB,EPC,AKBE,DVBP,FBMO,
     *FEMO,FBM,FEM,T,TB,TE,YBO,YEO,YB1,YE1,GENB,GENE)
C
C     THIS SUBPROGRAM IS USED TO CALCULATE THE SO2 AND NOX
C     CONCENTRATIONS IN THE BED
C
      D1= ((1.-ETUBE-EPC)*AM*AKE/TE+AKBE*EPB/T)*PAV/RG*DVBP+FEM
      ALF=AKBE*EPB*DVBP*PAV/(D1*RG*T)
      D2 = FBM+ALF*FEM+((EPC-EPB)*AKB/TB+
     1ALF*(1.0-EPC-ETUBE)*AKE/TE)*DVBB*AM*PAV/RG
      IF (D2 .EQ. 0.0) YB1 = 0.0
      IF (D2 .NE. 0.0) YB1=(FBMO*YBO+GENB+ALF*FEMO*YEO)/D2
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      YE1=(YEO*FEMO+GENE)/D1+ALF*YB1
      RETURN
      END
      SUBROUTINE HAREA ( ATI, DTI, ZI )
      COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
     2UO(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKBE(60),YB(60),
     3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
     4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
      COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
     1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
     2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
     3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFBC,NTC
C
C     CALCULATION OF THE HEIGHT GIVEN THE CROSS SECTIONAL AREA
C
      RI = SQRT ( ATI / PI )
      DTI = 2.0 * RI
                                  DO 10 J = 1 , MTB
      IF ( ATI .GT. ATB(J) )  GO TO 10
      A1 = SQRT ( ATI / ATB(J-1) ) - 1.0
      B1 = SQRT ( ATB(J) / ATB(J-1) ) - 1.0
      C = ZB(J) - ZB(J-1)
      ZI = ZB(J-1) + A1 * C / B1
      GO TO 20
   10                             CONTINUE
   20 CONTINUE
      RETURN
      END
      FUNCTION HEIGHT (VV)
      COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
     2UO(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKBE(60),YB(60),
     3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
     4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
      COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
     1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
     2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
     3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFBC,NTC
C
C     CALCULATION OF THE HEIGHT GIVEN THE EFFECTIVE VOLUME OF THE BED
C     (EXCLUDING THE VOLUME OCCUPIED BY THE TUBES)
C
      HT = 0.0
      SUM = 0.0
                                  DO 100 I = 2 , NTC
      SUM = SUM + DVBEFF(I)
      HT = HT + DZAV
      IF ( SUM .LT. VV )  GO TO 100
      HT = ( VV - SUM ) * DZAV / DVBEFF(I) + HT
      GO TO 110
  100                             CONTINUE
  110 CONTINUE
      HEIGHT = HT
      RETURN
      END
      SUBROUTINE HYDRO
      REAL MGAS
      COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
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          2UO(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKPE(60),YB(60),
          3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
          4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
           COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
          1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
          2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
          3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFBC,NTC
           COMMON /C/ DPSE(30),DPWE(30),DCSE(30),DCWE(30),WEA(30),WEC(30),
          1HB(30),WCHOLD(30),WAHOLD(30),KT
           DIMENSION DTUBEI(60),PHI(60),PVI(60),IARRNG(60)
C
C          CALCULATION OF BUBBLE HYDRODYNAMICS
C
           LAST = 0
           SUM=0.0
           SUMEFF=0.0
           BEDVOL = 0.0
           SUMV = 0.0
           ICR = 0
           HCR = 0.0
           IFBC = 0
           DTUBEI(1) = 0.0
           DBAV(1) = 0.0
           H(1) = 0.0
           AT(1) = ATB(1)
           DT(1) = SQRT(4.0*AT(1)/PI)
           DVBB(1)= 0.0
           DVBBEF(1) = 0.0
           IARRNG(1) = 0.0
           ETUBE(1) = 0.0
           ETUBE(2) = 0.0
           RHOGAS = PAV*MGAS/(RG*T(2))
           VISC = 3.72E-6*T(2)**0.676
           A1 = 33.7**2+0.0408*DPSVB**3*G*(RHOBED-RHOGAS)*RHOGAS/VISC**2
           UMF(2) = VISC/(DPSVB*RHOGAS) * (SQRT(A1)-33.7)
           UMF(1) = UMF(2)
           UO(2) = FMF*MGAS/RHOGAS/(AT(1)*(1.-ETUBE(2)))
           DBO = 0.347*(AT(1)*(1.-ETUBE(2))*(UO(2)-UMF(2))/AND)**0.4
           DBA = DBO
           H(2) = DBO
C
C          ASSUMING THE COMPARTMENT SIZE, BUBBLE SIZE IS COMPUTED IN THAT
C          COMPARTMENT. ITERATION IS CONTINUED TILL THE ASSUMED COMPARTMENT
C          SIZE AND THE CALCULATED BUBBLE SIZE IN THAT COMPARTMENT AGREE
C
                                      DO 200 I = 2,100
           IF (I .EQ. 2) GO TO 16
           DDB = 5.0
           INDEX = 0
           EMAX = 0.1
           DBA = H(I-1)-H(I-2)
16                                    DO 250 K = 1,30
           IF (I .LE. M1) GO TO 5
           T(I) = T(M1)
           X(I) = X(M1)
           YB(I) = YB(M1)
           YE(I) = YE(M1)
5          CONTINUE
           H(I) = H(I-1) +  DBA
C
```

```
C      IDENTIFICATION OF COOLING TUBES IN THE COMPARTMENT
C
       DO 210 J = 1,MTHE
       IF (ZHE(J) .LE. H(I) .AND. ZHE(J+1) .LT. H(I)) GO TO 210
       IF (ZHE(J) .LE. H(I-1) .AND. ZHE(J+1) .GE. H(I)) GO TO 220
       F1 = (H(I)-ZHE(J))/DBA
       F2 = (ZHE(J)-H(I-1))/DBA
       AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)
       DTUBEI(I) = F1*DTUBE(J)+F2*DTUBE(J-1)
       GO TO 230
220    AHEAV(I) = AHE(J)
       DTUBEI(I) = DTUBE(J)
230    PVI(I) = PV(J)
       PHI(I) = PH(J)
       IARRNG(I) = IARR(J)
       GO TO 240
210    CONTINUE
240    CALL AREA(H(I),DT(I),AT(I))
       HAV = 0.5*(H(I-1)+H(I))
       CALL AREA (HAV,DTAV,ATAV)
       DVBB(I) = 0.5*(AT(I-1)+AT(I))*DBA
       DVBBEF(I) = DVBB(I)*(1.-0.25*AHEAV(I)*DTUBEI(I))
       ETUBE(I) = 1.0 - DVBBEF(I)/DVBB(I)
       IF (I .EQ. 2) GO TO 260
       RHOGAS = PAV*MGAS/(RG*T(I))
       VISC = 3.72E-6*T(I)**0.676
       A1 = 33.7**2+0.0408*DPSVB**3*G*(RHOBED-RHOGAS)*RHOGAS/VISC**2
       UMF(I) = VISC/(DPSVB*RHOGAS)*(SQRT(A1)-33.7)
       UO(I) = FMO*MGAS/RHOGAS/(ATAV*(1.-ETUBE(I)))
       IF (IFBC .GT. 0) GO TO 125
       IF (ABS(UO(I)-UMF(I)) .LE. 0.01*UMF(I)) GO TO 18
       IF (UO(I) .LT. UMF(I)) GO TO 10
       GO TO 17
18     ICR = 1
17     DBMAX = 0.652*(ATAV*(1.-ETUBE(I))*ABS(UO(I)-UMF(I)))**0.4
       IF (DBMAX .GT. DTAV) DBMAX = DTAV
       DBC = DBMAX - (DBMAX-DBO)*EXP(-0.3*HAV/DTAV)
       IF (IARRNG(I).GT.2 .AND. PHI(I).GE.DBAV(I-1) .AND. DBC.GE.
      1PHI(I))  DBC = PHI(I)
       IF (LAST .GT. 0) GO TO 260
       ER = DBC - DBA
       IF(K .EQ. 1.AND. DBC .LT. DBA) DDB = -DDB/2.0
       CALL CRRECT (K,INDEX,DDB,X1,X2,DBA,E1,E2,ER,EMAX)
       IF (INDEX .EQ. 2) GO TO 260
250    CONTINUE
260    CONTINUE
       DBAV(I) = DBA
       AKBE(I) = 11.0/DBAV(I)
C
C      CALCULATIONS FOR UBR --- BUBBLE RISING VEL.AT MIN.FLUDIZATION,
C                       UBS --- BUBBLE VEL. AT SLUGGING CONDITIONS,
C                       UB ---- ABS.BUBBLE RISING VELOCITY,
C                       EPB --- BUBBLE FRATION,
C                       EPC --- CLOUD FRACTION
C
       UBR = 0.711 * SQRT ( G * DBAV(I) )
       UBS = 0.355 * SQRT ( G * DTAV )
       IF (UBR .GT. UBS) UBR = UBS
       UB(I) = UO(I)-UMF(I)+UBR
       EPB(I) = ( UO(I)-UMF(I) ) / UB(I)*(1.0-ETUBE(I))
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      ALFB = EMF * UBR / UMF(I)
      EPC(I) = EPB(I) * ALFB / ( ALFB - 1.0 )
      IF (EPB(I) .GT. 0.7) EPB(I) = 0.7
      IF (EPC (I) .GT. (0.99 - ETUBE(I)) ) EPC(I) = 0.99 - ETUBE(I)
      IF ( (EPC(I)-EPB(I)) .GT. 0.01) EPC(I) = EPB(I) + 0.01
      BEDVOL = BEDVOL + DVBB(I)
      SUMV = SUMV + DVBBEF(I)
      SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)
      SUMEFF = SUMEFF + SOLVOL
      SUM = SUM + SOLVOL / ( 0.5 * (AT(I)+AT(I-1)) )
      IF (ICR .GT. 0) GO TO 35
      IF (LAST .GT. 0) GO TO 125
      IF (HLF .NE. 0.0) GO TO 20
C
C     TEST FOR CONVERGENCY
C
      IF (ABS(SUMEFF-VMF) .LT. 0.01*VMF) GO TO 125
      IF (SUMEFF .LT. VMF) GO TO 200
      VOL = SUMV-(SUMEFF-VMF) * (1.0 - ETUBE(I)) / (1.0-EPB(I)-ETUBE(I))
      H(I) = HEIGHT(VOL)
      CALL AREA ( H(I),DT(I),AT(I) )
      BEDVOL = BEDVOL - DVBB(I)
      SUMV = SUMV - DVBBEF(I)
      SUMEFF = SUMEFF - SOLVOL
      SUM = SUM - SOLVOL / (0.5*(AT(I)+AT(I-1)))
      LAST = 1
      DBA = H(I)-H(I-1)
      GO TO 16
   20 CONTINUE
C
C     TEST FOR CONVERGENCY
      IF (ABS(H(I)-HLF) .LE. 1.0E-3*HLF) GO TO 125
      IF (ABS(H(I)-HLF) .LE. 0.5 * (H(I)-H(I-1))) GO TO 50
      IF (H(I) .LT. HLF) GO TO 200
   50 H(I) = HLF
      BEDVOL = BEDVOL - DVBB(I)
      SUMV = SUMV - DVBBEF(I)
      SUMEFF = SUMEFF - SOLVOL
      SUM = SUM - SOLVOL / (0.5*(AT(I) + AT(I-1)))
      CALL AREA ( H(I),DT(I),AT(I) )
      LAST = 1
      DBA = H(I)-H(I-1)
      GO TO 16
   10 UO(I) = UMF(I)
      ATAV  = FMO * RG * T(I) / ( PAV * UO (I) * (1.0-ETUBE(I))  )
      CALL HAREA ( ATAV,DTAV,HAV )
      H(I) = 2.0*HAV - H(I-1)
      ICR = 1
      LAST = 1
      DBA = H(I)-H(I-1)
      GO TO 16
  200                          CONTINUE
      IF (IFBC .EQ. 0) GO TO 125
   35 CONTINUE
      HCR = H(I)
      IF (ABS(H(I)-HLF) .LE. 1.0E-3*HLF) GO TO 125
      IF ( ABS(VMF-SUMEFF) .LE. 0.01 * VMF ) GO TO 125
      I = I + 1
      DBAV(I) = 0.0
      UB(I) = 0.0
```

```
      AKBE(I) = 1000.0
      EPB(I) = 0.0
      EPC(I) = 0.0
      IF (VMF .EQ. 0.0) GO TO 45
C
C     FIXED BED CONDITIONS
C
      VOL = SUMV + ( VMF - SUMEFF )
      H(I) = HEIGHT(VOL)
 45   CONTINUE
      IF (VMF .EQ. 0.0) H(I) = HLF
      IF (I .LE. M1) GO TO 6
      T(I) = T(M1)
      X(I) = X(M1)
      YB(I) = YB(M1)
      YE(I) = YE(M1)
 6    CONTINUE
      DO 310 J = 1,MTHE
      IF (ZHE(J) .LE. H(I) .AND. ZHE(J+1) .LT. H(I)) GO TO 310
      IF (ZHE(J) .LE. H(I-1) .AND. ZHE(J+1) .GE. H(I)) GO TO 320
      F1 = (H(I)-ZHE(J))/(H(I)-H(I-1))
      F2 = (ZHE(J)-H(I-1))/(H(I)-H(I-1))
      AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)
      DTUBEI(I) = F1*DTUBE(J)+F2*DTUBE(J-1)
      PVI(I) = F1*PV(J)+F2*PV(J-1)
      PHI(I) = F1*PH(J)+F2*PH(J-1)
      GO TO 330
 320  AHEAV(I) = AHE(J)
      DTUBEI(I) = DTUBE(J)
      PVI(I) = PV(J)
      PHI(I) = PH(J)
 330  IARRNG(I) = IARR(J)
      GO TO 340
 310  CONTINUE
 340  CALL AREA(H(I),DT(I),AT(I))
      DVBB(I) = 0.5*(AT(I-1)+AT(I))*(H(I)-H(I-1))
      DVBBEF(I) = DVBB(I)*(1.-0.25*AHEAV(I)*DTUBEI(I))
      ETUBE(I) = 1.0 - DVBBEF(I)/DVBB(I)
      RHOGAS = PAV*MGAS/(RG*T(I))
      VISC = 3.72E-6*T(I)**0.676
      A1 = 33.7**2+0.0408*DPSVB**3*G*(RHOBED-RHOGAS)*RHOGAS/VISC**2
      UMF(I) = VISC/(DPSVB*RHOGAS)*(SQRT(A1)-33.7)
      HAV = 0.5*(H(I-1)+H(I))
      CALL AREA (HAV,DTAV,ATAV)
      UO(I) = FMO*MGAS/RHOGAS/(ATAV*(1.-ETUBE(I)))
      BEDVOL = BEDVOL + DVBB(I)
      SUMV = SUMV + DVBBEF(I)
      SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)
      SUMEFF = SUMEFF + SOLVOL
      SUM = SUM + SOLVOL / ( 0.5 * (AT(I)+AT(I-1)) )
      IFBC = 1
 125  M1 = I
      TETUBE = 1.0 - SUMV/BEDVOL
      EFFVOL = SUMV
      SOLVOL = SUMEFF
      M = M1 - 1
      DO 460 K = 2,KT
      I = I + 1
      H(I) = H(M1)+HB(K)
                                DO 410 J = 1,MTHE
```

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```
      IF (ZHE(J).LE.H(I).AND.ZHE(J+1).LT.H(I)) GO TO 410
      IF (ZHE(J).LE.H(I-1).AND.ZHE(J+1).GE.H(I)) GO TO 420
      F1 = (H(I)-ZHE(J))/(H(I)-H(I-1))
      F2 = (ZHE(J)-H(I-1))/(H(I)-H(I-1))
      AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)
      DTUBEI(I) = F1*DTUBE(J)+F2*DTUBE(J-1)
      PVI(I) = F1*PV(J)+F2*PV(J-1)
      PHI(I) = F1*PH(J)+F2*PH(J-1)
      GO TO 430
420   AHEAV(I) = AHE(J)
      DTUBEI(I) = DTUBE(J)
      PVI(I) = PV(J)
      PHI(I) = PH(J)
430   IARRNG(I) = IARR(J)
      GO TO 440
410                               CONTINUE
440   CALL AREA (H(I),DT(I),AT(I))
      DVBB(I) = 0.5*(AT(I-1)+AT(I))*(H(I)-H(I-1))
      DVBBEF(I) = DVBB(I) * (1.-0.25*AHEAV(I)*DTUBEI(I))
      ETUBE(I) = 1. - DVBBEF(I)/DVBB(I)
460   CONTINUE
      MT = I
      HFB = H(MT)-H(M1)
      RETURN
      END
      SUBROUTINE SIMQ(A,B,N,NN,KS)
      DIMENSION A(NN),B(N)
C
C     FORWARD SOLUTION
C
      TOL=0.0
      KS=0
      JJ=-N
                                  DO 65 J=1,N
      JY=J+1
      JJ=JJ+N+1
      BIGA=0.
      IT=JJ-J
                                  DO 30 I=J,N
C
C     SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
C
      IJ=IT+I
      IF( ABS(BIGA) - ABS(A(IJ)))20,30,30
   20 BIGA=A(IJ)
      IMAX=I
   30 CONTINUE
C
C     TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
C
      IF( ABS(BIGA) - TOL) 35,35,40
   35 KS=1
      WRITE(6,100) KS
  100 FORMAT(/' NO SOLUTION',' KS=',I2)
      STOP
C
C     INTERCHANGE ROWS IF NECESSARY
C
   40 I1=J+N*(J-2)
      IT=IMAX-J
```

```
                                  DO 50 K=J,N
      I1=I1+N
      I2=I1+IT
      SAVE=A(I1)
      A(I1)=A(I2)
      A(I2)=SAVE
C
C     DIVIDE EQUATION BY LEADING COEFFICIENT
C
   50 A(I1)=A(I1)/BIGA
      SAVE=B(IMAX)
      B(IMAX)=B(J)
      B(J)=SAVE/BIGA
C
C    ELIMINATE NEXT VARIABLE
C
      IF( J - N) 55,70,55
   55 IQS=N*(J-1)
                                  DO 65 IX=JY,N
      IXJ=IQS+IX
      IT=J-IX
                                  DO 60 JX=JY,N
      IXJX=N*(JX-1)+IX
      JJX=IXJX+IT
   60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))
   65 B(IX)=B(IX)-B(J)*A(IXJ)
C
C     BACK SOLUTION
C
   70 NY=N-1
      IT=N*N
                                  DO 80 J=1,NY
      IA=IT-J
      IB=N-J
      IC=N
                                  DO 80 K=1,J
      B(IB)=B(IB)-A(IA)*B(IC)
      IA=IA-N
   80 IC=IC-1
      RETURN
      END
      SUBROUTINE VEL(VISC,RHOGAS,G,RHOS,DPAR,UM,UT)
C
C     THIS SUBROUTINE CALCULATES THE MINIMUM FLUIDIZATION VELOCITY AND
C     THE TERMINAL VELOCITY OF THE PARTICLE
C
      A1 = 33.7**2+0.0408*DPAR**3*G*(RHOS-RHOGAS)*RHOGAS/VISC**2
      UM = VISC/(DPAR*RHOGAS)*(SQRT(A1)-33.7)
      UT = (4.0*(RHOS-RHOGAS)**2*G**2/225.0/RHOGAS/VISC)**(1./3.)*DPAR
      REP = DPAR*RHOGAS*UT/VISC
      IF (REP .GT. 0.4 .AND. REP .LE. 500.0) GO TO 210
      UT = G*(RHOS-RHOGAS)*DPAR**2/18./VISC
      REP = DPAR*RHOGAS*UT/VISC
      IF(REP.LE.0.4) GO TO 210
      UT = SQRT(3.1*G*(RHOS-RHOGAS)*DPAR/RHOGAS)
210   RETURN
      END
      FUNCTION VOLUME (ZZ)
      COMMON /A/ ZHE(10),AHE(10),FV(10),PH(10),ZF(10),FFC(10),DTUBE(10),
     1DVB(60),DVBEFF(60),FFAD(10),ZDIS(10),FD(10),AHEAV(60),ETUBE(60),
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```
     2U0(60),UMF(60),H(60),AT(60),DT(60),T(60),X(60),AKHE(60),YB(60),
     3YE(60),YCOE(60),EPB(60),EPC(60),DVBB(60),DVBBEF(60),DBAV(60),
     4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(60),ZAVG(60),IARR(10)
      COMMON /B/ YBO(60),YEO(60),DB(60),DPSVB,DPWMB,DCSVB,DCWMB,RHOCH,
     1HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,RHOBED,
     2EMF,PAV,HCR,BEDVOL,EFFVOL,SOLVOL,TETUBE,HLMF,PI,AND,DNZL,
     3FW,FSW,DZAV,MFEED,MDIS,MTHE,MTB,MT,M1,M,ICR,IFBC,NTC
C
C     CALCULATON OF THE EFFECTIVE VOLUME OF THE BED GIVEN THE HEIGHT
C
      N = IFIX (ZZ/DZAV)+1
      IF (N.EQ.1) N = 2
      SUM = 0.0
      ZN = FLOAT(N-1)*DZAV
                                    DO 100 I = 2 , N
      SUM = SUM + DVBEFF(I)
      IF ( I .LT. N ) GO TO 100
      A1 = ( ZZ - ZN ) / DZAV
      SUM = SUM + DVBEFF(I) * A1
100                                 CONTINUE
      VOLUME = SUM
      RETURN
      END
```

INPUT TO COMBUSTION PROGRAM

```
12345678901234567890123456789012345678901234567890123456789012345678901234567890

KT
4
 HB(1)    DPSE(1)   DPWE(1)   WEA(1)    HB(2)     DPSE(2)   DPWE(2)   WEA(2)
 0.0      0.0509    0.06139   193.3     56.43     0.0295    0.03409   9.527
 HB(3)    DPSE(3)   DPWE(3)   WEA(3)    HB(4)     DPSE(4)   DPWE(4)   WEA(4)
 112.9    0.02067   0.02651   1.446     138.1     0.01679   0.02386   0.7261
 DCSE(1)  DCWE(1)   WEC(1)    DCSE(2)   DCWE(2)   WEC(2)    DCSE(3)   DCWE(3)
 0.0464   0.07726   0.587     0.04491   0.05237   0.1387    0.04069   0.04673
 WEC(3)   DCSE(4)   DCWE(4)   WEC(4)
 0.05128  0.04769   0.05      0.02685
 WDIS     WELUA     CELU      EFF       DPSVB     DPWMB     DCSVB     DCWMB
 0.852    0.726     0.02685   0.9927    0.0746    0.1001    0.0787    0.1049
 DASVF    DAWMF     DCSVF     DCWMF
 0.0758   0.1287    0.0677    0.1004
A1  A2  A3  A4
NASA LEWIS
MTB
4
 ZB(1)    ATB(1)    ZB(2)     ATB(2)    ZB(3)      ATB(3)   ZB(4)     ATB(4)
 0.0      405.0     62.7      405.0     81.3       670.0    280.0     2193.0
MTHE
5
 ZHE(2)   AHE(1)    DTUBE(1)  PV(1)     PH(1)        IARR(1)
 24.0     0.0       0.0       0.0       0.0                0
 ZHE(3)   AHE(2)    DTUBE(2)  PV(2)     PH(2)        IARR(2)
 40.0     0.1744    1.27      8.0       2.86               3
 ZHE(4)   AHE(3)    DTUBE(3)  PV(3)     PH(3)        IARR(3)
 48.0     0.0       0.0       0.0       0.0                0
 ZHE(5)   AHE(4)    DTUBE(4)  PV(4)     PH(4)        IARR(4)
 56.0     0.1744    1.27      8.0       2.86               3
 ZHE(6)   AHE(5)    DTUBE(5)  PV(5)     PH(5)        IARR(5)
 280.0    0.0       0.0       0.0       0.0                0
MFEED
1
 ZF(1)    FFC(1)    FFAD(1)
 6.91     1.0       1.0
MDIS
1
 ZDIS(1)  FD(1)
 142.0    1.0
 AND      DNZL      FW        FSW
 84.0     0.198     0.075     0.1
NAMEL1  NAMEL2
LIMEST13
 XCAO     XMGO      XSIO2     XCO2
 0.557    0.003     0.006     0.434
NAMEC1  NAMEC2
PTGHCOAL
 XC       XH        XN        XS        XO        XW        XA        VM
 0.754    0.051     0.015     0.02      0.076     0.022     0.084     0.412
 HCOAL    XACAO
 7300.0   0.08
 HLMF     HLF       FAV       TAV       TSTA      TWIN      TWOUT     TWALLA
 0.0      141.9     5.15      1151.0    1250.0    298.0     310.0     298.0
 UHEAV1   UHEAV2    UWALL1    UWALL2    TF        TSF       PF
 0.00765  0.0025    0.0021    0.00025   298.0     298.0     5.4
 WCOAL    WAD       CAS       UO        FMF       EXAIR
 4.51     0.0       1.67      0.0       0.0       0.639
IGNITE,ISO2,INOX,ITEMP,IPRES
11111

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```

NASA LEWIS

HT.ABOVE DISTRIBUTOR.CM	CROSS SECTIONAL AREA OF BED.SQ.CM.
0.0	405.000
62.7000	405.000
81.3000	670.000
280.0000	2193.000

HEIGHT.CM	SP.HEAT TRANS.AREA.SQ.CM/CU.CM	DIA.OF TUBES.CM	VER.PITCH.CM	HOR.PITCH.CM	TUBES ARRNGT
24.00	0.0	0.0	0.0	0.0	0
40.00	0.1744	1.270	8.000	2.860	3
48.00	0.0	0.0	0.0	0.0	0
56.00	0.1744	1.270	8.000	2.860	3
280.00	0.0	0.0	0.0	0.0	0

SOLIDS FEED LEVEL	FRACTION COAL FED	FRACTION LIMESTONE FED
6.91	1.0000	1.0000

SOLIDS DISCHARGE LEVEL	FRACTION DISCHARGED
142.00	1.0000

NO.OF DISTRIBUTOR HOLES = 84.0

NOZZLE DIAMETER = 0.1980 CM

FW = 0.075

FSW = 0.100

```
LIMEST13      XCAO =  0.557        XMGO =  0.003        XSIO2 =  0.006        XCO2 =  0.434

    SURFACE VOL MEAN DIA.OF ADDITIVES FEED = DASVF =      0.0758   CM     WEIGHT MEAN DIA. = DAWMF =      0.1287   CM

PITHCOAL    XCF = 0.575   XCV = 0.179   XH = 0.051   XN = 0.015   XS = 0.020   XO = 0.076   XW = 0.022   XW = 0.084
            VM = 0.412    V = 0.305    HCOAL =  7300.00   CALS/GM    XACAO = 0.080

            SURFACE VOL MEAN DIA OF COAL FEED = DCSVF =      0.0677   CM     WT.MEAN DIA. = DCWMF =      0.1004   CM
```

K	FREEBOARD Ft.	DPSE	DPWE	WEA	DCSE	DCWE	WEC
1	0.0	5.090E-02	6.139E-02	1.933E 02	4.640E-02	7.726E-02	5.870E-01
2	5.643E 01	2.950E-02	3.409E-02	9.527E 00	4.491E-02	5.237E-02	1.387E-01
3	1.129E 02	2.067E-02	2.651E-02	1.446E 00	4.069E-02	4.673E-02	5.128E-02
4	1.381E 02	1.679E-02	2.386E-02	7.261E-01	4.769E-02	5.000E-02	2.685E-02

```
&BPCF
HLMF= 0.0        ,HLF=  141.89999     ,PAV=  5.1499996     ,TAV=  1151.0000     ,TSTA=  1250.0000     ,TWIN=  298.00000     ,TWOUT=
 310.00000     ,TWALLA=  298.00000     ,UHEAV1= 0.76499991E-02,UHEAV2= 0.24999999E-02,UWALL1= 0.20999999E-02,UWALL2= 0.24999981E-03,
TF=  298.00000     ,TSF=  298.00000     ,WCCAL=  4.5099993     ,WAD= 0.46351516     ,CAS=  1.6699991     ,EXAIR= 0.63900000     ,WGAS=
 29.599724     ,FMTH=  1.5620272     ,FMF=  2.5601540     ,FMU=  2.6296120     ,H2SV= 0.54268312E-01,ANH3V= 0.93031347E-01,RHOCH=
 0.99230257     ,RHOBFD=  2.6564837     ,RVGAS= 0.62061697E-02,RCHAR= 0.67313063     ,OVGAS=  409974.13     ,OVCO=  356196.25     ,
DCLIN=  423.09209
&END
```

RESULTS .ALL TEMPERATURES IN CENTIGRADE

ITC.XAV.TAV.ITRIAL = 0.9928E 00 0.2324E-02 0.0705E 03 2

I	HT	YB	YE	YVE	YCOE	YCO2E	YCO2B	X	ZAVG
2	4.1203E 00	1.9433E-01	1.5000E-01	0.0	4.4329E-04	4.5813E-02	3.6070E-03	3.6553E-03	2.0602E 00
3	9.8807E 00	1.8336E-01	0.0	0.0	7.4665E-03	1.3840E-01	1.3707E-02	3.7087E-03	7.0005E 00
4	1.7026E 01	1.7237E-01	2.8000E-02	0.0	2.7338E-04	1.2175E-01	2.1555E-02	3.3083E-03	1.3453E 01
5	2.5717E 01	1.6303E-01	4.2000E-02	0.0	1.3115E-04	1.1334E-01	2.8321E-02	2.8563E-03	2.1372E 01
6	3.6065E 01	1.5493E-01	4.8000E-02	0.0	1.2708E-04	1.1076E-01	3.4297E-02	2.4532E-03	3.0891E 01
7	4.8112E 01	1.4716E-01	4.8000E-02	0.0	1.0918E-04	1.1128E-01	4.0057E-02	2.1070E-03	4.2088E 01
8	6.1827E 01	1.4000E-01	4.8000E-02	0.0	9.3365E-05	1.1515E-01	4.5365E-02	1.8168E-03	5.4969E 01
9	7.7819E 01	1.3217E-01	4.4000E-02	0.0	7.0108E-05	1.1712E-01	5.1383E-02	1.5781E-03	6.9830E 01
10	9.7037E 01	1.2372E-01	3.4000E-02	0.0	4.5380E-05	1.2738E-01	5.8124E-02	1.4296E-03	8.7443E 01
11	1.1903E 02	1.1498E-01	2.6000E-02	0.0	3.3544E-05	1.3478E-01	6.5194E-02	1.3141E-03	1.0804E 02
12	1.4190E 02	1.0600E-01	2.0000E-02	0.0	2.7508E-05	1.4040E-01	7.2053E-02	1.2573E-03	1.3047E 02

I	HT	YB	YV	YCO	YCO2	T	TPB	TPE	ZAVG

2	4.120E 00	1.877E-01	0.0	4.713E-05	9.951E-03	9.652E 02	1.394E 03	1.343E 03	2.060E 00
3	9.881E 00	1.540E-01	0.0	1.156E-05	3.368E-02	9.031E 02	1.371E 03	9.073E 02	7.001E 00
4	1.703E 01	1.492E-01	0.0	3.208E-05	3.771E-02	8.927E 02	1.344E 03	9.740E 02	1.345E 01
5	2.572E 01	1.436E-01	0.0	2.102E-05	4.195E-02	8.817E 02	1.318E 03	1.010E 03	2.137E 01
6	3.606E 01	1.378E-01	0.0	2.038E-05	4.656E-02	8.707E 02	1.295E 03	1.019E 03	3.089E 01
7	4.811E 01	1.313E-01	0.0	1.751E-05	5.148E-02	8.743E 02	1.274E 03	1.006E 03	4.209E 01
8	6.183E 01	1.252E-01	0.0	1.450E-05	5.598E-02	8.674E 02	1.254E 03	9.852E 02	5.497E 01
9	7.785E 01	1.180E-01	0.0	1.126E-05	6.194E-02	8.544E 02	1.232E 03	9.571E 02	6.984E 01
10	9.704E 01	1.093E-01	0.0	7.202E-06	6.925E-02	8.516E 02	1.207E 03	9.098E 02	8.744E 01
11	1.190E 02	1.007E-01	0.0	5.394E-06	7.630E-02	8.482E 02	1.179E 03	8.873E 02	1.080E 02
12	1.419E 02	9.267E-02	0.0	4.427E-06	8.305E-02	8.459E 02	1.152E 03	8.750E 02	1.305E 02
13	1.903E 02	8.861E-02	0.0	1.840E-06	8.711E-02	8.495E 02	1.138E 03	1.138E 03	1.701E 02
14	2.540E 02	8.775E-02	0.0	0.0	8.797E-02	7.931E 02	1.081E 03	1.081E 03	2.266E 02
15	2.800E 02	8.766E-02	0.0	0.0	8.806E-02	7.574E 02	1.027E 03	1.027E 03	2.674E 02

(ETS,FS,CAS,CASE)=
0.6269E 00 0.3300E 00 0.1670E 01 0.1066E 01

HT.	YSO2B	YSO2E	ZAVG	YSO2	RELB	RELE
4.1203E 00	3.5220E-06	3.3427E-04	2.0602E 00	5.3237E-05	8.2846E-06	1.9224E-04
9.8807E 00	2.2974E-05	2.5514E-03	7.0005E 00	4.2799E-04	1.1232E-05	1.4098E-03
1.7026E 01	1.4572E-04	1.0660E-03	1.3453E 01	4.2135E-04	1.1290E-05	4.7455E-05
2.5717E 01	2.2919E-04	1.4484E-03	2.1372E 01	4.2460E-04	1.1070E-05	7.9037E-05
3.6065E 01	2.8736E-04	1.1906E-03	3.0891E 01	4.3219E-04	1.0624E-05	8.6146E-06
4.8112E 01	3.3041E-04	1.0098E-03	4.2088E 01	4.3939E-04	9.9031E-06	9.3890E-05
6.1827E 01	3.6200E-04	8.8014E-04	5.4969E 01	4.4515E-04	9.2195E-06	8.7107E-05
7.7849E 01	3.8464E-04	7.6488E-04	6.9838E 01	4.4570E-04	1.0999E-05	1.1549E-04
9.7037E 01	3.9542E-04	6.1272E-04	8.7443E 01	4.3033E-04	1.4829E-05	1.4011E-04
1.1903E 02	3.9593E-04	4.5828E-04	1.0804E 02	4.0596E-04	1.7126E-05	1.3578E-04
1.4190E 02	3.8911E-04	3.3658E-04	1.3047E 02	3.8066E-04	1.8130E-05	1.2612E-04
1.9813E 02	0.0	0.0	1.7011E 02	3.8501E-04	8.0197E-05	0.0
2.5400E 02	0.0	0.0	2.2656E 02	3.9036E-04	1.7052E-05	0.0
2.8000E 02	0.0	0.0	2.6740E 02	3.9105E-04	1.8595E-06	0.0

FXAIR,TAV,ETA,ENOX,ENOEX =
0.6390E 00 0.8705E 03 0.9165E 00 0.1501E-03 0.8753E-04

HT	YNOXB	YNOXE	X	CARCON	ZAVG	YNOX	RELB	RELE
4.1203E 00	5.6924E-06	1.0545E-04	3.6553E-03	1.5030E-03	2.0602E 00	2.0686E-05	1.4202E-05	3.2955E-04
9.8807E 00	1.5340E-05	2.2052E-03	3.7887E-03	1.7010E-03	7.0005E 00	3.7895E-04	1.9255E-05	2.4167E-03
1.7026E 01	6.7791E-05	7.9408E-04	3.3083E-03	1.4963E-03	1.3453E 01	1.8416E-04	1.9354E-05	8.1352E-05
2.5717E 01	8.2931E-05	3.2609E-04	2.8563E-03	1.2996E-03	2.1372E 01	1.2190E-04	1.8977E-05	1.3549E-04
3.6063E 01	8.8404E-05	2.1274E-04	2.4532E-03	1.0774E-03	3.0891E 01	1.0834E-04	1.8213E-05	1.4768E-04
4.8112E 01	9.1122E-05	1.8763E-04	2.1070E-03	9.7148E-04	4.2088E 01	1.0660E-04	1.7114E-05	1.6095E-04
6.1827E 01	9.3541E-05	1.9276E-04	1.8168E-03	3.2914E-04	5.4969E 01	1.0946E-04	1.5805E-05	1.4933E-04
7.7849E 01	9.5633E-05	1.9499E-04	1.5781E-03	8.8332E-04	6.9838E 01	1.1159E-04	1.8855E-05	1.9798E-04
9.7037E 01	9.8050E-05	1.7612E-04	1.4296E-03	1.0549E-03	8.7443E 01	1.1059E-04	2.5422E-05	2.4018E-04
1.1903E 02	1.0046E-04	1.4715E-04	1.3141E-03	1.0831E-03	1.0804E 02	1.0797E-04	2.9350E-05	2.3276E-04
1.4190E 02	1.0260E-04	1.4904E-04	1.2573E-03	1.1451E-03	1.3047E 02	1.0525E-04	3.1093E-05	2.1621E-04
1.9813E 02	0.0	0.0	4.8580E-03	7.9956E-06	1.7011E 02	1.4028E-04	1.3748E-04	0.0
2.5400E 02	0.0	0.0	1.3149E-02	1.2380E-06	2.2656E 02	1.4909E-04	2.9232E-05	0.0
2.8000E 02	0.0	0.0	2.7577E-02	3.1091E-07	2.6740E 02	1.5012E-04	3.1877E-06	0.0

OUTLET GAS CONCENTRATION

O2	CO2	SO2	H2O	CO
0.8766E-01	0.8806E-01	0.3911E-03	0.4487E-01	0.0

PRESSURE DROP ACROSS THE DISTRIBUTOR = 7.3568E 02

COMP.NO	PRESSURE DROP IN THE BED
2	1.6942E 00
3	2.5061E 00
4	3.2317E 00
5	3.9708E 00
6	5.0537E 00
7	5.5546E 00
8	6.4784E 00
9	8.5680E 00
10	1.4159E 01
11	1.8129E 01
12	2.0025E 01

PRESSURE DROP IN THE FIXED BED SECTION = 0.0

```
&LC
HDIS= 0.05200000 ,WELUA= 0.72599995 ,CCLU= 0.26809996E-01,EFF= 0.99269998 ,DPSVB= 0.74599981E-01,DPWHD= 0.10009998
DCSVB= 0.78699946E-01,DCWHD= 0.10489994 ,GFLOW= 77.833176 ,U0= 115.91977 ,CLOSS= 0.23999073E-01,CCHAR= 0.85392314
HCHAR= 0.0 ,OCHAR= 0.0 ,NCHAR= 0.10005482E-01,SCHAR= 0.13340615E-01,TARC= 0.34254539
&END
&DPCF1
ICR= 0,IFBC= 0,NTC= 10,HCR= 0.0 ,HLF= 141.89999 ,HLMF= 96.116150 ,VMF= 45559.746,
```

```
BEDVOL=  66058.125    ,ELEVOL=  80316.608    ,SOLVOL=  45590.740    ,TETUMF= 0.39401054F-02,HAREA=  1417.1987    ,DTRANS=
 9057.1406        ,OVEL= 0.10451573       ,QAREA=  6.3900760    ,HFD=  130.09976       ,BLDCOM=  2.1036196    ,FACOM= 0.18477947    ,TCRATE=
 2.7986190        ,XC2=  2.9793720       ,X02C=  3.4059245
 END
```

I	HEIGHT	ZAVG	AV.BUBBLE DIA	BUBBLE VEL.	BUBBLE FRAC.	CLOUD FRAC.	SUP.VELOCITY	MIN.FLU.VEL.
2	4.120	2.060	4.1203E 00	1.4595E 02	6.9043E-01	7.0043E-01	1.1917E 02	1.8395E 01
3	9.881	7.001	9.7603E 00	1.5069E 02	6.6199E-01	6.7199E-01	1.2214E 02	1.8416E 01
4	17.076	13.433	7.1454E 00	1.5954E 02	6.5950E-01	6.6950E-01	1.2100E 02	1.8501E 01
5	25.717	21.372	8.6910E 00	1.5161E 02	6.5603E-01	6.6603E-01	1.2023E 02	1.8589E 01
6	36.065	30.891	1.0347E 01	1.6018E 02	6.3220E-01	6.4230E-01	1.2509E 02	1.8675E 01
7	48.112	42.088	1.2047E 01	1.5257E 02	6.5287E-01	6.6207E-01	1.1833E 02	1.8723E 01
8	61.827	54.969	1.3715E 01	1.5114E 02	6.3438E-01	6.5438E-01	1.1995E 02	1.8771E 01
9	77.847	69.838	1.6022E 01	1.3240E 02	5.7698E-01	5.8858E-01	9.5393E 01	1.8791E 01
10	97.037	87.443	1.9189E 01	1.0546E 02	4.4447E-01	4.5447E-01	6.7464E 01	1.8811E 01
11	119.033	108.039	2.1796E 01	1.0193E 02	3.7341E-01	3.8946E-01	5.7511E 01	1.8834E 01
12	141.900	130.467	2.2867E 01	5.5971E 01	3.1435E-01	3.2436E-01	4.9017E 01	1.8848E 01

COMPT.NO.	HEIGHT	BED DIA.	BED C/S AREA
1	0.0	2.271E 01	4.050E 02
2	4.12	2.271E 01	4.050E 02
3	9.88	2.271E 01	4.050E 02
4	17.03	2.271E 01	4.050E 02
5	25.72	2.271E 01	4.050E 02
6	36.06	2.271E 01	4.050E 02
7	48.11	2.271E 01	4.050E 02
8	61.83	2.271E 01	4.050E 02
9	77.85	2.800E 01	6.158E 02
10	97.04	3.108E 01	7.586E 02
11	119.03	3.370E 01	8.917E 02
12	141.90	3.642E 01	1.041E 03
13	198.33	4.313E 01	1.461E 03
14	254.00	4.984E 01	1.951E 03
15	280.00	5.284E 01	2.193E 03

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APPENDIX VII

MANUAL FOR THE COMPUTER PROGRAMS

In this appendix, explanation for the main programs for elutriation and combustion calculations are given followed by the alphabetical list of subprograms used in both the programs. Except for the subroutine SIMQ which is the duplication of one of the subroutines in SSP supplied by IBM, explanation is given for each subprogram.

1. Elutriation Main Program

In the first part of the program, FBC design data and operating conditions are specified as input. From CN 89 (Card Number 89), the composition and the amount of volatiles and char produced are calculated. At CN 178, ELUT subprogram is called in to perform the elutriation calculations. Calculated results of particle size distributions of limestone and char in the bed and in the entrained solids, solids withdrawal rate, char elutriation rate and combustion efficiency are printed out.

2. Combustion Main Program

Computed results from the elutriation program are used as input in combustion calculations. From CN 64 to CN 84, all the input variables are specified. Then, the devolatilization of coal is considered. Knowing the average temperature of FBC, the yield of volatiles and char and their respective compositions are calculated. The input variables and calculated results so far are printed out.

The combustion of coal is specified by the indicator IGNITE. If IGNITE equals to zero, there is no combustion, and bubble hydrodynamics alone is calculated. Otherwise, the combustion calculations are started from CN 248. First the boundary conditions are specified.

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Hydrodynamic calculations are then performed using the assumed temperature profile. The log mean temperature of the cooling medium is calculated knowing the inlet and outlet temperatures. Then, the axial distribution of solids feed is calculated in CN 281/302. Based on the solids mixing parameter f_w, the amount of volatiles released near the coal feed point and throughout the bed are calculated in CN 310/311. The flow rate of gas through the bubble and emulsion phases are computed.

Before proceeding with the combustion calculations, the combustion efficiency is assumed. From the combustion efficiency, the average carbon weight fraction is calculated in CN 350 using the overall carbon material balance. The gas phase material balance is performed and the axial distribution of concentrations of various gaseous species are calculated. Then, based on oxygen material balance, combustion efficiency is calculated.

$$\text{Combustion efficiency} = \frac{O_2 \text{ in} - O_2 \text{ in the exit gas}}{\text{Stoichiometric } O_2 \text{ required}} \qquad \text{(A.VII.1)}$$

The criterion for the convergency of the gas phase balance is that the assumed combustion efficiency based on carbon balance should agree with the calculated combustion efficiency based on oxygen balance. Then, the axial distribution of the solids withdrawal rate, the solids mixing rate and the net flow rate of solids are computed in CN 429/460. Carbon material balance calculations for each compartment are then performed, and the equations are solved by the subroutine SIMQ in CN 486. The solution of the equations gives the carbon concentration in each compartment. Knowing the solids withdrawal rate, the carbon concentration in the bed and the char elutriation rate the overall combustion efficiency is calculated in CN 502. Using the computed carbon concentration profile, the gas phase material balance is performed again from CN 510/555 to accurately estimate the concentrations of the gaseous species along the combustor. Then, the equations obtained for energy balance are solved using SIMQ subroutine. The temperature calculations converge when the assumed ($T_{i,OLD}$) and calculated (T_i) temperatures agree with each other within the specified tolerance limit. The results are printed out in CN 674/677.

SO_2 retention calculations are done in CN 696/775 if the indicator ISO2 is greater than zero. Total feed rate of sulfur is estimated in CN 698. SO_2 generated from the burning volatiles and char is estimated in CN 718/721. SO_2 retention calculations are iterative. First, SO_2 retention efficiency is assumed, and hence the reactivity of the limestone particle is calculated. SO_2 material balance is performed and from the exit SO_2 concentration, SO_2 capture efficiency is calculated as

$$SO_2 \text{ capture efficiency} = 1 - \frac{\text{Sulfur in flue gas}}{\text{Total sulfur fed}} \quad . \qquad (A.VII.2)$$

If the assumed and calculated efficiencies agree, iteration is stopped, and the results are printed out.

If the INOX indicator is greater than zero NO_x material balance calculations are performed. NO_x release due to volatiles and char combustion is calculated in CN 783/786. NO_x balances in the bed and in the freeboard are done in CN 795/824 and the calculated results are printed out.

If IPRES is greater than zero, pressure drop calculations are performed from CN 854/876. Pressure drop across the distributor, across the fluidized bed and if there is a fixed bed section above the fluidized bed, then, pressure drop across the fixed bed section are calculated using the equations provided by Kunii and Levenspiel (1969). The final results are printed out in CN 881/891.

3. <u>Subprogram AKAD</u>

This function subprogram calculates the overall rate constant for limestone-SO_2 reaction. This subprogram is designed based on the data of Borgwardt (1970) for Type 4 limestone. The overall reaction rate constant for limestone-SO_2 reaction is calculated by the equation

$$k_{v\ell} = k'_{v\ell}\, S_g\, \lambda_\ell \qquad 1/\text{sec} \qquad \text{(A.VII.3)}$$

where $k'_{v\ell}$ is defined as:

$$k'_{v\ell} = 490 \exp(-17500/RT) \qquad \text{gm/cm}^3\text{.sec} \qquad \text{(A.VII.4)}$$

S_g is the specific surface area of limestone, and is equal to

$$S_g = 35.9\ T - 3.67 \times 10^4\ \frac{\text{cm}^2}{\text{gm}},\ T < 1253\ °K \qquad \text{(A.VII.5)}$$

$$= -38.43\ T + 5.64 \times 10^4\ \frac{\text{cm}^2}{\text{gm}},\ T \geq 1253\ °K \qquad \text{(A.VII.6)}$$

and λ_ℓ is the reactivity of limestone as a function of CaO utilization, particle temperature and size. The reactivity of limestone is calculated using the grain model developed by Ishida and Wen (1971). The results are stored in the subprogram. The effect of temperature on the limestone reactivity is minimal for the range of temperatures encountered in the FBC. The reactivity of limestone for any intermediate particle size and conversion is calculated by linear interpolation on semilogarithmic scale as follows:

$$\lambda_{\ell a} = \left(\frac{\lambda_{\ell a2}}{\lambda_{\ell a1}}\right)^{\frac{f_\ell - f_1}{f_2 - f_1}} \times \lambda_{\ell a1} \qquad \text{(A.VII.7)}$$

$$\lambda_{\ell b} = \left(\frac{\lambda_{\ell b2}}{\lambda_{\ell b1}}\right)^{\frac{f_\ell - f_1}{f_2 - f_1}} \times \lambda_{\ell b1} \qquad \text{(A.VII.8)}$$

$$\lambda_{\ell} = \left(\frac{\lambda_{\ell a}}{\lambda_{\ell b}}\right)^{\frac{\ell n(d_\ell/d_{\ell b})}{\ell n(d_{\ell a}/d_{\ell b})}} \times \lambda_{\ell b} \qquad \text{(A.VII.9)}$$

where λ_ℓ is the reactivity of limestone, f_ℓ is the fractional conversion of limestone and d_ℓ is the limestone particle diameter. Subscripts a and b refer to the successive particle sizes for which the reactivity profiles are specified (for the same conversion). Subscripts 1 and 2 refer to the successive particle conversions for which the reactivity profiles are specified (for the same particle size).

4. Subprogram AKK

Overall rate constants for char combustion and C-CO_2 reaction are calculated in this subroutine subprogram. Char particle temperature is calculated using the equation (V.38) by a trial and error procedure using Regula-Falsi method. The values of parameters used in this subprogram are given below:

Emissivity of the char particle, $\varepsilon_m = 1.0$

Thermal conductivity of the surrounding gas, λ

$$= 6.32 \times 10^{-6}\, T_m^{0.5}/\{1 + \frac{245 \times 10^{(-12/T_m)}}{T_m}\}, \frac{\text{cals}}{\text{sec.cm.}^\circ\text{C}} \qquad \text{(A.VII.10)}$$

Stefan-Boltzman constant, $\sigma = 1.36 \times 10^{-12}\ \frac{\text{cals}}{\text{sec.cm}^2.^\circ\text{K}^4}$

$$\text{Diffusivity of } O_2\text{-}N_2 = 4.26\ \left(\frac{T_m}{1800}\right)^{1.75}/P \qquad \text{(A.VII.11)}$$

$$\text{Diffusivity of } CO_2\text{-}N_2 = 3.26\ \left(\frac{T_m}{1800}\right)^{1.75}/P \qquad \text{(A.VII.12)}$$

5. Subprogram AREA

By using this subroutine subprogram, cross sectional area of the combustor at any height above the distributor can be calculated. A set of data Z_j and $A_{t,j}$, $j = 1\sim MTB$ is fed into subroutine DESIGN and stored in the common address before subroutine AREA is called. The given height Z is searched between Z_{j-1} and Z_j so that

$$Z_{j-1} \leqslant Z < Z_j$$

Then, cross sectional area A_t corresponding to height Z is obtained as follows:

$$A_t = \pi r^2 \tag{A.VII.13}$$

$$\text{where} \quad r = [1 + (\frac{Z - Z_{j-1}}{Z_j - Z_{j-1}}) \{(\frac{A_{t,i}}{A_{t,j-1}})^{1/2} - 1\}] r_{j-1} \tag{A.VII.14}$$

$$r_{j-1} = (A_{t,j-1}/\pi)^{1/2} \tag{A.VII.15}$$

r = radius of the combustor at height Z above the distributor, cm

6. Subprogram ATTR

This subroutine subprogram calculates the burning time of a char particle of given size, and hence the size reduction constant due to combustion. Char particle temperature is first calculated using the Equation (V.38) by a trial and error procedure using Regula-Falsi method. The burning time, t_b, of a char particle is calculated using the Equation (V.51). The values of parameters used in this subprogram are:

Emissivity of the char particle, $\varepsilon_m = 1.0$

Stefan-Boltzman constant, $\sigma = 1.36 \times 10^{-12}$, cals/sec.cm^2.°K^4

Thermal conductivity of the surrounding gas, and the diffusivity of O_2-N_2 are calculated by Equations (A.VII.10) and (A.VII.11) respectively. Char size reduction rate constant is equal to $(1/t_b)$.

7. Subprogram CRRECT

This subroutine subprogram provides the initial value for the unknown variable to be used in the next iteration of Regula Falsi method, and also judges if the iteration has converged. The Regula Falsi iteration has two periods.

Period 1: the root is not found in the interval (INDX = 0)

Period 2: the root is found in the interval (INDX = 1) as shown in Fig. 26.

The parameter INDX is an indicator for the two periods, and if INDX = 2, it means the iteration has converged. During the period 1, the search for the root is continued by proceeding in one direction indicated by the sign of increment for the variable. Once the root is found in the interval, Newton-Raphson method is applied to arrive at the exact value.

To use this subroutine, the following statements must be prepared in the program from where CRRECT is called.

1) Initial assumption for the unknown variable, X
2) Value of increment, DX
3) Tolerance limit for error, EMAX
4) Difference between the assumed and calculated values for the variable, E
5) Initial value for INDX, INDX = 0
6) DO loop for iteration
7) A statement to get off the DO loop when INDX = 2

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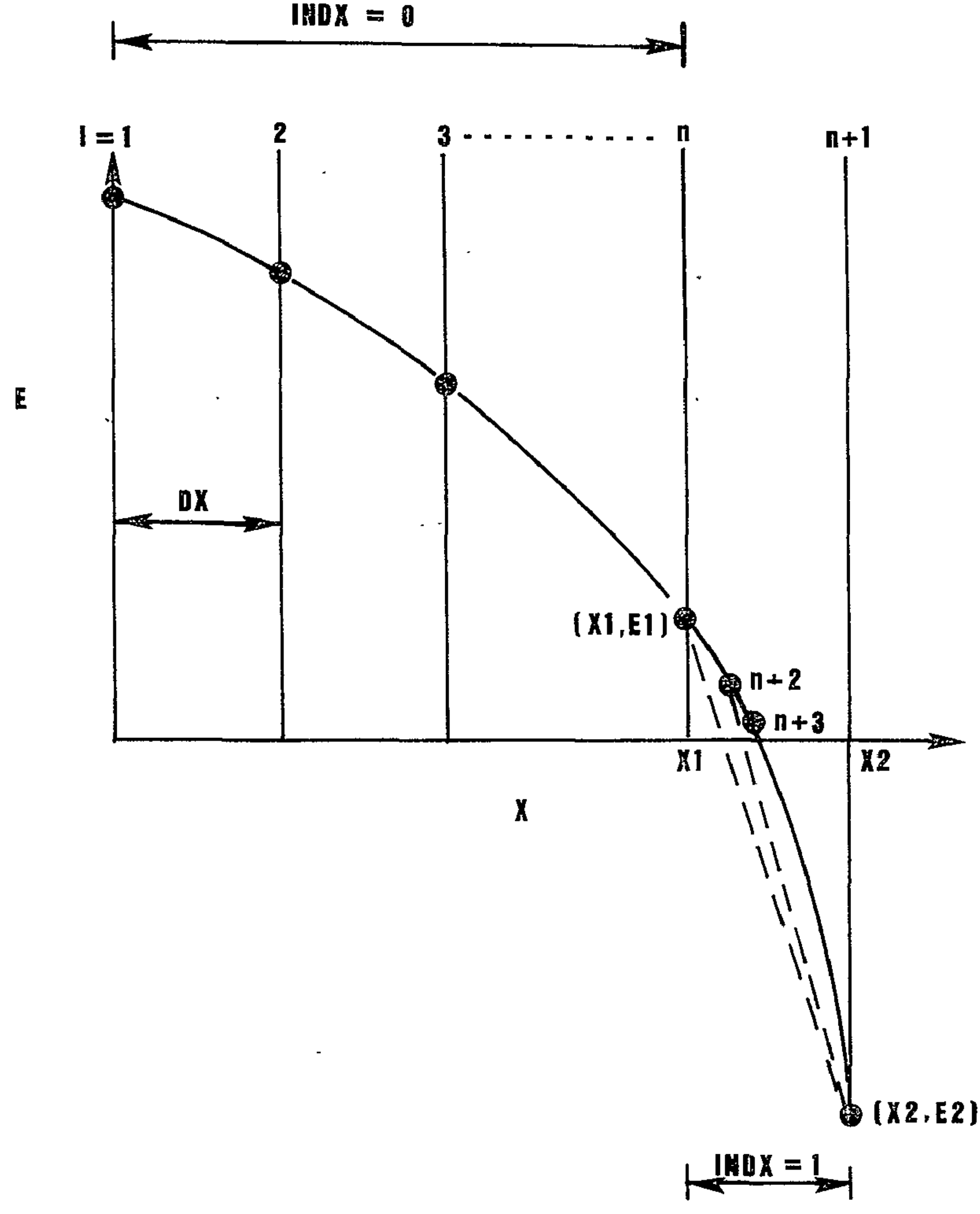

Fig. 26 Illustration for Regula Falsi Method

The initial value of X and the sign of DX are very important factors to get a successful result from the iteration. If there are multiple roots, special consideration for choosing these values is needed. In the ordinary case it is recommended to start from either the maximum or minimum possible value of the unknown variable, X.

8. Subprogram DESIGN

Values of the design variables are fed into the main program by calling this subroutine. The axial variation of the bed cross section as a function of height above the distributor (A_t V_s Z), the locations of heat transfer tubes, the specifications of the tubes (specific heat transfer area based on outside diameter of the tube, tube diameter (o.d.), vertical pitch, horizontal pitch, tubes arrangement), solids feed locations and the fraction of total feed through each nozzle, solids discharge locations and the fraction of materials discharged through each nozzle, number of orifices in the distributor, orifice diameter, the solids mixing parameter, f_w and the fraction of wake solids thrown into the freeboard, f_{sw} are the input variables in this subprogram.

Specific heat transfer area of the coils in a section of the bed refers to the outside surface area of the coils available for heat transfer per unit volume of the bed in that section. If the specific heat transfer area is not given, but the tube diameter is given, the former can be calculated.

For the triangular arrangement of the tubes (Fig. 27),

$$a_{HE} = \frac{\text{Heat transfer area}}{\text{Volume of bed}}$$

$$= \frac{(\frac{1}{2})\ \pi d_o\ \Delta Z}{(\frac{1}{2})(P_H\ P_V\ \Delta Z)} = \frac{\pi d_o}{P_H P_V} \qquad \text{(A.VII.16)}$$

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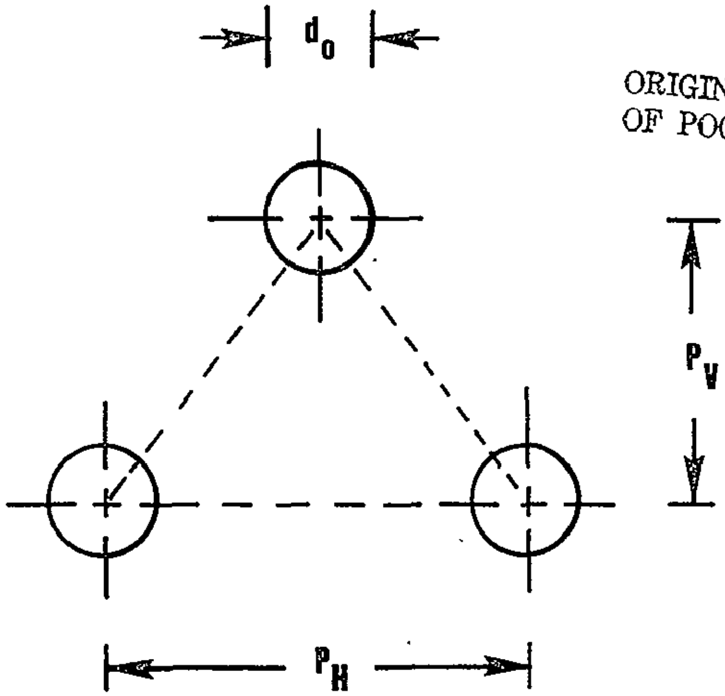
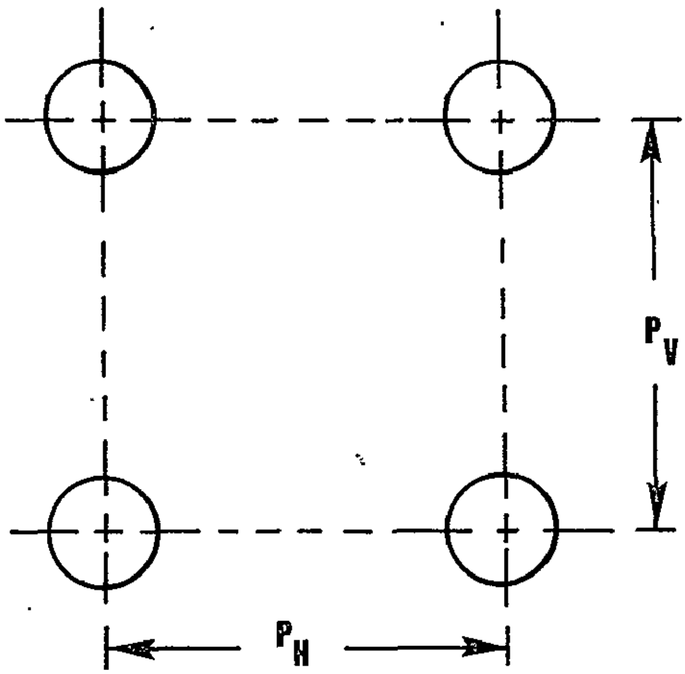


(a) TRIANGULAR ARRANGEMENT



(b) RECTANGULAR ARRANGEMENT

Fig.27 Arrangement of Cooling Tubes

For the rectangular arrangement (Fig. 27),

$$a_{HE} = \frac{\pi d_o \ \Delta Z}{P_H P_V \ \Delta Z} = \frac{\pi d_o}{P_H P_V} \qquad \text{(A.VII.17)}$$

For design purposes, the height of an elemental volume of the combustor corresponding to each compartment is chosen. The height should be so chosen that the total number of compartments in the combustor is always less than the maximum dimensions allowed by the program. Then, heat transfer tubes specifications for each compartment is calculated along with the diameter and cross sectional area. The differential volume of each compartment, and the effective volume (excluding the volume occupied by the tubes) are computed.

Volume occupied by the tubes per unit volume of bed is given as follows:

(for triangular arrangement): $$\frac{\frac{1}{2}(\frac{\pi}{4} d_o^2)\Delta Z}{\frac{1}{2} P_H P_V \ \Delta Z} = \frac{d_o}{4} \ a_{HE} \qquad \text{(A.VII.18)}$$

(for rectangular arrangement): $$\frac{(\frac{\pi}{4} d_o^2)\Delta Z}{P_H P_V \ \Delta Z} = \frac{d_o}{4} \ a_{HE} \qquad \text{(A.VII.19)}$$

Volume fraction of tubes is then equal to

$$\varepsilon_{tube} = 1 - \text{effective volume/total volume} \qquad \text{(A.VII.20)}$$

For each compartment, tube diameter, specific heat transfer area, tube fraction, volume and effective volume are calculated.

9. Subprogram ELUT

This subroutine subprogram is the basis for the entrainment calculations. Entrainment calculations for limestone are performed first followed by char entrainment calculations.

From the bed operating conditions, total bed weight is known.

Initially, the size distribution of the bed is assumed knowing the feed particles size distribution. Based on the assumed bed size distribution, mass balance calculations for each close size fraction are performed, and the bed weight and the new bed size distribution are calculated. If the calculated bed weight equals the known bed weight, the iteration is stopped; otherwise, procedure is repeated using the calculated bed size distribution for the next iteration.

The axial gas dispersion coefficient in the freeboard is then calculated from Reynolds number and Peclet number. From the dispersion coefficient, number of compartments and hence the compartment size in the freeboard are calculated. At each freeboard height, the solids entrainment rate and the average particle sizes are computed.

A similar procedure with slight modification is adopted for char entrainment calculations. To start with, carbon combustion efficiency is assumed and the average carbon concentration (weight fraction) in the bed is calculated based on carbon balance. Knowing the bed weight and carbon concentration in the bed, the weight of char in the bed is calculated. From the coal particle feed size distribution, the bed char size distribution is assumed. Mass balance for each close size fraction of char is performed. Based on the bed char size distribution, entrainment rate along the freeboard height is calculated. The effect of diminishing char particle size due to combustion is taken into account in the char entrainment calculations. The char leaving the combustor unburnt is calculated. The combustion efficiency is calculated again. If the assumed and calculated efficiencies equal, the iteration is stopped; otherwise, procedure is repeated by assuming a new initial value for combustion efficiency. The calculated results will give the size distribution of limestone and char in the bed, the average particle sizes of limestone and char, and their entrainment rates along the freeboard height, bed solids withdrawal rate, char elutriation rate, solids elutriation rate and the combustion efficiency.

10. Subprogram FBC

This subroutine subprogram considers the freeboard char combustion and solves the material balance equations for oxygen in the freeboard. There will be two cases in the calculations (i) oxygen rich or excess air conditions and (ii) oxygen starved conditions. For the oxygen rich case, Regula Falsi method is applied to calculate the oxygen concentration since the calculations involve a trial and error procedure.

11. Subprogram GPB

The material balance equations for oxygen in the emulsion phase and in the bubble phase are solved in this subroutine using the subroutine SIMQ. Two different cases are encountered in the solution: (i) the oxygen concentration in the emulsion phase is zero and (ii) the volatiles concentration in the emulsion phase is zero. The equations are solved by trial and error procedure.

12. Subprogram GPHASE

This subroutine is designed for solving the material balance equations in the emulsion phase and in the bubble phase for SO_2 and NO (nitric oxide).

13. Subprogram HAREA

This subprogram calculates the height of the specific compartment above the distributor for the given cross sectional area of that

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compartment. The idea is basically the same as that of subprogram AREA. The height Z, corresponding to the area, A_t, is calculated by the equation

$$Z = Z_{j-1} + \frac{(A_t/A_{j-1})^{1/2} - 1}{(A_j/A_{j-1})^{1/2} - 1} (Z_j - Z_{j-1}) \tag{A.VII.21}$$

This subroutine is called from subroutine HYDRO to determine the height of the bed where $U_o = U_{mf}$. This situation does not occur at the cylindrical section, but occurs only at the tapered section. Therefore, $A_j > A_{j-1}$, and the error of dividing by zero is automatically avoided.

14. <u>Subprogram HEIGHT</u>

This function subprogram calculates the height of the bed for the given effective volume of the bed. Effective volume is the total volume of the bed minus the volume occupied by the tubes.

15. <u>Subprogram HYDRO</u>

This subroutine subprogram essentially calculates the bubble hydrodynamics of the bed. In the first part of the calculations, the compartment size is assumed and hence the bubble size. Then, from the correlation, bubble size in that compartment is calculated. If the assumed and calculated bubble sizes are equal to each other, then the iteration is stopped; otherwise, a new compartment size is assumed and the procedure repeated. For each compartment, cooling tubes specifications, effective volume, total volume, height above the distributor and the cross sectional area at that height are calculated. After the bubble size calculation, the hydrodynamic calculations are done using the equations listed in Table 2.

The program is also designed to take into consideration the formation of a fixed bed section over the fluidized bed section. First, the volume of bed at minimum fluidization is evaluated in the case when the expanded bed height is not given. (Either the minimum fluidization height or the expanded bed height has to be specified in the input). Subroutine HYDRO is called inside the temperature iteration loop. Depending upon the temperature of the bed, the hydrodynamic parameters and the bed height are determined. If more number of compartments are needed than that of the earlier iteration, then for the excess number of compartments the temperature, carbon concentration, bubble and emulsion phase oxygen concentrations are taken as those corresponding to the last compartment in the earlier iteration.

Knowing the temperature, density and viscosity of the gas, minimum fluidizing velocity and superficial velocity are calculated for each compartment. U_o is compared with U_{mf}. If the cross-sectional area of the bed increases as the height increases (for tapered geometry), the superficial velocity decreases. If at any instance, U_o is less than or equal to U_{mf}, it represents the end of fluidized section and the beginning of a fixed bed section. Then different calculations are to be performed for the fixed bed section. Four different cases are analyzed:

(i) Expanded bed height given, no fixed bed section:

For each compartment, the bubble hydrodynamics is calculated. The iteration is performed till the height of the last compartment reaches the expanded bed height.

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(ii) Expanded bed height given, fixed bed section present:

The bubble hydrodynamics is calculated for each compartment. As the height increases, U_o is decreasing, and when it is smaller than U_{mf}, critical height has been reached. The critical height corresponds to the height of the bed above the distributor at which the fixed bed section starts. At this location U_o is equal to U_{mf}. Above this height, there is no fluidization, and the bubble fraction is zero. The presence of critical height and fixed bed are tagged by the symbols ICR and IFBC. If they are greater than zero, critical height and fixed bed section are present.

For each compartment the volume of solids (including the voids) and the effective height of the solids are calculated. Sum of these heights would be the height of the bed at minimum fluidization.

(iii) Height at minimum fluidization given, no fixed bed section:

Instead of basing the convergency criterion directly on the minimum fluidization height, the volume of the bed at minimum fluidization is used. This would help avoid any inacurracy involved in the calculation of the effective solids height in each compartment. Also, it would be easy to determine the total bed height when the effective volume of solids in the bed equals the volume at the minimum fluidization. The sum of each compartment volume, effective volume of solids (excluding the bubbles and tubes) and the effective height of solids are computed. The iteration continues till the effective solids volume equals the volume at minimum fluidization. If it exceeds volume at minimum fluidization, the excess solid volume, corrected for the expansion and tube fraction, is subtracted from the effective volume of the bed to give the correct volume of the bed. From this effective volume of the bed, the expanded bed height is calculated.

(iv) Height at minimum fluidization given, fixed bed section present:

As before, computations are performed till U_o becomes smaller than U_{mf}. In the fixed bed section, the bubble fraction is zero. Fixed bed is equivalent to the condition of minimum fluidization. Total volume of the bed is the sum of the effective volume of solids in the fluidized bed section and the difference in the minimum fluidization volume and the volume of solids in the fluidized section. Total height of the bed is computed from the total volume of the bed.

16. Subprogram SIMQ

A copy of this SSP (Scientific Subrouting Package) subroutine supplied by IBM is attached.

17. Subprogram VEL

This subprogram calculates the minimum fluidization velocity and the terminal velocity of the particle. The terminal velocity is calculated from (Kunii and Levenspiel, 1969):

$$U_t = \frac{g(\rho_s - \rho_g)d_p^2}{18\mu} \quad \text{for } R_{e,p} \leq 0.4 \tag{A.VII.22}$$

$$U_t = \left[\frac{4}{225} \frac{(\rho_s - \rho_g)^2 g^2}{\rho_g \mu}\right]^{1/3} d_p \quad \text{for } 0.4 < R_{e,p} < 500 \tag{A.VII.23}$$

$$U_t = \left[\frac{3.1\ g\ (\rho_s - \rho_g)d_p}{\rho_g}\right]^{1/2} \quad \text{for } 500 < R_{e,p} \tag{A.VII.24}$$

$$R_{e,p} = d_p\ \rho_g\ U_t/\mu \tag{A.VII.25}$$

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Subroutine SIMQ

```
C
C     ..................................................................
C
C        SUBROUTINE SIMQ
C
C        PURPOSE
C           OBTAIN SOLUTION OF A SET OF SIMULTANEOUS LINEAR EQUATIONS,
C           AX=B
C
C        USAGE
C           CALL SIMQ(A,B,N,KS)
C
C        DESCRIPTION OF PARAMETERS
C           A - MATRIX OF COEFFICIENTS STORED COLUMNWISE.  THESE ARE
C               DESTROYED IN THE COMPUTATION.  THE SIZE OF MATRIX A IS
C               N BY N.
C           B - VECTOR OF ORIGINAL CONSTANTS (LENGTH N). THESE ARE
C               REPLACED BY FINAL SOLUTION VALUES, VECTOR X.
C           N - NUMBER OF EQUATIONS AND VARIABLES. N MUST BE .GT. ONE.
C           KS - OUTPUT DIGIT
C                0 FOR A NORMAL SOLUTION
C                1 FOR A SINGULAR SET OF EQUATIONS
C
C        REMARKS
C           MATRIX A MUST BE GENERAL.
C           IF MATRIX IS SINGULAR , SOLUTION VALUES ARE MEANINGLESS.
C           AN ALTERNATIVE SOLUTION MAY BE OBTAINED BY USING MATRIX
C           INVERSION (MINV) AND MATRIX PRODUCT (GMPRD).
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           METHOD OF SOLUTION IS BY ELIMINATION USING LARGEST PIVOTAL
C           DIVISOR. EACH STAGE OF ELIMINATION CONSISTS OF INTERCHANGING
C           ROWS WHEN NECESSARY TO AVOID DIVISION BY ZERO OR SMALL
C           ELEMENTS.
C           THE FORWARD SOLUTION TO OBTAIN VARIABLE N IS DONE IN
C           N STAGES. THE BACK SOLUTION FOR THE OTHER VARIABLES IS
C           CALCULATED BY SUCCESSIVE SUBSTITUTIONS. FINAL SOLUTION
C           VALUES ARE DEVELOPED IN VECTOR B, WITH VARIABLE 1 IN B(1),
C           VARIABLE 2 IN B(2),........, VARIABLE N IN B(N).
C           IF NO PIVOT CAN BE FOUND EXCEEDING A TOLERANCE OF 0.0,
C           THE MATRIX IS CONSIDERED SINGULAR AND KS IS SET TO 1. THIS
C           TOLERANCE CAN BE MODIFIED BY REPLACING THE FIRST STATEMENT.
C
C     ..................................................................
C
      SUBROUTINE SIMQ(A,B,N,KS)
      DIMENSION A(1),B(1)
C
C        FORWARD SOLUTION
C
      TOL=0.0
      KS=0
      JJ=-N
      DO 65 J=1,N
      JY=J+1
      JJ=JJ+N+1
      BIGA=0
      IT=JJ-J
      DO 30 I=J,N
C
C        SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
C
      IJ=IT+I
      IF(ABS(BIGA)-ABS(A(IJ))) 20,30,30
   20 BIGA=A(IJ)
      IMAX=I
   30 CONTINUE
C
C        TEST FOR PIVOT LESS THAN TOLERANCE (SINGULAR MATRIX)
C
      IF(ABS(BIGA)-TOL) 35,35,40
   35 KS=1
      RETURN
C
C        INTERCHANGE ROWS IF NECESSARY
C
   40 I1=J+N*(J-2)
      IT=IMAX-J
      DO 50 K=J,N
      I1=I1+N
      I2=I1+IT
      SAVE=A(I1)
      A(I1)=A(I2)
      A(I2)=SAVE
C
C        DIVIDE EQUATION BY LEADING COEFFICIENT
C
   50 A(I1)=A(I1)/BIGA
      SAVE=B(IMAX)
      B(IMAX)=B(J)
      B(J)=SAVE/BIGA
C
C        ELIMINATE NEXT VARIABLE
C
      IF(J-N) 55,70,55
   55 IQS=N*(J-1)
      DO 65 IX=JY,N
      IXJ=IQS+IX
      IT=J-IX
      DO 60 JX=JY,N
      IXJX=N*(JX-1)+IX
      JJX=IXJX+IT
   60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))
   65 B(IX)=B(IX)-(B(J)*A(IXJ))
C
C        BACK SOLUTION
C
   70 NY=N-1
      IT=N*N
      DO 80 J=1,NY
      IA=IT-J
      IB=N-J
      IC=N
      DO 80 K=1,J
      B(IB)=B(IB)-A(IA)*B(IC)
      IA=IA-N
   80 IC=IC-1
      RETURN
      END
```

18. Subprogram VOLUME

This function subprogram calculates the effective volume of the bed (excluding the tubes, including the voids) for a given height above the distributor.

APPENDIX VIII

NOMENCLATURE FOR THE COMPUTER PROGRAMS

MAIN PROGRAM COMBUSTION

FORTRAN Symbol	Mathematical Symbol	Description
AAA	-	Matrix coefficients
AE	-	Activation energy of char-NO reduction reaction, cals/gmole
AHE	(SEE DESIGN)	
AHEAV	a_{HE}	Specific heat transfer area of the tubes, cm^2/cm^3 FBC volume
AHEW	a_{HEW}	Specific heat transfer area of the walls, cm^2/cm^3 FBC volume
AK	k_{v1}	Overall volume reaction rate constant for limestone - SO_2 reaction, 1/sec
AKB	$k_{c,B}$	Overall rate constant for char combustion in bubble phase, cm/sec
AKBE	K_{BE}	Gas exchange coefficient, 1/sec
AKC	k_c	Overall rate constant for char combustion, 1/sec
AKCO2	-	Overall rate constant for C-CO_2 reaction, cm/sec
AKE	$k_{c,E}$	Overall rate constant for char combustion in emulsion phase, cm/sec
AKNO	k_{NO}	NO reduction rate constant, cm/sec
ALFA	-	Temperature matrix coefficients
AMODF	a_m	Defined by Equation (VI.12)
AND	n_d	Number of orifices in the distributor
ANH3V	-	NH_3 content in the volatiles, gmole NH_3/gmole volatiles
ANITRO	-	Nitrogen released during char combustion, gatom/sec
AT	A_t	Cross sectional area of the bed, cm^2

FORTRAN Symbol	Mathematical Symbol	Description
ATB	(SEE DESIGN)	
BBB	-	Matrix coefficients
BEDCOM	-	Char combustion rate in the bed, gm/sec
BEDVOL	-	Total bed volume, cm^3
BETA	-	Temperature matrix coefficients
CADF	C_{Sf}	Heat capacity of feed additives, cals/gm·°C
CARCON	-	Carbon concentration, gm carbon/cm^3 bed volume (including tubes)
CAS	-	Ca/S molar ratio in feed solids
CASE	-	Effective Ca/S molar ratio (including Ca in ash)
CCF	C_{cf}	Heat capacity of coal feed, cals/gm·°C
CCHAR	C_{ch}	Carbon content in char, gm carbon/gm char
CELU	-	Char elutriated from the combustor, gms/sec
CGM	C_{gm}	Molar heat capacity of gas, cals/gmole °C
CGMF	-	Molar heat capacity of feed gas, cals/gmole °C
CHARC	-	Carbon content in char, gmole carbon/gm coal
CHARH	-	Hydrogen content in char, gatom hydrogen/gm coal
CHARN	-	Nitrogen content in char, gatom nitrogen/gm coal
CHARO	-	Oxygen content in char, gatom oxygen/gm coal
CHARS	-	Sulfur content in char, gatom sulfur/gm coal
CH4	CH_4	Wt. fraction CH_4 in the volatiles; CH_4 released during devolatilization, gmole CH_4/gm coal
CLOSS	-	Total carbon loss (elutriated + withdrawn), gm/sec
CO	CO	Wt. fraction CO in the volatiles; CO released during devolatilization, gmole CO/gm coal
COALC	-	Carbon content in coal, gatom carbon/gm coal (d.b.)

FORTRAN Symbol	Mathematical Symbol	Description
COALH	-	Hydrogen content in coal, gatom hydrogen/gm coal (d.b.)
COALN	-	Nitrogen content in coal, gatom nitrogen/gm coal (d.b.)
COALO	-	Oxygen content in coal, gatom oxygen/gm coal (d.b.)
COALS	-	Sulfur content in coal, gatom sulfur/gm coal (d.b.)
COB	-	Carbon monoxide burnt in each compartment, gmole/sec
COV	-	CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles
COVB	-	CO produced during volatiles combustion, gmole CO/gmole volatiles
CO2	-	Wt. fraction CO_2 in the volatiles; CO_2 released during devolatilization, gmole CO_2/gm coal
CO2V	-	CO_2 released during devolatilization per mole of volatiles released, gmole CO_2/gmole volatiles
CO2VB	-	CO_2 produced during volatiles combustion, gmole CO_2/gmole volatiles
CS	C_S	Heat capacity of solids, cals/gm °C
CTAR	-	Carbon content in char, gm carbon/gm coal fed
DASVF	-	Surface volume mean particle diameter of additives in the feed, cm
DAWMF	-	Weight mean particle diameter of additives in the feed, cm
DBAV	D_B	Bubble diameter in each compartment, cm
DCSE	d_{ce}	Surface volume mean diameter of char particles in the freeboard, cm
DCSVB	d_c	Surface volume mean diameter of char particles in the bed, cm

FORTRAN Symbol	Mathematical Symbol	Description
DCSVF	-	Surface volume mean diameter of coal particles in the feed, cm
DCWE	-	Weight mean diameter of char particles in the freeboard, cm
DCWMB	-	Weight mean diameter of char particles in the bed, cm
DCWMF	-	Weight mean diameter of coal particles in the feed, cm
DELT	-	Temperature matrix coefficients
DETC	-	Increment in combustion efficiency
DETS	-	Increment in sulfur dioxide retention efficiency
DNZL	-	Diameter of orifice holes in the distributor, cm
DPDIS	-	Pressure drop across the distributor, cm H_2O
DPFIX	-	Pressure drop across the fixed bed section, cm H_2O
DPFLU	-	Pressure drop across the fluid bed section, cm H_2O
DPSE	$d_{\ell e}$	Surface volume mean particle diameter of additives entrained in the freeboard, cm
DPSVB	d_{ℓ}	Surface volume mean particle diameter of additives in the bed, cm
DPWE	-	Weight mean particle diameter of additives entrained in the freeboard, cm
DPWMB	-	Weight mean particle diameter of additives in the bed, cm
DTUBE	(SEE DESIGN)	
DVBB	-	Volume of each compartment, cm^3

FORTRAN Symbol	Mathematical Symbol	Description
DT	D_t	Diameter of the combustor, cm
EETCM	-	Tolerance limit for combustion efficiency convergency
EETSM	-	Tolerance limit for sulfur dioxide retention efficiency convergency
EFF	-	Combustion efficiency calculated from elutriation calculations
EFFVOL	-	Volume of bed (excluding tubes), cm^3
EINDEX	-	Nitric oxide emission index, gmole NO/gm coal burnt
EMF	ε_{mf}	Void fraction at minimum fluidization
ENOX	-	Nitric oxide emission, mole fraction
EPB	ε_B	Bubble fraction
EPC	ε_c	Cloud fraction including bubble
ETC	-	Carbon combustion efficiency
ETCA	-	Assumed carbon combustion efficiency
ETCC	-	Carbon combustion efficiency based carbon balance
ETCG	-	Carbon combustion efficiency based on oxygen balance
ETN	-	NO_x emission efficiency
ETC	-	Sulfur dioxide retention efficiency
ETSC	-	Calculated sulfur dioxide retention efficiency
ETUBE	ε_{tube}	Volume fraction of tubes in each compartment
EXAIR	-	Excess air, fraction

FORTRAN Symbol	Mathematical Symbol	Description
FBCOM	-	Char combustion rate in the freeboard, gm/sec
FBM	F_{BM}	Molar flow rate of gas in the bubble phase, gmole/sec
FD	-	Fraction of solids withdrawn from the bed at each location
FEM	F_{EM}	Molar flow rate of gas in the emulsion phase, gmole/sec
FFAD	-	Fraction of total additives fed at each location
FFC	-	Fraction of total coal fed at each location
FMF	-	Molar feed rate of fluidizing air, gmole/sec
FMTH	-	Stoichiometric air feed rate, gmole/sec
FMO	F_{MT}	Total molar flow rate of gas in the combustor, gmole/sec
FR	-	Frequency factor for char-NO reaction, cm/sec
FRN	-	Feed rate of fuel nitrogen, gatom/sec
FRS	-	Feed rate of fuel sulfur, gatom/sec
FS	f_{ℓ}	Fractional conversion of limestone
FSW	(SEE DESIGN)	
FW	f_w	Solids mixing parameter, ratio of wake volume to the bubble volume including the wakes
G	g	Acceleration due to gravity, cm/sec^2
GAMA	-	Temperature matrix coefficients
GB	g_B	Volatiles burning rate in the bubble phase, gmole/sec
GE	g_E	Volatiles burning rate in the emulsion phase, gmole/sec
GENB	-	SO_2 or NO_x release rate in the bubble phase or in the freeboard due to volatiles combustion, gmole/sec

FORTRAN Symbol	Mathematical Symbol	Description
GENE	-	SO_2 or NO_x release rate in the emulsion phase or in the freeboard due to volatiles combustion, gmole/sec
GFLOW	G	Gas flow rate, gms/sec
H	-	Height above the distributor, cms
HB	h	Height above the bed surface, cms
HAREA	-	Total heat transfer area of cooling tubes (based on outside diameter of tube), cm^2
HCHAR	-	Hydrogen content in char, gm hydrogen/gm char
HCOAL	-	Lower heating value of coal, cals/gm
HCR	-	Critical bed height above which there is a fixed bed section, cm
HFB	-	Freeboard height, cm
HLF	-	Expanded bed height, cm
HLMF	-	Bed height at minimum fluidization, cm
HTAR	-	Hydrogen content in tar, gm hydrogen/gm coal fed
H2	H_2	Wt. fraction H_2 in the volatiles; H_2 released during devolatilization, gmole H_2 /gm coal
H2O	H_2O	Wt. fraction H_2O in the volatiles; H_2O released during devolatilization, gmole H_2O/gm coal
H2SV	-	H_2S content in the volatiles, gmole H_2S/gmole volatiles
IARR	(SEE DESIGN)	
ICR	-	Indicator for cirtical bed height
IFBC	-	Indicator for fixed bed section
IGNITE	-	Indicator for combustion calculations
INOX	-	Indicator for NO_x calculations
IPRES	-	Indicator for pressure drop calculations

FORTRAN Symbol	Mathematical Symbol	Description
ISO2	-	Indicator for SO_2 calculations
ITEMP	-	Indicator for temperature calculations
ITRIAL	-	Number of trials made in the combustion calculations
KT	-	Number of compartments in freeboard
MAIR	-	Molecular weight of air, gms/gmole
MC	-	Atomic weight of carbon, gms/gatom
MCAO	-	Molecular weight of calcium oxide, gms/gmole
MCACO3	-	Molecular weight of calcium carbonate, gms/gmole
MCASO4	-	Molecular weight of calcium sulfate, gms/gmole
MCO	-	Molecular weight of carbon monoxide, gms/gmole
MCO2	-	Molecular weight of carbon dioxide, gms/gmole
MDIS	-	No. of solids withdrawal locations
MFEED	-	No. of solids feed locations
MGAS	-	Molecular weight of combustion gases, gms/gmole
MH2	-	Molecular weight of hydrogen, gms/gmole
MH2O	-	Molecular weight of water, gms/gmole
MH2S	-	Molecular weight of hydrogen sulfide, gms/gmole
MMGCO3	-	Molecular weight of magnesium carbonate, gms/gmole
MMGO	-	Molecular weight of magnesium oxide, gms/gmole
MN	-	Atomic weight of nitrogen, gms/gatom

FORTRAN Symbol	Mathematical Symbol	Description
MNO	-	Molecular weight of nitric oxide, gms/gmole
MN2	-	Molecular weight of nitrogen, gms/gmole
MO2	-	Molecular weight of oxygen, gms/gmole
MS	-	Atomic weight of sulfur, gms/gatom
MSO2	-	Molecular weight of sulfur dioxide, gms/gmole
MTAR	-	Average molecular weight of tar in the volatiles, gms/gmole
MTB	(SEE DESIGN)	
MTHE	(SEE DESIGN)	
M1	-	No. of compartments in the bed + 1
NA	-	No. of additive particles in the freeboard
NAMEC1 NAMEC2	-	Name of coal
NAMEL1 NAMEL2	-	Name of limestone
NC	-	No. of char particles in the freeboard
NCHAR	-	Nitrogen content in char, gm nitrogen/ gm char
NTC	-	Total number of compartments in the combustor using DZAV + 1
OCHAR	-	Oxygen content in char, gm oxygen/gm char
OTAR	-	Oxygen content in tar, gm oxygen/gm coal fed
PAV	P	Average pressure in the combustor, atm
PF	-	Pressure of fluidizing air at the inlet to the distributor, atm
PH	(SEE DESIGN)	
PHIB	ϕ_B	Mechanism factor in the freeboard
PHIE	ϕ_E	Mechanism factor in the emulsion phase
PI	π	3.14159265
PV	(SEE DESIGN)	

FORTRAN Symbol	Mathematical Symbol	Description
QAREA	-	Heat transfer rate to the tubes per unit heat transfer area of tubes, cals/cm^2.sec
QCHAR	-	Heat of combustion of char, cals/gm
QCLCN	-	Heat of calcination of limestone, cals/gm
QCO	-	Heat of combustion of carbon monoxide, cals/gmole
QTRANS	-	Total heat transferred to the cooling medium, cals/sec
QVCO	-	Heat of partial combustion of volatiles, cals/gmole
QVGAS	-	Heat of combustion of volatiles, cals/gmole
QVOL	-	Heat transfer rate per unit volume of bed, cals/cm^3
R	A	Defined by Equation (V.2)
RC	-	Fraction of carbon remaining in char after devolatilization, gm carbon/gm carbon in coal
RCHAR	R_{ch}	Char produced per unit gm of coal fed, gm/gm
RELB	-	Total release rate of SO_2 or NO_x in the bubble phase, gmole/sec
RELE	-	Total release rate of SO_2 or NO_x in the emulsion phase, gmole/sec
RG	R_g	Gas constant, 82.06 atm$\cdot$$cm^3$/gmole.°K
RH	-	Fraction of hydrogen remaining in char after devolatilization, gm hydrogen/gm hydrogen in coal
RHOAD	-	Density of additives, gms/cm^3
RHOASH	-	Density of ash, gms/cm^3
RHOBED	ρ_b	Density of the bed materials, gms/cm^3
RHOC	-	Density of coal, gms/cm^3

FORTRAN Symbol	Mathematical Symbol	Description
RHOCH	ρ_{ch}	Density of char, gms/cm^3
RHOGAS	ρ_g	Density of gas, gms/cm^3
RHOFG	-	Density of the fluidizing air at the inlet to the distributor, gms/cm^3
RN	-	Fraction of nitrogen remaining in char after devolatilization, gm nitrogen/gm nitrogen in coal
RO	-	Fraction of oxygen remaining in char after devolatilization, gm oxygen/gm oxygen in coal
RR	-	Rate of combustion of char in each compartment per unit weight fraction of carbon in the bed, gms/sec; heat generation rate minus heat of calcination in each compartment, gms/sec
RRB	-	Rate of combustion of char in the bubble phase, gms/sec
RRE	-	Rate of combustion of char in the emulsion phase, gms/sec
RS	-	Fraction of sulfur remaining in char after devolatilization, gm sulfur/gm sulfur in coal
RVGAS	-	Volatiles released during devolatilization per unit gm of coal, gmole volatiles/gm coal
SCHAR	-	Sulfur content in char, gm sulfur/gm char
SOLVOL	-	Volume of solids in the bed (including voids) which is equal to volume of bed at minimum fluidization (excluding the internals), cm^3
SULFUR	-	Sulfur released during char combustion, gatom/sec
T	T	Temperature, °K
TAR	Tar	Wt. fraction tar in the volatiles; tar released during devolatilization per unit gm of coal, gmole tar/gm coal
TARC	-	Stoichiometric air required per unit gm of char, gmole/gm char

FORTRAN Symbol	Mathematical Symbol	Description
TAV	-	Mean bed temperature, °K
TAVB	T_B	Mean temperature in the boundary layer of the char particles in the bubble phase, °K; also in the freeboard, °K
TAVE	T_E	Mean temperature in the boundary layer of the char particles in the emulsion phase, °K
TCRATE	-	Total char combustion rate, gm/sec
TETUBE	-	Total volume fraction of tubes in the bed
TF	-	Temperature of fluidizing air at the inlet to the distributor, °K
TFC	-	Total char feed rate, gms/sec
TNORM	-	Temperature criterion for convergency
TOLD	-	Bed temperature in the previous iteration, °K
TPB	-	Char particle temperature in the bubble phase, °K; also in the freeboard, °K
TPE	-	Char particle temperature in the emulsion phase, °K
TSF	-	Temperature of feed solids, °K
TSTA	-	Starting temperature (assumed) for iteration, °K
TW	-	Cooling water temperature, °K
TWALL	-	Wall temperature, °K
TWALLA	-	Average wall temperature used for heat losses, °K
TWAV	-	Log mean temperature of the cooling water
TWIN	-	Inlet water temperature, °K
TWOUT	-	Outlet water temperature, °K

FORTRAN Symbol	Mathematical Symbol	Description
UB	U_B	Bubble velocity, cm/sec
UHE	U	Bed to tube heat transfer coefficient, cals/sec·cm^2·°C
UHEAV1	-	Bed to tube heat transfer coefficient (average) within the bed, cals/sec·cm^2°C
UHEAV2	-	Bed to tube heat transfer coefficient (average) in the freeboard, cals/sec·cm^2 °C
UHEW	U_W	Bed to wall heat transfer coefficient, cals/sec·cm^2°C
UMF	U_{mf}	Minimum fluidization velocity, cm/sec
UO	U_o	Superficial gas velocity as a function of bed height, cm/sec
UOR	-	Orifice velocity, cm/sec
UT	U_t	Terminal velocity of the particle, cm/sec
UWALL1	-	Bed to wall heat transfer coefficient (average) within the bed, cals/sec cm2°C
UWALL2		Bed to wall heat transfer coefficient (average) in the freeboard, cals/sec cm^2 °C
UO	-	Superficial gas velocity at the distributor, cm/sec
V	-	Volatiles yield during devolatilization, gms volatiles/gm coal (daf); also gms volatiles/gm coal
VAHOLD	-	Volumetric additives holdup in the freeboard; cm^3 solid volume
VCHOLD	-	Volumetric char hold-up in the freeboard, cm^3 solid volume
VGASN	-	Volatile nitrogen in coal, gatom/gm coal (d.b.)
VGASS	-	Volatile sulfur in coal, gatom/gm coal (d.b.)
VISC	μ	Viscosity of gas, gm/cm·sec

FORTRAN Symbol	Mathematical Symbol	Description
VM	-	Proximate volatile matter in coal, gm/gm coal (daf)
VMF	-	Bed volume at minimum fluidization (excluding the internals), cm^3
VPROD	-	Volatiles released in each compartment, gmole/sec
WAD	$W_{f,a}$	Additives feed rate, gms/sec
WAHOLD	-	Additives hold-up in the freeboard, gms
WB	M_b	Weight of bed materials, gms
WCHOLD	-	Char hold-up in the freeboard, gms
WCOAL	-	Coal feed rate as received basis, gms/sec
WD	-	Solids withdrawal rate at each location, gms/sec
WDIS	W_D	Solids withdrawal rate, gms/sec
WEA	-	Additives entrainment rate in the freeboard, gms/sec
WEC	-	Char entrainment rate in the freeboard, gms/sec
WELUA	-	Solids (excluding char) elutriation rate from the combustor, gms/sec
WFAD	$W_{f,a}$	Additives feed rate in each compartment, gms/sec
WFC	$W_{f,c}$	Coal feed rate in each compartment, gms/sec
WMIX	W_{mix}	Solids mixing rate, gms/sec
WNET	W_{net}	Net flow rate of solids, gms/sec
WW	B	Defined by Equation (V.3)
X	X	Weight fraction carbon in the bed
XA	-	Ash content in coal as received basis, gm ash/gm coal
XACAO		Calcium oxide content in ash, gm CaO/gm ash

FORTRAN Symbol	Mathematical Symbol	Description
XAV	-	Average weight fraction of carbon in the bed
XC	-	Carbon content in coal, gm carbon/gm coal (d.b.)
XCAO	-	Calcium oxide content in limestone, gm CaO/gm limestone
XCF	-	Fixed carbon content in coal, gm carbon/gm coal (d.b.)
XCO2	-	Carbon dioxide content in limestone, gm CO_2/gm limestone
XCV	-	Volatile carbon content in coal, gm carbon/gm coal (d.b.)
XH	-	Hydrogen content in coal, gm hydrogen/gm coal (d.b.)
XMGO	-	Magnesium oxide content in limestone, gm MgO/gm limestone
XN	-	Nitrogen content in coal, gm nitrogen/gm coal (d.b.)
XO	-	Oxygen content in coal, gm oxygen/gm coal (d.b.)
XO2	X_{O_2}	Oxygen required for partial combustion of volatiles, gmole O_2/gmole volatile
XO2C	$X_{O_2,c}$	Oxygen required for complete combustion of volatiles, gmole O_2/gmole volatile
XS	-	Sulfur content in coal, gm sulfur/gm coal (d.b.)
XSIO2	-	Silicon dioxide content in limestone, gm SiO_2/gm limestone
XW	-	Moisture content in coal as received basis, gm H_2O/gm coal
YAV	-	Average O_2 concentration (assumed) for iteration, mole fraction
YB	-	Mole fraction O_2 or SO_2 or NO in the bubble phase

FORTRAN Symbol	Mathematical Symbol	Description
YBO	Y_B	Mole fraction O_2 in the bubble phase
YCO	Y_{CO}	Mole fraction CO
YCOE	$Y_{E,CO}$	Mole fraction CO in the emulsion phase
YCO2	Y_{CO_2}	Mole fraction CO_2
YCO2B	Y_{B,CO_2}	Mole fraction CO_2 in the bubble phase
YCO2E	Y_{E,CO_2}	Mole fraction CO_2 in the emulsion phase
YE	-	Mole fraction O_2 or SO_2 or NO in the emulsion phase
YEO	Y_E	Mole fraction O_2 in the emulsion phase
YGO	-	Gaseous species concentrations at the exit, mole fraction
YH2O	Y_{H_2O}	Mole fraction H_2O
YNOX	Y_{NO}	Mole fraction NO
YO	Y_O	Mole fraction O_2
YSO2	Y_{SO_2}	Mole fraction SO_2
YV	Y_v	Mole fraction volatiles
YVE	$Y_{E,v}$	Mole fraction volatiles in the emulsion phase
ZAVG	-	Average height of each compartment above the distributor, cm
ZB	(SEE DESIGN)	
ZF	-	Locations of solids feed ports, cms
ZHE	(SEE DESIGN)	
ZDIS	(SEE DESIGN)	

MAIN PROGRAM ELUTRIATION

FORTRAN Symbol	Mathematical Symbol	Description
AHE	(SEE DESIGN)	
ATB	A_t	Cross sectional area of the bed, cm^2
CAS	-	Ca/S molar ratio in feed solids
CCHAR	C_{ch}	Carbon content in char, gm carbon/ gm char
CELU	-	Char elutriated from the combustor, gms/sec
CHARC	-	Carbon content in char, gmole carbon/ gm coal
CHARH	-	Hydrogen content in char, gatom hydrogen/gm coal
CHARN	-	Nitrogen content in char, gatom nitrogen/gm coal
CHARO	-	Oxygen content in char, gatom oxygen/gm coal
CHARS	-	Sulfur content in char, gatom sulfur/gm coal
CH4	CH_4	Wt. fraction CH_4 in the volatiles; CH_4 released during devolatilization, gmole CH_4/gm coal
CO	CO	Wt. fraction CO in the volatiles; CO released during devolatilization, gmole CO/gm coal
COALC	-	Carbon content in coal, gatom carbon/ gm coal (d.b.)
COALH	-	Hydrogen content in coal, gatom hydrogen/gm coal (d.b.)
COALN	-	Nitrogen content in coal, gatom nitrogen/gm coal (d.b.)
COALO	-	Oxygen content in coal, gatom oxygen/gm coal (d.b.)
COALS	-	Sulfur content in coal, gatom sulfur/gm coal (d.b.)

FORTRAN Symbol	Mathematical Symbol	Description
COV	-	CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles
COVB	-	CO produced during volatiles combustion, gmole CO/gmole volatiles
CO_2	-	Wt. fraction CO_2 in the volatiles; CO_2 released during devolatilization, gmole CO_2/gm coal
CO2V	-	CO_2 released during devolatilization per mole of volatiles released, gmole CO_2/gmole volatiles
CO2VB	-	CO_2 produced during volatiles combustion, gmole CO_2/gmole volatiles
CTAR	-	Carbon content in tar, gm carbon/gm coal fed
DASVF	-	Surface volume mean particle diameter of additives in the feed, cm
DAWMF	-	Weight mean particle diameter of additives in the feed, cm
DCSE	d_{ce}	Surface volume mean diameter of char particles in the freeboard, cm
DCSVB	d_c	Surface volume mean diameter of char particles in the bed, cm
DCSVF	-	Surface volume mean diameter of coal particles in the feed, cm
DCWE	-	Weight mean diameter of char particles in the freeboard, cm
DCWMB	-	Weight mean diameter of char particles in the bed, cm
DCWMF	-	Weight mean diameter of coal particles in the feed, cm
DIA(I)	-	Feed particle diameter of ith fraction based on seiving screen size

FORTRAN Symbol	Mathematical Symbol	Description
DP	d_x	Mean diameter of the particles of x th size fraction, cm
DPSE	$d_{\ell e}$	Surface volume mean particle diameter of additives entrained in the freeboard, cm
DPSVB	d_ℓ	Surface volume mean particle diameter of additives in the bed, cm
DPWE	-	Weight mean particle diameter of additives entrained in the freeboard, cm
DPWMB	-	Weight mean particle diameter of additives in the bed, cm
DTUBE	(SEE DESIGN)	
EMF	ε_{mf}	Void fraction at minimum fluidization
EXAIR	-	Excess air, fraction
FMF	-	Molar feed rate of fluidizing air, gmole/sec
FMO	F_{MT}	Total molar flow rate of gas in the combustor, gmole/sec
FMTH	-	Stoichiometric air feed rate, gmole/sec
FRACTA	-	Weight fraction of additives feed of x th size fraction
FRACTC	-	Weight fraction of coal feed of x th size fraction
G	g	Acceleration due to gravity, cm/sec^2
GFLOW	G	Gas flow rate, gms/sec
HCHAR	-	Hydrogen content in char, gm hydrogen/gm char
HFB	-	Freeboard height, cm
HLF	-	Expanded bed height, cm

FORTRAN Symbol	Mathematical Symbol	Description
HLMF	-	Bed height at minimum fluidization, cm
HTAR	-	Hydrogen content in tar, gm hydrogen/gm coal fed
H2	H_2	Wt. fraction H_2 in the volatiles; H_2 released during devolatilization gmole H_2/gm coal
H2O	H_2O	Wt. fraction H_2O in the volatiles; H_2O released during devolatilization, gmole H_2O/gm coal
IARR	(SEE DESIGN)	
MAIR	-	Molecular weight of air, gms/gmole
MC	-	Atomic weight of carbon, gms/gatom
MCAO	-	Molecular weight of calcium oxide, gms/gmole
MCASO4	-	Molecular weight of calcium sulfate, gms/gmole
MCO	-	Molecular weight of carbon monoxide, gms/gmole
MCO2	-	Molecular weight of carbon dioxide, gms/gmole
MGAS	-	Molecular weight of combustion gases, gms/gmole
MH2	-	Molecular weight of hydrogen, gms/gmole
MH2O	-	Molecular weight of water, gms/gmole
MH2S	-	Molecular weight of hydrogen sulfide, gms/gmole
MNO	-	Molecular weight of nitric oxide, gms/gmole
MN2	-	Molecular weight of nitrogen, gms/gmole
MO2	-	Molecular weight of oxygen, gms/gmole
MS	-	Atomic weight of sulfur, gms/gatom

FORTRAN Symbol	Mathematical Symbol	Description
MSO2	-	Molecular weight of sulfur dioxide, gms/gmole
MTAR	-	Average molecular weight of tar in the volatiles, gms/gmole
MTB MTHE	(SEE DESIGN)	
NCHAR	-	Nitrogen content in char, gm nitrogen/gm char
NDP	-	Number of size fractions
OCHAR	-	Oxygen content in char, gm oxygen/gm char
OTAR	-	Oxygen content in tar, gm oxygen/gm coal fed
PAV	P	Average pressure in the combustor, atm
PH	(SEE DESIGN)	
PI	π	3.14159265
PV	(SEE DESIGN)	
R	A	Defined by Equation (V.2)
RC	-	Fraction of carbon remaining in char after devolatilization, gm carbon/gm carbon in coal
RCHAR	R_{ch}	Char produced per unit gm of coal fed, gm/gm
RG	R_g	Gas constant, 82.06 atm·cm^3/gmole·°K
RH	-	Fraction of hydrogen remaining in char after devolatilization, gm hydrogen/gm hydrogen in coal
RHOAD	-	Density of additives, gms/cm^3
RHOASH	-	Density of ash, gms/cm^3
RHOBED	ρ_b	Density of the bed materials, gms/cm^3
RHOC	-	Density of coal, gms/cm^3
RHOCH	ρ_{ch}	Density of char, gms/cm^3
RN	-	Fraction of nitrogen remaining in char after devolatilization, gm nitrogen/gm nitrogen in coal

FORTRAN Symbol	Mathematical Symbol	Description
RO	-	Fraction of oxygen remaining in char after devolatilization, gm oxygen/gm oxygen in coal
RS	-	Fraction of sulfur remaining in char after devolatilization, gm sulfur/gm sulfur in coal
RVGAS	-	Volatiles released during devolatilization per unit gm of coal gmole volatiles/gm coal
SCHAR	-	Sulfur content in char, gm sulfur/gm char
TAR	Tar	Wt. fraction tar in the volatiles; tar released during devolatilization per unit gm of coal, gmole tar/gm coal
TAV	-	Mean bed temperature, °K
TDHC	TDH	Transport disengaging height, cms
UO	U_o	Superficial gas velocity as a function of bed height, cms/sec
V	-	Volatiles yield during devolatilization, gms volatiles/gm coal (daf); also, gms volatiles/gm coal
VM	-	Proximate volatile matter in coal, gm/gm coal (daf)
VMF	0	Bed volume at minimum fluidization (excluding the internals), cm^3
WAD	$W_{f,a}$	Additives feed rate, gms/sec
WB	M_b	Weight of bed materials, gms
WBC	-	Weight of bed materials calculated, gms
WCOAL	$W_{f,c}$	Coal feed rate as received basis, gms/sec
WDIS	W_D	Solids withdrawal rate, gms/sec

FORTRAN Symbol	Mathematical Symbol	Description
WELUA	-	Solids (excluding char) elutriation rate, gms/sec
WW	B	Defined by Equation (V.3)
XA	-	Ash content in coal, gm ash/gm coal
XC	-	Carbon content in coal, gm carbon/gm coal (d.b.)
XCAO	-	Calcium oxide content in limestone, gm CaO/gm limestone
XCF	-	Fixed carbon content in coal, gm carbon/gm coal (d.b.)
XCO2	-	Carbon dioxide content in limestone, gm CO_2/gm limestone
XCV	-	Volatile carbon content in coal, gm carbon/gm coal (d.b.)
XH	-	Hydrogen content in coal, gm hydrogen/gm coal (d.b.)
XMGO	-	Magnesium oxide content in limestone, gm MgO/gm limestone
XN	-	Nitrogen content in coal, gm nitrogen/gm coal (d.b.)
XO	-	Oxygen content in coal, gm oxygen/gm coal (d.b.)
XS	-	Sulfur content in coal, gm sulfur/gm coal (d.b.)
XSIO2	-	Silicon dioxide content in limestone, gm SiO_2/gm limestone
XW	-	Moisture content in coal as received basis, gm H_2O/gm coal
ZB	(SEE DESIGN)	
ZHE	(SEE DESIGN)	

SUBPROGRAM AKAD

FORTRAN Symbol	Mathematical Symbol	Description
ALIME	λ_ℓ	Reactivity of lime
AKAD	$k_{v\ell}$	Overall volume reaction rate constant for limestone SO_2 reaction, 1/sec
DP	d_p	Particle diameter, cm
DP1 DP2 DP3	-	Specified particle diameter for which the limestone reactivity is given, cm
FS	f_ℓ	Fractional conversion of limestone
FB	-	Limestone reactivity (given)
RR	-	Mean reactivity of limestone particles of size, DP1
RB	-	Mean reactivity of limestone particles of size, DP2
RC	-	Mean reactivity of limestone particles of size, DP3
SG	S_g	Effective specific surface area of limestone, cm^2/gm
T	T	Temperature in the bed, °K

SUBPROGRAM AKK

FORTRAN Symbol	Mathematical Symbol	Description
AKCO2	-	Overall rate constant for $C-CO_2$ reaction, cm/sec
AKF	k_{cf}	Gas film diffusion rate constant for O_2, $gm/cm^2 \cdot sec \cdot atm$
AKFCO2	-	Gas film diffusion rate constant for CO_2, $gm/cm^2 \cdot sec \cdot atm$

FORTRAN Symbol	Mathematical Symbol	Description
AKRCO2	k_{CO_2}	C-CO_2 chemical reaction rate constant, cm/sec
AKR	k_c	Overall rate constant for char combustion, cm/sec
AKS	k_{cR}	Chemical reaction rate constant for char combustion, cm/sec
COND	λ	Thermal conductivity of the gas, cals/sec.cm.°C
D	D	Molecular diffusivity for O_2-N_2, cm^2/sec; for CO_2-N_2, cm^2/sec
DC	-	Diameter of char particle, cm
DTS	-	Increment in temperature, °K
EM	ε_m	Emissivity of the char particle
ETS	-	Difference between assumed and calculated temperatures, °K
ETSMAX	-	Tolerance limit for temperature convergency, °K
MC	-	Atomic weight of carbon, gms/gatom
P	-	Pressure in the combustor, atm
PHI	ϕ	Mechanism factor for char combustion
Q	-	Heat of combustion of char, cals/gm char
RG	R_g	Gas constant, 82.06 atm. cm^3/gmole.°K
SIGM	σ	Stefan-Boltzman constant, cal/s.cm^2.°K^4
T	T	Temperature in the bed, °K
TAV	T_m	Mean temperature in the boundary layer of the particle, °K
TP	T_c	Char particle temperature, °K
YO2	-	Mole fraction oxygen
Z	p	Defined by Equation (V.16)

SUBPROGRAM AREA

FORTRAN Symbol	Mathematical Symbol	Description
ATB	-	Bed cross sectional area at height ZB above the distributor, cm^2
ATI	-	Bed cross sectional area at height ZI above the distributor, cm^2
DTI	D_t	Diameter of the combustor at height ZI above the distributor, cms
MTB	-	Number of locations along the combustor where the cross sectional areas are specified.
PI	π	3.14159265
RI	-	Radius of the combustor at height ZI above the distributor, cms
ZB	-	Height above the distributor at which the cross sectional area is specified, cms
ZI	-	Height above the distributor, cms

SUBPROGRAM ATTR

FORTRAN Symbol	Mathematical Symbol	Description
AKF	k_{cf}	Gas film diffusion rate constant, $gm/cm^2 \cdot sec \cdot atm$
AKR	k_c	Overall rate constant for char combustion, cm/sec
AKS	k_{cR}	Chemical reaction rate constant for char combustion, $gm/cm^2.sec.atm$
COND	λ	Thermal conductivity of the gas, cals/ $sec \cdot cm \cdot {}^\circ C$
D	D	Molecular diffusivity for O_2-N_2 cm^2/sec
DC	-	Diameter of the char particle, cm
DTS	-	Increment in temperature, °K
EM	ε_m	Emissivity of the char particle

C-3

FORTRAN Symbol	Mathematical Symbol	Description
ETS	-	Difference between assumed and calculated temperatures, °K
ETSMAX	-	Tolerance limit for temperature convergency, °K
MC	M_c	Atomic weight of carbon, gms/gatom
P	-	Pressure in the combustor, atm
PHI	ϕ	Mechanism factor for char combustion
Q	-	Heat of combustion of char, cals/gm char
RG	R_g	Gas constant, 82.06 atm.cm^3/gmole·°K
RHOCCH	$\rho_{c,ch}$	Density of carbon in char, gms/cm^3
RKI	-	Size reduction constant for char (due to combustion), 1/sec
SIGM	σ	Stefan-Boltzman constant, cal/s.cm^2.K^4
T	T	Temperature in the bed, °K
TAV	T_m	Mean temperature in the boundary layer layer of the char particle, °K
TB	t_b	Burning time of a char particle, sec
TP	T_c	Char particle temperature, °K
YO2	-	Mole fraction oxygen
Z	p	Defined by Equation (V.16)

SUBROUTINE CRRECT

FORTRAN Symbol	Mathematical Symbol	Description
DX	-	Increment in the variable, x
E	-	Difference between the assumed and calculated values of the variable, x
EMAX	-	Tolerance limit for convergency
E1	-	Value of E in the iteration, I
E2	-	Value of E in the iteration, I+1

FORTRAN Symbol	Mathematical Symbol	Description
I	-	Iteration or step number
INDX	-	Indicator for convergency interval
X	-	Variable for which the assumed and calculated values should be equal
X1	-	Value of x in the iteration, I
X2	-	Value of x in the iteration, I+1

SUBPROGRAM DESIGN

A1,A2,A3,A4	-	Alphanumeric characters
ABED	A_t	Cross sectional area of the combustor, cm^2
AHE	a_{HE}	Specific heat transfer area of the tubes, cm^2/cm^3 FBC volume
AND	n_d	Number of orifices in the distributor
ATB	-	Bed cross sectional area at height ZB above the distributor, cm^2
DBED	D_t	Diameter of the combustor, cm
DNZL	-	Diameter of orifice holes in the distributor, cm
DTUBE	d_o	Diameter of cooling tubes, cm
DVB	-	Volume of each compartment based on DZAV, cm^3
DVBEFF	-	Volume of each compartment excluding the tubes, cm^3
DZAV	-	Average compartment size used in design calculations, cm
FD	-	Fraction of solids withdrawn from the bed at each location
FFAD	-	Fraction of total additives fed at each location

FORTRAN Symbol	Mathematical Symbol	Description
FFC	-	Fraction of total coal fed at each location
FSW	f_{sw}	Fraction of wake solids thrown into the freeboard
FW	f_w	Ratio of wake volume to the bubble volume including the wakes
IARR	-	Tubes arrangement code
MDIS	-	No. of solids withdrawal locations
MFEED	-	No. of solids feed locations
MTB	-	No. of locations along the combustor where the cross sectional areas are specified
MTHE	-	No. of locations of cooling tubes
NTC	-	Total number of compartments in the combustor using DZAV + 1
PI	π	3.14159265
PH	P_H	Horizontal pitch distance between the tubes, cm
PV	P_V	Vertical pitch distance between the tubes, cm
ZB	-	Height above the distributor at which the cross sectional area is specified, cms
ZDIS	-	Locations of solids withdrawal ports, cms
ZF	-	Locations of solids feed ports, cms
ZHE	-	Locations of cooling tubes, cms

SUBPROGRAM ELUT

BB	-	Weight of bed material of x th size fraction, gms

FORTRAN Symbol	Mathematical Symbol	Description
CBED	-	Weight of char in the bed, gms
CBEDC	-	Weight of char in the bed (calculated), gms
CCHAR	C_{ch}	Carbon content in char, gm carbon/gm char
CELU	-	Char elutriated from the combustor, gms/sec
CENT	-	Char entrained in the freeboard, gms/sec
CU	-	Fraction finer than size, d_x
DCSE	d_{ce}	Surface volume mean diameter of char particles in the freeboard, cm
DCSVB	d_c	Surface volume mean diameter of char particles in the bed, cm
DCWE	-	Weight mean diameter of char particles in the freeboard, cm
DCWMB	-	Weight mean diameter of char particles in the bed, cm
DETC	-	Increment in combustion efficiency
DP	d_x	Mean diameter of the particles of x th size fraction, cm
DPSE	$d_{\ell e}$	Surface volume mean particle diameter of additives entrained in the freeboard, cm
DPSVB	d_ℓ	Surface volume mean particle diameter of additives in the bed, cm
DPWE	-	Weight mean particle diameter of additives entrained in the freeboard, cm
DPWMB	-	Weight mean particle diameter of additives in the bed, cm
DWDIS	-	Increment in the solids withdrawal rate, gms/sec

FORTRAN Symbol	Mathematical Symbol	Description
E	E_x	Elutriation rate constant, gm/sec
EETC	-	Tolerance limit for combustion efficiency convergency
EMF	ε_{mf}	Void fraction at minimum fluidization
ENTA	-	Entrainment rate of additives of x th size fraction in the freeboard, gm/sec
ENTC	-	Entrainment rate of char of x th size fraction in the freeboard, gm/sec
ERR	-	Difference between assumed and calculated combustion efficiencies
ETCA	-	Assumed combustion efficiency
ETCC	-	Calculated combustion efficiency
EWB	-	Tolerance limit for bed height convergency
FCE	-	Weight fraction of char particles of x th size fraction entrained
FFI	a_x	Proportion of total abrasion fines in the x th size fraction
FO	-	Solids entrainment rate at the bed surface of x th size fraction, gms/sec
FRA	b_x	Weight fraction of bed materials in the x th size fraction
FRACTA	-	Weight fraction of additives feed of x th size fraction
FRACTC	-	Weight fraction of coal feed of x th size fraction
FRAEL	-	Weight fraction of additives of x th size fraction elutriated from the combustor
FRAEN	-	Weight fraction of additives of x th size fraction entrained in the freeboard

FORTRAN Symbol	Mathematical Symbol	Description
FRC	-	Weight fraction of char particles of x th size fraction in the bed
FSC	-	Fraction of solids in the cloud region
FSW	f_{sw}	Fraction of wake solids thrown into the freeboard
FW	f_{sw}	Volume fraction of wake to bubble (including wakes)
GFLOW	G	Gas flow rate, gms/sec
HB	h	Height above the bed surface, cms
HFB	-	Freeboard height, cm
HLF	-	Expanded bed height, cm
HLMF	-	Bed height at minimum fluidization, cm
MGAS	-	Molecular weight of gas, gms/gmole
MTB	-	No. of locations along the combustor where the cross sectional areas are specified
NDP	-	Number of size fractions
P1	p_1	Proportion of fines recycled to the bed from the primary cyclone
P2	p_2	Proportion of fines recycled to the bed from the secondary cyclone
PAV	P	Average pressure of the FBC, atm
PFA	-	Gain of fines in the x th size fraction due to abrasion, gms/sec
Q1	q_{1x}	Collection efficiency of the primary cyclones for the x th size fraction
Q2	q_{2x}	Collection efficiency of the secondary cyclones for the x th size fraction
R	-	Entrainment rate of particles of size d_x, gms/sec
RCHAR	R_{ch}	Char produced per unit gm of coal fed, gm/gm

FORTRAN Symbol	Mathematical Symbol	Description
RG	R_g	Gas constant, 82.06 atm.cm^3/gmole·°K
RHOAD	-	Density of additives, gms/cm^3
RHOBED	ρ_b	Density of bed materials, gms/cm^3
RHOCCH	$\rho_{c,ch}$	Density of carbon in char, gms/cm^3
RHOCH	ρ_{ch}	Density of char, gms/cm^3
RHOGAS	ρ_g	Density of gas, gms/cm^3
RK	K	Attrition rate constant, 1/cm
RKI	-	Size reduction constant for char (due to combustion), 1/sec
RT	-	Residence time of solids in the freeboard, sec
TAV	-	Mean bed temperature, °K
TB	t_b	Burning time of a char particle, sec
TDH	TDH	Transport Disengaging Height, cm; if TDH > HFB, TDH = HFB
TDHC	TDH	Transport Disengaging Height, cm
UMF	U_{mf}	Minimum fluidization velocity, cm/sec
UO	U_o	Superficial gas velocity at the bed surface, cm/sec
UTA	-	Terminal velocity of additive particles of size d_x, cm/sec
UTC	-	Terminal velocity of char particles of size d_x, cm/sec
VISC	μ	Viscosity of gas, gm/cm.sec
VMF	-	Bed volume at minimum fluidization (excluding the internals), cm^3
W	W_x	Rate of transfer of particles from size fraction x to fraction x+1 by size reduction, gms/sec

FORTRAN Symbol	Mathematical Symbol	Description
WAD	$W_{f,a}$	Additives feed rate, gms/sec
WB	M_b	Weight of bed materials, gms
WBC	-	Weight of bed materials calculated, gms
WCOAL	$W_{f,c}$	Coal feed rate, gms/sec
WDIS	W_D	Solids withdrawal rate, gms/sec
WEA	-	Additives entrainment rate in the freeboard, gms/sec
WEC	-	Char entrainment rate in the freeboard, gms/sec
WELUA	-	Solids (excluding char) elutriation rate, gms/sec
WF	$W_{f,x}$	Solids feed rate of x th size fraction, gms/sec
WTF	-	Feed rate of (limestone + ash in coal)
XA	-	Ash content in coal, gm ash/gm coal
XAV	-	Weight fraction carbon in the bed (average), gm carbon/gm bed material
YO2	-	Mole fraction oxygen
ZB	-	Height above the distributor at which the cross sectional area is specified, cms

SUBPROGRAM FBC

FORTRAN Symbol	Mathematical Symbol	Description
AKC	k_c	Overall rate constant for char combustion, cm/sec
AKCO2	-	Overall rate constant for $C-CO_2$ reaction, cm/sec
AKP	k'	Defined by Equation (VI.32)

FORTRAN Symbol	Mathematical Symbol	Description
COB	-	Carbon monoxide burnt in each compartment, gmole/sec
COVB	-	CO produced during volatiles combustion, gmole CO/gmole volatiles
CO2VB	-	CO_2 produced during volatiles combustion, gmole CO_2/gmole volatiles
DCSVE	d_{ce}	Surface volume mean diameter of char particles in the freeboard, cm
DVBB	-	Volume of each compartment, cm^3
DYO	-	Increment in O_2 mole fraction
ER	-	Difference between assumed and calculated O_2 concentrations, mole fraction
ETUBE	ε_{tube}	Volume fraction of tube in each compartment
EYO	-	Tolerance limit for O_2 concentration convergency
FMO	F_{MT}	Total molar flow rate of gas in the combustor, gmole/sec
G	g	Acceleration due to gravity, cm/sec^2
GB	g_B	Volatiles burning rate in the bubble phase, gmole/sec
GE	g_E	Volatiles burning rate in the freeboard, gmole/sec
NC	-	No. of char particles in the freeboard
PAV	P	Average pressure in the combustor, atm
PHIB	ϕ_B	Mechanism factor in the freeboard
PI	π	3.14159265
RG	R_g	Gas constant, 82.06 atm.cm^3/gmole.°K
RVGAS	-	Volatiles released during devolatilization per unit gm of coal, gmole volatiles/gm coal

FORTRAN Symbol	Mathematical Symbol	Description
T	T	Temperature, °K
TAVB	T_B	Mean temperature in the boundary layer of the char particles in the freeboard, °K
XO2	X_{O_2}	Oxygen required for partial combustion of volatiles, gmole O_2/gmole volatile
YCO	Y_{CO}	Mole fraction CO
YCO0	-	Mole fraction CO in the bottom compartment
YCO2	-	Mole fraction CO_2 in the bottom compartment
YH2O	Y_{H_2O}	Mole fraction H_2O
YO	Y_O	Mole fraction oxygen
YOC	-	Mole fraction oxygen calculated
YO0	-	Mole fraction oxygen in the bottom compartment
YV	Y_V	Mole fraction volatiles
YV0	-	Mole fraction volatiles in the bottom compartment

SUBPROGRAM GPB

FORTRAN Symbol	Mathematical Symbol	Description
A	-	Matrix coefficients
AA	-	Matrix coefficients
AKB	$k_{c,B}$	Overall rate constant for char combustion in bubble phase, cm/sec
AKBE	K_{BE}	Gas exchange coefficient, 1/sec
AKCO2	-	Overall rate constant for C-CO_2 reaction, cm/sec
AKE	$k_{c,E}$	Overall rate constant for char combustion in emulsion phase, cm/sec

FORTRAN Symbol	Mathematical Symbol	Description
AKP	k	Defined by Equation (VI.24)
AMODF	a_m	Defined by Equation (VI.12)
B	-	Matrix coefficients
BB	-	Mtrix coefficients
COB	-	Carbon monoxide burnt in each compartment, gmole/sec
COV	-	CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles
COVB	-	CO produced during volatiles combustion, gmole CO/ gmole/volatiles
CO2V	-	CO_2 released during devolatilization per mole of volatiles released, gmole CO_2/gmole volatiles
CO2VB	-	CO_2 produced during volatiles combustion, gmole CO_2/gmole volatiles
DVBB	-	Volume of each compartment, cm^3
DYE	-	Increment in oxygen concentration in emulsion phase, mole fraction
EMAX	-	Tolerance limit for oxygen concentration convergency
EMF	ε_{mf}	Void fraction at minimum fluidization
EPB	ε_B	Bubble fraction
EPC	ε_c	Cloud fraction including bubble
FBM	F_{BM}	Molar flow rate of gas in the bubble phase, gmole/sec
FBMO	-	Molar flow rate of gas in the bubble phase in the bottom compartment, gmole/sec
FEM	F_{EM}	Molar flow rate of gas in the emulsion phase, gmole/sec
FEMO	-	Molar flow rate of gas in the emulsion phase in the bottom compartment, gmole/sec

FORTRAN Symbol	Mathematical Symbol	Description
GB	g_B	Volatiles burning rate in the bubble phase, gmole/sec
GE	g_E	Volatiles burning rate in the emulsion phase, gmole/sec
PAV.	P	Average pressure in the combustor, atm.
PHIE	ϕ_E	Mechanism factor in the emulsion phase
RG	R_g	Gas constant, 82.06 atm.cm^3/gmole.°K
RVGAS	-	Volatiles released during devolatilization per unit gm of coal, gmole volatiles/gm coal
T	T	Temperature in the bed, °K
TAVB	T_B	Mean temperature in the boundary layer of the char particles in the bubble phase,°K
TAVE	T_E	Mean temperature in the boundary layer of the char particles in the emulsion phase,°K
VPROD	-	Volatiles released in each compartment, gmole/sec
X	X	Weight fraction carbon in the bed
XO2	X_{O_2}	Oxygen required for partial combustion of volatiles, gmole O_2/gmole volatiles
XO2C	$X_{O_2,c}$	Oxygen required for complete combustion of volatiles, gmole O_2/gmole volatiles
YB	Y_B	Mole fraction oxygen in the bubble phase
YBO	-	Mole fraction oxygen in the bubble phase in the bottom compartment
YCOE	$Y_{E,CO}$	Mole fraction CO in the emulsion phase
YCOEO	-	Mole fraction CO in the emulsion phase in the bottom compartment
YCO2B	Y_{B,CO_2}	Mole fraction CO_2 in the bubble phase
YCO2BO	-	Mole fraction CO_2 in the bubble phase in the bottom compartment

YCO2E	Y_{E,CO_2}	Mole fraction CO_2 in the emulsion phase
YCOEO	-	Mole fraction CO_2 in the emulsion phase in the bottom compartment
YE	Y_E	Mole fraction oxygen in the emulsion phase
YEC	-	Mole fraction oxygen calculated
YEO	-	Mole fraction oxygen in the bottom compartment
YH2O	Y_{H_2O}	Mole fraction H_2O
YVE	$Y_{E,v}$	Mole fraction volatiles in the emulsion phase
YVEO	-	Mole fraction volatiles in the emulsion phase in the bottom compartment

<u>SUBPROGRAM GPHASE</u>

AKB	-	Reaction rate constant in bubble phase
AKBE	K_{BE}	Gas exchange coefficient, 1/sec
AKE	-	Reaction rate constant in emulsion phase
AM	a_m	Defined by Equation (VI.12) for NO_x reduction reaction; = $(1-\varepsilon_{mf})$ for SO_2 absorption reaction
DVBB	-	Volume of each compartment, cm^3
EPB	ε_B	Bubble fraction
EPC	ε_c	Cloud fraction including bubble
ETUBE	ε_{tube}	Volume fraction of tubes in each compartment
FBM	F_{BM}	Molar flow rate of gas in the bubble phase, gmole/sec
FBMO	-	Molar flow rate of gas in the bubble phase in the bottom compartment, gmole/sec
FEM	F_{EM}	Molar flow rate of gas in the emulsion phase, gmole/sec
FEMO	-	Molar flow rate of gas in the emulsion phase in the bottom compartment, gmole/sec

FORTRAN Symbol	Mathematical Symbol	Description
GENB	-	SO_2 or NO_x release rate in the bubble phase, gmole/sec
GENE	-	SO_2 or NO_x release rate in the emulsion phase, gmole/sec
PAV	P	Average pressure in the combustor, atm
RG	R_g	Gas constant, 82.06 atm.cm^3/gmole.°K
T	T	Temperature in the bed, °K
TB	T_B	Mean temperature in the boundary layer of the particles, °K
TE	T_E	Mean temperature in the boundary layer of the particles, °K
YB0	-	Gas concentration in the bubble phase in the bottom compartment, mole fraction
YB1	-	Gas concentration in the bubble phase, mole fraction
YE0	-	Gas concentration in the emulsion phase in the bottom compartment, mole fraction
YE1	-	Gas concentration in the emulsion phase, mole fraction

SUBPROGRAM HAREA

FORTRAN Symbol	Mathematical Symbol	Description
ATB	-	Bed cross sectional area at height ZB above the distributor, cm^2
ATI	-	Bed cross sectional area at height ZI above the distributor, cm^2
DTI	D_t	Diameter of the combustor at height ZI above the distributor, cm
MTB	-	Number of locations along the combustor where the cross sectional areas are specified
PI	π	3.14159265
RI	-	Radius of the combustor at height ZI above the distributor, cms

FORTRAN Symbol	Mathematical Symbol	Description
ZI	-	Height above the distributor, cms
		SUBPROGRAM HEIGHT
DBVEFF	-	Volume of each compartment excluding the tubes, cm^3
DZAV	-	Average compartment size used in design calculations, cm
HEIGHT	-	Height above the distributor, cm
HT	-	Height above the distributor, cm
NTC	-	Total number of compartments in the combustor using DZAV + 1
VV	-	Volume of bed (excluding tubes) at any height, cm^3
		SUBPROGRAM HYDRO
AHE	a_{HE}	Specific heat transfer area of the tubes, cm^2/cm^3 (DESIGN input) FBC volume
AHEAV	a_{HE}	Specific heat transfer area of the tubes in each compartment, cm^2/cm^3, FBC volume
AKBE	K_{BE}	Gas exchange coefficient, 1/sec
ALFB	α_b	$=\varepsilon_{mf}\ U_B/U_{mf}$
AND	n_d	Number of orifices in the distributor
AT	A_t	Cross sectional area of the bed, cm^2
ATAV	-	Average cross sectional area used in calculations for each compartment
BEDVOL	-	Total bed volume, cm^3
DBA	-	Bubble diameter in each compartment assumed, cm
DBAV	D_B	Bubble diameter in each compartment, cm

FORTRAN Symbol	Mathematical Symbol	Description
DBC	-	Bubbld diameter (calculated), cm
DBMAX	D_{BM}	Fictitious maximum bubble diameter, cm
DBO	D_{BO}	Bubble diameter at the distributor level, cm
DDB	-	Increment in bubble size, cm
DPSVB	-	Surface volume mean particle diameter of additives in the bed, cm
DT	D_t	Diameter of the combustor, cm
DTAV	-	Average diameter used in calculations for each compartment
DTUBE	d_o	Diameter of cooling tubes (DESIGN input), cm
DTUBEI	-	Diameter of cooling tubes in each compartment, cm
DVBB	-	Volume of each compartment, cm^3
DVBBFF	-	Volume of each compartment (excluding the tubes), cm^3
EFFVOL	-	Volume of the bed (excluding the tubes), cm^3
EMAX	-	Tolerance limit for bubble diameter convergency
EMF	ε_{mf}	Void fraction at minimum fluidization
EPB	ε_B	Bubble fraction
EPC	ε_c	Cloud fraction including bubble
ETUBE	ε_{tube}	Volume fraction of tubes in each compartment
FMO	F_{MT}	Total molar flow rate of gas in the combustor, gmole/sec
G	g	Accelaration due to gravity, cm/sec^2

FORTRAN Symbol	Mathematical Symbol	Description
H	-	Height above the distributor, cms
HAV	-	Average height of the compartment, cms
HB	h	Height above the bed surface, cm
HCR	-	Critical bed height above which there is a fixed bed section, cm
HFB	-	Freeboard height, cm
HLF	-	Expanded bed height, cm
IARR	-	Tubes arrangement code (DESIGN input)
IARRNG	-	Tubes arrangement code in each compartment
ICR	-	Indicator for critical bed height
IFBC	-	Indicator for fixed bed section
LAST	-	Indicator for the last compartment in the bed
M	-	Number of compartments in the bed
MGAS	-	Molecular weight of gas, gms/gmole
MT	-	Total number of compartments in FBC + 1
MTHE	-	No. of locations of cooling tubes
M1	-	M + 1
PAV	P	Average pressure in the combustor, atms
PH	P_H	Horizontal pitch distance between the tubes (DESIGN input), cm
PHI	P_H	Horizontal pitch distance between the tubes in each compartment, cm
PV	P_V	Vertical pitch distance between the tubes (DESIGN input), cm
PVI	P_V	Vertical pitch distance between the tubes in each compartment, cm

FORTRAN Symbol	Mathematical Symbol	Description
RG	R_g	Gas constant, 82.06 atm.cm^3/gmole.°K
RHOBED	ρ_b	Density of bed materials, gm/cm^3
RHOGAS	ρ_g	Density of gas, gm/cm^3
SUM	-	Height that would be occupied by solids alone in each compartment, cm
SUMEFF	-	Effective volume of bed (solids volume alone), cm^3
SUMV	-	Volume of bed, cm^3
SOLVOL	-	Volume of solids in each compartment (including voids), cm^3
T	T	Temperature in the bed, °K
TETUBE	-	Total volume fraction of tubes in the bed
UB	U_B	Bubble velocity, cm/sec
UBR	-	Bubble rising velocity, cm/sec
UBS	-	Bubble rising velocity under slugging conditions, cm/sec
UMF	U_{mf}	Minimum fluidization velocity, cm/sec
UO	U_o	Superficial gas velocity, cm/sec
VISC	μ	Viscosity of gas, gm/cm.sec
VMF	-	Bed volume at minimum fluidization (excluding internals), cm^3
X	X	Weight fraction carbon in the bed
YB	Y_B	Mole fraction oxygen in the emulsion phase
ZHE	-	Locations of cooling tubes, cm

SUBPROGRAM VEL

DPAR	d_p	Particle diameter, cm

FORTRAN Symbol	Mathematical Symbol	Description
G	g	Acceleration due to gravity, cms/sec^2
REP	$R_{e,p}$	Particle Reynolds number
RHOGAS	ρ_g	Density of gas, gm/cm^3
RHOS	ρ_s	Density of solids, gm/cm^3
UM	U_{mf}	Minimum fluidization velocity, cm/sec
UT	U_t	Terminal velocity of the particle, cms/sec
VISC	μ	Viscosity of gas, gm/cm.sec
		SUBPROGRAM VOLUME
DVBEFF	-	Volume of each compartment excluding the tubes, cm^3
DZAV	-	Average compartment size used in design calculations, cm
VOLUME	-	Volume of bed (excluding tubes) at any height ZZ, cm^3
ZZ	-	Height above the distributor, cms