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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<tr>
<td>G</td>
<td>Acceleration due to gravity, (\text{cms/sec}^2)</td>
</tr>
<tr>
<td>REP</td>
<td>Particle Reynolds number</td>
</tr>
<tr>
<td>RHOGAS</td>
<td>Density of gas, (\text{gm/cm}^3)</td>
</tr>
<tr>
<td>RHOS</td>
<td>Density of solids, (\text{gm/cm}^3)</td>
</tr>
<tr>
<td>UM</td>
<td>Minimum fluidization velocity, (\text{cm/sec})</td>
</tr>
<tr>
<td>UT</td>
<td>Terminal velocity of the particle, (\text{cm/sec})</td>
</tr>
<tr>
<td>VISC</td>
<td>Viscosity of gas, (\text{gm/cm.sec})</td>
</tr>
</tbody>
</table>

**SUBPROGRAM/VOLUME**

<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>DVBEFF</td>
<td>Volume of each compartment excluding the tubes, (\text{cm})</td>
</tr>
<tr>
<td>DZAV</td>
<td>Average compartment size used in design calculations, (\text{cm})</td>
</tr>
<tr>
<td>VOLUME</td>
<td>Volume of bed (excluding tubes) at any height (\text{ZZ}), (\text{cm})</td>
</tr>
<tr>
<td>ZZ</td>
<td>Height above the distributor, (\text{cm})</td>
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NOMENCLATURE

\( A \quad \text{Defined by equation (V.2)} \)

\( A_t \quad \text{Cross sectional area of the bed, cm}^2 \)

\( a_{B,NO} \quad \text{Defined by equation (VI.51)} \)

\( a_{B,SO_2} \quad \text{Defined by equation (VI.49)} \)

\( a_{E,NO} \quad \text{Defined by equation (VI.47)} \)

\( a_{E,SO_2} \quad \text{Defined by equation (VI.45)} \)

\( a_{HE} \quad \text{Specific heat transfer area of the tubes, cm}^2/\text{cm}^3 \text{ FBC volume} \)

\( a_{HEW} \quad \text{Specific heat transfer area of the walls, cm}^2/\text{cm}^3 \text{ FBC volume} \)

\( a_{NO} \quad \text{Defined by equation (VI.55)} \)

\( a_{SO_2} \quad \text{Defined by equation (VI.53)} \)

\( a_m \quad \text{Defined by equation (VI.12)} \)

\( a_x \quad \text{Proportion of total abrasion fines in the xth size fraction} \)

\( a_1 \quad \text{Defined by equation (VI.9)} \)

\( a_2 \quad \text{Defined by equation (VI.15)} \)

\( a_3 \quad \text{Defined by equation (VI.25)} \)

\( a_4 \quad \text{Defined by equation (VI.21)} \)

\( a_1' \quad \text{Defined by equation (VI.33)} \)

\( a_2' \quad \text{Defined by equation (VI.30)} \)

\( a_4' \quad \text{Defined by equation (VI.33)} \)

\( B \quad \text{Defined by equation (V.3)} \)

\( b_x \quad \text{Weight fraction of bed material in the xth size fraction} \)

\( C_{ccf} \quad \text{Heat capacity of coal feed, cals/gm.}^\circ\text{C} \)

\( C_{CO_2} \quad \text{Concentration of carbon dioxide, gmole/cm}^3 \)
\( C_{NO} \) Concentration of nitric oxide, g/mole/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, g/mole/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 \\
\( C_{H_4} \) Wt. fraction \( C_4 \) in the volatiles \\
\( C_O \) Wt. fraction \( C_O \) in the volatiles \\
\( C_{O_2} \) Wt. fraction \( C_{O_2} \) 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 \\
\( d_{Le} \) 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 \( x \)th size fraction, cm \\
\( E_x \) Elutriation rate constant, gm/sec \\
\( E_2 \) Dispersion coefficient in the freeboard, l/sec \\
\( E_{BM} \) Molar flow rate of gas in the bubble phase, g/mole/sec \\
\( F_{EM} \) Molar flow rate of gas in the emulsion phase, g/mole/sec \\
\( F_T \) Total molar flow rate of gas in the combustor, g/mole/sec \\
\( F_{j} \) Solids entrainment rate at the bed surface, g/m/sec
$f_k$ 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 $x$th size fraction, $1/sec$
\( K' \) Defined by Equation (VI.32)

\( K'_{vl} \) Chemical reaction rate constant for limestone-SO\(_2\) reaction, \( \text{l/sec} \)

\( M \) 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

\( P_{02} \) 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

\( q_{\text{cal}} \) Heat of calcination of limestone, cals/gm

\( q_{\text{ch}} \) Heat of combustion of char, cals/gm

\( q_{\text{v}} \) Heat of combustion of volatiles (complete burning), cals/gmole

\( q_{v,\text{CO}} \) Heat of combustion of volatiles (partial burning), cals/gmole
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
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<tbody>
<tr>
<td>$q_{1x}$</td>
<td>Collection efficiency of the primary cyclones for the xth size fraction</td>
</tr>
<tr>
<td>$q_{2x}$</td>
<td>Collection efficiency of the secondary cyclones for the xth size fraction</td>
</tr>
<tr>
<td>$R$</td>
<td>Gas constant, 1.987 cals/gmole °K</td>
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<tr>
<td>$R_{B,NO,c}$</td>
<td>NO release rate in the bubble phase due to char combustion, gmole/sec</td>
</tr>
<tr>
<td>$R_{B,NO,V}$</td>
<td>NO release rate in the bubble phase due to volatiles combustion, gmole/sec</td>
</tr>
<tr>
<td>$R_{B,SO_2,c}$</td>
<td>SO$_2$ release rate in the bubble phase due to char combustion, gmole/sec</td>
</tr>
<tr>
<td>$R_{B,SO_2,V}$</td>
<td>SO$_2$ release rate in the bubble phase due to volatiles combustion, gmole/sec</td>
</tr>
<tr>
<td>$R_{CO}$</td>
<td>CO released during devolatilization, gmole/sec</td>
</tr>
<tr>
<td>$R_{CO_2}$</td>
<td>CO$_2$ released during devolatilization, gmole/sec</td>
</tr>
<tr>
<td>$R_{E,NO,c}$</td>
<td>NO release rate in the emulsion phase due to char combustion, gmole/sec</td>
</tr>
<tr>
<td>$R_{E,NO,V}$</td>
<td>NO release rate in the emulsion phase due to volatiles combustion, gmole/sec</td>
</tr>
<tr>
<td>$R_{E,SO_2,c}$</td>
<td>SO$_2$ release rate in the emulsion phase due to char combustion, gmole/sec</td>
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<td>$R_{E,SO_2,V}$</td>
<td>SO$_2$ release rate in the emulsion phase due to volatiles combustion, gmole/sec</td>
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<tr>
<td>$R_{e,p}$</td>
<td>Particle Reynolds number, defined by equations (A.VII.22-24)</td>
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<tr>
<td>$R_{NO}$</td>
<td>NO release rate, gmole/sec</td>
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<tr>
<td>$R_{SO_2}$</td>
<td>SO$_2$ release rate, gmole/sec</td>
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<tr>
<td>$R_a$</td>
<td>Attrition rate, gms/sec</td>
</tr>
<tr>
<td>$R_{ch}$</td>
<td>Char produced per unit gm of coal fed, gm/gm</td>
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<tr>
<td>$R_V$</td>
<td>Volatiles released, gmole/sec</td>
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<tr>
<td>$R_g$</td>
<td>Gas constant, 82.06 atm.cm$^3$/gmole °K</td>
</tr>
<tr>
<td>$r_{CO}$</td>
<td>Rate of combustion of CO, gmole/cm$^3$ sec</td>
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<tr>
<td>$r_i$</td>
<td>Char combustion rate in ith compartment, gms/sec</td>
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</table>
Char combustion rate, g mol/sec·particle

Effective specific surface area of limestone, cm$^2$/gm

Temperature in the bed, °K

Mean temperature in the boundary layer of the char particle in the bubble phase, °K; also in the freeboard, °K

Transport Disengaging Height, cms

Mean temperature in the boundary layer of the char particle in the emulsion phase, °K

Wt. fraction tar in the volatiles

Char particle temperature, °K

Mean temperature in the boundary layer of the char particle, °K

Solids feed temperature, °K

Cooling water temperature, °K

Average FBC wall temperature, °K

Temperature, °C

Burning time of a char particle, sec

Bed to tube heat transfer coefficient, cals/sec·cm$^2$·°C

Bubble velocity, cms/sec

Minimum fluidization velocity, cms/sec

Superficial gas velocity or fluidization velocity, cms/sec

Average superficial gas velocity in the freeboard, cms/sec

Terminal velocity of the particle, cms/sec

Bed to wall heat transfer coefficient, cals/sec·cm$^2$·°C

Volatiles yield during devolatilization, % of coal daf

Proximate volatile matter in the coal, % of coal daf

CO produced due to volatiles burning, g mol CO/g mol 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; $\Delta Z$ compartment size, cms

Greek Symbols

$\varepsilon_B$ Bubble fraction

$\varepsilon_c$ Cloud fraction including bubble

$\varepsilon_m$ Emissivity of the char particle

$\varepsilon_{mf}$ Void fraction at minimum fluidization

$\varepsilon_{tube}$ Volume fraction of tubes

$\theta$ Time, sec

$\lambda$ Thermal conductivity of the gas, cals/sec.cm$^\circ$C

$\lambda_L$ Reactivity of limestone

$\mu$ Viscosity of gas, gm/cm.sec

$\Pi$ 3.14159265

$\rho_B$ Density of the bed materials, gms/cm$^3$

$\rho_{C,CH}$ Density of carbon in char, gms/cm$^3$

$\rho_{CH}$ Density of char, gms/cm

$\rho_g$ Density of gas, gms/cm$^3$

$\rho_s$ Density of solids, gms/cm$^3$

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

$\phi$ Mechanism factor of char combustion
\( \phi_B \) Mechanism factor in the freeboard

\( \phi_E \) Mechanism factor in the emission phase

**Subscript**

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<td>( x )th size fraction</td>
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<tr>
<td>( i )</td>
<td>( i )th compartment</td>
</tr>
</tbody>
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**Abbreviation**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tr>
<td>d.b.</td>
<td>dry basis</td>
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<tr>
<td>daf</td>
<td>dry ash free basis</td>
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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:

$$\text{CaO} + \text{SO}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{CaSO}_4$$

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&EE), Morgantown Energy Technology Center (MBTC), 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 \( d_p < 50 \mu m \) 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:
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).

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).

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).

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 mathematical 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 Wer, 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

<table>
<thead>
<tr>
<th>Model Description</th>
<th>Investigators</th>
<th>Bubble Phase</th>
<th>Emulsion Phase</th>
<th>Solids mixing in the bed</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two phase bubbling bed model</td>
<td>Avedesian and Davidson (1973)</td>
<td>a) Plug Flow</td>
<td>Plug Flow</td>
<td>Complete Mixing</td>
<td>1) Bubble diameter is assumed to be uniform throughout the bed in most cases and is an adjustable parameter</td>
</tr>
<tr>
<td></td>
<td>Gibbs (1975)</td>
<td>b) Plug Flow</td>
<td>Complete Mixing</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Campbell and Davidson (1975)</td>
<td>c) Complete</td>
<td>Complete Mixing</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Gordon and Amundson (1976)</td>
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<td></td>
<td>Baron, et al. (1977)</td>
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<tr>
<td></td>
<td>Horio, et al. (1977)</td>
<td>Complete</td>
<td>Complete Mixing</td>
<td>Complete mixing within each</td>
<td>1) Bubbles grow along the bed height.</td>
</tr>
<tr>
<td>Two phase compartment in series</td>
<td>Rengarajan, et al. (1977)</td>
<td>mixing</td>
<td>within</td>
<td>within each compartment</td>
<td></td>
</tr>
<tr>
<td>model</td>
<td>Horio and Wen (1978)</td>
<td>within each compartment</td>
<td></td>
<td>with backflow of solids from one compartment to another</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Rajan, et al. (1978)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Three phase bubbling bed model</td>
<td>Chen and Saxena (1977)</td>
<td>Plug Flow</td>
<td>Plug Flow</td>
<td>Complete Mixing</td>
<td>1) Cloud-wake is treated as a separate phase and is in plug flow</td>
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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.
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.,

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.
Axial bed temperature profile.

O₂, CO, CO₂, SO₂ and NOₓ concentration profiles.

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, SO₂, NOₓ 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 SO₂ and NOₓ 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) SO₂ and NOₓ release during the combustion of char and volatiles and the simultaneous absorption of SO₂ by limestone and reduction of NOₓ 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.
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):

\[ V = VM - A - B \quad \text{(V.1)} \]
\[ A = \exp(26.41 - 3.961 \ln t + 0.0115 VM) \quad \text{(V.2)} \]
\[ B = 0.2(VM - 10.9) \quad \text{(V.3)} \]

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):

\[ CH_4 = 0.201 - 0.469 VM + 0.241 VM^2 \quad \text{(V.4)} \]
\[ H_2 = 0.157 - 0.868 VM + 1.388 VM^2 \quad \text{(V.5)} \]
\[ CO_2 = 0.135 - 0.900 VM + 1.906 VM^2 \quad \text{(V.6)} \]
\[ CO = 0.428 - 2.653 VM + 4.845 VM^2 \quad \text{(V.7)} \]
\[ H_2O = 0.409 - 2.389 VM + 4.554 VM^2 \quad \text{(V.8)} \]
\[ \text{Tar} = -0.325 + 7.279 VM - 12.880 VM^2 \quad \text{(V.9)} \]
Fig. 1 Schematic Illustration of the FBC
Volatile nitrogen released during devolatilization is expressed as (Fine, et al. 1974):

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

and volatile sulfur is expressed as:

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

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 volatile 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 \( \text{CO}_2 \) because of excess oxygen present in the bubble phase.

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

\[ \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2, \quad r_{\text{CO}} = 3 \times 10^{10} \left( \frac{p}{R T} \right)^{1.8} \exp\left(-16000/C/RT\right)Y_{\text{H}_2\text{O}}^{0.5} \times \frac{Y_{\text{CO}}^{17.5} Y_0^{1+24.7 Y_0}}{\text{gmole/m}^3\text{sec}} \quad (V.12) \]
Residual char burns according to the reaction:

\[
C + \frac{1}{2} O_2 \rightarrow (2 - \frac{2}{\phi})CO + \frac{2}{\phi}CO_2
\]  

(V.13)

where \(\phi\) 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, \(\phi\), 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, \(\phi\) is expressed as:

\[
\phi = \frac{2p + 2}{p + 2} \quad \text{for } d_c \leq 0.005 \text{ cm} \quad \text{(V.14)}
\]

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

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

\[
p = CO/CO_2 = 2500 \exp(-12400/RT) \quad \text{(V.16)}
\]

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

\[
r_* = \pi d_c^2 k_c C_{O_2} \quad \text{g mole/sec particle} \quad \text{(V.17)}
\]

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

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

\[
k_{cR} = \text{chemical reaction rate constant}
\]

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

\[
k_{cf} = \text{diffusion rate constant}
\]

\[
= 24 \phi D/d_c R_g T_m, \quad \text{gm/cm}^2 \cdot \text{sec} \cdot \text{atm} \quad \text{(V.20)}
\]
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). CO₂ formed during combustion reacts with char according to the following reaction:

\[
C + CO_2 \rightarrow 2 CO
\]  

(V.21)

and the rate expression for the above reaction is \( r_{CO_2} = \pi d_c^2 k_{CO_2} C_{CO_2} \) g mole/sec . particle, where \( k_{CO_2} = 4.1 \times 10^3 \exp(-59200/RT) \) cm/sec (Caram and Amundson, 1977).

2. Sulfur Dioxide - Limestone Reaction:

When limestone is added to a fluidized bed burning coal, the SO₂ released from the combustion of coal reacts with calcined limestone according to the reaction:

\[
CaO + SO_2 + \frac{1}{2} O_2 \rightarrow CaSO_4
\]  

(V.22)

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

\[
x_k = \frac{\pi}{6} d_k^3 \frac{d}{\nu} C_{SO_2}
\]  

(V.23)

where \( k_{\nu} \) is the overall volumetric reaction rate constant and is a rapidly decreasing function of limestone conversion, \( f_k \). The overall reaction rate constant, \( k_{\nu} \), is calculated by the equation:

\[
k_{\nu} = k_{N_\nu} S_g \lambda_k
\]  

(V.24)

where \( k_{\nu} \) is equal to \( 490 \exp(-17500/RT) \) g 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:

\[ S_g = -38.4 T + 5.6 \times 10^4, \text{ cm}^2/\text{gm for } T > 1253^\circ K \quad \text{(V.25)} \]

\[ = 35.9 T - 3.67 \times 10^4, \text{ cm}^2/\text{gm for } T < 1253^\circ K \quad \text{(V.26)} \]

\( \lambda_h \), 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 heterogeneouse 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

\[ C + 2 NO \rightarrow CO_2 + N_2 \quad \text{(V.27)} \]

The rate expression for NO reduction is

\[ r_{NO} = \pi d_c^2 k_{NO} C_{NO}, \text{ g mole NO/sec-particle} \quad \text{(V.28)} \]

where \( k_{NO} = 5.24 \times 10^7 \exp(-34000/RT_m) \text{ cm/sec} \) (Oguma, et al. 1977, Horio, et al. 1977).
TEMPERATURE = 850 °C

d_1 = 100 μm

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 \((U_0 - U_{mf})\) and also to the bed weight. The rate of production of fines is correlated as:

\[ R_a = K(U_0 - U_{mf})M_b \text{ gm/sec} \quad (V.29) \]

The value of \(K\) is dependent on the friability of the material. The values of \(K\) lie in the range \(9.11 \times 10^{-8}\) for ash and \(2.73 \times 10^{-8}\) 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:

\[ R_x = E_x b_x \text{ gms/sec} \quad (V.30) \]

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:

\[
E_x = 6 \exp[-10.4 \left( \frac{U_t}{U_o} \right)^{0.5} \left( \frac{U_{mf}}{U_o - U_{mf}} \right)^{0.25}] \text{ gm/sec} \quad (V.31)
\]

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:

\[
R_x = F_{0,x} \cdot \exp \left[ \frac{h}{275.0} \cdot \ln \left( \frac{E_x \cdot b_x}{F_{0,x}} \right) \right] \text{ gms/sec} \quad (V.32)
\]

where \( F_{0,x} \) 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).

\[
F_{0h} = A_t \cdot (U_o - U_{mf}) f_w \cdot (1 - \varepsilon_{mf}) \rho_s \cdot f_{sw} \text{ gms/sec} \quad (V.33)
\]

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.

\[ \text{TDH} = 0.429 \overline{U}_o^{1.2} (11.43 - 1.2 \ln \overline{U}_o) \text{ cms} \]  

(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:

\[ U_{mf} = \left( \frac{\mu}{\rho_g} \right) \left\{ \left[ 33.7^2 + \frac{0.0408 \rho_s \rho_g}{\rho_s - \rho_g} \right]^{1/2} - 33.7 \right\} \]  

(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):

\[ \frac{dD_B}{dz} = \frac{0.3}{D_t} (D_{BM} - D_B) \]  

(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:

\[ D_{BM} = 0.652 \left[ A_t (U_o - U_{mf}) \right]^{0.4} \]  

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):

\[ U_b = U_o - U_{mf} + 0.711 \sqrt{gD_B} \]  

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

\[ K_{BE} = 11.0/D_B \]  

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, \( \dot{W}_{mix} \), caused by the lifting of particles by bubble wakes is expressed as:

\[ \dot{W}_{mix} = (U_o - U_{mf}) A_t \frac{f_w}{(1 - \varepsilon_{mf})} \rho_s \]  

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:

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

where $\varepsilon_m$ is the emissivity of the char particle (taken as 1.0 Field, et al., 1967), $\lambda$ is the thermal conductivity of the surrounding gas and $\sigma$ 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$^2$.°C (40 to 80 Btu/hr.ft$^2$.°F). 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
<table>
<thead>
<tr>
<th>CATEGORY I</th>
<th>CATEGORY II</th>
</tr>
</thead>
<tbody>
<tr>
<td>(bulk circulation)</td>
<td>(local mixing)</td>
</tr>
</tbody>
</table>

**GROSS MIXING**

**DRIFT MOTION**

**Fig. 5 Two Modes of Solids Mixing**

particle trajectory after the passage of the bubble
Fig. 6 Schematic Illustration of the Solid Phase Model

$X_i, T_i$ : solids in compartment $i$

$W_{mix,i}$ : solids mixing rate in compartment $i$

$W_{mix,2}$ : solids mixing rate in compartment 2

$W_{net,i}$ : net flow rate of solids in compartment $i$

$W_{net,2}$ : net flow rate of solids in compartment 2

$X : \text{wt. fraction carbon}$

$T : \text{temperature}$

$W_{mix} : \text{solids mixing rate}$

$W_{net} : \text{net flow rate of solids}$
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)

\[
N_{Re} = \frac{D_t}{\bar{U}_o} \frac{\rho_g}{\mu_g} \quad (V.42)
\]

\[
N_{Pe} = \frac{\bar{U}_o \ D_t}{E_z} \quad (V.43)
\]

\[
N_{Sc} = \frac{\mu_g}{D} \frac{\rho_g}{\bar{U}_o} \quad (V.44)
\]

\[
\frac{1}{N_{Pe}} = \frac{1}{N_{Re}} \frac{N_{Sc}}{192} + \frac{N_{Re} \cdot N_{Sc}}{192} \quad \text{for } N_{Re} < 2000 \quad (V.45)
\]

\[
\frac{1}{N_{Pe}} = \frac{3 \times 10^7}{2.1 \ \frac{N_{Re}}{N_{Sc}}} + \frac{1.35}{1.8 \ \frac{N_{Re}}{N_{Sc}}} \quad \text{for } N_{Re} > 2000 \quad (V.46)
\]

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

\[
\Delta Z = 2 \ \frac{E_z}{\bar{U}_o} \quad (V.47)
\]

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 $\Delta Z/(\bar{U}_o - \bar{U}_r)$ where $\Delta Z$ is the compartment size. Solids hold-up in each compartment is then obtained from

\[
\text{Solids hold-up in each compartment} = \frac{(\text{upward+downward}) \text{ flow rate of solids x residence time of solids in that compartment}}{} \quad (V.48)
\]

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):

\[ t_b = \text{burning time of a char particle} \]

\[ = \frac{\rho_{c,\text{ch}} R_g T_m d_c^2}{(96 \phi D P_{O_2})} \]
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:

\[
W_{f,x} + W_{x-1} + a_x k_x M_x = M_x \frac{W_D}{M_b} + R_x q_{1x} (1-p_1) + R_x q_{2x} (1-q_{1x}) (1-p_2) \\
+ R_x (1-q_{1x})(1-q_{2x}) + k_x M_x \\
+ W_x
\]

\((VI.1)\)
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:

$$\frac{dM}{dt} = -k_x M(U_o - U_m)$$  \hspace{1cm} (VI.2)

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

$$\frac{dd_x}{dt} = -\frac{k_x}{3} d_x (U_o - U_m)$$  \hspace{1cm} (VI.3)

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

$$\frac{dM}{dd_x} = \frac{3M}{d_x}$$  \hspace{1cm} (VI.4)

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

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

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

Therefore, $W_x = \left[W_{f_{x+1}} + a_x K(U_o - U_m)M_o + W_{x-1}\right]\left(\frac{d_{x+1}}{d_x}\right)^3$.  \hspace{1cm} (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, CO₂, oxygen, SO₂ 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:**

\[ Y_{E,i} = 0.0 \]  \hspace{1cm} (VI.7)

**Volatile:**

\[ \frac{F_{E_{M,i}} Y_{E,v,i}}{Y_{E,i}} = \frac{F_{E_{M,i-1}} Y_{E,v,i-1}}{Y_{E,i-1}} - a_1 \frac{Y_{E,v,i-1}}{X_{O_2}} \]

(Volatiles out) \hspace{.5cm} (Volatiles in) \hspace{1cm} (Volatiles Exchanged to Bubble Phase)  \hspace{1cm} (VI.8)

\[ F_{E_{M,i-1}} Y_{E,v,i-1} + a_1 \frac{Y_{B,i}}{X_{O_2}} + R_{v,i} \]

(Volatiles Burnt) \hspace{1cm} (Volatiles Released during Devolutilization)

where \[ a_1 = K_{BE,i} A_{t,i} \Delta Z_i e_{E,i} \frac{P}{gT_i}, \text{ g mole/sec} \]  \hspace{1cm} (VI.9)

**Carbon monoxide:**

\[ F_{E_{M,i}} Y_{E,CO,i} = F_{E_{M,i-1}} Y_{E,CO,i-1} - a_1 Y_{E,CO,i} \]

(CO out) \hspace{1cm} (CO in) \hspace{1cm} (CO Exchanged to Bubble Phase)
\((\text{CO Produced by Volatiles}) + \text{(CO Released during Burning)}\)

\[\text{CO} + R_{\text{CO},i} + 2 a_4 Y_{E,\text{CO}_2,i}\]

\((\text{CO Produced by C-CO}_2 \text{ Reaction})\)

\[\text{where}\]

\[a_4 = a_m A_{x,i} \Delta N_i (1 - \epsilon_{c,i} - \epsilon_{\text{tube},i}) \left( k_{\text{CO}_2,i} \frac{P}{R T_{E,i}} \right) X_i \text{, gmole/sec}\]

\[a_m = \frac{6 \rho_b (1 - \epsilon_{mf})}{d_c \rho_{ch} c_{ch}}\]

\(\text{Carbon dioxide:}\)

\[F_{\text{EM},i} Y_{E,\text{CO}_2,i} = F_{\text{EM},i-1} Y_{E,\text{CO}_2,i-1} - a_1 (Y_{E,\text{CO}_2,i} - Y_{B,\text{CO}_2,i}) + R_{\text{CO}_2,i} + a_4 Y_{E,\text{CO}_2,i}\]

\((\text{CO}_2 \text{ out}) \quad (\text{CO}_2 \text{ in}) \quad (\text{CO}_2 \text{ Exchanged to Bubble Phase})\)

\[\text{(CO}_2 \text{ Released during Devolatilization) \quad (CO}_2 \text{ Consumed by C-CO}_2 \text{ Reaction)}\]

\(\text{Oxygen:}\)

\[F_{\text{BM},i} Y_{B,i} = F_{\text{BM},i-1} Y_{B,i-1} - a_1 Y_{B,i}\]

\((\text{Oxygen out}) \quad (\text{Oxygen in}) \quad (\text{Oxygen Exchanged to Emulsion Phase})\)
\[ -a_2 Y_{B,i} = \frac{a_1 Y_{E,CO,i}}{2} - a_1 Y_{E,v,i} X_{O_2,c} \quad \text{(VI.14)} \]

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

where

\[ a_2 = a_m \Delta Z_i (\varepsilon_{c,i} - \varepsilon_{B,i}) k_{CB,i} \frac{P}{R_{B,i}} T_i \quad \text{(VI.15)} \]

Carbon dioxide:

\[ F_{BM,i} Y_{B,CO_2,i} = F_{BM,i-1} Y_{B,CO_2,i-1} - a_1 (Y_{B,CO_2,i} - Y_{E,CO_2,i}) \quad \text{(CO_2 out)} \]

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

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

**FREEBOARD EQUATIONS**

Oxygen:

\[ Y_{O,i} = 0.0 \quad \text{(VI.17)} \]
Volatile:
\[ F_{MT} Y_{v,i} = F_{MT} Y_{v,i-1} - F_{MT} Y_{0,i-1}/X_{O_2} \]  
(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)

\[ + F_{MT}(Y_{v,i-1} - Y_{v,i})V_{CO} \]  
(CO Produced by Volatiles Burning)

where \( a_4 = \frac{P}{R T_B} N_{c_1} d^2 k_{CO_2,i} \) g mole/sec  
(VI.20)

Carbon dioxide:
\[ F_{MT} Y_{CO_2,i} = F_{MT} Y_{CO_2,i-1} - a_4 Y_{CO_2,i} \]  
(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

Volatile:
\[ Y_{E,v,i} = 0.0 \]  
(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)
- \( a_3 \frac{Y_{E,i}}{\phi_{E,i}} - (F_{EM,i-1} Y_{E,v,i-1} + R_{v,i})X_0^2 \)

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

\[- k \frac{17.5 Y_{E,i}}{1 + 24.7 Y_{E,i}} (VI.23)\]

(Oxygen Consumed by CO)

where

\[ k = 3 \times 10^{10} \exp\left(-\frac{16000}{RT_i}\right) \frac{P}{R g_{E,i}}^{1.8} Y_{H_2O}^{0.5} A_{t,i} \Delta Z_i (1 - \varepsilon_c, i - \varepsilon_{tube,i}) \varepsilon_{mf} \]

\[ a_3 = a_m A_{t,i} \Delta Z_i (1 - \varepsilon_c, i - \varepsilon_{tube,i}) \frac{k_{E,i} P}{R g_{E,i}} X_i \]  

\[ (VI.24) \]

**Carbon monoxide:**

\[ F_{EM,i} Y_{E,CO,i} = F_{EM,i-1} Y_{E,CO,i-1} - k \frac{17.5 Y_{E,i}}{1 + 24.7 Y_{E,i}} \]

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

\[ + (F_{EM,i-1} Y_{v,i-1} + R_{v,i})Y_{CO} + R_{CO,i} \]

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

\[ + 2 a_4 Y_{E,CO_2,i} \]

(CO Produced by C-CO\(_2\) Reaction) (CO Produced by Char Combustion)

\[ a_3 (2 - \frac{2}{\phi_{E,i}}) Y_{E,i} \]  

\[ (VI.26) \]

**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)
\[
+ k Y_{E, CO_i} \frac{17.5 Y_{E_i}}{1 + 24.7 Y_{E_i}} + R_{CO_2_i}
\]

\begin{align*}
&\text{(CO}_2\text{ Produced by CO Combustion)} & \text{(CO}_2\text{ Released during Devolatilization)} \\
&\text{(CO}_2\text{ Consumed by C-CO}_2\text{ Reaction)} & \text{(CO}_2\text{ Produced by Char Combustion)} \\
&\varepsilon_4 Y_{E, CO_2_i} + a_3 \left(\frac{2}{\Phi_{E_i}} - 1\right) Y_{E_i} \\
\end{align*}

\[(VI.27)\]

**Bubble Phase Equations**

**Oxygen:**

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

\[(Oxygen \text{ out}) \quad (Oxygen \text{ in}) \quad (Oxygen \text{ Exchanged to Emulsion Phase})\]

\[- a_2 Y_{B, i} - a_1 Y_{E, CO_i}/2 \]

\[(VI.28)\]

**Carbon dioxide:**

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

\[(CO_2 \text{ out}) \quad (CO_2 \text{ in}) \quad (CO_2 \text{ Exchanged to Emulsion Phase})\]

\[+ a_2 Y_{B, i} + a_1 Y_{E, CO_i} \]

\[(VI.29)\]

**Freeboard Equations**

**Volatiles:**

\[Y_{V, i} = 0.0\]

\[(VI.30)\]

**Oxygen:**

\[
F_{MT} Y_{O, i} = F_{MT} Y_{O, i-1} - F_{MT} Y_{V, i-1} X_{O_2}
\]

\[(Oxygen \text{ out}) \quad (Oxygen \text{ in}) \quad (Oxygen \text{ Consumed by Volatiles})\]
\[
-k' Y_{CO,1} \left( \frac{17.5 Y_{0,i}}{1+24.7 Y_{0,i}} \right)/2 - a_2' Y_{0,i}/\phi_{B,i}
\]

\[(VI.31)\]

(Oxygen Consumed by CO Combustion)

where

\[
k' = 3 \times 10^{10} \exp(-16000/RT) \frac{P}{g T_i} 0.8 \frac{D_{H,2 \sigma}}{A_{t,1}} (1 - \varepsilon_{tube,i}) \text{ g mole/sec} \quad (VI.32)
\]

\[
a_2' = \frac{P}{R \phi_{B,i}} N_c i \pi d^2 k_n i \text{ g mole/sec} \quad (VI.33)
\]

**Carbon monoxide:**

\[
F_{MT} Y_{CO,i} = F_{MT} Y_{CO,i-1} + 2 a'_4 Y_{CO,i}
\]

\[(CO \text{ out}) \quad (CO \text{ in}) \quad (CO \text{ Produced by C-CO}_2 \text{ Reaction})\]

\[
+ F_{MT} Y_{v,i-1} V_{CO} + a'_2 Y_{0,i} \left( 2 - \frac{2}{\phi_{B,i}} \right)
\]

\[(CO \text{ Produced by Volatiles Burning}) \quad (CO \text{ Produced by Char Combustion})\]

\[
- k' Y_{CO,i} \left( \frac{17.5 Y_{0,i}}{1+24.7 Y_{0,i}} \right) \quad (VI.34)
\]

\[(CO \text{ Burnt})\]

**Carbon dioxide:**

\[
F_{MT} Y_{CO_2,i} = F_{MT} Y_{CO_2,i-1} - a'_3 Y_{CO_2,i}
\]

\[(CO_2 \text{ out}) \quad (CO_2 \text{ in}) \quad (CO_2 \text{ Consumed by C-CO}_2 \text{ Reaction})\]

\[
+ a'_2 Y_{C,i} \left( \frac{2}{\phi_{B,i}} - 1 \right) + k' Y_{CO_2,i} \left( \frac{17.5 Y_{0,i}}{1+24.7 Y_{0,i}} \right) \quad (VI.35)
\]

\[(CO_2 \text{ Produced by Char Combustion}) \quad (CO_2 \text{ Produced by CO Combustion})\]
The boundary conditions are:

\[ Y_{B,1} = 0.21 \frac{F_{MF}}{F_{MT}} \]  
\[ Y_{E,1} = Y_{B,1} \]  
\[ Y_{E,v,1} = 0.0 \]  
\[ Y_{E,CO_2,1} = 0.0 \]  
\[ Y_{B,CO_2,1} = 0.0 \]

**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°C (Fine, et al. 1974) and is expressed as:

\[ V_N = 0.001T - 0.6 \]  

Similarly the sulfur content in the volatiles is expressed as:

\[ V_S = 0.001T - 0.6 \]

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**

\[ F_{EM,i} Y_{E,SO_2,i} = F_{EM,i-1} Y_{E,SO_2,i-1} - a_i (Y_{E,SO_2,i} - Y_{B,SO_2,i}) \]

(SO\(_2\) out) (SO\(_2\) in) (SO\(_2\) Exchanged to Bubble Phase)
\[-a_{E,SO_2,i} Y_{E,SO_2,i} + R_{E,SO_2,c,i} + R_{E,SO_2,V,i} \quad (VI.44)\]

(SO$_2$ Absorbed by Limestone)\hspace{2cm} (SO$_2$ Released during Char Combustion)\hspace{2cm} (SO$_2$ Released during Volatiles Combustion)

where

\[a_{E,SO_2,i} = A_t, i \Delta Z_i (1 - \varepsilon_c, i - \varepsilon_{tube,i})(1 - \varepsilon_{mf}) k_{E,i} \frac{P}{R T_i}, \text{ gmole/sec} \quad (VI.45)\]

\[F_{EM,i} Y_{E,NO,i} = F_{EM,i-1} Y_{E,NO,i-1} - a_{1}(Y_{E,NO,i} - Y_{B,NO,i}) \quad (NO \text{ out}) \hspace{2cm} (NO \text{ in}) \hspace{2cm} (NO \text{ Exchanged to Bubble Phase})\]

\[-a_{E,NO,i} Y_{E,NO,i} + R_{E,NO,c,i} + R_{E,NO,V,i} \quad (VI.46)\]

(NO Reduced by Char)\hspace{2cm} (NO Released during Char Combustion)\hspace{2cm} (NO Released during Volatiles Combustion)

where

\[a_{E,NO,i} = a_{m} A_t, i \Delta Z_i (1 - \varepsilon_c, i - \varepsilon_{tube,i}) k_{E,NO,i} \frac{P}{R T_i}, X_{1}, \text{ gmole/sec} \quad (VI.47)\]

**BUBBLE PHASE EQUATIONS**

\[F_{BM,i} Y_{B,SO_2,i} = F_{BM,i-1} Y_{B,SO_2,i-1} - a_{1}(Y_{B,SO_2,i} - Y_{E,SO_2,i}) \quad (SO_2 \text{ out}) \hspace{2cm} (SO_2 \text{ in}) \hspace{2cm} (SO_2 \text{ Exchanged to Emulsion Phase})\]

\[-a_{B,SO_2,i} Y_{B,SO_2,i} + R_{B,SO_2,c,i} + R_{B,SO_2,V,i} \quad (VI.48)\]

(SO$_2$ Absorbed by Limestone)\hspace{2cm} (SO$_2$ Released during Char Combustion)\hspace{2cm} (SO$_2$ Released during Volatiles Combustion)

where

\[a_{B,SO_2,i} = A_t, i \Delta Z_i (\varepsilon_c, i - \varepsilon_{B,i})(1 - \varepsilon_{mf}) k_{E,i} \frac{P}{R T_i}, \text{ gmole/sec} \quad (VI.49)\]
\[ F_{BM,i} Y_{B,NO,i} = F_{BM,i-1} Y_{B,NO,i-1} - a_i(Y_{B,NO,i} - Y_{E,NO,i}) \]

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

\[ - a_{B,NO,i} Y_{B,NO,i} + R_{B,NO,c,i} + R_{B,NO,V,i} \]  

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

where

\[ a_{B,NO,i} = a_m A_t,i \Delta z_i (e_{c,i} - e_{tube,i}) k_{B,NO,i} \frac{p}{R T_{B,i}} X_i, \text{ gmole/sec} \]  

FREEBOARD EQUATIONS

\[ F_{MT} Y_{SO_2,i} = F_{MT} Y_{SO_2,i-1} + R_{SO_2,i} - a_{SO_2,i} Y_{SO_2,i} \]

(SO\textsuperscript{2} out)  (SO\textsuperscript{2} in)  (SO\textsuperscript{2} Released)  (SO\textsuperscript{2} Absorbed by Limestone)

where

\[ a_{SO_2,i} = \left( \frac{p}{R T_i} \right) N_{A,i} d_{e,i}^{2} e_{i,k,i} \text{ gmole/sec} \]

\[ F_{MT} Y_{NO,i} = F_{MT} Y_{NO,i-1} + R_{NO,i} - a_{NO,i} Y_{NO,i} \]

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

where

\[ a_{NO,i} = \left( \frac{p}{R T_{B,i}} \right) N_{c,i} d_{e,i}^{2} e_{i,k,NO,i} \text{ gmole/sec} \]

The boundary conditions are:

\[ Y_{E,SO_2,i} = Y_{B,SO_2,i} = Y_{E,NO,i} = Y_{B,NO,i} = 0.0 \]

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:
The boundary condition is \( W_{\text{net},1} = 0.0 \).

The material balance for the carbon in the \( i \)th compartment is given as follows by introducing the backmix flow, \( W_{\text{mix}} \):

\[
(W_{\text{mix},i} - W_{\text{net},i})X_{i+1} - [W_{\text{mix},i-1} - W_{\text{net},i-1} + W_{\text{mix},i} - W_{D,i}]X_i
+ W_{\text{mix},i-1} = r_i - W_{fc,i} C_{\text{ch}} M_{c} \tag{VI.58}
\]

where \( X_i \) is the weight fraction of carbon in the \( i \)th compartment.

The boundary conditions are:

\[
W_{\text{mix},1} = W_{\text{mix}} M_l = 0.0 \tag{VI.59}
\]

The energy balance for the \( i \)th compartment is given as follows:

\[
C_s (W_{\text{mix},i} - W_{\text{net},i}) T_{i+1}
- C_s (W_{\text{mix},i-1} - W_{\text{net},i-1} + W_{\text{mix},i} - W_{D,i}) T_i + C_s W_{\text{mix},i-1} + C_{gm} F_{\text{MT}} T_i
+ [C_s W_{\text{mix},i-1} + C_{gm} F_{\text{MT}}] T_{i-1}
+ r_i q_{\text{ch}}
+ g_{E,i} q_{V,CO} + g_{B,i} q_{V} + g_{CO,i} q_{CO}
\]

(heat generated by char combustion)

(heat generated by volatiles combustion in emulsion phase) (heat generated by CO combustion)
\(-q_{cal} W_{fa,i} + (W_{fa,i}C_{sf} + W_{fc,i}C_{cf})T_{sf,i}\)

(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 \(i\)th compartment.

\[
(W_{ent,i}C_s + C_{gm} F_{MT}) T_{i-1} + T_i q_{ch}
\]

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

\[+ g_{E,i} q_{V,CO} + g_{CO,i} q_{CO}\]

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

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

(heat out from \(i\)th cell) (heat removed by cooling tubes)

\[+ A_{t,i} \Delta Z_i a_{HEW,i} U_{w,i} (T_i - T_{wall,i})\]

(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, \( C_S = 0.215 \text{ cals/gm.}^\circ \text{C} \)

Heat capacity of gas, \( C_g = 6.8 + 0.5 \times 10^{-3} t(\circ \text{C}) \)

Density of limestone = 2.4 gms/cm³

Density of coal = 1.4 gms/cm³

Minimum fluidization velocity,

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

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

where

\[
D_{BM} = 0.652 \left\{ A_t (U - U_{mf}) \right\}^{0.4},
\]

\[
D_{BO} = 0.347 \left\{ A_t (U - U_{mf})/n_d \right\}^{0.4}.
\]

Bubble velocity, \( U_B = U - U_{mf} + 0.711 \sqrt{gD_B} \)

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

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, $f_w = 0.075$~$0.3$
Fraction of wake solids thrown into the freeboard, $f_{sw} = 0.1$~$0.5$
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
ASSUME COMBUSTION EFFICIENCY. ETCA

CALCULATE XAV

→ WEIGHT OF CHAR IN THE BED

ASSUME SIZE DISTRIBUTION OF CHAR IN THE BED

MASS BALANCE FOR EACH SIZE FRACTION → CHAR SIZE DISTRIBUTION IN THE BED

ENTRAINMENT AND FREEBOARD COMBUSTION

CHAR ELUTRIATION

→ ETCC = 1 - \frac{\text{CARBON LOSS}}{\text{CARBON FED}}

ETCA = ETCC

→ YES

PRINT

NO

SUBROUTINE CORRECT

Fig. 8 Logic Diagram for the Computation of Char Entrainment
Elutriation Results

Design Data → Input

Operating Conditions → Operating Conditions

Combustion

Yes

Initial Values
ETCA, Ti, Xi
Ti, old : Ti

Hydrodynamics

Gas Phase Material Balance
ETCG: \( \frac{O_2 \text{ in} - O_2 \text{ out}}{\text{Stoichiometric } O_2} \)

Subroutine
CRRECT

No

ETCA: ETCG

Yes

Carbon Balance
Xi

Gas Phase Balance

Energy Balance \( \rightarrow T_i \)

\[
TNORM: \frac{\sum |T_{i, \text{old}} - T_i|}{M}
\]

TAV: \( \sum T_i / M \)

TNORM ≤ 1% TAV

No

Yes

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>
<thead>
<tr>
<th>Type</th>
<th>Bed Cross-section (sizes in cms)</th>
<th>Specific surface area $cm^2/cm^3$ bed</th>
<th>Tube Outside Diameter cms</th>
<th>Vertical Pitch cms</th>
<th>Horizontal Pitch cms</th>
<th>Tube configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>NCB</td>
<td>90</td>
<td>0.15</td>
<td>3.4</td>
<td>9.9</td>
<td>11.4</td>
<td>Horizontal - staggered</td>
</tr>
<tr>
<td>Gibbs, et al. (1975)</td>
<td>30</td>
<td>-</td>
<td>1.25</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Exxon Mini Plant</td>
<td>30</td>
<td>0.205</td>
<td>1.9</td>
<td>-</td>
<td>5.5</td>
<td>Horizontal serpentine</td>
</tr>
<tr>
<td>NASA</td>
<td></td>
<td>0.1744</td>
<td>1.25</td>
<td>8.0</td>
<td>2.86</td>
<td>Horizontal In line</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
A &= 52.8 \\
B &= 29.2 \\
C &= 22.7 \\
D &= 25.9 \\
E &= 81.3 \\
F &= 62.7
\end{align*}
\]
Fig. 10 Size Distributions of the Particles in the FBC

- Bed Height = 67.1 cms
- Bed Temp. = 749 °C
- Fluidizing Vel. = 120 cms/sec
- Limestone 18
- No Recycle
- NCB Data
- Predicted
- Elutriated
- Feed
- Bed
Fig. 11 Simulation of Axial Bed Temperature Profile

EXXON DATA (1978)

SIMULATED

* HORIZONTAL COILS

- - - - VERTICAL COILS

EXCESS AIR : 13.4%

FLUIDIZING VEL. : 190 cms/SEC

PRESSURE : 9 atm.

HEIGHT ABOVE THE DISTRIBUTOR, cms
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 $\text{CO}_2$, 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 $\text{CO}_2$ 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-$\text{CO}_2$ reaction takes place. Hence the $\text{CO}_2$ concentration in the emulsion phase along the bed height decreases until all the volatiles are burnt. Once CO and char combustion start, $\text{CO}_2$ concentration increases in the emulsion phase. On the other hand, $\text{CO}_2$ 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.
In CO\textsubscript{1} CONCENTRATION, mole percent
CD\textsubscript{-}IM 0
ow
MCC
anw
00
~~0*-' -
C
CO\textsubscript{2} VOLATILE CONCENTRATION, mole percent

Fig. 14 CO, CO\textsubscript{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 determining 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 SO₂ Retention

LIMESTONE 18 (-1680 μm)
FLUIDIZING VELOCITY = 120 cms/sec
BED TEMPERATURE = 850 °C
BED HEIGHT = 67 cms
*NCB DATA
— PREDICTED
LIMESTONE 18 (-1680 µm)

PREDICTED

NCB DATA

FLUIDIZING VELOCITY = 120 cms/sec

Ca/S RATIO = 2.2

BED HEIGHT = 67 cms

Fig. 16 Effect of Temperature on SO₂ Retention
Figure 17: Effect of Fluidizing Velocity on \( \text{SO}_2 \) Retention

- HCB Data
- Predicted
- Limestone 18 (\(-1680\) μm)
- Bed Temperature = 800 °C
- Bed Height = 67 cms
- Ca/S Ratio = 2.2

SO\(_2\) Retention Efficiency, %

Fluidizing Velocity, cms/sec
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.
PRESSURE = 5.15 atm.
EXCESS AIR = 63.9 %
BED TEMP. = 876°C
LIMESTONE 1359 (-2830 μm)

Fig. 18 $SO_2$ Concentration Profile in the Combustor
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\textsubscript{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.
GIBBS ET AL. (1975)

PREDICTED

EXCESS AIR = 10 - 20%
BED HEIGHT = 61 cms (EXPANDED)
FLUIDIZING VELOCITY = 90 cms/sec

Fig. 19 Effect of Temperature on NO Emission
Fig. 20 NO and Carbon Concentration Profiles in the Bed

GIBBS ET AL. (1975) NEAR THE WALL B : BUBBLE PHASE
EXCESS AIR = 17%
BED TEMP. = 804°C
FLUIDIZING VEL. = 90 cms/sec

NO CONCENTRATION - ppm (dry)
CARBON CONCENTRATION - gm/cm³
HEIGHT ABOVE THE DISTRIBUTOR - cms
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).

$$ F_0 = A_t (U_o - U_{mf}) f_w (1 - \varepsilon_{mf}) \rho_s f_{sw} \, \text{gm/sec} \quad (VIII.1) $$
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 cal/ sec.cm$^2$,°C (56 Btu/hr.ft$^2$,°F), assuming a lower heat transfer coefficient of 0.0063 cal/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
NASA FBC
PRESSURE = 5.15 atm
EXCESS AIR = 64%
U = 0.00765 cal/sec.cm²°C

f_{SW} = 0.1
U_{W(bed)} = 0.002 cal/sec.cm²°C
U_{W(freeboard)} = 0.00025 cal/sec.cm²°C

Fig. 22 Effect of Solids Entrainment on the Temperature Profile
![Graph](image)

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

- **U = 0.0063 cal/sec.cm²°C** (46 Btu/hr.ft²°F)
- **COMPRESSED BED HEIGHT = 142 cms**
- **U_W = 0.002 cal/sec.cm²°C**
- **NASA DATA**
- **PRESSURE = 5.15 atm**
- **COAL FEED**
- **HEIGHT ABOVE THE DISTRIBUTOR, cms**
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 (or Compartment Size) on the Bed Temperature Profile

NASA DATA
VARYING BUBBLE SIZE (PRESENT WORK)

EQN. V.36

PRESSURE = 5.15 atm.
EXCESS AIR = 64%
EXPANDED BED HEIGHT = 142 cms
C: COOLING TUBES

BED TEMPERATURE °C

BED TEMPERATURE °C

HEIGHT ABOVE THE DISTRIBUTOR cms

HEIGHT ABOVE THE DISTRIBUTOR cms

0 50 100 150

0 50 100 150

D_B = 5 cms

7

10

15

C: COOLING TUBES
Fig. 25 Effect of location of Cooling Tubes on the Bed Temperature Profile

- Location of Cooling Tubes
- Specific Heat Transfer
- Area of Tubes: 0.174 cm²
- Pressure: 5.15 atm
- Excess Air: 64%
- Expanded Bed Height: 142 cms
- Coal Feed Point: 50 cm above the distributor.
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 O₂, CO, CO₂ 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 SO₂ 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%.
REFERENCES


APPENDIX I
ELUTRIATION PROGRAM

A GENERAL MODEL FOR FBC ELUTRIATION CALCULATIONS

PROGRAMMED BY
RENGA RAJAN
AT
WEST VIRGINIA UNIVERSITY

REAL MCMH2,MS,M02MN2,MNOMH2O,MSO2,MH25,MCO,MCO2,MCAO,MGAS,MV6S
COMMON /A/ZHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZU(30),
UNA(30),VUH(30),DVBEFF(30),UTA(30),UTC(30),
2EAF6,6,PT,HLMP,HLF,PAV,TAV,FMD,ROHCH,RHOED,BZAV,VHF,XAV,ETCC,
3DPSUB,PMUB,DCSUB,DCWMB,UO,MGAS,HTB
COMMON /C/ DIA(30),FRACF(30),FRACTC(30),DP(30),FRI(30),FRA(30),
LUF(30),QI(30),Q2(30),BR(30),RN(30),WI(30),E(30),ENTA(30),ELUA(30),
2ENTC(30),30),FRAS(30),FRAEL(30),CU(30),
3PFAF(30),GFLOW,WCOAL,WAD,WBC,WELU,WCEU,EFN,XC,HG,
4XASW,RCHAR,CHAR,MDIS,RHOAD,TDHC,HFB,NDF
NAMELIST /OPCF/ HLMF,VMF,HLF,WAD,WBC,WELU,WCEU,EFN,XC,HG,
1/RES/ WDIS,WELUA,CELU,EFN,DPSUB,DPWMB,DCSUB,DCWMB,
2/DASVF,DAMVF,DCSUF,DCWVF
DATA MC,MCMH2,MS,M02MN2,MNOMH2O,MSO2,MH25,MCO,MCO2,MCAO,MCAS04
1/12.,2.,32.,32.,28.,30.,18.,34.,28.,44.,56.,08.,136.,14/
DATA RHOCRHOASH/I.4,1.4/
EMF = 0.5
R = 82.05
G = 980.1
PI = 3.141593

FBC DESIGN DATA AND FEED PARTICLE SIZE DISTRIBUTION

CALL DESIGN
READ(5,1000) NDP,(DIA(I),I=INDP)
READ(5,1001) (FRACTA(I),I=INDP)
READ(5,1001) (FRACTC(I),I=INDP)
DP(I) = DIA(I)
SUMA = 0.0
SUMB = 0.0
SUMC = 0.0
SUMD = 0.0
DO 10 I = 2,NDP
DP(I) = (DIA(I-1)+DIA(I))/2
SUMA = SUMA + FRACTA(I)/DP(I)
SUMB = SUMB + FRACTA(I)*DP(I)
SUMC = SUMC + FRACTC(I)/DP(I)
SUMD = SUMD + FRACTC(I)*DP(I)
CONTINUE
DASVF = 1./SUMA
DAMVF = SUMB
DCSUF = 1./SUMC
DCWVF = SUMD

ORIGINAL PAGE IS OF POOR QUALITY
LIMESTONE COMPOSITION

READ(S1010)NAME1,NAME2,XCAO,XMG0,XSIO2,XCO2

COMPOSITION AND NET HEATING VALUE OF COAL

---------------------------------------------------------------

XC F : FIXED CARBON
XCY : VOLATILE CARBON
XH : HYDROGEN
X S : SULPHUR
XO : OXYGEN
XN : NITROGEN
XM : MOISTURE

--------------------- DRY BASIS ---------------------

READ(S1010)NAMEC1,NAMEC2,XC1,XH1,XS1,XO1,XN1,XM1,

OPERATING CONDITIONS 1 (RED CONDITION)

READ(S1001)HLMF,HLF,PAY,YAV

OPERATING CONDITION 2 (SOLIDS AND GAS FEEDS)

READ(S1001)HCOR,YAR,CASH0,FMD,EXAIR

CALCULATION OF VOLATILES YIELD AND THE COMPOSITION OF VOLATILES

W = 0.2*EXP(100.*0.0419-10.9)

V = (100.*XVM - R - W)*0.01

RN = 1.6 - 0.01*TAV

RN GT. 1, RN = 1.0

RN LT. 0.5, RN = 0.5

RS = RN

RO = 0.0

RN = 0.0

CH4 = 0.204*0.469*VM*0.241*VM*0.02

JH2 = 0.157*0.868*VM*0.133*VM*0.02

CO2 = 0.135*0.900*VM*0.901*VM*0.02

H2O = 0.423*2.655*VM*0.845*VM*0.02

TAR = -3.3257 - 2.79*VM*13.89*VM*0.02

HTAR = XH*(1.0 RH)+(1.0 XV) - VM*CH4/16.*H2/2.0 + H2O/18.*0.5

QTAR = XV*(1.0 HQ) - VM*(CO2/44.*CO/28.*H2O/18.*0.5)*32.0

MTAR = 120.0

CH4 = VM*CH4/16.*0

H2 = VM*H2/2.0

CO2 = VM*CO2/44.*0

H2O = VM*H2O/18.*0

TAR = (MCAR - HTAR + QTAR)

COV = CO/VRAGAS

C02V = CO2/VRAGAS

C02V = COV
110. \( \chi_{CV} = \chi_{CTAR} + (\chi_{CH4} + \chi_{CO2} + \chi_{CO}) \times 12.0 \)
121. \( \chi_{CF} = \chi_C - \chi_{CV} \)
122. \( \chi_{RC} = \chi_{XCF} / \chi_C \)
123. \( \chi_{COALC} = \chi_C / 12.0 \)
124. \( \chi_{COALH} = \chi_X \)
125. \( \chi_{COALO} = \chi_O / 16.0 \)
126. \( \chi_{COALN} = \chi_N / 14.0 \)
127. \( \chi_{COALs} = \chi_S / 32.0 \)
128. \( \chi_{CHARC} = \chi_{RC} \times \chi_{COALC} \)
129. \( \chi_{CHAM} = \chi_{RH} \times \chi_{COALH} \)
130. \( \chi_{CHAMR} = \chi_{RN} \times \chi_{COALN} \)
131. \( \chi_{CHAMS} = \chi_{RS} \times \chi_{COALS} \)
132. \( \chi_{HAIR} = 0.21 \times \chi_{M02} + (1.0 - 0.21) \times \chi_{MN2} \)
133. \( \chi_{A2} = \chi_{XC} / \chi_{MC} + \chi_{XH} / \chi_{MH2} \times 0.5 + \chi_{XS} / \chi_{MS} + \chi_{XN} / \chi_{MN2} - \chi_{XO} / \chi_{MO2} \)
134. \( \chi_{FMTH} = \chi_{WCOAL} \times (1.0 - \chi_{W}) \times \chi_{A2} / 0.21 \)
135. IF (EXAIR .GT. 0.) FMF = FMTH \times (1.0 + EXAIR)
136. IF (EXAIR .EQ. 0.) FMF = ATB(1) \times UO \times PAV / RG / \chi_{TAV}
137. \( \chi_{UO} = FMF \times RG \times \chi_{TAV} / PAV / ATB(1) \)
138. IF (CAS .GT. 0.0) \chi_{AI} = 0.85 / CAS
139. IF (\chi_{AI} .GT. 0.4) \chi_{AI} = 0.4
140. \( \chi_{RHOBED} = (1.0 - \chi_{CO2} + \chi_{XCAO} + \chi_{MCASO4}) \times \chi_{RHOAD} \)
141. IF (CAS .EQ. 0.0) \chi_{RHOBED} = \chi_{RHOAD}
142. WRITE (6) \chi_{DIA(I)}, \chi_{FRACTA(I)}, I = 1 \chi_{NDP}
143. WRITE (6) \chi_{DASVF}, \chi_{DAMWF}
144. WRITE (6) \chi_{NAME1}, \chi_{NAME2}, \chi_{XCAO}, \chi_{XMGO}, \chi_{XSIO2}, \chi_{XCO2}, \chi_{XH}
145. *) \chi_{DIA(I)}, \chi_{FRACTC(I)}, I = 1 \chi_{NDP}
146. WRITE (6) \chi_{DASVF}, \chi_{DAMWF}
147. WRITE (6) \chi_{NAME1}, \chi_{NAME2}, \chi_{XCF}, \chi_{XCV}, \chi_{XH}, \chi_{XN}, \chi_{XO}, \chi_{XW}, \chi_{XA}, \chi_{VN}, \chi_{V}
148. WRITE (6) \chi_{DIA(I)}, \chi_{FRACTC(I)}, I = 1 \chi_{NDP}
149. WRITE (6) \chi_{DASVF}, \chi_{DAMWF}
150. IF (HLF .GT. 0.0) \chi_{VHM} = \chi_{VOLUME(HLMF)}
151. IF (HLF .EQ. 0.0) \chi_{VHM} = \chi_{VHM} \times \chi_{WCOAL} \times \chi_{FMTH} \times 0.21 \times \chi_{EXAIR} \times \chi_{MO2}
152. IF (CAS .EQ. 0.0) \chi_{RHOBED} = \chi_{RHOAD}
153. WRITE (6, DPCF)
180. WRITE(*,RES)
181. 1000 FORMAT(12//*(BF10.0))
182. 1001 FORMAT(1F10.0)
183. 1010 FORMAT(2A4/(SF10.0))
184. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
185.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
186. 180. WRITE(6,RES)
187. 180 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
188.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
189. 180 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
190.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
191. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
192.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
193. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
194.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
195. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
196.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
197. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
198.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
199. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
200.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
201. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
202.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
203. 190. FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
204.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
205. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
206.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
207. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
208.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
209. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
210.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
211. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
212.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
213. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
214.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
215. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
216.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
217. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
218.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
219. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
220.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
221. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
222.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
223. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
224.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
225. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
226.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
227. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
228.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
229. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
230.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
231. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
232.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
233. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
234.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
235. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
236.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
237. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
238.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
239. 2000 FORMAT('O',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
240.  *XSIDC = ',F6.3,10X,'XCO2 = ',F6.3,10X)
0 = 0.26 * (TAV / 1800.) ** 1.75 / P

COND = 0.63 * SQR(TAV) / (1. + 245. / TAV * 10. ** (-12. / TAV))

Z = 250. * EXP(-12400. / 1.986 / TAV)

IF (DC .LE. 0.005) PHI = 1. / (Z + 1.) ** (2. + Z + 1.)

IF (DC .GT. 0.005) PHI = 1.0

G = 7900.0 * (2. / PHI - 1.) + 2340.0 * (2. - 2. / PHI)

AKF = 24. * PHI / (DC * RG * TAV)

RHS = AKF * PT * YO2 * MC / (DC / (2.0 * COND))

ETS = T - T - RHOS * DC / (2.0 * COND)

CALL CRRECT(I, INDEX, X1, X2, XNEW, E1, E2, E, EMAX)

IF (INDEX .EQ. 2) GO TO 110

100 CONTINUE

WRITE (6, 4000)

4000 FORMAT ('O', 10X, 'TP CALCULATION HAS NOT CONVERGED. S.NO.=4000',/)

110 CONTINUE

TB = RHOCCH * RG * TAV * DC / (1. / PHI + PHI)

RHI = 1. / TB

RETURN

END

SUBROUTINE CRRECT(I, INDEX, X1, X2, XNEW, E1, E2, E, EMAX)

C I: NUMBER OF THIS TRIAL, 1 FOR FIRST TRIAL

C INDEX: INDEX OF THE TRIAL LEVEL

C INDEX=0: JUST PROCEEDING

C INDEX=1: THE ROOT HAS BEEN CAUGHT BETWEEN X1 AND X2

C INDEX=2: THE ITERATION HAS CONVERGED

I.EQ.0 GO TO 5

INDEX = 1

IF (INDEX .EQ. 1) GO TO 150

10 XI = X2

E1 = E2

XNEW = XNEW + DX

RETURN

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),

IATB(30), UMF(30), BVH(30), BVHEFF(30), UTA(30), UTC(30),

EMF, RG, RP, MLN, MPL, PAV, THM, RHCH, RHOBED, HZAV, VMF, XAV, ETCC,

DPSVB, DPWMB, DCSVB, DCWMB, UO, MGAS, MTB

COMMON /C/ DIAT(30), FRACTA(30), FRACTC(30), DPA(30), FRC(30), FRAC(30),

ILF(30), G1(30), G2(30), BB(30), RMI(30), W(30), E(30), ENTA(30), ELUA(30),

ORIGINAL PAGE IS OF POOR QUALITY
DIMENSION IARR(30)

C AXIAL VARIATION OF BED CROSS SECTION

READ (5,100) A1, A2, A3, A4

READ (5,1001) MTB, ZB(J), ATB(J), J = 1, MTB

C IARR(1) = 1, 2, 3

1   2   ---- VERTICAL INLINE ARRANGEMENT

3   4   ---- VERTICAL STAGGERED ARRANGEMENT

1   2   ---- HORIZONTAL INLINE ARRANGEMENT

3   4   ---- HORIZONTAL STAGGERED ARRANGEMENT

C HEAT EXCHANGE TUBES

READ (5,1002) MTHE, ZHE(J+1), AHE(J), DTUBE(J), PV(J), PH(J), ZB(J),

IARR(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) = PTUBE(J) / DTUBE(J) / PH(J).

CONTINUE 100

WRITE (6,200) 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),

1 J = 1, MTHE

Z1 = ZB(1)

ZBED1 = ATB(1)

DBED1 = SORT(4.0 * ZBED1 / PI)

PV(1) = 0.0

DVBEFF(1) = 0.0

ZHE(1) = 0.0

DZAV = ZA0.0

N. = IFIX(ZB(MTB)/DZAV)

DO 10 I = 1, N.

Z2 = Z1 + DZAV

DO 20 J = 1, MTHE

IF (ZHE(J) .LE. Z2 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) - Z2) / DZAV

AH = F1 * AHE(J) + F2 * AHE(J-1)

DIAT = F1 * DTUBE(J) + F2 * DTUBE(J-1)

GO TO 40

AH = AHE(J)

DIAT = DTUBE(J)

CONTINUE 350

40 CONTINUE

GO TO 50

350 CONTINUE

CALL AREA(Z2, DBED1, ABED)

DVBEFF(I+1) = 0.5 * (ABED+ABED1) * DZAV

DVBEFF(I+1) = DVBEFF(I+1) * (1.0 - 0.25 * AH * DIAT)

Z1 = Z2

ABED1 = ABED
CONCINUE

FORMAT (4A4)

FORMAT (I1/I0F10.0)

FORMAT (1FS10.0,I10)

FORMAT ('T',20X,4A4,/

FORMAT (',T41,'HT.ABOVE DISTRIBUTOR,CM',T85,'CROSS SECTIONAL

AREA OF BED, SQ.CM./')

FORMAT (T49,F8.4,T96,F10.3)

FORMAT (',T6,'HEIGHT,CM',T20,'SF.HEAT TRANS.AREA, SQ.CM./CU.CM/',

T59,'DIA. OF TUBES[CM]',T70,'VER.PITCH,CM',T95,'HOR.PITCH,CM/',

T70,'T113,'TUBES ARRNGT./')

FORMAT (T91,F8.4,T41,'HT.ABOVE DISTRIBUTOR',T85,'CROSS SECTIONAL

AREA OF BED, SQ.CM./')

FORMAT (T49,F8.4,/) FORM (I1/(GFiO.0)-)

FORMAT (11/(SF10.0,I10))

2000 FORMAT ('I',20X,4A4, //)

2001 FORMAT ('O',T41,'HT.ABOVE DISTRIBUTOR',CM',T85,'CROSS SECTIONAL

AREA OF BED, SQ.CM./')

2002 FORMAT (T49,F8.4,T96,F10.3)

2003 FORMAT (',T6,'HEIGHT,CM',T20,'SF.HEAT TRANS.AREA, SQ.CM./CU.CM/',

T59,'DIA. OF TUBES[CM]',T70,'VER.PITCH,CM',T95,'HOR.PITCH,CM/',

T70,'T113,'TUBES ARRNGT./')

2004 FORMAT (T91,F8.4,/) FORM (I1/(GFi0.0)-)

RETURN

END

SUBROUTINE ELUT

C THIS SUBROUTINE PERFORMS THE ENTRAINMENT AND ELUTRIATION CALCULATIONS

USING THE MASS BALANCE FOR EACH SIZE FRACTION OF THE PARTICLES

REAL MGAS

COMMON /A/ ZHE(30),AHE(30),DTUBE(30),PV30),PH(30),ZB(30),

ATB(30),UMF(30),DV(30),VOLUME(HLMF),HLF,PAV,TAV,FOH,ROHBD,DIAY,VMF,XAV,ETCC,

3DPV,3BV,3DC,3UB,3DVMAG,3TB

COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),3FRA(30),

1WF(30),Q1(30),Q2(30),EB(30),RKL(30),W(30),E(30),ENF(30),ELUA(30),

2I(30),3FRAEN(30),3FRAEL(30),C(30);

3FRA(30),FRAEN(30),FRAEL(30),CU(30),

3PPA(30),GFLOW,WCAL,WAD,WBC,WELUA,CEL,EF,FC,CF,

4XAR/RCHAR,RCHAR,WD,S,THDH,THDC,HFB,NDF

DIMENSION FFI(30),R(30),FU(30),HP(30),DPSE(30),DPWE(30),DCSE(30),

1DCWE(30),DC(30),FCE(30),WEA(30),WEC(30)

IF (HLMF .GT. 0.0) GO TO 1

HLMF = 0.5*HLF

1

VMF = VOLUME(HLMF)

W8 = VMF*(1.0-EMF)*ROHBD

CONTINUE

2

WTF = W8*CAL*RHO/RHOB

3

BB(I) = 0.0

CONTINUE

4

BB(NDF) = 0.0

CONTINUE

5

DO 25 I = 2,NDF

2

FFI(I) = 0.0

25 CONTINUE

CONTINUE

6

F8 = 0.075

7

FSW = 0.1

8

P1 = 0.0

9

P2 = 0.0

10

IF (HLF .LE. 0.0) HLF = 2.0*HLMF

11

HT = HLF

12

AREA(HLT,DT,CSAREA)

13

RHOB = PAV*MGAS/RG/TAV

14

VISC = 3.72E-5*TAV**0.676

15

UO = GFLOW/CSAREA/RHOB

16

TDH = 0.429*(UO**1.2)*(11.43-1.2*ALOG(UO))

17

TDH = TDH

18

HFB = ZB(NDF)*HLF

19

IF (TDH .GT. HFB) TDH = HFB

20

DO 10 I = 1,NDF
CALL VEL(VISC,RHOGAS,G,RHOBED,DP(I),UMF(I),UTA(I))
WF(I) = FRACTA(I)*WAD+RHOBED/RHOGAS+FRACTB(I)*WCOAL*WA
Q1(I) = WF(I)/WTF
Q2(I) = 0.0
Q3(I) = 0.0
CONTINUE

WRITE(6,I11) (I,UTA(I),UMF(I),I=1,NDP)
FORMAT ('0',5X,'r,UTA,UMF = ',rS,IP2EI2.3)

WDXS = 0.01

CK = 0.003/3600./30.48

WUB = 0.02*WB

WDIS = 0.3*WUB

INDEX = 0

W(I) = 0.0

DO 30 L = 1,100

30 CONTINUE

SUMA = 0.0

DO 5 I = 2,NDP

IF ((UTA(I)-UQ) .LT. 0.2*UQ) 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 = U0-UMF(I)
PFA(I) = FFI(I)*RK*DIFF*WB

IF (FRA(I) .EQ. 0.0) GO TO 55

CU(I) = 1.0

DO 45 K = 2,NDP

CU(I) = CU(I-1)*FRA(K)

45 CONTINUE

IF (UMF(I) .GE. UQ) DIFF = 0.0

W(I) = (WF(I)+PFA(I)+W(I-1))*((DP(I+1)/DP(I))*3

DR = Q1(I)*Q1(I-1)+Q1(I)*Q1(I)*Q1(I-1)Q(I-1)+Q1(I)+Q2(I)*Q1(I-1)Q(I-1)

IF (UMF(I) .GE. UQ) GO TO 56

ARG = -10.4*SORT(UTA(I)/UQ)*(UMF(I)/DIFF)*Q0.5

E(I) = (18.0*EXP(ARG))*GFLOW

FO(I) = DIFF*CSAREA*FW*FSW*(1.-EMF)*RHOBED*FRA(I)

R(I) = FO(I)*EXP(TDHC/1275.0*ALOG(E(I)*FRA(I)/FO(I)))

56 CONTINUE

ANR = WF(I)+PFA(I)+U(I-1)

1-W(I)-RL*DIFF*WB*FRA(I)*CF(I)*R(I-1)=R(I)*DR

IF (ANR .GT. 0.0) GO TO 57

FRA(I) = FRA(I)*0.5

57 CONTINUE

BB(I) = WB*ANR*WDIS

CONTINUE

55 CONTINUE

WBC = WBC + PB(I)

WRITE(6,I10)I,FRA(I),ANR,E(I),BB(I),WF(I),W(I),CU = ',I2,1P7E11.3

I10 FORMAT (2X,'I,FRA,ANR,E,BB,WF,W,CU = ',I2,1P7E11.3)
C WRITE (6,111) L,WB,WBC,WDIS
111 FORMAT ('0',5X,'L, WB, WBC, WDIS = ',I2,1P3E12.3)
ERR = WBC-WB
CALL CRRECT (L,INDEX,WDIS,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
C REY = DT*UO*RHOGAS/VISC
IF (REY .LT. 2000.0) GO TO 300
PECI = 3.37/REY**2.1 + 1.35/REY**0.125
GO TO 310
300 D = 4.26*(TAU/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 SOLIDS ENTRAINMENT RATE ALONG THE FREEBOARD IS CALCULATED
C
HB(C) = 0.0
DO 320 K = 1,30
   IF (N.GT.1) HB(K) = HB(K-1) + DZ
   IF (HB(K) .GE. TDH) HB(K) = TDH
311 DO 340 I = 2,NDP
   R(I) = 0.0
312 DIFF = UO - UMF(I)
313 IF (FRA(I) .EQ. 0.0) GO TO 340
315 IF (UMF(I) .GE. UO) GO TO 340
316 ARG = -10.4*SLRT<UTA(I/UO)*(UMF(I)/DIFF)**0.25
317 E(I) = 18.0*EXP(ARG)*GFLOW
318 R(I) = DIFF*CSAREA*FW*FSW*(I.-EMF)*RHOBED*FRA(I)
319 F(I) = DIFF/275.0*ALOG(E(I)*FRA(I)/F(I))
320 340 CONTINUE
321 WENTA = 0.0
322 DO 350 I = 2,NDP
323 ENTA(I) = R(I)
324 IF (FRA(I) .EQ. 0.0 .AND. UO .GT. 0.833*UTA(I))
325 1 ENTA(I) = WF(I) + PFA(I)
326 WENTA = WENTA + ENTA(I)
327 350 CONTINUE
328 WEA(K) = WENTA
329 DO 360 I = 2,NDP
330 FRAEN(I) = ENTA(I)/WENTA
331 IF (FRAEN(I) .LT. 1.E-3) FRAEN(I) = 0.0
332 360 CONTINUE
333 SUMA = 0.0
334 SUMB = 0.0
335 DO 370 I = 2,NDP
336 SUMA = SUMA + FRAEN(I)/DP(I)
337 SUMB = SUMB + FRAEN(I)*DP(I)
338 370 CONTINUE
339 DPSE(K) = 1./SUMA
IF (HB(h) \( \leq \) TDH) GO TO 380
CONTINUE

DATA TBH \= 541.

320 CONTINUE

DO 80 I = 2, NDP

80 CONTINUE

DO 90 I = 2, NDP

90 CONTINUE

IF (FRAEL(I) \( \lt \) 1.E-3) FRAEL(I) \= 0.0

CONTINUE

DO -80 I \( = \) 2, NDP

ELUA(I) \= (1. \(-\) Q1(I)) \*(1. \(-\) Q2(I)) \* ENTA(I)

WELUA \= WELUA \(+\) ELUA(I)

CONTINUE

DO 100 I \( = \) 2, NDP

100 CONTINUE

DPWMB \= SUMB

DPWME \= SUMC

DPWME \= SUMD

WRITE (*,101) WDIS, WTF, WELUA, DPWDB, DPWMB,

1(DP(I), FRA(I), FRAEL(I) \( = \) 2, NDP)

101 FORMAT ('O', TIO, 'WDIS, WTO, WELUA, DPWDB, DPWMB, '

/ (TIO, IPEI0.3, T30, 'BED SIZE FRACTION', T60, 'ELUT.

2 SIZE FRACTION', '/ (TIO, IPEI0.3, T30, 'BED SIZE FRACTION', '/)

SIMILAR ENTRAINMENT CALCULATIONS ARE PERFORMED FOR CHAR

DO 210 I \( = \) 1, NDP

WF(I) \= FRACTC(I) \* WCOAL

FRC(I) \= FRACTC(I)

CALL VEL(VISC, RHODAS, G, RHOCH, DP(I), UMF(I), UTC(I))

210 CONTINUE

ETCA \= 0.9995

ETC0 \= -0.001

ECTC \= 0.001

CENT \= 0.0

DO 200 L \( = \) 1, 30

200 CONTINUE

SUMA \= 0.0

DO 150 I \( = \) 2, NDP

150 CONTINUE

IF ((UTC(I) \(-\) UO) \( \lt \) 0.2 \* UO) FRC(I) \= 0.0

SUMA \= SUMA \(+\) FRC(I)

CONTINUE

DO 160 I \( = \) 1, NDP

160 CONTINUE

XAV \= ((WCOAL \* RCHAR \(-\) CENT) \* CCHAR \( = \) 1. \(-\) ETCA) \* WDIS

CBED \= XAV \* WBC \* CCHAR

CELU \= 0.0

CENT \= 0.0
93

CBEDC = 0.0
00 220 I = 2, NDP
B(I) = FRC(I)*CBED
R(I) = 0.0
DIFF = U0-UMF(I)
FFA(I) = FFI(I)*R(I)*DIFF*CBED/CCHAR
FSC = 0.01
IF (FRC(I) .EQ. 0.0) GO TO 256
DO 252 K = 2, NDP
CU(K) = CU(K-1)-FRC(K)
IF (UMF(I) .GE. U0) DIFF = 0.0
W(I) = (WF(I)+FFA(I)+W(I-1))*(DP(I+1)/DP(I))*0.25
DR = U1(I)*(1.-P1)+Q2(I)*(1.-Q1(I))*(1.-P2)+Q1(I)*(1.-Q2(I))
ARS = -10.4*SQRT(UTC(I)/U0)*(UMF(I)/DIFF)*0.25
E(I) = (18.0*EXP(ARG)*XAV)**0.25
F0(I) = DIFF*CSAREA*FW*FSW*FRC(I)
R(I) = F0(I)*EXP(DTHC/275.0)*ALOG(E(I)*FRC(I)/FO(I)))
CONTINUE
Y02 = 0.15
RHOCCH = RHOCCH*CCHAR
CALL ATTR(RHOCCH,TAV,DP(I),PAU,Y02,RG+TB,RKI(I))
ANR = WF(I)+FFA(I)+W(I-1)-W(I)
IF (ANR .GT. 0.0) GO TO 175
R(I) = FRC(I)*0.5
GO TO 211
FRC(I) = FRC(I)*0.5
CONTINUE
BB(I) = WB*ANR/WDIS
CONTINUE
C = CBEDC + CBEDC
WRITE(6,i70)IFRC(I),ANR,E(I),BB(I),W(I),WF(I),RKI(I)
I70 FORMAT (2X,'IFRAANR,EBR,W,WF,RKI
RT',I2,P7EZ1.3)
CONTINUE
-DO 400 I = 2, NDP
DIFF = U0-UMF(I)
IF (FRC(I) .EQ. 0.0) GO TO 410
IF (UMF(I) .GE. U0) GO TO 410
ARG = -10.4*SQRT(UTC(I)/U0)*(UMF(I)/DIFF)*0.25
E(I) = 18.0*EXP(ARG)*XAV
F0(I) = DIFF*CSAREA*FW*FSW*FRC(I)
GO TO 415
F0(I) = 0.0
ENTC(1,I) = F0(I)
IF (FRC(I) .EQ. 0.0 .AND. U0 .GT. 0.833*UTC(I)) ENTC(1,I) = WF(I)*
IF (FRC(I) .EQ. 0.0 .AND. U0 .GT. 0.833*UTC(I)) ENTC(1,I) = WF(I)*
ENTC(1,I) = CENT + ENTC(1,I)
CENT = CENT + ENTC(1,I)
CONTINUE
C
CHAR ENTRAINMENT RATE AS A FUNCTION OF THE FREEBOARD HEIGHT IS
CALCULATED TAKING INTO ACCOUNT THE DECREASING PARTICLE SIZE DUE TO
CHAR COMBUSTION

WE(I) = CENT
400 CONTINUE
401 CONTINUE
410 CONTINUE
415 CONTINUE
420 CONTINUE
430 CONTINUE
DO 440 I = 2, NDP
IF (DCE(J-1,I) .GT. 0.0) GO TO 435
RT = 1.E8
TB = 0.0
GO TO 436.
435 CONTINUE
CALL VEL(VISC,RHOGAS,GRHOCH,DCE(J-1,I),UMF(I),UTC(I))
HT = HLF + HB(J)
CALL AREA (HT,DT,CSAREA)
UAV = GFLW/CSAREA/RHOGAS
RT = (HB(J)-HB(J-1))/ABS(UAV-UTC(I))
YO2 = 0.09
CALL ATT(RHOCCH,TAY,DCE(J-1,I),PAV,YO2,RJ,TB,RI(J))
IF (TB.GT.RT) DCE(J,I) = (1.-RT/TB)**0.5*DCE(J-1,I)
CONTINUE
436 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,GRHOCH,DCE(J,I),UMF(I),UTC(I))
RT = HB(J)/ABS(UO-UTC(I))
DIFF = UO-UMF(D)
IF (UMF(I) .GE. UO) GO TO 431
ARG = -10.4*SQRT(UTC(I)/UO)**0.25
E(I) = 19.0*EXP(ARG)*GFLW
IF (FO(I) .GT. 0.0) R(I) = FO(I)*EXP(HB(J)/275.0*ALOG(E(I)*
IFRC(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)
433 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
WRITE(6,190)CELU,CENTDCSVBDCWMB,(AD(I),FRC(I),DC(JI),C$i( ,fl
420 CONTINUE
DO 460 N = 1,KT
SUMA = 0.0
SUMB = 0.0
460 CONTINUE
WRITE(6,190)CELU,CENTDCSVBDCWMB,(AD(I),FRC(I),DC(JI),C$i( ,fl
420 CONTINUE
IF (SUMA .GT. 0.0) DCSE(k) = 1./SUMA
DCWE(k) = SUMB
CONTINUE
CELU = WEC(k)
ETCC = 1.- WDIS*XAV/((WCOAL*RCHAR-CENT)*CCHAR)
XAV = ((WCOAL*RCHAR-CENT)*CCHAR*(I-ETCC))/WDIS
C WRITE (6,190) L,CBED,CELU,CENT
C 1IP7E12.3
ERR = ETCA - ETCC
CALL CRRECT(L,IND,DETQ,XI,X2,ETCA,E,E2,ERR,ETEC)
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 = I./SUMB
DCUMB = SUMA
WRITE (6,190) L,CBED,DCSVB,DCUMB,(DP(I),FRC(I),OCEKTI)
IFCE(KT,I),I=2,NDP)
WRITE (6,390) (NHB(K),DPSE(l)UDPWE(N),WCA(K),K=fT)
WRITE (6,490) (K,HB(K)DCSE(K),DCWE(K),WEC(K),K=1,T)
490 FORMAT ('0',9X,'FREEBOARD HT.',9X,'DCSE',I2X,'DCWE'12X,'ENT.
R.A.',//,(TIO,PEII.3,T31,1PEI.3,51PEli.3,vT74,1PE11.3,/))
390 FORMAT ('O',X'K',9X,'FREEBOARD HT.',9X,°DPSE',2X,'DPWE',12X,'-EN
R.A.',//,(9X,12,SX,IPEI.3,6XIPEI1.3,6X,IPE11.3))
190 FORMAT ('O',9X,'CELUCENT,DCSVB,DCWMB = ''IP4EI2.3,
1'O',9X,'BED PAR.DIA.,CM',SXP'BED SIZE FRACTION',SX,'ENT.PAR.DIA.r
2CM',SX,'ENT.SIZE FRACTION',/,'O',(TIO,PEII.3,T31,1PEI.1.3))
RETURN
END
SUBROUTINE VEL(VISCRHOGASYGRHOSDPAR,UMUT)
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*(G3*(RHOS-RHOGAS)*RHOGAS/VISC**2
UM = VISC/(DPAR*RHOGAS)*(SQRT(A1)-33.7)
UT = (4.0*(RHOS-RHOGAS)**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 = 6*(RHOS-RHOGAS)*DPAR**2/199/VISC
REP = DPAR/RHOGAS/UT/VISC
IF(REP.LE.0.4) GO TO 210
UT = SQRT(3.1*G*(RHOS-RHOGAS)*DPAR/RHOGAS)
RETURN
END
FUNCTION VOLUME (ZZ)
COMMON /A/ ZHE(30),AHE(30),DTUE430).PV(30),PH(30),ZB(30),
EMF,RG,G,PIHLNFHLFPAV,TAV,FMORHOCH,RHOBED,DZAV,VMF,XAV-ETCC,
CALCULATION OF THE EFFECTIVE VOLUME OF THE BED GIVEN THE HEIGHT

N = IFIX (ZZ/DZA AV) + 1
IF (N.EQ.1) N = 2
SUM = 0.0
ZN = FLOAT(N-1)*DZA V
DO 100 I = 2, N
SUM = SUM + DVB E FF(I)
IF (I .LT. N) GO TO 100
A1 = (ZZ - ZN) / DZ AV
SUM = SUM + DVB EF F(I) * A1
CONTINUE
100
VOLUME = SUM
RETURN
END
### APPENDIX II

**INPUT TO ELUTRIATION PROGRAM**

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<tr>
<th></th>
<th>ATB(1)</th>
<th>ZB(1)</th>
<th>ATB(2)</th>
<th>ZB(2)</th>
<th>ATB(3)</th>
<th>ZB(3)</th>
<th>ATB(4)</th>
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**MTB**

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**NAME1** | **NAME2**

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**NAMEC1** | **NAMEC2**

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<th>XN</th>
<th>XS</th>
<th>XD</th>
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**Wcoal**

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<th>FMF</th>
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1234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
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<th>HEIGHT, CM</th>
<th>SP. HEAT TRANS. AREA, SQ. CM/CU. FT</th>
<th>DIAM. TUBES, CM</th>
<th>VERT. PITCH, CM</th>
<th>CONS. PITCH, CM</th>
<th>TUBES ARRANG.</th>
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<tr>
<td>24.00</td>
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<td>1.270</td>
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**DIAMETER, CM**

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<tr>
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<td>0.1600</td>
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**WEIGHT MEAN DIA. = DAWF = 0.0576 CM**

**WEIGHT MEAN DIA. = DAWF = 0.1287 CM**

**DIAMETER, CM**

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<thead>
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**WEIGHT MEAN DIA. = DAWF = 0.0677 CM**

**WEIGHT MEAN DIA. = DAWF = 0.1004 CM**
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<td>2.10E+01</td>
<td>2.71E-02</td>
<td>0.00E-01</td>
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<tr>
<td>1.90E+01</td>
<td>6.60E-02</td>
<td>0.00E-01</td>
</tr>
<tr>
<td>1.45E+01</td>
<td>1.62E-01</td>
<td>0.00E-01</td>
</tr>
<tr>
<td>1.30E+01</td>
<td>4.79E-01</td>
<td>0.00E-01</td>
</tr>
<tr>
<td>1.00E+01</td>
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<td>0.00E-01</td>
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<tr>
<td>9.00E+00</td>
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<tr>
<td>8.10E+00</td>
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</tr>
<tr>
<td>7.40E+00</td>
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<td>0.00E-01</td>
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<tr>
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<tr>
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<td>6.00E+01</td>
<td>0.00E-01</td>
</tr>
<tr>
<td>4.30E+00</td>
<td>1.09E+02</td>
<td>0.00E-01</td>
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<tr>
<td>3.50E+00</td>
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<td>0.00E-01</td>
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<tr>
<td>3.20E+00</td>
<td>4.40E+02</td>
<td>0.00E-01</td>
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<tr>
<td>3.00E+00</td>
<td>9.00E+02</td>
<td>0.00E-01</td>
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<tr>
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<td>2.00E+00</td>
<td>0.00E+00</td>
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</tbody>
</table>
1. C***************************************************************
2. C A GENERAL MODEL OF FLUIDIZED BED COAL COMBUSTOR
3. C***************************************************************
4. C PROGRAMMED BY
5. C RENGA RAJAN
6. C AT
7. C WEST VIRGINIA UNIVERSITY
8. C***************************************************************
9. C***************************************************************
10. REAL MC, MH2, MS, MO2, MN2, MH2O, MO2, MH2S, MCO, MCO2, MCAO3, MCAO, MCAS04
11. 1, MNC03, M2G0, MAIR, MGAS, MVGAS, MN, NC, HA, HMO, NCCHAR, NTAR
12. COMMON /A/ ZHE(IO), AHE(IO), PV(10), FH(IO), ZF(IO), FFC(IO), DTUBE(IO),
13. 1DBV(IO), 1DBVEF(IO), FFFAD(IO), ZDIS(IO), FD(IO), AHEAV(IO), ETUBE(a0),
14. 2UB(a0), UFMB(IO), H(MIO), AT(MIO), DT(MIO), T(MIO), X(MIO), AHBE(MIO), YB(MIO),
15. 3YE(MIO), YCOE(MIO), EPB(MIO), EPC(MIO), DVBB(MIO), DVBBEF(MIO), DBAV(MIO),
16. 4UB(MIO), UTC(MIO), UTA(MIO), ZB(MIO), ATB(MIO), YVE(MIO), ZAVG(MIO), IARR(IO),
17. COMMON /B/ YBDO(MIO), YEDO(MIO), DB(MIO), DPSVB, DPWMB, DCXSVB, DNBWB, RHOCH,
18. 1HLF, VNF, PFM, UFM, UF, FT, RG, MGAS, DFIX, DPFLU, DPDIS, RHOED,
19. 3EUF, PAV, HCHR, RADEVOL, EFVOL, BOLVOL, TETUBE, HLMF, EF, AND, BNIL,
20. COMMON /C/ DPSE(30), DPWEC(30), DCEC(30), DCWEO(30), WEAO(30), UHEAV(30),
21. IHB(30), WOHOLD(30), WAIHOLD(30), KT
22. DIMENSION ALFA(60), BETA(60), GAMMA(60), DELT(60), UHE(60), GB(60),
23. 1BE(60), CDB(60), WHX(60), UWE(60), WOF(60), WFAI(60), WD(60), YCO2(60),
24. 2TW(60), YGCC(50), TO(60), YCO(60), YVE(60), YCO2(60), YNOX(60),
25. 3YPRD(60), RELB(60), RELG(60), TPB(60), TPE(60), RCOG(60),
26. 4RR(60), RRB(60), RR(60), TOLD(60), AAA(3600), BBB(60), FEN(60), FBM(60),
27. SYCO2(60), YCO2E(60), YHEW(60), YHEW(60), TAWALL(60),
28. NAMELIST /OPCF/ HLMF, HLF, HLMF, VMF, VGF, VGF, HLMF, PFM, FMO,
29. *HUEVF, WMHOLD(30), WAIHOLD(30), EF, TSW, WCAL, WAD, CAS, EXAIR, MGAS, FTH, VNF, FMO,
30. H2SV, ANH2V, RHOC, RHOCH, RVGAS, VCHAR, VGAS, QVCO, QCLCN
31. *OPCF1, ICR, IFBC, NTC, HCR, HLF, HLMF, VGF, BEDVOL, EFVOL, SOLVOL, TETUBE,
32. *HAREA, QTRAN, QARE, HFB, EDCOM, FBCOM, TCRATE, X02, X03
33. NAMELIST /DC/ UD5, WELC, CELU, EFF, DPSVB, DPWMB, DCXSVB, DNBWB, GFLOW,
34. 1U5, CLSS5, SCHAR, HCHAR, SCHAR, NCHAR, SCHAR, TARC
35. DATA MG, MH2, MS, MO2, MH2O, MO2, MH2S, MCO, MCO2, MCAO3, MCAO, MCAS04
36. 1, MNC03, M2G0, MAIR, MGAS, MVGAS, MN, NC, HA, HMO, NCCHAR, NTAR
37. DATA AAA, BBB, 3600, 0, /RHOC, RHAS, ROHAD, 1, 1, 1, 1, 2, 2, /HAREA, QTRAN,
38. *QVOL, QARE, R(A), R(RE), R(RE) /7*0.0, *
39. *CADF, CCF, GMN, 0, 198, 0.0, 193, 6.79/
40. M1 = 100
41. M1old = M1
42. ENF = 0.5
43. RG = 32.05
44. S = 980.1
45. PI = 3.141593
46. ETUBE(1) = 0.
47. EPR(1) = 0.
48. EPC(1) = 0.
49. DBAV(1) = 0.
50. U(1) = 0.
51. DAVB(1) = 0.
52. AHEAV(1) = 0.
FC DESIGN DATA

INPUT DATA FROM ENTRAINMENT CALCULATIONS

READ (5, 1000) KT
READ (5, 1001) (HB(K), DSE(K), DPWE(K), WEA(K), K = 1, KT),
1(DCE(K), DCWE(K), WEC(K), K = 1, KT)
READ (5, 1001) WDIS, UELUA, CELU, EFF, DPSVB, DPWMB, DCSVB, DCWMB,
1(DASVF, DAWMF, DCSVF, DCWVF)
CALL DESIGN

COMPOSITION OF LIMESTONE

READ (5, 1010) NAME1, NAME2, XCAO, XHGO, XSI02, XCO2

COMPOSITION AND NET HEATING VALUE OF COAL

READ (5, 1010) NAMEC, NAMEC2, XC, XH, XN, XS, XO, XA, VM, HCOAL, XCAO

OPERATING CONDITIONS

READ (5, 1001) HLMT, HLF, PAV, TAV, TSTA, TWINT, TWOUT, TWALL, UHEA1, UHEA2,
1(T, WALL2, TF, TSF, F)
READ (5, 1001) WCOAL, WAD, CAS, U0, F, EXAIR
READ (5, 1000) Ignite, ISO, INOX, TEMP, IPRES

CALCULATION OF VOLATILES YIELD AND THE COMPOSITION OF VOLATILES

WU = 0.2*(100.*VM - 10.9)
R = EXP(26.41 - 3.961*ALOG(TAV-273.)) + 0.0115*100.*VM
V = (100.*VM - R - WU)*0.01
RN = 1.6 - 0.001*TWALL
IF (RN .GT. 1.) RN = 1.0
IF (RN .LT. 0.0) RN = 0.0
RS = RN
VGAS = XS*(1.-XW)*(1.-RS)/32.0
VGASN = XN*(1.-XW)*(1.-RN)/14.0
R0 = 0.0
RH = 0.0
OCHR = 7000.0
OC = 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*H20/18.)*0.5*32.0
MTAR = 120.0
CTAR = V*CH4/16.0
H2 = V*H2/2.0
CO2 = V*CO2/44.0
CO = V*CO/28.0
H2O = V*H20/18.0
CTAR = V*CH4/16.0
H2 = V*H2/2.0
CO2 = V*CO2/44.0
CO = V*CO/28.0
H2O = V*H20/18.0
CTAR = V*CH4/16.0
H2 = V*H2/2.0
CO2 = V*CO2/44.0
CO = V*CO/28.0
H2O = V*H20/18.0
CTAR = V*CH4/16.0
H2 = V*H2/2.0
CO2 = V*CO2/44.0
CO = V*CO/28.0
H2O = V*H20/18.0
CTAR = V*CH4/16.0
H2 = V*H2/2.0
CO2 = V*CO2/44.0
CO = V*CO/28.0
H2O = V*H20/18.0
120. \[ CO_{2V} = \frac{CO_{2}}{RVGAS} \]
121. \[ CO_{2V} = \frac{CH_{4}+CTAR}{12.0}/RVGAS \]
122. \[ CO_{2} = \frac{CH_{4}+CTAR}{12.0}/RVGAS \]
123. \[ X_{02} = \frac{CH_{4}+CO_{2}+CO}{12.0}/RVGAS \]
124. \[ \frac{CH_{4}}{12.0} + \frac{H}{2.0} \times 0.5 - \frac{OTAR}{32.0} + \frac{VGAS}{RVGAS} + \frac{VGAS}{RVGAS} \]
125. \[ X_{02} = \frac{CH_{4}+CO_{2}+CO}{12.0}/RVGAS \]
126. \[ X_{CF} = X_{C} - X_{CV} \]
127. \[ X_{CV} = \frac{CH_{4}+CO_{2}+CO}{12.0}/RVGAS \]
128. \[ R_{CH_{4}} = X_{C} - X_{CF} \]
129. \[ Lill = \frac{H_{2}S}{RVGAS} \]
130. \[ ANH_{3} = \frac{ANH_{3}}{RVGAS} \]
131. \[ COALC = \frac{XC}{12.0} \]
132. \[ COALH = \frac{XH}{14.0} \]
133. \[ COALO = \frac{XO}{16.0} \]
134. \[ COALN = \frac{XN}{14.0} \]
135. \[ COALS = \frac{XS}{32.0} \]
136. \[ CH_{2} = \frac{CH_{2}}{32.0} \]
137. \[ CHARC = \frac{RC}{RCHAR} \]
138. \[ CHARH = \frac{RH}{RCHAR} \]
139. \[ CHARO = \frac{RO}{RCHAR} \]
140. \[ CHARN = \frac{RN}{RCHAR} \]
141. \[ CHARS = \frac{RS}{RCHAR} \]
142. \[ R_{CHAR} = \frac{1.0}{V-XW} \]
143. \[ CCH_{2} = \frac{CH_{2}}{RCHAR} \]
144. \[ RCCH = \frac{RC}{RCHAR} \]
145. \[ RCHAR = \frac{RCH}{RCHAR} \]
146. \[ RCH = \frac{RCH}{RCHAR} \]
147. \[ SCHAR = \frac{SCHAR}{RCHAR} \]
148. \[ TARC = \frac{RCH}{RCHAR} \]
149. \[ QV_{GAS} = (HCOAL - RCHAR * QCHAR - QCO * COB) / RVGAS \]
150. \[ QCBO = QV_{GAS} - QCO * COB \]
151. \[ T(1) = TF \]
152. \[ IF(WCOAL.EQ.0.) IGNITE=0 \]
153. \[ IF(WCOAL.EQ.0.) IGNITE=0 \]
154. \[ C \] IGNITE 0 1 \]
155. \[ C \] NO COMBUSTION \]
156. \[ C \] COMBUSTION \]
157. \[ MAIR = 0.21*MCO2*(1.0-0.21)*MN2 \]
158. \[ MC = \frac{MC}{MH2}+MH2/12.0+XS/MS+MN2-XM/H2O2 \]
159. \[ FNTH = WCOAL*12.0*MC/2.1 \]
160. \[ IF (EXAIR.EQ.0.) FMF = FMF*1.0+EXAIR \]
161. \[ IF (EXAIR.EQ.0.) FMF = ATB(1)*UO*PAV/ATB \]
162. \[ IF (EXAIR.EQ.0.) EXAIR = FMF*FMF - 1. \]
163. \[ UO = FMF*RCH*PAV/ATB \]
164. \[ FHO = FMF*1.0-0.21)*(XC/MC+MH2+XS/MS)*0.1+MO2*(1-XW)/MN2+XW)*WCOAL \]
165. \[ XW/MH20*XWCOAL*EFF*FMF*0.21*EXAIR \]
166. \[ GFLOW = FMF*1.0-0.21)*(MC/MC2+MH2+XM2+XS/MS)*0.21*XW \]
167. \[ XW/MH20*XWCOAL*EFF*FMF*0.21*EXAIR \]
168. \[ MGAS = GFLOW/FHO \]
169. \[ C \] FMO : AVERAGE FLOW RATE OF GAS IN THE BED \]
170. \[ C \] MOLE/SEC \]
171. \[ C \] FBC \]
172. \[ C \] FBC \]
173. \[ C \] FBC \]
174. \[ C \] FBC \]
175. \[ C \] FBC \]
176. \[ C \] FBC \]
177. \[ C \] FBC \]
178. \[ C \] FBC \]
179. \[ C \] FBC \]
104. 
IQAD=CAS*(WCOAL,(1.-XWbKXS/MS)/(XCAO/MCAO)

115. Ai = 0.85/CAS

182. IF(CAS .GT. 0.0)
    Ai = 0.4

183. RHOBED=(±.-XO02+XCAO/MCAO*Ai*MCASO4)MRHOAD

185. IF (CAS .EQ. 0.0) RHOBED = RHOAD

186. RHOGAS=PAV*MGAS/(RG*TAV)

187. VISC=3,72E-6*(TAV**0.676)

C
QCLCN : HEAT OF CALCINATION PER GRAM ADDITIVE

C
QCLCN=(<2500.0*XC02/MCAO + 23810.0*XMGO/MGO)
   CS=0.315

C
MAIN OUTPUT 2

C

WRITE (6,2000) NAMELI,NAMEL2,XCAO,XMEO,XSIO2,XCO2

WRITE (6,2010) DAVF,DAWMF

WRITE (6,2020) NAMEC1,NAMEC2,XCF,XCV,XH,XN,XS,XG,XV,XA,VM,V,HCAO

C

WRITE (6,2040) DCSVF,DCWMF

WRITE (6,2050) (K,HB(K),DPSE(K),DPWE(K),YWEA(I),ICSE(K),DCWE(K),

115. IWEC(K),K=IKT)

WRITE (6,OPCF)

ZAVG(1) = 0.0

X(i) = 0.0

IF (rTEMP .GT. 0)
    TAU = TSTA

DO 20 I=2,60
    T(I)=TAV

20 CONTINUE

C
INITIAL BUBBLE HYDRODYNAMIC CALCULATION

C
IF (HLF .EQ. 0.0) VMF = VOLUME(HLMF)

C
IF (HLMF .GT. 0.0) WS = VMF*(1.-EMF)*RHOBEU

C
IF(IGNITE.EQ.0)GO TO 41

CALL HYDRO

DO 35 1=2,M

ZAVG(I) = H(I) + H(I-1) * .5

35 CONTINUE

ETC=0.

YAV=0.21

XAV=WCOAL*X/C/(WCOAL+WAD)*1.-XW

FMO=FMF

IF (WAD.EQ.0.0 .AND. IGNITE .EQ. 0) GO TO 900

C
FOR CONDITIONS OF NO COAL COMBUSTION, IGNITION IS ZERO AND

C
MATERIAL AND ENERGY BALANCES CALCULATIONS ARE SKIPPED

YB(1) = YAV

YE(1) = YB(1)

FEN(1) = UMF(1) * AT(1) * PAV / (RG*T(2))

FBM(1) = FMO - FEN(1)

DO 115 I = 2,60

115 RBB(I) = 0.0

RE(I) = 0.0

YB(I) = YAV

YE(I) = YAV

X(I) = XAV

IF (1 .GT. 1) GO TO 115

FEM(I) = UMF(I)*AT(I)*(1.0-ETUBE(I))*PAV / (RG*T(I))
FBM(I) = FM0 - FEM(I)
IF (UO(I) .LE. UMF(I)) FEM(I) = 0.0
CONTINUE
IF (IGNITE .EQ. 0) GO TO 630
CONTINUE
C BOUNDARY CONDITIONS FOR GAS CONCENTRATIONS
YO(1) = 0.21
YV(1) = 0.0
YC02(1) = 0.0
YN02(1) = 0.0
YB(1) = FMF*0.21/FMO
YE(1) = YB(1)
YV(1) = 0.0
YCO2(1) = 0.0
YB(1) = 0.0
YCO2B(1) = 0.0
YCO2E(1) = 0.0
YB(1) = 0.0
C FROM HERE TO THE STATEMENT NO.600 : TEMPERATURE ITERATION LOOP
DO 600 ITrial = 1,30
C CALCULATION OF LOG MEAN TEMPERATURE OF THE COOLING WATER
A1 = TWOUT - TWIN
A2 = ALOG((TAV-TWIN)/(TAV-TWOUT))
TAV = TAV - A1/A2
CALL HYDRO
DO 25 I = 1,MT
TW(I) = TAV
IF (I .LE. M1) UHE(I) = UHEAV1
IF (I .GT. M1) UHE(I) = UHEAV2
IF (I .LE. M1) UWALL(I) = UWALL1
IF (I .GT. M1) UWALL(I) = UWALL2
AHEW(I) = 4.0/DT(I)
T WALL(I) = T WALLA
CONTINUE
MP1 = M1 + 1
IF(ITRIAL .GT. 1 .AND. M1.EQ.M10LD)GO TO 170
J1 = 1
DO 56 I = 1, 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
CONTINUE
55 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)
FEM(I) = UMF(I) * AT(I) * (1.0 - ETUBE(I)) * PAV / (RG * T2)

\[ F_{\text{NuI}} = F_{\text{MF}} - F_{\text{EA}(1)} \]

DO 133 I=2,M1

TOLD(I) = T(I)

133 CONTINUE

INDEX = 0

DETCA = -0.0001

DO 200 NT = 1,30

XAV = ((COAL * RCHAR - CELE) * TCRATE) / WDIS

DO 1 I = 1,M1

If (I .LT. MI) YAV = 0.16

YB(I) = YAV

YE(I) = YAV

YO(I) = YAV

CONTINUE

175 CONTINUE

DO 233 I = 2,M1

CALL AK(T(I),FAV,DCSVB,TPB(I),YR(I),RG,MC,AHCO2,PHIB)

TAVB = (T(I) + TPB(I)) / 2.
360. CALL ANK(ANE(I),PAV,DCSVB,TPB,TH(I),YE(I),RG,MC,AKCO2,PHIE)
361. TAVE=(T(I)+TPB)/2.
362. I=I+1
363. CALL GPB(YH2O,AKB,ANE,ANEI,AKMODF,DCVB,EMF,EPB,EPB(I),EPB(I),
364. THUE(I),FBM(I),FBM(I),FEM(I),GB(I),GB(I),GE(I),PAV,
365. EPHIE,RG,RGAS(TH,TAUB,TAUE,UPROD(I)X(I),XO2,XO2C,YB(I),YB(I),
366. 3YE(II),3YE(II),YE(I),YE(II),YVE(I),YVE(II),AKCO2,COV+COV2+COV8+
367. 4CO2VYCO2B(II),YCO2B(II),YCO2B(II),YCO2B(II),YCO2B(II),YCO2B(I),
368. AM=DCVB(I)*AKMODF(I)*MC
369. RR(I)=AM*(PAV/RG)*(EPC(I)-EPB(I))*YB(I)*AKB/TAVB/CCHAR
370. RRE(I)=AM*(PAV/RG/TAVE)*(1.-EPC(I)-ETUBE(1))/CCHAR*(YB(I)*AKB+
371. 1YCO2E(I)*AKCO2)
372. RR(I)=(RRB(I)+RRE(I))/X(I)
373. TCRATE=TCRATE+RR(I)*X(I)
374. YO(I)=(FEM(I)*YE(I)+FBM(I)*YB(I))/FM0
375. YC02(I)=(FEM(I)*YCO2E(I)+FBM(I)*YCO2B(I))/FM0
376. YV(I)=(FEM(I)*YE(I))/FM0
377. YCO(I)=FEM(I)*YE(I)/FM0
378. CONTINUE
379.
380. C GAS PHASE MATERIAL BALANCE IN THE FREEBOARD
381.*
382. DO 334 I=MI,MT
383. J=I-MI
384. K=J+1
385. HAV=(HI-1+H(I))/2.0
386. CALL AREA(HAV,DTAV,ATAV)
387. RHOGAS=PAV*MGAS/RG/T(I)
388. VISC=3.72E-6*TR(I)**0.676
389. DCSV=0.5*(DCSV(E(I)+DCSV(E(K))
390. DCWE=0.5*(DCWE(I)+DCWE(K))
391. CALL VEL(VISC,RHOGAS,G,RHCH,DCSV,UMFAV,UTAV)
392. UO(I)=FM0*MGAS/RHOGAS/ATAV/(1.-ETUBE(I))
393. RT=(HB(K)-HB(J))/ABS(UO(I)-UTAV)
394. WCHOLD(I)=(2.0*WEC(J)-WEC(K))*RT
395. YCO(I)=WCHOLD(I)/RHOCH
396. NC=VCHOLD*6.0/(PI*DCSV**3)
397. CALL AKK(ANK+TH(I),PAV,DCSV,TPB(YO(I),YD(I),RG,MC,AKCO2,PHIB)
398. TPE(I)=TPB(I)
399. TAVB=(T(I)+TPB(I))/2.0
400. I=I+1
401. CALL FBC(YH2O,AKC,DCSV,DCVB,ETUBE(I),FMO,GB(I)*COB(I),
402. 1GE(I),NC,PAV,PHIB,P1,GB,RGAS(TH,TAUB,TAUE,YCO(I),YD(I),
403. 2YO(I),YV(I),YV(I),AKC02,COV2,COV8,YCO2B(I),YCO2E(I))
404. RRB(I)=MC*NC*PI*DCSV**3*PAV/RGAV/CCHAR*(YD(I)*AKCO2+
405. YCO2B(YCO2B(I))
406. RRE(I)=0.0
407. TCRATE=TCRATE+RRB(I)
408. CONTINUE
409.
410. C WRITE(6,205) (I,YB(I),YE(I),YCOE(I),YVE(I),H(I),YCO2E(I),YCO2B(I),
411. 1UO(I),UMF(I),I=1,HI)
412. C FORMAT ('O',TS,'I',TT2,'YB',T3S,'YE',T46,'YVE',T70,'H',T70,'YCOE',T82,'YCO2E',T94,'YCO2B',T106,'UMF',//,(15,1PE12.3)
413. 1A1=FM0/0.21+WCOAL*(I.-XW)*XO/M2-FMO*YO(MT)
414. 1ETCO=ETCA-ETCG
415. C WRITE(6,209) NT,ETCA,ETCG,XTAV
416. C FORMAT ('O',10X,NT,ETCA,ETCG,XTAV=*,I4,1P1B12.3)
417. ER=ETCO-ETCA
418. CALL CRECTNT(INDEX,ETCA,ETC1,ETC2,ETCA,E1,E2,ER,ETECH)
419. IF (INDEX .EQ. 2) GO TO 236
A FORTRAN subroutine has been written to calculate the carbon concentration profile in a bed. The subroutine, named SIMO, solves the simultaneous solution of algebraic equations to estimate the combustion rate of gas-phase material. Knowing this and the solids mixing rate, carbon balance equations are solved by SIMO. The solution gives the carbon concentration profile in the bed.

The subroutine begins with initializing variables:

- WMIX(I) = 0
- WNET(I) = 0
- J = 1
- W(D) = 0

Then, a DO loop is executed from I = 2 to M1:

1. If(J1 > MDIS) go to 63
2. For J = J1 to MDIS:
   - W(D) = W(D) + WDIS * FD(J)
   - J2 = J + 1
3. Continue

Next, the DO loop is executed from J = 1 to MDIS:

1. If(J1 > MDIS) go to 63
2. For J = J1 to MDIS:
   - W(D) = W(D) + WDIS * FD(J)
3. Continue

The subroutine then calculates UMIX, which is the solid mixing flow which is superposed on the flow of solids. WNET(I) is the net flow rate of solid from the top of I-th compartment. The positive value means the upward flow.

The carbon mass balance equation is then solved for the carbon concentration calculation.

The subroutine concludes by printing the carbon concentration profile.
I = I + 1

481. AAA(II) = -WMIX(I1) - WMIX(I1) + WNET(I1)
482. 1 - WD(I1) - RR(I1)
483. AAA(II-M) = WMIX(I1) - WMIX(I1) + WNET(I1)
484. AAA(II-M) = WNET(I1) + WMIX(I1)

270 CONTINUE

486. CALL SIMQ(AABB, M, MM, H)
487. SUM = 0.
488. X(I1) = BBB(I1)
489. SUM = SUM + X(I1)
490. 280 CONTINUE

XAV = SUM / FLOAT(M)

C286 FORMAT ('0', ' ', XAV = ', F12.3, /', 'I, X, H = ', 15, '1P2E12.3')

SUM = 0.

DO 285 I = 2, M

CARCON(I) = X(I) * RR(M) * ETUBE(I) * EPB(I) / (1. - ETUBE(I))

295 CONTINUE

CLOS = SUM + CCEL * CCHAR

ETCC = 1.0 - SUM / ((WCOAL * RCHL - CCEL) * CCHAR)

HAVING OBTAINED THE CORRECT CARBON CONCENTRATIONS IN THE BED,

GAS PHASE MATERIAL BALANCE IS REPERFORMED TO ARRIVE AT THE CORRECT

CONCENTRATION PROFILES FOR THE VARIOUS GASEOUS SPECIES

GAS PHASE MATERIAL BALANCE IN BED

TCRATE = 0.0

DO 235 I = 2, M

CALL ANK(AK, I, PAV, DCSV, TPB(I), YB(I), RG, MC, AKC02, PHIE)

TAVB = (T(I) + TPB(I)) / 2.

CALL ANK(AK, I, PAV, DCSV, TPE(I), YE(I), RG, MC, AKC02, PHIE)

TAVE = (T(I) + TPE(I)) / 2.

AM = DCSV(I) * AMODF * X(I) * MC

RRB(I) = AM * (PAV/RG) * (EP(I) - EPB(I)) * YB(I) * AKB / TAVB / CCHAR

RR(I) = AM * (PAV/RG/TAVE) * (1. - EP(I) - ETUBE(I)) / (CCHAR * YE(I) * AKC02 / CCHAR)

1YCOE(I) = AKCO2 / CCHAR

I = I + 1

DO 235 I = 2, M

BEDCOM = TCRATE

GAS PHASE MATERIAL BALANCE IN THE FREEBOARD

DO 237 I = MP1, MT

J = I - M1

\ = J + 1
DCSVE = 0.5*(DCSE(J)+DCSE(K))

VCHOLD = VCHOLD(I)/RHOCH

NC = VCHOLD(I)/0.5*(DCSVE(I)+DCSVE)**3

CALL AAH(AKCT(I),PAV,DCSVE,TPB(I),T0(I),RG,MC,ANCO2,PHIB)

TPE(I) = TPB(I)

TAVB = (T(I)+TPB(I))/2.0

II = I-1

CALL FBC(YH2O,AKC,DCSVE,TVBB(I),ETUBE(I),FMO,GB(I),CGB),

1#(I),NC,PAV,PHIB,P1,RP,+RUGAS,T(I),TAVB,XO(I),YCO(I),YO(I),

2Y0(I),YU(I),YV(I),YN(I),YV0(I),YV(I),YV(I)

3#(I) = MC*N*C%%PI*DCSVE**2+PAV/RG/TAVB/CCHAR*(YO(I)*AH.C +

1ANCO2*YCO2(I))

4#RBI(I) = 0.0

553. TCRATE = TCRATE + RR(I)

554. 237 CONTINUE

FBCOM = TCRATE - BEPCOM

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.

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*WFA(I)/RHOAD

295 CONTINUE

DO 300 I = MP1, MT

RR(I) = RR(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 CALCULATION OF TEMPERATURE

AI = CADF

A2 = CCF

CGM = 6.0+0.5E-3*(TAV-273)

A3 = CGM*FM0

ALFA(2) = (WMIX(2)+WD(2))#CS+A3+UHE(2)*AHEAV(2)*DVBB(2)

BETA(2) = (WMIX(2)+WD(2))*CS

AIHFW(2) = WMIX(2)*CS+A3+UHE(2)*AHEAV(2)*DVBB(2)

CVM(2) = WMIX(2)*CS+A3+UHE(2)*AHEAV(2)*DVBB(2)*

I*(TW(2)-273.)

DO 310 I=1, M

AI = -1

ALFA(I) = -UNET(I)+WMIX(I)+WMIX(I)+WD(I)

BETA(I) = (WMIX(I)+WMIX(I))*CS

GAMA(I) = WMIX(I)+CS+A3

DELT(I) = RR(I)+AI*WFA(I)+A2*WFC(I)*(TSE-273.)+UHE(2)*AIHEAV(I)*

1DVBB(I)*X(I)-273.)+UHE(2)*AIHEAV(I)*DVBB(I)*(TWALL(I)-273.)

310 CONTINUE

DO 310 I=3, M

AI = 1

ALFA(I) = -UNET(I)+WMIX(I)+WMIX(I)+WD(I)

BETA(I) = (WMIX(I)+WMIX(I))*CS

GAMA(I) = WMIX(I)+CS+A3

DELT(I) = RR(I)+AI*WFA(I)+A2*WFC(I)*(TSE-273.)+UHE(2)*AIHEAV(I)*

1DVBB(I)*X(I)-273.)+UHE(2)*AIHEAV(I)*DVBB(I)*(TWALL(I)-273.)

310 CONTINUE

ALFA(M1) = -UNET(M)+WMIX(M)+WD(M1)*CS+A3

BETA(M1) = 0.

GAMA(M1) = (WMIX(M))*CS+A3
OR1CAI%.At PAGm

OYPOOR

f

600. OELT(MI)=RR(MI)+AI*WFAD(MI)+A2*WFC(MI)*(TSF-273.)

601. L+UHE(M1)*AHEAV(M1)*DVBB(M1)*(TW(M1)-273.)

602. Z+UHEW(M1)*AHEW(M1)*DVBB(M1)*(TWALL(M1)-273.)

603. C TEMPERATURE SOLUTION BY SIMQ

604. C

605. DO 501 I=1,MM

606. 501 AAA(I)=0.

607. DO 502 I=1,M

608. 502 BBB(I)=DELT(I+1)

609. AAA(I)=ALFA(2)

610. AAA(MI)= -BETA(2)

611. AAA(MM)= ALFA(M1)

612. AAA(MM-M)=GAMA(M1)

613. DO 503 I=2,M0

614. II=(I-1)+M1

615. AAA(II)=ALFA(I+1)

616. AAA(II+M)=GAMA(I+1)

617. AAA(II+M)=BETA(I+1)

618. 503 CONTINUE

619. CALL SIMQ(AAA,BBB,M,MM,KM)

620. TNORM=0.

621. TAV=0.

622. DO 504 I=2,MM

623. T(I)=BBB(I-1)+273.

624. TAV=TAV+T(I)

625. TNORM=TNORM+ABS(T(I)-TOLD(I))

626. CONTINUE

627. TAV=TAV/FLOAT(M)

628. TNORM=TNORM/FLOAT(M)

629. WRITE (6,208) TNORM,TAV,BEDCOM,FBCOM

630. 208 FORMAT ('0',10X,'TNORM,TAV,BEDCOM,FBCOM

631. C HEAT BALANCE IN THE FREEBOARD

632. DO 320 I = MP1,MT

633. J = I-M1

634. WENTI = WEA(J)+WEJ(J)

635. ANR = (WENTI*CS+A3)*(T(I-1)-273.)+RR(I)+DVBB(I)*UHE(I)*AHEAV(I)*

636. I(TW(I)-273.)+DVBB(I)*UHEW(I)*AHEW(I)*DVBB(I)*(TWALL(I)-273.)

637. DR = WENTI*CS+A3+DVBB(I)*UHE(I)*AHEAV(I)+DVBB(I)*UHEW(I)*AHEW(I)

638. T(I) = ANR/DR + 273.0

639. 320 CONTINUE

640. C CONVERGENCY CRITERION FOR TEMPERATURE CALCULATION

641. IF(TNORM.LT.0.01*TAV) GO TO 610

642. MIOLD = MI

643. 600 CONTINUE

644. WRITE (6,3003) 3003 FORMAT ('0','10X,’GAUSS SEIDEL TEMPERATURE TRIAL HAS NOT CONVERGED.

645. 1 S.NO. = 3003’,/)

646. 610 CONTINUE

647. A1 = AHEAV(I) * DVBB(I)

648. HAREA = HAREA + A1

649. 600 CONTINUE

650. WRITE (6,3005) 3005 FORMAT ('0','10X,’GAUSS SEIDEL TEMPERATURE TRIAL HAS NOT CONVERGED.

651. 1 S.NO. = 3005’,/)

652. 610 CONTINUE

653. DO 620 I = 2,MT

654. A1 = AHEAV(I) * DVBB(I)

655. HAREA = HAREA + A1

656. QTRANS = UHE(I) * A1 * ( T(I)-TW(I) ) + QTRANS-

657. RR(I) = RR(I) / DVBBEF(I)

658. ZAVG(I) = ( H(I-1) + H(I) ) * 0.5

659. 620 CONTINUE
QVOL = QTRANS/BEVOL
HFB = H(MI) - 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
612 CONTINUE
T(I) = T(I) - 273.
TPB(I) = TPB(I) - 273.
TPE(I) = TPE(I) - 273.
DO 613 I = 1, MT
613 CONTINUE
YBO(I) = YO(MT)
C
C MAIN OUTPUT 3
WRITE (6,2001) ETC,XAV,TAV,ITRIAL,(I,H(I),YB(I),YE(I),YVE(I),
1 YCO(I),YCO2(I),YCO2B(I),X(I),ZAVG(I),I=2,MT)
WRITE (6,2002) (I,H(I),YO(I),YV(I),YCO(I),YCO2(I),T(I),TPB(I),
1 TPE(I),ZAVG(I),I=2,MT)
DO 710 I = 2, MT
710 CONTINUE
IF (IGNITE.EQ.0.) TCRATE = 0.0
DO 710 I = 1,MT
710 CONTINUE
IF (I .GE. M1) GO TO 709
709 YEO(I) = YE(I)
710 YBO(I) = YB(I)
711 YB(I) = 0.
712 YE(I) = 0.
713 IF (ISO2 .EQ. 0.) GO TO 811
714 CONTINUE
FRS = WCOAL*XS/MS*FLOAT(IGNITE)*(1.-XW)
IF (FRS .LE. 1.E-6) GO TO 810
FRS = WCOAL*XS/MS*FLOAT(IGNITE)*(1.-XW)
CASE = (WAD*XCAO+WCOAL*XAKA)/HCAO/FRS
IF (CASE.EQ.0.) GO TO 811
SULFUR = WCOAL*(1.-XW)*XS*RS/MS - CLOSS*SCHAR/CCHAR/MS
RELB(I) = 0.0
RELE(I) = 0.0
YE(I) = YB(I)
ETS = 0.0
DB = 0.1
EETS = 0.005
INDEX = 0.
DO 711 I = 2, MT
711 CONTINUE
RELB(I) = 0.0
RELE(I) = 0.0
IF (TCRATE .LE. 0.) GO TO 711
GENE = GB(I)*VXAS/VRAS
GENE = GE(I)*VXAS/VRAS
REL:B(I) = RRB(I)/TCRATE*SULFUR+GENB
    REL:E(I) = REI(I)/TCRATE*SULFUR+GENE
    CONTINUE
    DO 800 ITRY=1,20
    FS=ETS/CASE
    FS : FRACTIONAL CONVERSION OF ADDITIVE
    ASSUMING THE SULFUR CAPTURE EFFICIENCY, FS IS CALCULATED AND HENCE
    THE LIMESTONE REACTIVITY, THEN S02 MATERIAL BALANCE IS PERFORMED.
    FROM THE EXIT S02 CONC. IN THE FLUE, S02 CAPTURE EFFICIENCY IS
    CALCULATED. ITERATION IS CONTINUED TILL THE ASSUMED AND THE
    CALCULATED SULFUR DIoxide RETENTION EFFICIENCIES AGREE.
    AK=AKAD(FS,DPSE,T(I))
    S02 BALANCE IN THE BED
    DO 540 I=1,M1
    AM=(I-1)-ENF
    CALL GPHASE(AK,AN,AM,FAV,RG,ETUBE(I),EPB(I),EPC(I),
    1A,BE(I),DVB(B(I),FMB(I),FEM(I),FHM(I),FEM(I),T(I),T(I),T(I),
    2YB(I),YE(I),YE(I),RELB(I),RELE(I))
    YSO2(I) = (FEM(I)*YE(I)+FMB(I)*YB(I))/FMO
    CONTINUE
    S02 BALANCE IN THE FREEBOARD
    DO 740 I=MT
    ;
    J = I-M1
    ;
    RHOGAS = PA*MGAS/RG/T(I)
    VISC = 3.72E-6*T(I)**0.675
    DPSE = 0.5*(DPWE(J)+DPWE(K))
    DPWE = 0.5*(DPSE(J)+DPSE(K))
    CALL VEL(VISC,RHOGAS,RHOBED,DPSE,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*DPSE**3)
    AK = AKAD(FS,DPSE,T(I))
    ANR = FMO*YSO2(I-1)+RELB(I)+RELE(I)
    DR = FMO + NA*PI*DPSE**3/6.0 *AN*PAV/RG/T(I)
    YSO2(I) = ANR/DR
    CONTINUE
    ETSC=I.-FMO*YSO2(MT)/FRS
    EE=ETS-ETSC
    CALL CRRECT(ITY,INDX,ETS,ETS1,ETS2,ET,EE,ETS1M)
    IF(INDX.EQ.2) GO TO 810
    ETSC=I.-FMO*YSO2(MT)/FRS
    EE=ETS-ETSC
    CALL CRRECT(ITY,INDX,ETS,ETS1,ETS2,ET,EE,ETS1M)
    IF(INDX.EQ.2) GO TO 810
    WRITE(6,Y3600)
    3600 FORMAT('0',10X,'ETS HAS NOT CONVERGED, S.NO. = 3600,')
    810 CONTINUE
    YSO2(I)=YSO2(MT)
    WRITE(6,Y3605)ETS,FS,CASE,INDX
    IF(INOX.EQ.40) GO TO 814
    YSO2(I)=YSO2(MT)
    WRITE(6,Y3605)ETS,FS,CASE,INDX
    IF(INOX.EQ.40) GO TO 814
    CONTINUE
    YSO2(I)=YSO2(MT)
    WRITE(6,Y3605)ETS,FS,CASE,INDX
    IF(INOX.EQ.40) GO TO 814
    CONTINUE
    NOX CALCULATIONS
    C
    C
    C
    C
    C
FRN = WCOAL * (1.-XU) * XN/HN * FLOAT(IGNITE)

ANITRO = WCOAL * (1.-XU) * XN & RN / MN - CO2*CHAR/CCHAR/MN

DO 750 I = 2,MT

GENB = GB(I)*VGASH/RVGAS
GENE = GE(I)*VGASH/RVGAS

RELB(I) = RGB(I)/TCRATE * ANITRO + GENB
RELE(I) = RRE(I)/TCRATE * ANITRO + GENE

CONTINUE

YB(I) = 0.0
YE(I) = 0.0

FR = 5.24E7
AE = 34000.0

C
NOX BALANCE IN THE BED
C
DO 760 I = 2,MT

C
I1 = I-1
TAVB = (T(I)+TPB(I))/2.0
TAVE = (T(I)+TPE(I))/2.0

C
ANB = FR*EXP(-AE/I.986/TAVB)
AKE = FR*EXP(-AE/I.986/TAVE)
ANDF = 6.0*RHOBED*(1.-EMF)/(DCSVE*RHOCHE/CHAR)

AM = ANDF*XCI

CALL GPHASE (AKBAKEiAMYRAVRG,ETUEI)EPB(I),EPC(I),AKBE(I),
LBB(I),FBM(II),FEM(I),FBM(U),FEM(I),T(I),TAVE,TA1B,YB(I),
YE(I),RELB(I),RELE(I))

YNOX(I) = (FBM(I)*YB(I)+FEM(I)*YE() )/FM0

CONTINUE

C
NOX BALANCE IN THE FREEBOARD
C
DO 770 I = M1,MT

C
TAVB = (T(I)+TPB(I))/2.9

C
J = I-M1
K = J+I

DCSVE = 0.5*(DCSVE(J)+DCSVE(K))

X(I) = WCHOLD(I)*CHAR/(WCHOLDI)+WAHOLD(I))
CARCH(I) = WCHOLD(I)*CCHAR/DVBEF(1)

VCHOLD = WCHOLD/I/RHOC1

HC = VCHOLD*6.0/(P00CSE**3)

AKNO = FR*EXP(-AE/I.986/TAVB)

ANR = FM0*YNOX(I-1) + RELB(I) + RELE(I)

DR = FM0 + NC*PI*DCSVE**2 *AKNO*PAV/RH/TAVB

YNOX(I) = ANR/DR

CONTINUE

ENOX = FM0*YNOX(MT)
EINDEX = ENOX/WCOAL

ETN = 1.0 - ENOX /FRN
ENOX = ENOX/FMO

WRITE (5,2007)EXAIR,TAH,TAV,ETN,YNOX,EINDEX,H(I),YB(I),YE(I),X(I),
ICARCH(I),TAVG(I),YNOX(I),RELB(I),RELE(I),I=2,MT

CONTINUE
C
MAIN OUTPUT 4
C

CONTINUE

YGO(2)=YCO2(MT)
YGO(4)=YH20
YGO(5)=YCO(MT)

WRITE(6,2006) (YGO(I),I=1,5)
I15

ORIGINAL PAGE IS
OF POOR QUALITY

940. IF (HLMF .EQ. 0.0) VMF = VOL
941. IF (HLMF .EQ. 0.0) HLMF = HEIGHT(VMF)
942. IF (HLF .EQ. 0.0) HLF = H(H1)
943. IF (IPRES .EQ. 0) CONTINUE
944. 900 CONTINUE
945. C PRESSURE DROP CALCULATION
946. C
947. C
948. C
949. C ALL THE PRESSURE DROP GIVEN IN CM OF WATER
950. C
951. C
952. C PRESSURE DROP CALCULATIONS ACROSS THE DISTRIBUTOR
953. C
954. C TEMP = T(2)
955. RHOFG = PF * MGAS / (PG*TEMP)
956. UOR = FMF * RG / TEMP / PF / (AND*0.25*PI*DML*2)
957. DDIS = (UOR/0.6) **2 ** RHOFG / (2.0*G)
958. WRITE (6,2050) DDIS
959. C
960. C PRESSURE DROP CALCULATIONS IN THE FLUIDIZED BED SECTION
961. C
962. WRITE (6,2051)
963. M1 = M1
964. IF (IFBC .EQ. 0) M1 = M1 - 1
965. DO 920 I = 2,M1
966. DPFLU = (1.0-EMF) * (1.0-EPB(I)) * (H(I)-H(I-1)) * RHOBED
967. WRITE (6,2052) I, DPFLU
968. 920 CONTINUE
969. IF (IFBC .EQ. 0) GO TO 930
970. C SECSTXRM ROUR:
971. C PRESSURE DROP CALCULATIONS IN THE FIXED BED SECTION
972. C
973. E1 = (H(M1) - H(M1-1)) / G
974. E2 = (1.0 - EMF) / EMF ** 3
975. DPFIX = E1 * (150.0 * (1.0 - EMF) * E2 * VISC * UO(M1)
976. I / DPSVR * 2 + 1.75 * E2 * RHOGAS * UO(M1)**2/DPSVR
977. 930 CONTINUE
978. IF (IFBC .EQ. 0) DPFIX = 0.0
979. WRITE (6,2053) DPFIX
980. 950 CONTINUE
981. WRITE (6,2053)
982. WRITE (6,2054)
983. WRITE (6,2055)
984. DO 910 I = 2,M1
985. WRITE(6,2070) I,H(I),ZAVB(I),DBAV(I),UB(I),EPB(I),EPC(I),UO(I),
986. UMFI(I)
987. 910 CONTINUE
988. WRITE (6,2075)
989. DO 940 I = 1,hT
990. WRITE (6,2080) I,H(I),DT(I),hT(I)
991. 940 CONTINUE
992. 1000 FORMAT(5I1)
993. 1001 FORMAT(8F10.0)
994. 1010 FORMAT(2A4/(8F10.0))
995. 2000 FORMAT('0',1X,XCAO,'XCAO = ',F6.3,10X,'XCA0 = ',F6.3,10X,'XMOO = ',F6.3,10X,
996. *XSID2 = ',F6.3,10X,'XDO = ',F6.3,10X,'XDI = ',F6.3,10X)
997. 2001 FORMAT('//10X,'"RESULTS ,ALL TEMPERATURES IN CENTIGRADE\"
998. */ETC,XAVTAV,ITRIAL,'"3E12.4',1X,I4,1X;
999. 12X,'1',6X,'HT',10X,'TB',10X,'TE',10X,'TB',8X,'YCOE',7X,'YCOE2';
FUNCTION AKAD(FS,DP,T)

C THIS SUBROUTINE CALCULATES LIMESTONE-SO2 REACTION RATE CONSTANT

C DIMENSION FB(15),RR(15),RB(15),RC(15)

DATA FB/0.0,0.05,0.1,0.2,0.25,0.3,0.35,0.4,0.45,0.475,0.5,
  0.525,0.55,0.6 / 

DATA RR/0.0,0.05,0.1,0.15,0.2,0.25,0.3,0.35,0.4,0.45,0.475,0.5,
  0.525,0.55,0.6 / 

DATA RB/0.0,0.05,0.1,0.15,0.2,0.25,0.3,0.35,0.4,0.45,0.475,0.5,
  0.525,0.55,0.6 / 

DATA RC/0.0,0.05,0.1,0.15,0.2,0.25,0.3,0.35,0.4,0.45,0.475,0.5,
  0.525,0.55,0.6 / 

C DB = 0.2

IF (DP > 0.6, DP = 0.6, DP = 0.2)

DO 30 1=2,13
  p=I

30  IF (FS < BE. I,0) RETURN

DO 40 1=2,13
  p=I

40  IF (FS > BE. I,0) RETURN

N=I

116
IF( FS .LE. FB(I) ) GO TO 11

10 CONTINUE

11 CONTINUE

N1=N+1

A=(FS-FP(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. 253.0) S5 = 3.51E04

IF (T .GT. 253.0)

S5 = -38.43*T + 5.64E04

IF (6*LT. 100.0 ) S5 100.0

AKAD = 490.0*EXP(-17500.0/1.987/T)*S5 * ALIME

RETURN

END

SUBROUTINE ANK(AKR, TPDC, TP, YO2, RGTAV, PHI

REAL MC

C THIS COMPUTES REACTION RATE CONSTANT FOR CHAR COMBUSTION AKR,

C RATE CONSTANT FOR C-C02 REACTION AND THE CHAR PARTICLE TEMPERATURE

C

EM=1.0

SIGN=1.36*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 = (TP+TP+.5)

D=4.25*(TAV/1800.0)**1.75/P

COND=0.632E-12*SQRT(TAV)/(1.0+245./TAV**10.0)**(-12./TAV)

Z = 2500.0*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 = 1.0/(Z+2.)*(2.*Z+2.)

IF (DC .GT. 0.10) PHI = 1.0

Q = 7900.0*(2./PHI-1)+1340.0*(2.-2./PHI)

AKF=24.*PHI*D/(DC*RGTAV)

AKR=(RG*TAV/HC)/(1/AKS+1./AKF)

RHS = AKR*YPY2*NCKZ/(RG*TAV) + EM*SIGN*(TP**A-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 ('O',IOX,'TP CALCULATION HAS NOT CONVERGED',/10X,'TP,ETS ','1 ',IP2E12.3)

110 CONTINUE

AKRCO2 = 4.1E08*EXP(-59200./1.987/TAV)

B = 3.25*(TAV/1800.0)**1.75/P

AKFCO2 = 2.*PHI*D/DC

AKC02 = 1./(1./AKRCO2+1./AKFCO2)

RETURN
SUBROUTINE AREA ( ZI, DTI, ATI )

COMMON /A/ ZHE(t,0),PV(u0),PH(IO),ZI=ZHE(IO),TBE<LO),IDVB'(60),DVBEFF(60),FFAD(1O),ZDIS(IO),FL(10),AHElV(60),ETUBE(60),
2UO(60),,UMF660'),HR60),AT(60)DT(60)

SUBROUTINE CPRRECT(I,,INDXDX,XIX2rXNEUEiE2EEMAX)

C NUMBER OF THIS TRIAL, I FOR FIRST TRIAL
C INDEX: INDEX OF THE TRIAL LEVEL
C INDEX=1: JUST PROCEEDING
C INDEX=1: THE ROOT HAS BEEN CAUGHT BETWEEN X1 AND X2
C INDEX=2: THE ITERATION HAS CONVERGED
C IF (ABSXI<GT.EMAX) GO TO 5
C INDEX=2
C RETURN

5 CONTINUE

SUBROUTINE DESIGN
COMMON /A/ ZHE(10),AHE(10),PV(10),PH(10),IF(10),FFC(10),DTUBE(10),
DVF(50),DVEFF(50),FFAD(10),ZDIS(10),FD(10),AHEAV(50),ETUBE(50),
2UD(60),UMF(60),H(50),AT(50),DT(60),T(60),X(50),AHE(50),YF(50),
3Y(50),YCOE(60),EPB(60),EPF(60),DVBB(60),DVEEF(50),DVE(50),
4UB(60),UTC(60),UTA(60),ZB(10),ATB(10),YVE(50),ZAVG(50),IARR(10),
COMMON /B/ YBO(60),YEO(60),DB(50),DPSVBDPWMB,DCSVB,DCWMB,RHCH,
1HLF,VMF,PM,FFP,FFP,TP,RB,SA,DAG,BPFI,DFLFL,DPDIS,RMDED,
EMF,PAV,HTC,EFFVOL,SOLVOL,TETUBE,HLMF,API,AND,DNZL,
3FW,FSD,DAV,MEED,MDIS,MTHE,MT,MI,H,IKC,IFFC,NTC

C AXIAL VARIATION OF BED CROSS SECTION
READ (5,1000) A1,A2,A3,A4
READ (5,1001) MTB(ZB(J),ATB(J),J = 1,MTB)
IARRNG 1 2 3
1 VERTICAL INLINE ARRANGEMENT
2 VERTICAL STAGGERED ARRANGEMENT
3 HORIZONTAL INLINE ARRANGEMENT
4 HORIZONTAL STAGGERED ARRANGEMENT

C HEAT EXCHANGE TUBES
READ (5,1002) MTHE,ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),
IARR(J),J = 1,MTHI

C LOCATION OF FEED AND DISCHARGE
READ (5,1001) MFEED,ZF(J),FFC(J),FFAD(J),J = 1,MFEED

C DISTRIBUTOR
READ (5,1003) ZDIS(J),FD(J),J = 1,MDIS

C DISTRIBUTOR
READ (5,1003) AND,DNZL,FW,FSD
DO 100 J = 1,MTHI
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))
CONTINUE

C CONDITION FOR COMPUTING AVERAGE CELL SIZE
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),
1 J = 1,MTHI
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,FSD
ZI = ZB(1)
ABED1 = ATB(1)
DBED1 = SORT(4.0 * ABED1 / PI)
DVB(1) = 0.0
DVEFF(1) = 0.0
ZHE(1.0) = 0.0
DZAV = 30.0
SUBROUTINE FBC(YH20ANC,DCSVE,DVBB,ETUBEFO,GBCB,GE,NC,IPAVPHIBPIPRVGASTTAVB,XO2,YCOO,'YCO,YOOYO,,YVOY,' '02,C02VB,CO2VB,YC020,YC02)

REAL NC

C THIS SUBPROGRAM PERFORMS THE GAS PHASE MATERIAL BALANCE FOR

C 02,C02 IN THE FREEBOARD

C

A2 = PAV/RG/TAUB*NC*PI*DCSVE**2*AKC

04 = PAV/RG/TAUB*NC*PI*DCSVE**2*AKC02

TV = YV0-Y00/X02

IF (YV .LT. 0.0) GO TO 100

Y0 = 0.0

C

120
OXYGEN RICH CONDITION

\[
YV = 0.0
\]
\[
YAP = 3. \times 10^{-9} \exp(-15000/1.787/T)**(PAV/RT)*1.3*YOC+1.5*DUBB*
\]
\[
I(1. - ETUBE)
\]
\[
INDEX = 0
\]
\[
YO = 0.0
\]
\[
DYO = 0.01
\]
\[
EYO = 0.001
\]

DO 110 I = 1, 20

ANR = FMO*YCO2+2.0*A4/(FMO+A4)*(FMO*YCO2+A2*YO)/(2./PHIB-1.))

IF (YCO < 1. E-6) GO TO 130

YCO2 = (FMO*YCO2+A2*YO)/(2./PHIB-1.))

1+A2*YO/FMO

YOC = YCO2+2.0*A4*AKP*(17.5*YO/(1.+24.7*YO))/(FMO+A4)

YOC = YOC/DR

IF (YOC < 0.0) YOC = 0.0

IF (YCO2 < 0.0) YCO2 = 0.0

GB = 0.0

GE = FMO*YVO

IF (YOC2 < 0.0) YOC2 = 0.0

IF (YOC < 0.0) YOC = 0.0

RETURN

SUBROUTINE FBC (YP, YOC, YCO, YCO2, YO, YOC2, YVO, YOC2, YCO2, YO2, YOC2, YCO2, YO2, YOC2, YCO2)

WRITE(6,190) 1, YCO, YCO2, YO, YOC

C190 FORMAT(SX, 'YCO, YCO2, YO, YOC - ',IPZE12.3)

END
DIMENSION A(25), B(5), AA(16), BB(4)

THIS SUBPROGRAM FORMS THE HEART OF THE CALCULATIONS FOR THE GAS PHASE BALANCES IN THE BED

\[
\begin{align*}
A_1 &= \text{ANBE} \times \text{DBBE} \times \text{EPB} \times \text{PAV} / (\text{RG} \times \text{TAV}) \times X \\
A_2 &= \text{AMDF} \times \text{DBBE} \times (1.0 - \text{EP} - \text{ETUBE}) \times \text{EPK} \times \text{PAV} / (\text{RG} \times \text{TAVE}) \times X \\
A_4 &= \text{AMDF} \times \text{DBBE} \times (1.0 - \text{EP} - \text{ETUBE}) \times \text{ARCO} \times \text{PAV} / (\text{RG} \times \text{TAVE}) \times X \\
\end{align*}
\]

DO 150 \( i = 1 \) to 25

OXYGEN CONCENTRATION IN EMULSION PHASE IS ZERO.

\[
\begin{align*}
A_{(i1)} &= 0.0 \\
A_{(i)} &= \text{FEM} + A_1 \\
A_{(i7)} &= -A_1 \times \text{CO} \times \text{VB} \\
A_{(i8)} &= A_1 \times \text{XO} \times \text{CC} \\
A_{(i9)} &= A_1 \times \text{XO} \times \text{CD} \\
A_{(i10)} &= A_1 / 2.0 \\
A_{(i12)} &= -2.0 \times \text{A} \times \text{A} \\
A_{(i13)} &= \text{FEM} + A_1 + A_4 \\
A_{(i14)} &= -A_1 \\
A_{(i18)} &= -A_1 \\
A_{(i19)} &= \text{FEM} + A_1 \\
A_{(i21)} &= A_1 / \text{XO} \\
A_{(i22)} &= -A_1 \times \text{CO} \times \text{VB} / \text{XO} \\
A_{(i23)} &= -A_2 \\
A_{(i25)} &= \text{FEM} + A_1 + A_2 \\
B_{(i1)} &= \text{FEM} \times \text{YVE} - \text{FEM} \times \text{YO} / \text{XO} + \text{VPROD} \\
B_{(i2)} &= \text{FEM} \times \text{YCOE} + \text{FEM} \times \text{YO} / \text{XO} + \text{VPROD} \times \text{CO} \\
B_{(i3)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i4)} &= \text{FEM} \times \text{YCOE} \\
B_{(i5)} &= \text{FEM} \times \text{YCOE} \\
B_{(i6)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i7)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i8)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i9)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i10)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i11)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i12)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i13)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i14)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i15)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i16)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i17)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i18)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i19)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i20)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i21)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i22)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i23)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i24)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
B_{(i25)} &= \text{FEM} \times \text{YCOE} + \text{VPROD} \times \text{CO} \\
\end{align*}
\]

OXYGEN CONCENTRATION IN EMULSION PHASE IS LARGE ENOUGH TO BURN THE VOLATILES RELEASED IN THAT COMPARTMENT


SUBROUTINE GPHASE(AhBAKEAMPAVR,ETUBE,EP,EPC,AKBE,BEFBO,FEMO,FTM,TTB,TE,YBO,YEO,Y91,YE1,GENB,GENE)

C
C THIS SUBPROGRAM IS USED TO CALCULATE THE SO2 AND NOX

D1 = ((1.-ETUBE-EPC)*AM*AKE/RE+ANBE*EPB/ TB)*PAV/RG*DBP+FEM
ALF=ANBE*EPB*DBP/PAV/(DIYRGT)

D2 = FEM+ALF*FEM+((EPC-EPB)*AM/ TB+
1ALF*(1.0-ETUBE)*MAKE/TE)*DVBB*AM*PAV/RG

IF ( (D2 .EQ. 0.0) YB1 = 0.0
IF ( (D2 .NE. 0.0) YDI = (FEMO*YBO+GENB+ALF*FEMO*YEO)/D2
1380. \( YEI = (YE*FEMO + GENE) / DI + ALF' = YE \)
1391. RETURN
1392. END
1393. SUBROUTINE HAREA (ATI, DTI, ZI)
1394. COMMON /A/ ZHE(10), AHE(10), PV(10), PH(10), ZF(10), FFC(10), DTUBE(10),
1395. 1DV(60), DVBEFF(60), FFAD(10), ZDIS(10), FDI(10), AHEAV(60), ETUBE(60),
1396. 2UD(60), UMF(60), R(60), AT(60), DT(60), T(60), X(60), YB(60),
1397. YB(60), YCOE(60), EPB(60), EPB(60),DVBB(60), DVBB(60), DVBB(60), DB(60),
1398. 2UB(60), UTC(60), UTB(60), ZB(10), ATB(10), YVE(60), ZAVB(60), IB(10)
1399. COMMON /B/ YBO(60), YE(60), DB(60), DSVB, DSVB, DSVB, DSVB, DSVB, DSVB,
1400. HOF, MIF, MHEF, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1401. 3MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1402. 4MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1403. 5MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1404. 6MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1405. 7MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1406. 8MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1407. 9MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1408. 10MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1409. 11MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1410. 12MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1411. 13MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1412. 14MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1413. 15MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1414. 16MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1415. 17MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1416. 18MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1417. 19MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1418. 20MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1419. 21MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1420. 22MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1421. 23MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1422. 24MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1423. 25MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1424. 26MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1425. 27MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1426. 28MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1427. 29MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1428. 30MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1429. 31MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1430. 32MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1431. 33MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1432. 34MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1433. 35MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1434. 36MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1435. 37MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1436. 38MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1437. 39MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1438. 40MF, FSW, DZAV, MFEDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE, MDE,
1440. COMMON /B/ YBO(60), YEO(60), IARRG(60)
1441. COMMON /C/ DPSE(30), DPWE(30), DCSE(30), WCSE(30), WEDC(30),
1442. 1HB(30), WCHOLD(30), WAHOLD(30), KT
1443. COMMON /B/ YBO(60), YEO(60), DB(10), YVE(60), 2V(60), IARRG(10)
1444. COMMON /B/ YBO(60), YEO(60), IARRG(60)
1445. COMMON /C/ YBO(60), YEO(60), EPB(60), EPC(60), VBB(60), DUBBEF(60), DUBBEF(60), DUM(60), UTA(60), ZB(10), ATB(10), YVE(60), 2V(60), IARRG(10)
1446. COMMON /C/ YBO(60), YEO(60), EPB(60), EPC(60), VBB(60), DUBBEF(60), DUBBEF(60), DUM(60), UTA(60), ZB(10), ATB(10), YVE(60), 2V(60), IARRG(10)
1447. COMMON /C/ YBO(60), YEO(60), EPB(60), EPC(60), VBB(60), DUBBEF(60), DUBBEF(60), DUM(60), UTA(60), ZB(10), ATB(10), YVE(60), 2V(60), IARRG(10)
1448. COMMON /C/ YBO(60), YEO(60), EPB(60), EPC(60), VBB(60), DUBBEF(60), DUBBEF(60), DUM(60), UTA(60), ZB(10), ATB(10), YVE(60), 2V(60), IARRG(10)
1449. COMMON /C/ YBO(60), YEO(60), EPB(60), EPC(60), VBB(60), DUBBEF(60), DUBBEF(60), DUM(60), UTA(60), ZB(10), ATB(10), YVE(60), 2V(60), IARRG(10)
1450. DIMENSION DTUBEI(60), PHI(60), PVI(60), IARRNG(60)
1451. C C CALCULATION OF BUBBLE HYDRODYNAMICS
1452. C
1453. LAST = 0
1454. SUM = 0.0
1455. SUMEFF = 0.0
1456. BEDVOL = 0.0
1457. SUMV = 0.0
1458. ICR = 0
1459. HCR = 0.0
1460. IFBC = 0
1461. DTUBEI(1) = 0.0
1462. DBAV(I) = 0.0
1463. H(1) = 0.0
1464. AT(I) = ATB(I)
1465. DT(I) = SQRT(4.0*AT(I)/PI)
1466. DBEV(1) = 0.0
1467. DBVEF(1) = 0.0
1468. IARRNG(1) = 0.0
1469. ETUBE(1) = 0.0
1470. ETUBE(2) = 0.0
1471. RHOGAS = PAV*MGAS/(RG*T(2))
1472. VISC = 3.72e-6*T(2)**0.676
1473. A1 = 33.7**2+0.0408*DPSE**3*(RHOBED-RHOGAS)*RHOGAS/VISC**2
1474. UMF(2) = VISC/(DPSE*RHOGAS) * (SQRT(A1)-33.7)
1475. UMF(1) = UMF(2)
1476. UO(2) = FMF*MGAS/RHOGAS/(AT(1)*1.ETUBE(2))
1477. DSO = 0.347*(AT(1)*1.ETUBE(2))*UO(2)-UMF(2))/AND)**0.4
1478. DBA = DB0
1479. H(2) = DB0
1480. C C ASSUMING THE COMPARTMENT SIZE, BUBBLE SIZE IS COMPUTED IN THAT
1481. C COMPARTMENT. ITERATION IS CONTINUED UNTIL THE ASSUMED COMPARTMENT
1482. C SIZE AND THE CALCULATED BUBBLE SIZE IN THAT COMPARTMENT AGREE
1483. C
1484. DO 200 I = 2, 190
1485. IF (I .EQ. 2) GO TO 16
1486. DBB = 5.0
1487. INDEX = 0
1488. EMAX = 0.1
1489. DBA = H(I-1) - H(I-2)
1490. IF (I .LE. M1) GO TO 5
1491. T(I) = T(M1)
1492. X(I) = X(M1)
1493. YB(I) = YB(M1)
1494. YE(I) = YE(M1)
1495. CONTINUE
1496. H(I) = H(I-1) + DBA
1497. C
IDENTIFICATION OF COOLING TUBES IN THE COMPARTMENT

DO 210 J = 1,NTHE
IF (ZH(J) .LE. H(I) .AND. ZH(J+1) .LT. H(I)) GO TO 210
IF (ZH(J) .LE. H(I-1) .AND. ZH(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)
210 GO TO 230

AHEAV(I) = AHE(J)
DTUBE(I) = DTUBE(J)
230 P'I(I) = PV(J)
PHICI) = PH(J)
IARRNG(I) = IARR(J)
GO TO 240

continuing...

CALCULATIONS FOR UBR --- BUBBLE RISING VEL. AT MIN. FLUIDIZATION,
UBS --- BUBBLE VEL. AT SLUGGING CONDITIONS,
UB --- ABS. BUBBLE RISING VELOCITY,
EPB --- BUBBLE FRACTION,
EPC --- CLOUD FRACTION

UBR = 0.711 * SORT ( G * DBAV(I) )
UBS = 0.355 * SORT ( G * DTAV )
IF (UBR .GT. UBS) UBR = UBS
UB(I) = UO(I)-UMF(I)+UBR
EPB(I) = ( UG(I)-UMF(I) ) / UB(I)**(1.0-ETUBE(I))
1560. \( \text{ALFB = EMF} \times \text{UBR} / \text{UMF(I)} \)
1561. \( \text{EPC(I)} = \text{EPB(I)} + \text{ALFB} / (\text{ALFB - 1.0}) \)
1562. IF (\text{EPC(I)} .GT. 0.7) \text{EPB(I)} = 0.7
1563. IF (\text{EPC(I)} .GT. (0.99 - \text{ETUBE(I)})) \text{EPC(I)} = 0.99 - \text{ETUBE(I)}
1564. IF ((\text{EPC(I)} - \text{EPB(I)}) .GT. 0.01) \text{EPC(I)} = \text{EPB(I)} + 0.01
1565. \text{BEDVOL = BEDVOL + DVBB(I)}
1566. \text{SUMV = SUMV + DVBBEF(I)}
1567. \text{SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)}
1568. \text{SUMEFF = SUMEFF + SOLVOL}
1569. \text{SUM = SUM + SOLVOL / (0.5 * (AT(I) + AT(I-1)))}

1570. IF (\text{ICR} .GT. 0) GO TO 35
1571. IF (\text{LAST} .GT. 0) GO TO 125
1572. IF (\text{HLF} .NE. 0.0) GO TO 20
1573. C
1574. C TEST FOR CONVERGENCE
1575. C
1576. IF (\text{ABS(SUMEFF-UMF)} .LT. 0.01*\text{UMF}) GO TO 125
1577. IF (\text{SUMEFF} .LT. \text{UMF}) GO TO 200
1578. \text{VOL = SUMV-\text{SUMEFF} * (1.0 - \text{ETUBE(I)}) / (1.0-\text{EPB(I)}-\text{ETUBE(I)})}
1579. \text{H(I) = HEIGHT(VOL)}
1580. \text{CALL AREA (H(I),BT(I),AT(I))}
1581. \text{BEDVOL = BEDVOL - DVBB(I)}
1582. \text{SUMV = SUMV - DVBBEF(I)}
1583. \text{SUMEFF = SUMEFF - SOLVOL}
1584. \text{SUM = SUM - SOLVOL / (0.5*(AT(I)+AT(I-1)))}
1585. \text{LAST = 1}
1586. \text{DBA = H(I)-H(I-1)}
1587. GO TO 16,
1588. 20 CONTINUE
1589. C
1590. C TEST FOR CONVERGENCE
1591. C
1592. IF (\text{ABS(H(I)-HLF)} .LE. 1.0E-3*\text{HLF}) GO TO 125
1593. IF (\text{ABS(H(I)-HLF)} .LE. 0.5*(H(I)-H(I-1))) GO TO 50
1594. \text{H(I) = HLF}
1595. \text{BEDVOL = BEDVOL - DVBB(I)}
1596. \text{SUMV = SUMV - DVBBEF(I)}
1597. \text{SUMEFF = SUMEFF - SOLVOL}
1598. \text{SUM = SUM - SOLVOL / (0.5*(AT(I)+AT(I-1)))}
1599. \text{CALL AREA (H(I),BT(I),AT(I))}
1600. \text{LAST = 1}
1601. \text{DBA = H(I)-H(I-1)}
1602. GO TO 16
1603. 10 \text{UO(I) = UMF(I)}
1604. \text{ATAV = FMO * RG * T(I) / (PAV * UO(I) * (1.0-ETUBE(I)))}
1605. \text{CALL MAREA (ATAV,DTAV,HAV)}
1606. \text{H(I) = 2.0*HAV - H(I-1)}
1607. \text{ICR = 1}
1608. \text{LAST = 1}
1609. \text{DBA = H(I)-H(I-1)}
1610. GO TO 16
1611. 200 CONTINUE
1612. IF (\text{IFBC .EQ. 0}) GO TO 125
1613. 35 CONTINUE
1614. \text{HCR = H(I)}
1615. IF (\text{ABS(H(I)-HLF)} .LE. 1.0E-3*\text{HLF}) GO TO 125
1616. IF (\text{ABS(UMF-SUMEFF)} .LE. 0.01 * \text{UMF}) GO TO 125
1617. I = I + 1
1618. \text{DBAV(I) = 0.0}
1619. \text{UB(I) = 0.0}
L620. AKBE(I) = 1000.0
L621. EPB(I) = 0.0
L622. EPC(I) = 0.0
L623. IF (VMF .EQ. 0.0) GO TO 45
L624. C
L625. C FIXED BED CONDITIONS
L626. C
L627. VOL = SUMV + (VMF - SUMEFF)
L628. H(I) = HEIGHT(VOL)
L629. CONTINUE
L630. IF (VMF .EQ. 0.0) H(I) = HLF
L631. IF (I .LE. M1) GO TO 6
L632. T(I) = T(M1)
L633. X(I) = X(M1)
L634. YB(I) = YB(M1)
L635. YE(I) = YE(M1)
L636. CONTINUE
L637. CONTINUE
L638. IF (ZHE(J) .LE. H(I) .AND. ZHE(J+1) .LT. H(I)) GO TO 310
L639. IF (ZHE(J) .LE. H(I-1) .AND. ZHE(J+1) .GE. H(I)) GO TO 320
L640. F1 = (H(I)-ZHE(J))/(H(I)-H(I-1))
L641. F2 = (ZHE(J)-H(I-1))/(H(I)-H(I-1))
L642. AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)
L643. DTUBEI(I) = F1*DTUBE(J)+F2*DTUBE(J-1)
L644. PV(I) = F1*PV(J)+F2*PV(J-1)
L645. PHI(I) = F1*PH(J)+F2*PH(J-1)
L646. CONTINUE
L647. CONTINUE
L648. AHEAV(I) = AHE(...
L649. DTUBEI(I) = DTUBE(J)
L650. PV(I) = PV(J)
L651. PHI(I) = PH(J)
L652. CONTINUE
L653. IARRNG(I) = IARR(J)
L654. CONTINUE
L655. CALL AREA(H(I),DT(I),AT(I))
L656. DVBB(I) = 0.5*(AT(I)+AT(I+1))*(H(I)-H(I-1))
L657. DVBBEF(I) = DVBB(I)*F1-0.5*AHEAV(I)*DTUBEI(I)
L658. ETUBE(I) = 1.0 - DVBBEF(I)/DVBB(I)
L659. RHOGAS = PAVG/RHOGAS
L660. VISC = 3.72E-6*T(I)**.676
L661. A1 = 33.7**2+0.0408*DPSVB**3*G*(RHOBE-RHOGAS)*RHOBE/VISC**2
L662. UMF(I) = VISC/(DPSVB*RHOGAS)*(SRT(A1)-33.7)
L663. CALL AREA(HAV,DTAV,ATAV)
L664. UC(I) = FMO*MGAS/RHOGAS/(ATAV*(1.-ETUBE(I)))
L665. BEDVOL = BEDVOL + DVBB(I)
L666. SUMU = SUMU + DVBBEF(I)
L667. SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)
L668. SUMEFF = SUMEFF + SOLVOL
L669. SUM = SUM + SOLVOL / (0.5 * (AT(I)+AT(I-1)))
L670. IFBE = 1
L671. M1 = I
L672. TETUBE = 1.0 - SUMU/BEDVOL
L673. EFFVOL = SUMV
L674. SOLVOL = SUMEFF
L675. M = M1 - 1
L676. DO 460 K = 2,KT
L677. I = I + 1
L678. H(I) = H(M1)+HB(K)
L679. DO 410 J = 1,MTHE
IF (ZHE(J) .LE. H(I)) AND ZHE(J+1).LT.H(I)) GO TO 110
IF (ZHE(J) .LE. H(I-1)) AND ZHE(J+1).LE.H(I)) GO TO 120
FI = (H(I)-ZHE(J))/(H(I)-H(I-1))
F2 = (ZHE(J)-H(I-1))/(H(I)-H(I-1))
AHEAV(I) = FI*AEHE(J)+F2*AEHE(J-1)
DTUBEI(I) = FI*DTUBE(J)+F2*DTUBE(J-1)
PV(I) = FI*PV(J)+F2*PV(J-1)
PHI(I) = FI*PH(J)+F2*PH(J-1)
GO TO 430
IF (ZHE(J) .LE. H(CIANIIZHE(J+1).GE.H(I))) GO TO 420
Fl = (H(I)-ZHE<J))/(H(U)-H(I-1))
F2 = (ZHE(J)-H(I-1))/(H(J-H(
AHEAV(I) = Fl*AHE(J)+F2*AHE(J-1)
DTUBEI(I) = Fl*DTUBE(J)+F2*DTUBE(J-1)
PV(I) = Fl*PV(J)+F2*PV(J-1)
PHI(I) = Fl*PH(J)+F2*PH(J-1)
GO TO 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) + (1.0-0.25*AHEAV(I)*DTUBEI(I))
ETUBE(I) = 1.0 - DVBBEF(I)/DVBB(I)
CONTINUE
MT = I
HFB = H(MT)-H(M1)
RETURN
SUBROUTINE SIMQ(A,B,N,NX,KS)
DIMENSION A(NN),B(N)
C FORWARD SOLUTION
C TOL=0.0
KS=0
JJ=-N
DO 65 J=1,N
JJ=JJ+N+1
BIGA=0.
IT=JJ-J
DO 30 I=J+N*(J-2)
IT=IT-IMAX
65 CONTINUE
C TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
C IF( ABS(BIGA) .LT. TOL) 35,35,40
C BIGA=A(IJ)
C IMAX=I
C 30 CONTINUE
C INTERCHANGE ROWS IF NECESSARY
C 35 KS=I
C WRITE(6,100) KS
C 100 FORMAT(/' NO SOLUTION',/' KS=',12)
C STOP
C 36
C 37
C 38
C 39
DO 50 I = J, N

I2 = I2 + N
SAVE = A(I2)
A(I2) = A(I2)

C DIVIDE EQUATION BY LEADING COEFFICIENT

DO 50 A(I1) = A(I1)/BIGA
SAVE = B(IMAX)
B(IMAX) = B(J)
B(J) = SAVE/BIGA

C ELIMINATE NEXT VARIABLE

IF(J - N) 55, 70, 55

TQS = N*(J/N(J-1))

DO 65 IX = JY, N

IXJ = IXS + IX
IT = J - IX

DO 60 JX = JY, N

IXJX = N*(IXJ-1) + IX
JJX = IXJX + IT

DO 60 A(IXJX) = A(IXJX) - ((IXJ)*A(JJX))

B(IX) = B(IX) - B(J)*A(IXJ)

C BACK SOLUTION

NY = N - 1
IT = N*NY

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

RETURN

END

SUBROUTINE VELYISCRHOGASG, RHOS, PARUM, UT

THIS SUBROUTINE CALCULATES THE MINIMUM FLUIDIZATION VELOCITY AND THE TERMINAL VELOCITY OF THE PARTICLE

A1 = 33.7*2 + 0.049*DPAR**3*(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)

RETURN

210 END

FUNCTION VOLUME (ZZ)

COMMON /A/ ZHE(IO), AHE(IO), PV(IO), PH(IO), ZF(IO), FFD(IO), DTUBE(IO),
1DS(V(60)), DVEFF(60), FFAD(IO), ZDIS(IO), FD(IO), AHEAV(60), ETUBE(60),
COMMON /YBG(60),YEO(60),DB(60),DPSVBDPWNB,DCSVBOC4MB,NOCH/

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
LO 100 I = 2 * N
SUM = SUM + DVBEFF(I)
IF ( I .LT. N ) GO TO 100
A1 = ( ZZ - ZN ) / DZAV
SUM = SUM + DVBEFF(I) * A1
CONTINUE
100 VOLUME = SUM
RETURN
APPENDIX V

INPUT TO COMBUSTION PROGRAM

132

12345678901234567890123456789012345678901234567890123456789012345678901234567890

KT

<table>
<thead>
<tr>
<th>HB(1)</th>
<th>DPSE(1)</th>
<th>DPWE(1)</th>
<th>WEA(1)</th>
<th>HB(2)</th>
<th>DPSE(2)</th>
<th>DPWE(2)</th>
<th>WEA(2)</th>
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<td>DPWE(3)</td>
<td>WEA(3)</td>
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<td>WEC(1)</td>
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WBIS WELUA CELU EFF DPSUB DPWB DCSUB DCWMB

| 0.0852 | 0.726  | 0.02685 | 0.9927 | 0.0746 | 0.1001 | 0.0787 | 0.1049 |
| DASVF DAWMF DCSVF DCWMB |
| 0.0758 | 0.1287 | 0.0677  | 0.1004 |

A1 A2 A3 A4
NASA LEWIS
MTB

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<th>ZB(2)</th>
<th>ATB(2)</th>
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MTHE

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NAME1 NAME2

LINITI3

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NAME1 NAME2

PTGHCQAL

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HCOAL XACAD

| 7300.0 | 0.08 |

HLMF

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UHEAV1 UHEAV2 UWALL1 UWALL2 TW TF TSF PF

| 0.000765 | 0.00025 | 0.00021 | 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,IS02,INOX,ITEMP,IPRES

111111

1234567890123456789012345678901234567890123456789012345678901234567890
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**Outlet Gas Concentration**

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**Pressure Drop Across the Distributor** = 7.3568E-02

**Pressure Drop in the Bed**

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<td>4</td>
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<tr>
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<td>8.9E+00</td>
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<tr>
<td>6</td>
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**Pressure Drop in the Fixed Bed Section** = 0.0

**Components**

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**Volume Flow Rate** = 14.18E+09
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.
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.

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

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.

\(\text{SO}_2\) retention calculations are done in CN 696/775 if the indicator IS02 is greater than zero. Total feed rate of sulfur is estimated in CN 698. \(\text{SO}_2\) generated from the burning volatiles and char is estimated in CN 718/721. \(\text{SO}_2\) retention calculations are iterative. First, \(\text{SO}_2\) retention efficiency is assumed, and hence the reactivity of the limestone particle is calculated. \(\text{SO}_2\) material balance is performed and from the exit \(\text{SO}_2\) concentration, \(\text{SO}_2\) capture efficiency is calculated as \(\text{SO}_2\) capture efficiency = \(1 - \frac{\text{Sulfur in flue gas}}{\text{Total sulfur fed}}\). (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, \(\text{NO}_x\) material balance calculations are performed. \(\text{NO}_x\) release due to volatiles and char combustion is calculated in CN 783/786. \(\text{NO}_x\) 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. **Subprogram AKAD**

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

$$k_{v_\ell} = k_{v_\ell} S_g \lambda_g \frac{1}{\text{sec}}$$  \hspace{1cm} \text{(A.VII.3)}

where $k_{v_\ell}$ is defined as:

$$k_{v_\ell} = 490 \exp(-17500/RT) \text{ gm/cm}^3\text{sec}$$  \hspace{1cm} \text{(A.VII.4)}

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

$$S_g = 35.9 T - 3.67 \times 10^4 \frac{\text{cm}^2}{\text{gm}}, T < 1253 \text{ °K}$$  \hspace{1cm} \text{(A.VII.5)}

$$= -38.43 T + 5.64 \times 10^4 \frac{\text{cm}^2}{\text{gm}}, T \geq 1253 \text{ °K}$$  \hspace{1cm} \text{(A.VII.6)}

and $\lambda_g$ 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:

$$\lambda_{\ell a} = \left(\frac{\lambda_{\ell a2}}{\lambda_{\ell a1}}\right)^{\frac{f_{\ell} - f_1}{f_2 - f_1}} \times \lambda_{\ell a1}$$  \hspace{1cm} \text{(A.VII.7)}
\[ \lambda_{lb} = \left( \frac{\lambda_{2b}}{\lambda_{b1}} \right) \frac{f_{2} - f_{1}}{f_{2} - f_{1}} \times \lambda_{b1} \quad (A.VII.8) \]

\[ \frac{\ln(d_{x}/d_{xb})}{\ln(d_{x}/d_{xb})} \]

\[ \lambda_{x} = \left( \frac{\lambda_{xa}}{\lambda_{xb}} \right) \times \lambda_{xb} \quad (A.VII.9) \]

where \( \lambda_{x} \) is the reactivity of limestone, \( f_{x} \) is the fractional conversion of limestone and \( d_{x} \) 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, \( \lambda \)

   \[ = 6.32 \times 10^{-6} \frac{T_{m}^{0.5}}{\left\{ 1 + \frac{245 \times 10^{-12} / T_{m}}{T_{m}} \right\}} \text{ cals/sec.cm}^\circ \text{C} \quad (A.VII.10) \]

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

   Diffusivity of O\(_2\)-N\(_2\) = 4.26 \( \left( \frac{T_{m}}{1800} \right)^{1.75} / P \) \quad (A.VII.11)

   Diffusivity of CO\(_2\)-N\(_2\) = 3.26 \( \left( \frac{T_{m}}{1800} \right)^{1.75} / P \) \quad (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 $A_{t,j}$, $j = 1$ to 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

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

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

$$A_t = \pi r^2$$  \hspace{1cm} (A.VII.13)

where

$$r = [1 + \left( \frac{Z - Z_{j-1}}{Z_j - Z_{j-1}} \right) \left( \frac{A_{t,j}}{A_{t,j-1}} \right)^{1/2} - 1]r_{j-1}$$  \hspace{1cm} (A.VII.14)

$$r_{j-1} = \left( \frac{A_{t,j-1}}{A_t} \right)^{1/2}$$  \hspace{1cm} (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 O₂-N₂ are calculated by Equations (A.VII.10) and (A.VII.11) respectively. Char size reduction rate constant is equal to \( \frac{1}{t_b} \).

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 \( \text{INDX} = 0 \)
- **Period 2:** the root is found in the interval \( \text{INDX} = 1 \)

as shown in Fig. 26.

The parameter \( \text{INDX} \) is an indicator for the two periods, and if \( \text{INDX} = 2 \), 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, \( E_{MAX} \)
4) Difference between the assumed and calculated values for the variable, \( E \)
5) Initial value for \( \text{INDX} \), \( \text{INDX} = 0 \)
6) DO loop for iteration
7) A statement to get off the DO loop when \( \text{INDX} = 2 \)
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, $f$, 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),

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

$$= \frac{\frac{1}{2} \pi d_0 \Delta Z}{\frac{1}{2} (p^H \cdot P^V \Delta Z)} = \frac{\pi d_0}{p^H P^V} \quad (A.VII.16)$$
Fig. 27 Arrangement of Cooling Tubes
For the rectangular arrangement (Fig. 27),

\[ a_{HE} = \frac{\pi d_o \Delta Z}{B H P V \Delta Z} = \frac{\pi d_o}{B H P V} \quad \text{(A.VII.17)} \]

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): \[
\frac{1}{2} \frac{\pi d_o^2}{B H P V} \frac{\Delta Z}{\Delta Z} = \frac{d_o}{4} \quad a_{HE} \quad \text{(A.VII.18)}
\]

(for rectangular arrangement): \[
\frac{\pi d_o^2}{B H P V} \frac{\Delta Z}{\Delta Z} = \frac{d_o}{4} \quad a_{HE} \quad \text{(A.VII.19)}
\]

Volume fraction of tubes is then equal to

\[ \varepsilon_{\text{tube}} = 1 - \text{effective volume/total volume} \quad \text{(A.VII.20)} \]

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 SO₂ 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
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 \( U = U_{mf} \). 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. **Subprogram HEIGHT**

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. **Subprogram HYDRO**

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. $U_0$ 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, $U_0$ 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.
(ii) Expanded bed height given, fixed bed section present:

The bubble hydrodynamics is calculated for each compartment. As the height increases, \( U_0 \) 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 \( U_0 \) 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 inaccuracy 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. \textbf{Subprogram SIMQ}

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

17. \textbf{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):

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

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

\[
U_t = \frac{3.1 g (\rho_s - \rho_g) d_p}{\rho_g} \quad \text{for } 500 < R_{e,p} \quad (A.VII.24)
\]

\[
R_{e,p} = d_p \rho_g U_t / \mu \quad (A.VII.25)
\]
Subroutine SIMQ

ORIGINAL PAGE IS
OF POOR QUALITY

SUBROUTINE SIMQ(X,Y,M,K5)

DIMENSION A(M,M),X(M),Y(K5)

C FORWARD SOLUTION

C GIVE SOLUTION AT END OF FORWARD SOLUTION

C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN

C TEST FOR PIVOT LESS THAN TOLERANCE (SINGULAR MATRIX)

C SHOULD AVOID DIVISION BY SMALL PIVOT

C UNEW EQUATION OF LEADING COEFFICIENT

C ELIMINATE NEXT VARIABLE

C BACK SOLUTION

C
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**

<table>
<thead>
<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AAA</td>
<td>-</td>
<td>Matrix coefficients</td>
</tr>
<tr>
<td>AE</td>
<td>-</td>
<td>Activation energy of char-NO reduction reaction, cals/gmole</td>
</tr>
<tr>
<td>AHE</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>AHEAV</td>
<td>( a_{HE} )</td>
<td>Specific heat transfer area of the tubes, ( \text{cm}^2/\text{cm}^3 ) FBC volume</td>
</tr>
<tr>
<td>AHEN</td>
<td>( a_{HEW} )</td>
<td>Specific heat transfer area of the walls, ( \text{cm}^2/\text{cm}^3 ) FBC volume</td>
</tr>
<tr>
<td>AK</td>
<td>( k_{v1} )</td>
<td>Overall volume reaction rate constant for limestone - SO(_2) reaction, 1/sec</td>
</tr>
<tr>
<td>AKB</td>
<td>( k_{c,B} )</td>
<td>Overall rate constant for char combustion in bubble phase, cm/sec</td>
</tr>
<tr>
<td>AKBE</td>
<td>( K_{BE} )</td>
<td>Gas exchange coefficient, 1/sec</td>
</tr>
<tr>
<td>AKC</td>
<td>( k_c )</td>
<td>Overall rate constant for char combustion, 1/sec</td>
</tr>
<tr>
<td>AKCO2</td>
<td>-</td>
<td>Overall rate constant for C-CO(_2) reaction, cm/sec</td>
</tr>
<tr>
<td>AKE</td>
<td>( k_{c,E} )</td>
<td>Overall rate constant for char combustion in emulsion phase, cm/sec</td>
</tr>
<tr>
<td>AKNO</td>
<td>( k_{NO} )</td>
<td>NO reduction rate constant, cm/sec</td>
</tr>
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<td>ALFA</td>
<td>-</td>
<td>Temperature matrix coefficients</td>
</tr>
<tr>
<td>AMDF</td>
<td>( a_m )</td>
<td>Defined by Equation (VI.12)</td>
</tr>
<tr>
<td>AND</td>
<td>( n_d )</td>
<td>Number of orifices in the distributor</td>
</tr>
<tr>
<td>ANH3V</td>
<td>-</td>
<td>( \text{NH}_3) content in the volatiles, gmole ( \text{NH}_3)/gmole volatiles</td>
</tr>
<tr>
<td>ANITRO</td>
<td>-</td>
<td>Nitrogen released during char combustion, gatom/sec</td>
</tr>
<tr>
<td>AT</td>
<td>( A_t )</td>
<td>Cross sectional area of the bed, ( \text{cm}^2 )</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>ATB</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>BFB</td>
<td>Matrix coefficients</td>
<td></td>
</tr>
<tr>
<td>BFB</td>
<td>Char combustion rate in the bed, gm/sec</td>
<td></td>
</tr>
<tr>
<td>BEDVOL</td>
<td>Total bed volume, cm³</td>
<td></td>
</tr>
<tr>
<td>BETA</td>
<td>Temperature matrix coefficients</td>
<td></td>
</tr>
<tr>
<td>CADP</td>
<td>Heat capacity of feed additives, cals/gm.°C</td>
<td></td>
</tr>
<tr>
<td>CARCON</td>
<td>Carbon concentration, gm carbon/cm³ bed volume (including tubes)</td>
<td></td>
</tr>
<tr>
<td>CAS</td>
<td>Ca/S molar ratio in feed solids</td>
<td></td>
</tr>
<tr>
<td>CASE</td>
<td>Effective Ca/S molar ratio (including Ca in ash)</td>
<td></td>
</tr>
<tr>
<td>CCF</td>
<td>Heat capacity of coal feed, cals/gm.°C</td>
<td></td>
</tr>
<tr>
<td>CHAR</td>
<td>Carbon content in char, gm carbon/gm char</td>
<td></td>
</tr>
<tr>
<td>CELU</td>
<td>Char elutriated from the combustor, gms/sec</td>
<td></td>
</tr>
<tr>
<td>CGM</td>
<td>Molar heat capacity of gas, cals/gmole °C</td>
<td></td>
</tr>
<tr>
<td>CMGF</td>
<td>Molar heat capacity of feed gas, cals/gmole °C</td>
<td></td>
</tr>
<tr>
<td>CHARC</td>
<td>Carbon content in char, gmoles carbon/gm coal</td>
<td></td>
</tr>
<tr>
<td>CHARNH</td>
<td>Hydrogen content in char, gatom hydrogen/gm coal</td>
<td></td>
</tr>
<tr>
<td>CHARN</td>
<td>Nitrogen content in char, gatom nitrogen/gm coal</td>
<td></td>
</tr>
<tr>
<td>CHARO</td>
<td>Oxygen content in char, gatom oxygen/gm coal</td>
<td></td>
</tr>
<tr>
<td>CHARS</td>
<td>Sulfur content in char, gatom sulfur/gm coal</td>
<td></td>
</tr>
<tr>
<td>CH4</td>
<td>Wt. fraction CH₄ in the volatiles; CH₄ released during devolatilization, gmoles CH₄/gm coal</td>
<td></td>
</tr>
<tr>
<td>CLOSS</td>
<td>Total carbon loss (elutriated + withdrawn), gm/sec</td>
<td></td>
</tr>
<tr>
<td>CO</td>
<td>Wt. fraction CO in the volatiles; CO released during devolatilization, gmoles CO/gm coal</td>
<td></td>
</tr>
<tr>
<td>COALC</td>
<td>Carbon content in coal, gatom carbon/gm coal (d.b.)</td>
<td></td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>COALH</td>
<td>-</td>
<td>Hydrogen content in coal, gatom hydrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALN</td>
<td>-</td>
<td>Nitrogen content in coal, gatom nitrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALO</td>
<td>-</td>
<td>Oxygen content in coal, gatom oxygen/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALS</td>
<td>-</td>
<td>Sulfur content in coal, gatom sulfur/gm coal (d.b.)</td>
</tr>
<tr>
<td>COB</td>
<td>-</td>
<td>Carbon monoxide burnt in each compartment, gmole/sec</td>
</tr>
<tr>
<td>COV</td>
<td>-</td>
<td>CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles</td>
</tr>
<tr>
<td>COVB</td>
<td>-</td>
<td>CO produced during volatiles combustion, gmole CO/gmole volatiles</td>
</tr>
<tr>
<td>CO2</td>
<td>-</td>
<td>Wt. fraction CO₂ in the volatiles; CO₂ released during devolatilization, gmole CO₂/gm coal</td>
</tr>
<tr>
<td>CO2V</td>
<td>-</td>
<td>CO₂ released during devolatilization per mole of volatiles released, gmole CO₂/gmole volatiles</td>
</tr>
<tr>
<td>CO2VB</td>
<td>-</td>
<td>CO₂ produced during volatiles combustion, gmole CO₂/gmole volatiles</td>
</tr>
<tr>
<td>GS</td>
<td>Cₛ</td>
<td>Heat capacity of solids, cals/gm °C</td>
</tr>
<tr>
<td>CTAR</td>
<td>-</td>
<td>Carbon content in char, gm carbon/gm coal fed</td>
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<td>DASVF</td>
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<td>Surface volume mean particle diameter of additives in the feed, cm</td>
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<tr>
<td>DAWMF</td>
<td>-</td>
<td>Weight mean particle diameter of additives in the feed, cm</td>
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<td>Dₐ</td>
<td>Bubble diameter in each compartment, cm</td>
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<tr>
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<td>dₙ</td>
<td>Surface volume mean diameter of char particles in the freeboard, cm</td>
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<td>dₗ</td>
<td>Surface volume mean diameter of char particles in the bed, cm</td>
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<td>Surface volume mean diameter of coal particles in the feed, cm</td>
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<td>Weight mean diameter of char particles in the freeboard, cm</td>
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<td>DCWMB</td>
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<td>Weight mean diameter of char particles in the bed, cm</td>
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<td>DCWMF</td>
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<td>Weight mean diameter of coal particles in the feed, cm</td>
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<td>DELT</td>
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<td>Temperature matrix coefficients</td>
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<td>DETC</td>
<td>-</td>
<td>Increment in combustion efficiency</td>
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<tr>
<td>DETS</td>
<td>-</td>
<td>Increment in sulfur dioxide retention efficiency</td>
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<td>Diameter of orifice holes in the distributor, cm</td>
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<td>Pressure drop across the distributor, cm H₂O</td>
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<td>DPFIX</td>
<td>-</td>
<td>Pressure drop across the fixed bed section, cm H₂O</td>
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<td>DPFLU</td>
<td>-</td>
<td>Pressure drop across the fluid bed section, cm H₂O</td>
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<td>dₑₑ</td>
<td>Surface volume mean particle diameter of additives entrained in the freeboard, cm</td>
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<td>(SEE DESIGN)</td>
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<td>Volume of each compartment, cm³</td>
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<td>$D_t$</td>
<td>Diameter of the combustor, cm</td>
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<td>EETSM</td>
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<td>Tolerance limit for sulfur dioxide retention</td>
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<td></td>
<td>elutriation calculations</td>
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<td>Volume of bed (excluding tubes), cm$^3$</td>
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<td>-</td>
<td>Nitric oxide emission index, gmole NO/gm coal</td>
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<td>EMF</td>
<td>$\varepsilon_{mf}$</td>
<td>Void fraction at minimum fluidization</td>
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<td>Nitric oxide emission, mole fraction</td>
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<td>$\varepsilon_B$</td>
<td>Bubble fraction</td>
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<td>ETCG</td>
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<td>Carbon combustion efficiency based on oxygen</td>
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<td>FBCOM</td>
<td>Char combustion rate in the freeboard, gm/sec</td>
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<td>Molar flow rate of gas in the bubble phase, gmole/sec</td>
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<td>Fraction of solids withdrawn from the bed at each location</td>
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<td>Molar flow rate of gas in the emulsion phase, gmole/sec</td>
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<td>FFAD</td>
<td>Fraction of total additives fed at each location</td>
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<tr>
<td>FFC</td>
<td>Fraction of total coal fed at each location</td>
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<td>FMF</td>
<td>Molar feed rate of fluidizing air, gmole/sec</td>
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<td>FMTH</td>
<td>Stoichiometric air feed rate, gmole/sec</td>
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<td>FMO</td>
<td>Total molar flow rate of gas in the combustor, gmole/sec</td>
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<td>FR</td>
<td>Frequency factor for char-NO reaction, cm/sec</td>
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<td>Feed rate of fuel nitrogen, gatom/sec</td>
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<tr>
<td>FRS</td>
<td>Feed rate of fuel sulfur, gatom/sec</td>
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<td>Fractional conversion of limestone</td>
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<td>Solids mixing parameter, ratio of wake volume to the bubble volume including the wakes</td>
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<td>FW</td>
<td>Solids mixing parameter, ratio of wake volume to the bubble volume including the wakes</td>
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<td>Acceleration due to gravity, cm/sec</td>
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<td>Temperature matrix coefficients</td>
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<td>Volatiles burning rate in the bubble phase, gmole/sec</td>
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<tr>
<td>GE</td>
<td>Volatiles burning rate in the emulsion phase, gmole/sec</td>
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<td>( \text{SO}_2 ) or ( \text{NO}_x ) release rate in the bubble phase or in the freeboard due to volatiles combustion, gmole/sec</td>
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<td>-</td>
<td>SO\textsubscript{2} or NO\textsubscript{x} release rate in the emulsion phase or in the freeboard due to volatiles combustion, gmole/sec</td>
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<tr>
<td>GFLOW</td>
<td>G</td>
<td>Gas flow rate, gms/sec</td>
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<tr>
<td>H</td>
<td>-</td>
<td>Height above the distributor, cms</td>
</tr>
<tr>
<td>HB</td>
<td>h</td>
<td>Height above the bed surface, cms</td>
</tr>
<tr>
<td>HAREA</td>
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<td>Total heat transfer area of cooling tubes (based on outside diameter of tube), cm$^2$</td>
</tr>
<tr>
<td>HCHAR</td>
<td>-</td>
<td>Hydrogen content in char, gm hydrogen/gm char</td>
</tr>
<tr>
<td>HCOAL</td>
<td>-</td>
<td>Lower heating value of coal, cals/gm</td>
</tr>
<tr>
<td>HCR</td>
<td>-</td>
<td>Critical bed height above which there is a fixed bed section, cm</td>
</tr>
<tr>
<td>HFB</td>
<td>-</td>
<td>Freeboard height, cm</td>
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<tr>
<td>HLF</td>
<td>-</td>
<td>Expanded bed height, cm</td>
</tr>
<tr>
<td>HLMF</td>
<td>-</td>
<td>Bed height at minimum fluidization, cm</td>
</tr>
<tr>
<td>HTAR</td>
<td>-</td>
<td>Hydrogen content in tar, gm hydrogen/gm coal fed</td>
</tr>
<tr>
<td>H2</td>
<td>H\textsubscript{2}</td>
<td>Wt. fraction H\textsubscript{2} in the volatiles; H\textsubscript{2} released during devolatilization, gmole H\textsubscript{2} /gm coal</td>
</tr>
<tr>
<td>H2O</td>
<td>H\textsubscript{2}O</td>
<td>Wt. fraction H\textsubscript{2}O in the volatiles; H\textsubscript{2}O released during devolatilization, gmole H\textsubscript{2}O/gm coal</td>
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<td>IARR</td>
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<td>(SEE DESIGN)</td>
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<td>-</td>
<td>Indicator for critical bed height</td>
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<tr>
<td>IFBC</td>
<td>-</td>
<td>Indicator for fixed bed section</td>
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<td>-</td>
<td>Indicator for combustion calculations</td>
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<tr>
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<td>-</td>
<td>Indicator for NO\textsubscript{x} calculations</td>
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<td>Indicator for pressure drop calculations</td>
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<td>Indicator for ( SO_2 ) calculations</td>
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<td>Indicator for temperature calculations</td>
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<td>Number of trials made in the combustion calculations</td>
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<td>Number of compartments in freeboard</td>
</tr>
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<td>MAIR</td>
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<td>Molecular weight of air, gms/gmole</td>
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<tr>
<td>MC</td>
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<td>Atomic weight of carbon, gms/gatom</td>
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<td>Molecular weight of calcium oxide, gms/gmole</td>
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<td>MCACO3</td>
<td>-</td>
<td>Molecular weight of calcium carbonate, gms/gmole</td>
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<td>MCASO4</td>
<td>-</td>
<td>Molecular weight of calcium sulfate, gms/gmole</td>
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<td>Molecular weight of carbon monoxide, gms/gmole</td>
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<td>Molecular weight of carbon dioxide, gms/gmole</td>
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<td>No. of solids withdrawal locations</td>
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<td>No. of solids feed locations</td>
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<td>Molecular weight of combustion gases, gms/gmole</td>
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<td>Molecular weight of hydrogen, gms/gmole</td>
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<td>Molecular weight of water, gms/gmole</td>
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<td>Molecular weight of hydrogen sulfide, gms/gmole</td>
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<td>Molecular weight of magnesium carbonate, gms/gmole</td>
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<td>Molecular weight of magnesium oxide, gms/gmole</td>
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<td>Molecular weight of nitrogen, gms/gmole</td>
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<tr>
<td>MO2</td>
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<td>Molecular weight of oxygen, gms/gmole</td>
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<td>Atomic weight of sulfur, gms/atom</td>
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<td>Molecular weight of sulfur dioxide, gms/gmole</td>
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<td>Average molecular weight of tar in the volatiles, gms/gmole</td>
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<td>MTHE</td>
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<tr>
<td>M1</td>
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<td>No. of compartments in the bed + 1</td>
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<td>-</td>
<td>No. of additive particles in the freeboard</td>
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<td>-</td>
<td>Name of coal</td>
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<td>-</td>
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</tr>
<tr>
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<td>-</td>
<td>Name of limestone</td>
</tr>
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<td>-</td>
<td>No. of char particles in the freeboard</td>
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<td>NCHAR</td>
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<td>Nitrogen content in char, gm nitrogen/gm char</td>
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<td>Total number of compartments in the combustor using DZAV + 1</td>
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<td>Oxygen content in char, gm oxygen/gm char</td>
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<td>OTAR</td>
<td>-</td>
<td>Oxygen content in tar, gm oxygen/gm coal fed</td>
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<td>P</td>
<td>Average pressure in the combustor, atm</td>
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<td>Pressure of fluidizing air at the inlet to the distributor, atm</td>
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<td>$\phi_B$</td>
<td>Mechanism factor in the freeboard</td>
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<td>$\phi_E$</td>
<td>Mechanism factor in the emulsion phase</td>
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<tr>
<td>QAREA</td>
<td>Q</td>
<td>Heat transfer rate to the tubes per unit heat transfer area of tubes, cals/cm².sec</td>
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<td>QCHAR</td>
<td>Q</td>
<td>Heat of combustion of char, cals/gm</td>
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<tr>
<td>QCLCN</td>
<td>Q</td>
<td>Heat of calcination of limestone, cals/gm</td>
</tr>
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<td>QCO</td>
<td>Q</td>
<td>Heat of combustion of carbon monoxide, cals/gmole</td>
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<td>Q</td>
<td>Total heat transferred to the cooling medium, cals/sec</td>
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<td>Q</td>
<td>Heat of partial combustion of volatiles, cals/gmole</td>
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<td>QVGAS</td>
<td>Q</td>
<td>Heat of combustion of volatiles, cals/gmole</td>
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<tr>
<td>QVOL</td>
<td>Q</td>
<td>Heat transfer rate per unit volume of bed, cals/cm³</td>
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<td>R</td>
<td>R</td>
<td>Defined by Equation (V.2)</td>
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<td>RC</td>
<td>R</td>
<td>Fraction of carbon remaining in char after devolatilization, gm carbon/gm carbon in coal</td>
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<tr>
<td>RCHAR</td>
<td>Rch</td>
<td>Char produced per unit gm of coal fed, gm/gm</td>
</tr>
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<td>RELB</td>
<td>R</td>
<td>Total release rate of SO₂ or NOₓ in the bubble phase, gmole/sec</td>
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<td>RELE</td>
<td>R</td>
<td>Total release rate of SO₂ or NOₓ in the emulsion phase, gmole/sec</td>
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<td>Gas constant, 82.06 atm.cm³/gmole.°K</td>
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<td>RH</td>
<td>R</td>
<td>Fraction of hydrogen remaining in char after devolatilization, gm hydrogen/gm hydrogen in coal</td>
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<td>Density of additives, gms/cm³</td>
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<tr>
<td>RHOASH</td>
<td></td>
<td>Density of ash, gms/cm³</td>
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<td>RHOBE D</td>
<td>ρ_b</td>
<td>Density of the bed materials, gms/cm³</td>
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<td>RHOC</td>
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<td>Density of coal, gms/cm³</td>
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<td>Mathematical Symbol</td>
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<td>RHOCH</td>
<td>$\rho_{\text{ch}}$</td>
<td>Density of char, gms/cm$^3$</td>
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<td>RHOGAS</td>
<td>$\rho_{g}$</td>
<td>Density of gas, gms/cm$^3$</td>
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<td>Density of the fluidizing air at the inlet to the distributor, gms/cm$^3$</td>
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<td>-</td>
<td>Fraction of nitrogen remaining in char after devolatilization, gm nitrogen/gm nitrogen in coal</td>
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<tr>
<td>RO</td>
<td>-</td>
<td>Fraction of oxygen remaining in char after devolatilization, gm oxygen/gm oxygen in coal</td>
</tr>
<tr>
<td>RR</td>
<td>-</td>
<td>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</td>
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<tr>
<td>RRB</td>
<td>-</td>
<td>Rate of combustion of char in the bubble phase, gms/sec</td>
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<tr>
<td>RRE</td>
<td>-</td>
<td>Rate of combustion of char in the emulsion phase, gms/sec</td>
</tr>
<tr>
<td>RS</td>
<td>-</td>
<td>Fraction of sulfur remaining in char after devolatilization, gm sulfur/gm sulfur in coal</td>
</tr>
<tr>
<td>RVGAS</td>
<td>-</td>
<td>Volatiles released during devolatilization per unit gm of coal, gmole volatiles/gm coal</td>
</tr>
<tr>
<td>SCHAR</td>
<td>-</td>
<td>Sulfur content in char, gm sulfur/gm char</td>
</tr>
<tr>
<td>SOLVOL</td>
<td>-</td>
<td>Volume of solids in the bed (including voids) which is equal to volume of bed at minimum fluidization (excluding the internals), cm$^3$</td>
</tr>
<tr>
<td>SULFUR</td>
<td>-</td>
<td>Sulfur released during char combustion, gatm/sec</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>Temperature, °K</td>
</tr>
<tr>
<td>TAR</td>
<td>Tar</td>
<td>Wt. fraction tar in the volatiles; tar released during devolatilization per unit gm of coal, gmole tar/gm coal</td>
</tr>
<tr>
<td>TARC</td>
<td>-</td>
<td>Stoichiometric air required per unit gm of char, gmole/gm char</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>TAV</td>
<td>-</td>
<td>Mean bed temperature, °K</td>
</tr>
<tr>
<td>TAVB</td>
<td>$T_B$</td>
<td>Mean temperature in the boundary layer of the char particles in the bubble phase, °K; also in the freeboard, °K</td>
</tr>
<tr>
<td>TAVE</td>
<td>$T_E$</td>
<td>Mean temperature in the boundary layer of the char particles in the emulsion phase, °K</td>
</tr>
<tr>
<td>TCRATE</td>
<td>-</td>
<td>Total char combustion rate, gm/sec</td>
</tr>
<tr>
<td>TETUBE</td>
<td>-</td>
<td>Total volume fraction of tubes in the bed</td>
</tr>
<tr>
<td>TF</td>
<td>-</td>
<td>Temperature of fluidizing air at the inlet to the distributor, °K</td>
</tr>
<tr>
<td>TFC</td>
<td>-</td>
<td>Total char feed rate, gms/sec</td>
</tr>
<tr>
<td>TNORM</td>
<td>-</td>
<td>Temperature criterion for convergency</td>
</tr>
<tr>
<td>TOLD</td>
<td>-</td>
<td>Bed temperature in the previous iteration, °K</td>
</tr>
<tr>
<td>TPB</td>
<td>-</td>
<td>Char particle temperature in the bubble phase, °K; also in the freeboard, °K</td>
</tr>
<tr>
<td>TPE</td>
<td>-</td>
<td>Char particle temperature in the emulsion phase, °K</td>
</tr>
<tr>
<td>TSF</td>
<td>-</td>
<td>Temperature of feed solids, °K</td>
</tr>
<tr>
<td>TSTA</td>
<td>-</td>
<td>Starting temperature (assumed) for iteration, °K</td>
</tr>
<tr>
<td>TW</td>
<td>-</td>
<td>Cooling water temperature, °K</td>
</tr>
<tr>
<td>TWALL</td>
<td>-</td>
<td>Wall temperature, °K</td>
</tr>
<tr>
<td>TWALLA</td>
<td>-</td>
<td>Average wall temperature used for heat losses, °K</td>
</tr>
<tr>
<td>TWAV</td>
<td>-</td>
<td>Log mean temperature of the cooling water</td>
</tr>
<tr>
<td>TWIN</td>
<td>-</td>
<td>Inlet water temperature, °K</td>
</tr>
<tr>
<td>TWOUT</td>
<td>-</td>
<td>Outlet water temperature, °K</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<td>----------------</td>
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<td>-------------</td>
</tr>
<tr>
<td>UB</td>
<td>U_B</td>
<td>Bubble velocity, cm/sec</td>
</tr>
<tr>
<td>UHE</td>
<td>U</td>
<td>Bed to tube heat transfer coefficient, cals/sec.cm^2°C</td>
</tr>
<tr>
<td>UHEAV1</td>
<td>-</td>
<td>Bed to tube heat transfer coefficient (average) within the bed, cals/sec.cm^2°C</td>
</tr>
<tr>
<td>UHEAV2</td>
<td>-</td>
<td>Bed to tube heat transfer coefficient (average) in the freeboard, cals/sec.cm^2°C</td>
</tr>
<tr>
<td>UHEW</td>
<td>U_W</td>
<td>Bed to wall heat transfer coefficient, cals/sec.cm^2°C</td>
</tr>
<tr>
<td>UMF</td>
<td>U_{mf}</td>
<td>Minimum fluidization velocity, cm/sec</td>
</tr>
<tr>
<td>UO</td>
<td>U_O</td>
<td>Superficial gas velocity as a function of bed height, cm/sec</td>
</tr>
<tr>
<td>UOR</td>
<td>-</td>
<td>Orifice velocity, cm/sec</td>
</tr>
<tr>
<td>UT</td>
<td>U_t</td>
<td>Terminal velocity of the particle, cm/sec</td>
</tr>
<tr>
<td>UWALL1</td>
<td>-</td>
<td>Bed to wall heat transfer coefficient (average) within the bed, cals/sec cm^2°C</td>
</tr>
<tr>
<td>UWALL2</td>
<td>-</td>
<td>Bed to wall heat transfer coefficient (average) in the freeboard, cals/sec cm^2°C</td>
</tr>
<tr>
<td>UO</td>
<td>-</td>
<td>Superficial gas velocity at the distributor, cm/sec</td>
</tr>
<tr>
<td>V</td>
<td>-</td>
<td>Volatiles yield during devolatilization, gms volatiles/gm coal (daf); also gms volatiles/gm coal</td>
</tr>
<tr>
<td>VAHOLD</td>
<td>-</td>
<td>Volumetric additives holdup in the freeboard; cm^3 solid volume</td>
</tr>
<tr>
<td>VCHOLD</td>
<td>-</td>
<td>Volumetric char hold-up in the freeboard, cm^3 solid volume</td>
</tr>
<tr>
<td>VGASN</td>
<td>-</td>
<td>Volatile nitrogen in coal, gatom/gm coal (d.b.)</td>
</tr>
<tr>
<td>VGASS</td>
<td>-</td>
<td>Volatile sulfur in coal, gatom/gm coal (d.b.)</td>
</tr>
<tr>
<td>VISC</td>
<td>( \mu )</td>
<td>Viscosity of gas, gm/cm·sec</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>--------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>VM</td>
<td></td>
<td>Proximate volatile matter in coal, gm/gm coal (daf)</td>
</tr>
<tr>
<td>VMF</td>
<td></td>
<td>Bed volume at minimum fluidization (excluding the internals), cm³</td>
</tr>
<tr>
<td>VPROD</td>
<td></td>
<td>Volatiles released in each compartment, gmole/sec</td>
</tr>
<tr>
<td>WAD</td>
<td>$W_{f,a}$</td>
<td>Additives feed rate, gms/sec</td>
</tr>
<tr>
<td>WAHOLD</td>
<td></td>
<td>Additives hold-up in the freeboard, gms</td>
</tr>
<tr>
<td>WB</td>
<td>$M_b$</td>
<td>Weight of bed materials, gms</td>
</tr>
<tr>
<td>WCHOLD</td>
<td></td>
<td>Char hold-up in the freeboard, gms</td>
</tr>
<tr>
<td>WCOAL</td>
<td></td>
<td>Coal feed rate as received basis, gms/sec</td>
</tr>
<tr>
<td>WD</td>
<td></td>
<td>Solids withdrawal rate at each location, gms/sec</td>
</tr>
<tr>
<td>WDIS</td>
<td>$W_D$</td>
<td>Solids withdrawal rate, gms/sec</td>
</tr>
<tr>
<td>WEA</td>
<td></td>
<td>Additives entrainment rate in the freeboard, gms/sec</td>
</tr>
<tr>
<td>WEC</td>
<td></td>
<td>Char entrainment rate in the freeboard, gms/sec</td>
</tr>
<tr>
<td>WELUA</td>
<td></td>
<td>Solids (excluding char) elutriation rate from the combustor, gms/sec</td>
</tr>
<tr>
<td>WFAD</td>
<td>$W_{f,a}$</td>
<td>Additives feed rate in each compartment, gms/sec</td>
</tr>
<tr>
<td>WFC</td>
<td>$W_{f,c}$</td>
<td>Coal feed rate in each compartment, gms/sec</td>
</tr>
<tr>
<td>WMIX</td>
<td>$W_{mix}$</td>
<td>Solids mixing rate, gms/sec</td>
</tr>
<tr>
<td>WNET</td>
<td>$W_{net}$</td>
<td>Net flow rate of solids, gms/sec</td>
</tr>
<tr>
<td>WW</td>
<td>B</td>
<td>Defined by Equation (V.3)</td>
</tr>
<tr>
<td>X</td>
<td>X</td>
<td>Weight fraction carbon in the bed</td>
</tr>
<tr>
<td>XA</td>
<td></td>
<td>Ash content in coal as received basis, gm ash/gm coal</td>
</tr>
<tr>
<td>XACAO</td>
<td></td>
<td>Calcium oxide content in ash, gm CaO/gm ash</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
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</tr>
<tr>
<td>XAV</td>
<td>-</td>
<td>Average weight fraction of carbon in the bed</td>
</tr>
<tr>
<td>XC</td>
<td>-</td>
<td>Carbon content in coal, gm carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>XCAO</td>
<td>-</td>
<td>Calcium oxide content in limestone, gm CaO/gm limestone</td>
</tr>
<tr>
<td>XCF</td>
<td>-</td>
<td>Fixed carbon content in coal, gm carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>XCO2</td>
<td>-</td>
<td>Carbon dioxide content in limestone, gm CO₂/gm limestone</td>
</tr>
<tr>
<td>XCV</td>
<td>-</td>
<td>Volatile carbon content in coal, gm carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>XH</td>
<td>-</td>
<td>Hydrogen content in coal, gm hydrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>XMGO</td>
<td>-</td>
<td>Magnesium oxide content in limestone, gm MgO/gm limestone</td>
</tr>
<tr>
<td>XN</td>
<td>-</td>
<td>Nitrogen content in coal, gm nitrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>X0</td>
<td>-</td>
<td>Oxygen content in coal, gm oxygen/gm coal (d.b.)</td>
</tr>
<tr>
<td>X02</td>
<td>X₀₂</td>
<td>Oxygen required for partial combustion of volatiles, gmole O₂/gmole volatile</td>
</tr>
<tr>
<td>X02C</td>
<td>X₀₂,c</td>
<td>Oxygen required for complete combustion of volatiles, gmole O₂/gmole volatile</td>
</tr>
<tr>
<td>XS</td>
<td>-</td>
<td>Sulfur content in coal, gm sulfur/gm coal (d.b.)</td>
</tr>
<tr>
<td>XSiO2</td>
<td>-</td>
<td>Silicon dioxide content in limestone, gm SiO₂/gm limestone</td>
</tr>
<tr>
<td>XW</td>
<td>-</td>
<td>Moisture content in coal as received basis, gm H₂O/gm coal</td>
</tr>
<tr>
<td>YAV</td>
<td>-</td>
<td>Average O₂ concentration (assumed) for iteration, mole fraction</td>
</tr>
<tr>
<td>YB</td>
<td>-</td>
<td>Mole fraction O₂ or SO₂ or NO in the bubble phase</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>YBO</td>
<td>Y_B</td>
<td>Mole fraction O₂ in the bubble phase</td>
</tr>
<tr>
<td>YCO</td>
<td>Y_CO</td>
<td>Mole fraction CO</td>
</tr>
<tr>
<td>YCOE</td>
<td>Y_E,CO</td>
<td>Mole fraction CO in the emulsion phase</td>
</tr>
<tr>
<td>YCO2</td>
<td>Y_CO₂</td>
<td>Mole fraction CO₂</td>
</tr>
<tr>
<td>YCO2B</td>
<td>Y_B,CO₂</td>
<td>Mole fraction CO₂ in the bubble phase</td>
</tr>
<tr>
<td>YCO2E</td>
<td>Y_E,CO₂</td>
<td>Mole fraction CO₂ in the emulsion phase</td>
</tr>
<tr>
<td>YE</td>
<td>-</td>
<td>Mole fraction O₂ or SO₂ or NO in the emulsion phase</td>
</tr>
<tr>
<td>YEO</td>
<td>Y_E</td>
<td>Mole fraction O₂ in the emulsion phase</td>
</tr>
<tr>
<td>YGO</td>
<td>-</td>
<td>Gaseous species concentrations at the exit, mole fraction</td>
</tr>
<tr>
<td>YH20</td>
<td>Y_H₂O</td>
<td>Mole fraction H₂O</td>
</tr>
<tr>
<td>YNOX</td>
<td>Y_NO</td>
<td>Mole fraction NO</td>
</tr>
<tr>
<td>YO</td>
<td>Y_O</td>
<td>Mole fraction O₂</td>
</tr>
<tr>
<td>YSO2</td>
<td>Y_SO₂</td>
<td>Mole fraction SO₂</td>
</tr>
<tr>
<td>YV</td>
<td>Y_V</td>
<td>Mole fraction volatiles</td>
</tr>
<tr>
<td>YVE</td>
<td>Y_E,V</td>
<td>Mole fraction volatiles in the emulsion phase</td>
</tr>
<tr>
<td>ZAVG</td>
<td>-</td>
<td>Average height of each compartment above the distributor, cm</td>
</tr>
<tr>
<td>ZB</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>ZF</td>
<td>-</td>
<td>Locations of solids feed ports, cms</td>
</tr>
<tr>
<td>ZHE</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>ZDIS</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<td>----------------</td>
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<td>-------------</td>
</tr>
<tr>
<td>AHE</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>ATB</td>
<td>$A_t$</td>
<td>Cross sectional area of the bed, cm$^2$</td>
</tr>
<tr>
<td>CAS</td>
<td></td>
<td>Ca/S molar ratio in feed solids</td>
</tr>
<tr>
<td>CCHAR</td>
<td>$C_{ch}$</td>
<td>Carbon content in char, gm carbon/gm char</td>
</tr>
<tr>
<td>CELU</td>
<td></td>
<td>Char elutriated from the combustor, gms/sec</td>
</tr>
<tr>
<td>CHARC</td>
<td></td>
<td>Carbon content in char, gmole carbon/gm coal</td>
</tr>
<tr>
<td>CHARN</td>
<td></td>
<td>Hydrogen content in char, gatom hydrogen/gm coal</td>
</tr>
<tr>
<td>CHARO</td>
<td></td>
<td>Nitrogen content in char, gatom nitrogen/gm coal</td>
</tr>
<tr>
<td>CHARS</td>
<td></td>
<td>Oxygen content in char, gatom oxygen/gm coal</td>
</tr>
<tr>
<td>CH4</td>
<td>$CH_4$</td>
<td>Wt. fraction $CH_4$ in the volatiles; $CH_4$ released during devolatilization, gmole $CH_4$/gm coal</td>
</tr>
<tr>
<td>CO</td>
<td>$CO$</td>
<td>Wt. fraction CO in the volatiles; CO released during devolatilization, gmole CO/gm coal</td>
</tr>
<tr>
<td>COALC</td>
<td></td>
<td>Carbon content in coal, gatom carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALH</td>
<td></td>
<td>Hydrogen content in coal, gatom hydrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALN</td>
<td></td>
<td>Nitrogen content in coal, gatom nitrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALO</td>
<td></td>
<td>Oxygen content in coal, gatom oxygen/gm coal (d.b.)</td>
</tr>
<tr>
<td>COALS</td>
<td></td>
<td>Sulfur content in coal, gatom sulfur/gm coal (d.b.)</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<td>----------------</td>
<td>---------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>COV</td>
<td>-</td>
<td>CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles</td>
</tr>
<tr>
<td>COVB</td>
<td>-</td>
<td>CO produced during volatiles combustion, gmole CO/gmole volatiles</td>
</tr>
<tr>
<td>CO₂</td>
<td>-</td>
<td>Wt. fraction CO₂ in the volatiles; CO₂ released during devolatilization, gmole CO₂/gm coal</td>
</tr>
<tr>
<td>CO₂V</td>
<td>-</td>
<td>CO₂ released during devolatilization per mole of volatiles released, gmole CO₂/gmole volatiles</td>
</tr>
<tr>
<td>CO₂VB</td>
<td>-</td>
<td>CO₂ produced during volatiles combustion, gmole CO₂/gmole volatiles</td>
</tr>
<tr>
<td>CTAR</td>
<td>-</td>
<td>Carbon content in tar, gm carbon/gm coal fed</td>
</tr>
<tr>
<td>DASVF</td>
<td>-</td>
<td>Surface volume mean particle diameter of additives in the feed, cm</td>
</tr>
<tr>
<td>DAWMF</td>
<td>-</td>
<td>Weight mean particle diameter of additives in the feed, cm</td>
</tr>
<tr>
<td>DCSE</td>
<td>d&lt;sub&gt;ce&lt;/sub&gt;</td>
<td>Surface volume mean diameter of char particles in the freeboard, cm</td>
</tr>
<tr>
<td>DCSVB</td>
<td>d&lt;sub&gt;c&lt;/sub&gt;</td>
<td>Surface volume mean diameter of char particles in the bed, cm</td>
</tr>
<tr>
<td>DCSVF</td>
<td>-</td>
<td>Surface volume mean diameter of coal particles in the feed, cm</td>
</tr>
<tr>
<td>DCWE</td>
<td>-</td>
<td>Weight mean diameter of char particles in the freeboard, cm</td>
</tr>
<tr>
<td>DCWMB</td>
<td>-</td>
<td>Weight mean diameter of char particles in the bed, cm</td>
</tr>
<tr>
<td>DCWMF</td>
<td>-</td>
<td>Weight mean diameter of coal particles in the feed, cm</td>
</tr>
<tr>
<td>DIA(I)</td>
<td>-</td>
<td>Feed particle diameter of ith fraction based on sieving screen size</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
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</tr>
<tr>
<td>DP</td>
<td>( d_x )</td>
<td>Mean diameter of the particles of ( x ) th size fraction, cm</td>
</tr>
<tr>
<td>DPSE</td>
<td>( d_{le} )</td>
<td>Surface volume mean particle diameter of additives entrained in the freeboard, cm</td>
</tr>
<tr>
<td>DPSVB</td>
<td>( d_L )</td>
<td>Surface volume mean particle diameter of additives in the bed, cm</td>
</tr>
<tr>
<td>DPWE</td>
<td>-</td>
<td>Weight mean particle diameter of additives entrained in the freeboard, cm</td>
</tr>
<tr>
<td>DPWMB</td>
<td>-</td>
<td>Weight mean particle diameter of additives in the bed, cm</td>
</tr>
<tr>
<td>DTUBE</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>EMF</td>
<td>( \varepsilon_{mf} )</td>
<td>Void fraction at minimum fluidization</td>
</tr>
<tr>
<td>EXAIR</td>
<td>-</td>
<td>Excess air, fraction</td>
</tr>
<tr>
<td>FMF</td>
<td>-</td>
<td>Molar feed rate of fluidizing air, gmole/sec</td>
</tr>
<tr>
<td>FMO</td>
<td>( F_{MT} )</td>
<td>Total molar flow rate of gas in the combustor, gmole/sec</td>
</tr>
<tr>
<td>FMTH</td>
<td>-</td>
<td>Stoichiometric air feed rate, gmole/sec</td>
</tr>
<tr>
<td>FRACTA</td>
<td>-</td>
<td>Weight fraction of additives feed of ( x ) th size fraction</td>
</tr>
<tr>
<td>FRACTC</td>
<td>-</td>
<td>Weight fraction of coal feed of ( x ) th size fraction</td>
</tr>
<tr>
<td>G</td>
<td>( g )</td>
<td>Acceleration due to gravity, ( \text{cm/sec}^2 )</td>
</tr>
<tr>
<td>GFLOW</td>
<td>G</td>
<td>Gas flow rate, gms/sec</td>
</tr>
<tr>
<td>HCHAR</td>
<td>-</td>
<td>Hydrogen content in char, gm hydrogen/gm char</td>
</tr>
<tr>
<td>HFB</td>
<td>-</td>
<td>Freeboard height, cm</td>
</tr>
<tr>
<td>HLF</td>
<td>-</td>
<td>Expanded bed height, cm</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
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<tr>
<td>HLMF</td>
<td>-</td>
<td>Bed height at minimum fluidization, cm</td>
</tr>
<tr>
<td>HTAR</td>
<td>-</td>
<td>Hydrogen content in tar, gm hydrogen/gm coal fed</td>
</tr>
<tr>
<td>H$_2$</td>
<td>H$_2$</td>
<td>Wt. fraction H$_2$ in the volatiles; H$_2$ released during devolatilization gmoles H$_2$/gm coal</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>H$_2$O</td>
<td>Wt. fraction H$_2$O in the volatiles; H$_2$O released during devolatilization gmoles H$_2$O/gm coal</td>
</tr>
<tr>
<td>IARR</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>MAIR</td>
<td>-</td>
<td>Molecular weight of air, gms/gmole</td>
</tr>
<tr>
<td>MC</td>
<td>-</td>
<td>Atomic weight of carbon, gms/gatom</td>
</tr>
<tr>
<td>MCAO</td>
<td>-</td>
<td>Molecular weight of calcium oxide, gms/gmole</td>
</tr>
<tr>
<td>MCASO$_4$</td>
<td>-</td>
<td>Molecular weight of calcium sulfate, gms/gmole</td>
</tr>
<tr>
<td>MCO</td>
<td>-</td>
<td>Molecular weight of carbon monoxide, gms/gmole</td>
</tr>
<tr>
<td>MCO$_2$</td>
<td>-</td>
<td>Molecular weight of carbon dioxide, gms/gmole</td>
</tr>
<tr>
<td>MGAS</td>
<td>-</td>
<td>Molecular weight of combustion gases, gms/gmole</td>
</tr>
<tr>
<td>MH$_2$</td>
<td>-</td>
<td>Molecular weight of hydrogen, gms/gmole</td>
</tr>
<tr>
<td>MH$_2$O</td>
<td>-</td>
<td>Molecular weight of water, gms/gmole</td>
</tr>
<tr>
<td>MH$_2$S</td>
<td>-</td>
<td>Molecular weight of hydrogen sulfide, gms/gmole</td>
</tr>
<tr>
<td>MNO</td>
<td>-</td>
<td>Molecular weight of nitric oxide, gms/gmole</td>
</tr>
<tr>
<td>MN$_2$</td>
<td>-</td>
<td>Molecular weight of nitrogen, gms/gmole</td>
</tr>
<tr>
<td>MO$_2$</td>
<td>-</td>
<td>Molecular weight of oxygen, gms/gmole</td>
</tr>
<tr>
<td>MS</td>
<td>-</td>
<td>Atomic weight of sulfur, gms/gatom</td>
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<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>---------------</td>
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</tr>
<tr>
<td>MSO2</td>
<td>-</td>
<td>Molecular weight of sulfur dioxide, gms/gmole</td>
</tr>
<tr>
<td>MTAR</td>
<td>-</td>
<td>Average molecular weight of tar in the volatiles, gms/gmole</td>
</tr>
<tr>
<td>MTB MTHE</td>
<td>(SEE DESIGN)</td>
<td>-</td>
</tr>
<tr>
<td>NCHAR</td>
<td>-</td>
<td>Nitrogen content in char, gm nitrogen/gm char</td>
</tr>
<tr>
<td>NDP</td>
<td>-</td>
<td>Number of size fractions</td>
</tr>
<tr>
<td>OCHAR</td>
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<td>Oxygen content in char, gm oxygen/gm char</td>
</tr>
<tr>
<td>OTAR</td>
<td>-</td>
<td>Oxygen content in tar, gm oxygen/gm coal fed</td>
</tr>
<tr>
<td>PAV</td>
<td>P</td>
<td>Average pressure in the combustor, atm</td>
</tr>
<tr>
<td>PH</td>
<td>(SEE DESIGN)</td>
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<td>PI</td>
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<td>PV</td>
<td>(SEE DESIGN)</td>
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<td>R</td>
<td>A</td>
<td>Defined by Equation (V.2)</td>
</tr>
<tr>
<td>RC</td>
<td>-</td>
<td>Fraction of carbon remaining in char after devolatilization, gm carbon/gm carbon in coal</td>
</tr>
<tr>
<td>RCHAR</td>
<td>$R_{\text{ch}}$</td>
<td>Char produced per unit gm of coal fed, gm/gm</td>
</tr>
<tr>
<td>RG</td>
<td>$R_g$</td>
<td>Gas constant, 82.06 atm·cm$^3$/g mole·°K</td>
</tr>
<tr>
<td>RH</td>
<td>-</td>
<td>Fraction of hydrogen remaining in char after devolatilization, gm hydrogen/gm hydrogen in coal</td>
</tr>
<tr>
<td>RHOAD</td>
<td>-</td>
<td>Density of additives, gms/cm$^3$</td>
</tr>
<tr>
<td>RHOASH</td>
<td>-</td>
<td>Density of ash, gms/cm$^3$</td>
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<tr>
<td>RHOBED</td>
<td>$\rho_b$</td>
<td>Density of the bed materials, gms/cm$^3$</td>
</tr>
<tr>
<td>RHOC</td>
<td>-</td>
<td>Density of coal, gms/cm$^3$</td>
</tr>
<tr>
<td>RHOCH</td>
<td>$\rho_{\text{ch}}$</td>
<td>Density of char, gms/cm$^3$</td>
</tr>
<tr>
<td>RN</td>
<td>-</td>
<td>Fraction of nitrogen remaining in char after devolatilization, gm nitrogen/gm nitrogen in coal</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<tr>
<td>RO</td>
<td>-</td>
<td>Fraction of oxygen remaining in char after devolatilization, gm oxygen/gm oxygen in coal</td>
</tr>
<tr>
<td>RS</td>
<td>-</td>
<td>Fraction of sulfur remaining in char after devolatilization, gm sulfur/gm sulfur in coal</td>
</tr>
<tr>
<td>RVGAS</td>
<td>-</td>
<td>Volatiles released during devolatilization per unit gm of coal, gmoles volatiles/gm coal</td>
</tr>
<tr>
<td>SCHAR</td>
<td>-</td>
<td>Sulfur content in char, gm sulfur/gm char</td>
</tr>
<tr>
<td>TAR</td>
<td>Tar</td>
<td>Wt. fraction tar in the volatiles; tar released during devolatilization per unit gm of coal, gmoles tar/gm coal</td>
</tr>
<tr>
<td>TAV</td>
<td>-</td>
<td>Mean bed temperature, °K</td>
</tr>
<tr>
<td>TDHC</td>
<td>TDH</td>
<td>Transport disengaging height, cms</td>
</tr>
<tr>
<td>UO</td>
<td>$U_o$</td>
<td>Superficial gas velocity as a function of bed height, cms/sec</td>
</tr>
<tr>
<td>V</td>
<td>-</td>
<td>Volatiles yield during devolatilization, gms volatiles/gm coal (daf); also, gms volatiles/gm coal</td>
</tr>
<tr>
<td>VM</td>
<td>-</td>
<td>Proximate volatile matter in coal, gm/gm coal (daf)</td>
</tr>
<tr>
<td>VMF</td>
<td>0</td>
<td>Bed volume at minimum fluidization (excluding the internals), cm$^3$</td>
</tr>
<tr>
<td>WAD</td>
<td>$W_{f,a}$</td>
<td>Additives feed rate, gms/sec</td>
</tr>
<tr>
<td>WB</td>
<td>$M_b$</td>
<td>Weight of bed materials, gms</td>
</tr>
<tr>
<td>WBC</td>
<td>-</td>
<td>Weight of bed materials calculated, gms</td>
</tr>
<tr>
<td>WCOAL</td>
<td>$W_{f,c}$</td>
<td>Coal feed rate as received basis, gms/sec</td>
</tr>
<tr>
<td>WDIS</td>
<td>$W_D$</td>
<td>Solids withdrawal rate, gms/sec</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>WELUA</td>
<td>-</td>
<td>Solids (excluding char) elutriation rate, gms/sec</td>
</tr>
<tr>
<td>WW</td>
<td>B</td>
<td>Defined by Equation (V.3)</td>
</tr>
<tr>
<td>XA</td>
<td>-</td>
<td>Ash content in coal, gm ash/gm coal</td>
</tr>
<tr>
<td>XC</td>
<td>-</td>
<td>Carbon content in coal, gm carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>XCAO</td>
<td>-</td>
<td>Calcium oxide content in limestone, gm CaO/gm limestone</td>
</tr>
<tr>
<td>XCF</td>
<td>-</td>
<td>Fixed carbon content in coal, gm carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>XCO2</td>
<td>-</td>
<td>Carbon dioxide content in limestone, gm CO$_2$/gm limestone</td>
</tr>
<tr>
<td>XCV</td>
<td>-</td>
<td>Volatile carbon content in coal, gm carbon/gm coal (d.b.)</td>
</tr>
<tr>
<td>XH</td>
<td>-</td>
<td>Hydrogen content in coal, gm hydrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>XMGO</td>
<td>-</td>
<td>Magnesium oxide content in limestone, gm MgO/gm limestone</td>
</tr>
<tr>
<td>XN</td>
<td>-</td>
<td>Nitrogen content in coal, gm nitrogen/gm coal (d.b.)</td>
</tr>
<tr>
<td>XO</td>
<td>-</td>
<td>Oxygen content in coal, gm oxygen/gm coal (d.b.)</td>
</tr>
<tr>
<td>XS</td>
<td>-</td>
<td>Sulfur content in coal, gm sulfur/gm coal (d.b.)</td>
</tr>
<tr>
<td>XS102</td>
<td>-</td>
<td>Silicon dioxide content in limestone, gm SiO$_2$/gm limestone</td>
</tr>
<tr>
<td>XW</td>
<td>-</td>
<td>Moisture content in coal as received basis, gm H$_2$O/gm coal</td>
</tr>
<tr>
<td>ZB</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>ZHE</td>
<td>(SEE DESIGN)</td>
<td></td>
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### SUBPROGRAM AKAD

<table>
<thead>
<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALIME</td>
<td>( \lambda_l )</td>
<td>Reactivity of lime</td>
</tr>
<tr>
<td>AKAD</td>
<td>( k_{vl} )</td>
<td>Overall volume reaction rate constant for limestone SO(_2) reaction, (1/\text{sec})</td>
</tr>
<tr>
<td>DP</td>
<td>( d_p )</td>
<td>Particle diameter, cm</td>
</tr>
<tr>
<td>DP1</td>
<td>-</td>
<td>Specified particle diameter for which the limestone reactivity is given, cm</td>
</tr>
<tr>
<td>DP2</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>DP3</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>FS</td>
<td>( f_l )</td>
<td>Fractional conversion of limestone</td>
</tr>
<tr>
<td>FB</td>
<td>-</td>
<td>Limestone reactivity (given)</td>
</tr>
<tr>
<td>RR</td>
<td>-</td>
<td>Mean reactivity of limestone particles of size, DP1</td>
</tr>
<tr>
<td>RB</td>
<td>-</td>
<td>Mean reactivity of limestone particles of size, DP2</td>
</tr>
<tr>
<td>RC</td>
<td>-</td>
<td>Mean reactivity of limestone particles of size, DP3</td>
</tr>
<tr>
<td>SG</td>
<td>( S_g )</td>
<td>Effective specific surface area of limestone, (\text{cm}^2/\text{gm})</td>
</tr>
<tr>
<td>T</td>
<td>( T )</td>
<td>Temperature in the bed, °K</td>
</tr>
</tbody>
</table>

### SUBPROGRAM AKK

<p>| AKCO2          | -                   | Overall rate constant for C-CO(<em>2) reaction, (\text{cm/sec}) |
| AKF            | ( k</em>{cf} )        | Gas film diffusion rate constant for (O_2), (\text{gm/cm}^2\cdot\text{sec} \cdot \text{atm}) |
| AKFCO2         | -                   | Gas film diffusion rate constant for (CO_2), (\text{gm/cm}^2\cdot\text{sec} \cdot \text{atm}) |</p>
<table>
<thead>
<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AKRC02</td>
<td>$k_{CO_2}$</td>
<td>C-CO$_2$ chemical reaction rate constant, cm/sec</td>
</tr>
<tr>
<td>AKR</td>
<td>$k_c$</td>
<td>Overall rate constant for char combustion, cm/sec</td>
</tr>
<tr>
<td>AKS</td>
<td>$k_{cR}$</td>
<td>Chemical reaction rate constant for char combustion, cm/sec</td>
</tr>
<tr>
<td>COND</td>
<td>$\lambda$</td>
<td>Thermal conductivity of the gas, cals/sec.cm°C</td>
</tr>
<tr>
<td>D</td>
<td>$D$</td>
<td>Molecular diffusivity for O$_2$-N$_2$, cm$^2$/sec; for CO$_2$-N$_2$, cm$^2$/sec</td>
</tr>
<tr>
<td>DC</td>
<td>$-$</td>
<td>Diameter of char particle, cm</td>
</tr>
<tr>
<td>DTS</td>
<td>$-$</td>
<td>Increment in temperature, °K</td>
</tr>
<tr>
<td>EM</td>
<td>$\varepsilon_m$</td>
<td>Emissivity of the char particle</td>
</tr>
<tr>
<td>ETS</td>
<td>$-$</td>
<td>Difference between assumed and calculated temperatures, °K</td>
</tr>
<tr>
<td>ETSMAX</td>
<td>$-$</td>
<td>Tolerance limit for temperature convergency, °K</td>
</tr>
<tr>
<td>MC</td>
<td>$-$</td>
<td>Atomic weight of carbon, gms/gatom</td>
</tr>
<tr>
<td>P</td>
<td>$-$</td>
<td>Pressure in the combustor, atm</td>
</tr>
<tr>
<td>PHI</td>
<td>$\phi$</td>
<td>Mechanism factor for char combustion</td>
</tr>
<tr>
<td>Q</td>
<td>$-$</td>
<td>Heat of combustion of char, cals/gm char</td>
</tr>
<tr>
<td>RG</td>
<td>$R_g$</td>
<td>Gas constant, 82.06 atm. cm$^3$/gmole.°K</td>
</tr>
<tr>
<td>SIGM</td>
<td>$\sigma$</td>
<td>Stefan-Boltzman constant, cal/s.cm$^2$.°K$^4$</td>
</tr>
<tr>
<td>T</td>
<td>$T$</td>
<td>Temperature in the bed, °K</td>
</tr>
<tr>
<td>TAV</td>
<td>$T_m$</td>
<td>Mean temperature in the boundary layer of the particle, °K</td>
</tr>
<tr>
<td>TP</td>
<td>$T_c$</td>
<td>Char particle temperature, °K</td>
</tr>
<tr>
<td>YO2</td>
<td>$-$</td>
<td>Mole fraction oxygen</td>
</tr>
<tr>
<td>Z</td>
<td>$p$</td>
<td>Defined by Equation (V.16)</td>
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### SUBPROGRAM AREA

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<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATB</td>
<td>-</td>
<td>Bed cross sectional area at height $Z_B$ above the distributor, cm$^2$</td>
</tr>
<tr>
<td>ATI</td>
<td>-</td>
<td>Bed cross sectional area at height $Z_I$ above the distributor, cm$^2$</td>
</tr>
<tr>
<td>DTI</td>
<td>$D_t$</td>
<td>Diameter of the combustor at height $Z_I$ above the distributor, cm$^2$</td>
</tr>
<tr>
<td>MTB</td>
<td>-</td>
<td>Number of locations along the combustor where the cross sectional areas are specified.</td>
</tr>
<tr>
<td>PI</td>
<td>$\pi$</td>
<td>3.14159265</td>
</tr>
<tr>
<td>RI</td>
<td>-</td>
<td>Radius of the combustor at height $Z_I$ above the distributor, cm$^2$</td>
</tr>
<tr>
<td>ZB</td>
<td>-</td>
<td>Height above the distributor at which the cross sectional area is specified, cm$^2$</td>
</tr>
<tr>
<td>ZI</td>
<td>-</td>
<td>Height above the distributor, cm$^2$</td>
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### SUBPROGRAM ATTR

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>AKF</td>
<td>$k_{cf}$ Gas film diffusion rate constant, gm/cm$^2$.sec.atm</td>
</tr>
<tr>
<td>AKR</td>
<td>$k_c$ Overall rate constant for char combustion, cm/sec</td>
</tr>
<tr>
<td>AKS</td>
<td>$k_{cR}$ Chemical reaction rate constant for char combustion, gm/cm$^2$.sec.atm</td>
</tr>
<tr>
<td>COND</td>
<td>$\lambda$ Thermal conductivity of the gas, cals/sec.cm.$^\circ$C</td>
</tr>
<tr>
<td>D</td>
<td>$D$ Molecular diffusivity for $O_2$-$N_2$ cm$^2$/sec</td>
</tr>
<tr>
<td>DC</td>
<td>- Diameter of the char particle, cm</td>
</tr>
<tr>
<td>DTS</td>
<td>- Increment in temperature, $^\circ$K</td>
</tr>
<tr>
<td>EM</td>
<td>$\epsilon_m$ Emissivity of the char particle</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
</tr>
<tr>
<td>----------------</td>
<td>--------------------</td>
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<tr>
<td>ETS</td>
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</tr>
<tr>
<td>ETSMAX</td>
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<td>MC</td>
<td>$M_c$</td>
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<td>P</td>
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<td>PHI</td>
<td>$\phi$</td>
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<tr>
<td>Q</td>
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<tr>
<td>RG</td>
<td>$R_g$</td>
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<td>$\rho_{c, ch.}$</td>
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<tr>
<td>SIGM</td>
<td>$\sigma$</td>
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<td>$T$</td>
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<tr>
<td>TAV</td>
<td>$T_m$</td>
</tr>
<tr>
<td>TB</td>
<td>$t_b$</td>
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<tr>
<td>TP</td>
<td>$T_c$</td>
</tr>
<tr>
<td>YO2</td>
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<td>Z</td>
<td>$p$</td>
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**SUBROUTINE CRRECT**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>DX</td>
<td>Increment in the variable, x</td>
</tr>
<tr>
<td>E</td>
<td>Difference between the assumed and calculated values of the variable, x</td>
</tr>
<tr>
<td>EMAX</td>
<td>Tolerance limit for convergency</td>
</tr>
<tr>
<td>E1</td>
<td>Value of E in the iteration, I</td>
</tr>
<tr>
<td>E2</td>
<td>Value of E in the iteration, I+1</td>
</tr>
</tbody>
</table>
### 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

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>A₁,A₂,A₃,A₄</td>
<td>Alphanumeric characters</td>
</tr>
<tr>
<td>ABED</td>
<td>Aₜ</td>
</tr>
<tr>
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**SUBPROGRAM ELUT**

<p>| BB             | -                   | Weight of bed material of x th size fraction, gms |</p>
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<td>Weight of char in the bed, gms</td>
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<td>$C_{ch}$</td>
<td>Carbon content in char, gm carbon/gm char</td>
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<td>Char elutriated from the combustor, gms/sec</td>
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<td>-</td>
<td>Char entrained in the freeboard, gms/sec</td>
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<td>CU</td>
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<td>Fraction finer than size, $d_x$</td>
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<td>Surface volume mean diameter of char particles in the freeboard, cm</td>
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<td>$d_c$</td>
<td>Surface volume mean diameter of char particles in the bed, cm</td>
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<td>Weight mean diameter of char particles in the bed, cm</td>
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<td>Increment in combustion efficiency</td>
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<td>Mean diameter of the particles of $x$ th size fraction, cm</td>
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<td>Surface volume mean particle diameter of additives entrained in the freeboard, cm</td>
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<td>Increment in the solids withdrawal rate, gms/sec</td>
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<td>E</td>
<td>$E_x$</td>
<td>Elutriation rate constant, gm/sec</td>
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<td>$-$</td>
<td>Tolerance limit for combustion efficiency convergency</td>
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<td>$\varepsilon_{mf}$</td>
<td>Void fraction at minimum fluidization</td>
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<td>Entrainment rate of additives of $x$th size fraction in the freeboard, gm/sec</td>
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<td>Entrainment rate of char of $x$th size fraction in the freeboard, gm/sec</td>
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<td>Difference between assumed and calculated combustion efficiencies</td>
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<td>ETCC</td>
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<td>Calculated combustion efficiency</td>
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<td>EWB</td>
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<td>Tolerance limit for bed height convergency</td>
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<td>Weight fraction of char particles of $x$th size fraction entrained</td>
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<td>Proportion of total abrasion fines in the $x$th size fraction</td>
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<td>Solids entrainment rate at the bed surface of $x$th size fraction, gms/sec</td>
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<td>$b_x$</td>
<td>Weight fraction of bed materials in the $x$th size fraction</td>
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<td>Weight fraction of additives feed of $x$th size fraction</td>
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<td>$-$</td>
<td>Weight fraction of coal feed of $x$th size fraction</td>
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<td>Weight fraction of additives of $x$th size fraction elutriated from the combustor</td>
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<td>Weight fraction of char particles of x th size fraction in the bed</td>
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<td>Fraction of solids in the cloud region</td>
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<td>$f_{SW}$</td>
<td>Fraction of wake solids thrown into the freeboard</td>
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<td>$f_{SW}$</td>
<td>Volume fraction of wake to bubble (including wakes)</td>
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<td>GFLOW</td>
<td>$G$</td>
<td>Gas flow rate, gms/sec</td>
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<tr>
<td>HB</td>
<td>$h$</td>
<td>Height above the bed surface, cms</td>
</tr>
<tr>
<td>HFB</td>
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<td>Freeboard height, cm</td>
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<tr>
<td>HLF</td>
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<td>Expanded bed height, cm</td>
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<tr>
<td>HLMF</td>
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<td>Bed height at minimum fluidization, cm</td>
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<tr>
<td>MGA$S$</td>
<td>-</td>
<td>Molecular weight of gas, gms/gmole</td>
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<tr>
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<td>-</td>
<td>No. of locations along the combustor where the cross sectional areas are specified</td>
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<td>Number of size fractions</td>
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<td>$P_1$</td>
<td>Proportion of fines recycled to the bed from the primary cyclone</td>
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<tr>
<td>P2</td>
<td>$P_2$</td>
<td>Proportion of fines recycled to the bed from the secondary cyclone</td>
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<td>$P$</td>
<td>Average pressure of the FBC, atm</td>
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<td>PFA</td>
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<td>Gain of fines in the x th size fraction due to abrasion, gms/sec</td>
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<td>Q1</td>
<td>$q_{1x}$</td>
<td>Collection efficiency of the primary cyclones for the x th size fraction</td>
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<td>$q_{2x}$</td>
<td>Collection efficiency of the secondary cyclones for the x th size fraction</td>
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<td>Entrainment rate of particles of size $d_x$, gms/sec</td>
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<td>Char produced per unit gm of coal fed, gm/gm</td>
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<td>RG</td>
<td>( R_g )</td>
<td>Gas constant, 82.06 atm.cm(^3)/gmole.-°K</td>
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<td>( \rho_{ad} )</td>
<td>Density of additives, gms/cm(^3)</td>
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<td>RHOBED</td>
<td>( \rho_b )</td>
<td>Density of bed materials, gms/cm(^3)</td>
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<td>RHOCC</td>
<td>( \rho_{c, ch} )</td>
<td>Density of carbon in char, gms/cm(^3)</td>
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<tr>
<td>RHOCH</td>
<td>( \rho_{ch} )</td>
<td>Density of char, gms/cm(^3)</td>
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<td>RHOGAS</td>
<td>( \rho_g )</td>
<td>Density of gas, gms/cm(^3)</td>
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<td>Attrition rate constant, 1/cm</td>
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<td>Size reduction constant for char (due to combustion), 1/sec</td>
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<td>Residence time of solids in the freeboard, sec</td>
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<td>Mean bed temperature, °K</td>
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<td>Burning time of a char particle, sec</td>
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<td>TDH</td>
<td>Transport Disengaging Height, cm; if TDH &gt; HFB, TDH = HFB</td>
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<td>TDH</td>
<td>Transport Disengaging Height, cm</td>
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<td>( U_{mf} )</td>
<td>Minimum fluidization velocity, cm/sec</td>
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<td>( U_o )</td>
<td>Superficial gas velocity at the bed surface, cm/sec</td>
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<td>Terminal velocity of additive particles of size ( d_x ), cm/sec</td>
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<td>Terminal velocity of char particles of size ( d_x ), cm/sec</td>
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<td>Viscosity of gas, gm/cm.sec</td>
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<td>Bed volume at minimum fluidization (excluding the internals), cm(^3)</td>
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<td>W</td>
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<td>Rate of transfer of particles from size fraction x to fraction x+1 by size reduction, gms/sec</td>
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<td>$W_{f,a}$</td>
<td>Additives feed rate, gms/sec</td>
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<td>Coal feed rate, gms/sec</td>
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<td>Solids withdrawal rate, gms/sec</td>
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<td>Additives entrainment rate in the freeboard, gms/sec</td>
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<td>Char entrainment rate in the freeboard, gms/sec</td>
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<td>Solids (excluding char) elutriation rate, gms/sec</td>
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<td>$W_{f,x}$</td>
<td>Solids feed rate of x th size fraction, gms/sec</td>
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<td>Feed rate of (limestone + ash in coal)</td>
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<td>Ash content in coal, gm ash/gm coal</td>
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<td>Weight fraction carbon in the bed (average), gm carbon/gm bed material</td>
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<td>Mole fraction oxygen</td>
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<td>Height above the distributor at which the cross sectional area is specified, cms</td>
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**SUBPROGRAM FBC**

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<td>AKCO2</td>
<td>Overall rate constant for C-CO$_2$ reaction, cm/sec</td>
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**SUBPROGRAM GPB**

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<td>COB</td>
<td>Carbon monoxide burnt in each compartment, gmole/sec</td>
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<tr>
<td>COV</td>
<td>CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles</td>
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<tr>
<td>COVB</td>
<td>CO produced during volatiles combustion, gmole CO/gmole volatiles</td>
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<tr>
<td>CO2V</td>
<td>CO$_2$ released during devolatilization per mole of volatiles released, gmole CO$_2$/gmole volatiles</td>
</tr>
<tr>
<td>CO2VB</td>
<td>CO$_2$ produced during volatiles combustion, gmole CO$_2$/gmole volatiles</td>
</tr>
<tr>
<td>DVBB</td>
<td>Volume of each compartment, cm$^3$</td>
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<tr>
<td>DYE</td>
<td>Increment in oxygen concentration in emulsion phase, mole fraction</td>
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<tr>
<td>EMAX</td>
<td>Tolerance limit for oxygen concentration convergency</td>
</tr>
<tr>
<td>EMF $\varepsilon_{mf}$</td>
<td>Void fraction at minimum fluidization</td>
</tr>
<tr>
<td>EPB $\varepsilon_B$</td>
<td>Bubble fraction</td>
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<tr>
<td>EPC $\varepsilon_C$</td>
<td>Cloud fraction including bubble</td>
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<td>Molar flow rate of gas in the bubble phase, gmole/sec</td>
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<td>Molar flow rate of gas in the bubble phase in the bottom compartment, gmole/sec</td>
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<tr>
<td>FEM $F_{EM}$</td>
<td>Molar flow rate of gas in the emulsion phase, gmole/sec</td>
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<tr>
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<td>Molar flow rate of gas in the emulsion phase in the bottom compartment, gmole/sec</td>
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**SUBPROGRAM GPHASE**

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**SUBPROGRAM HAREA**

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<tr>
<td>ATB</td>
<td>Bed cross sectional area at height ZB above the distributor, cm²</td>
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<tr>
<td>ATI</td>
<td>Bed cross sectional area at height ZI above the distributor, cm²</td>
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<tr>
<td>DTI</td>
<td>Diameter of the combustor at height ZI above the distributor, cm</td>
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<tr>
<td>MTB</td>
<td>Number of locations along the combustor where the cross sectional areas are specified</td>
</tr>
<tr>
<td>BI</td>
<td>π</td>
</tr>
<tr>
<td>RI</td>
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<tr>
<td>ZI</td>
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<td>Height above the distributor, cms</td>
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**SUBPROGRAM HEIGHT**

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<th>Symbol</th>
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<tr>
<td>DBVEFF</td>
<td>Volume of each compartment excluding the tubes, cm$^3$</td>
</tr>
<tr>
<td>DZAV</td>
<td>Average compartment size used in design calculations, cm</td>
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<tr>
<td>HEIGHT</td>
<td>Height above the distributor, cm</td>
</tr>
<tr>
<td>HT</td>
<td>Height above the distributor, cm</td>
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<tr>
<td>NTC</td>
<td>Total number of compartments in the combustor using $DZAV + 1$</td>
</tr>
<tr>
<td>VV</td>
<td>Volume of bed (excluding tubes) at any height, cm$^3$</td>
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**SUBPROGRAM HYDRO**

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<tr>
<td>AHE</td>
<td>Specific heat transfer area of the tubes, cm$^2$/cm$^3$ (DESIGN input) FBC volume</td>
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<tr>
<td>AHEAV</td>
<td>Specific heat transfer area of the tubes in each compartment, cm$^2$/cm$^3$, FBC volume</td>
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<tr>
<td>AKBE</td>
<td>Gas exchange coefficient, l/sec</td>
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<tr>
<td>ALFB</td>
<td>$\alpha_b = \varepsilon_{mf} \frac{U_B}{U_{mf}}$</td>
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<tr>
<td>AND</td>
<td>Number of orifices in the distributor</td>
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<tr>
<td>AT</td>
<td>Cross sectional area of the bed, cm$^2$</td>
</tr>
<tr>
<td>ATAV</td>
<td>Average cross sectional area used in calculations for each compartment</td>
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<tr>
<td>BEDVOL</td>
<td>Total bed volume, cm$^3$</td>
</tr>
<tr>
<td>DBA</td>
<td>Bubble diameter in each compartment assumed, cm</td>
</tr>
<tr>
<td>DBAV</td>
<td>Bubble diameter in each compartment, cm</td>
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<td>FORTRAN Symbol</td>
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<td>PVI</td>
<td>P_V</td>
</tr>
</tbody>
</table>
### FORTRAN Symbol | Mathematical Symbol | Description
--- | --- | ---
\( R_G \) | \( R_g \) | Gas constant, 82.06 atm.cm\(^3\)/gmole,\(^{\circ}\)K
\( \rho_{BED} \) | \( \rho_b \) | Density of bed materials, gm/cm\(^3\)
\( \rho_{GAS} \) | \( \rho_g \) | Density of gas, gm/cm\(^3\)
\( \text{SUM} \) | – | Height that would be occupied by solids alone in each compartment, cm
\( \text{SUMEFF} \) | – | Effective volume of bed (solids volume alone), cm\(^3\)
\( \text{SUMV} \) | – | Volume of bed, cm\(^3\)
\( \text{SOLVOL} \) | – | Volume of solids in each compartment (including voids), cm\(^3\)
\( T \) | \( T \) | Temperature in the bed, \(^{\circ}\)K
\( \text{TETUBE} \) | – | Total volume fraction of tubes in the bed
\( U_B \) | \( U_B \) | Bubble velocity, cm/sec
\( U_{BR} \) | – | Bubble rising velocity, cm/sec
\( U_{BS} \) | – | Bubble rising velocity under slugging conditions, cm/sec
\( U_{MF} \) | \( U_{mf} \) | Minimum fluidization velocity, cm/sec
\( U_O \) | \( U_O \) | Superficial gas velocity, cm/sec
\( \nu \) | \( \mu \) | Viscosity of gas, gm/cm.sec
\( V_{MF} \) | – | Bed volume at minimum fluidization (excluding internals), cm\(^3\)
\( X \) | \( X \) | Weight fraction carbon in the bed
\( Y_B \) | \( Y_B \) | Mole fraction oxygen in the emulsion phase
\( Z \) | \( Z \) | Locations of cooling tubes, cm

**SUBPROGRAM VEL**

\( \text{DPAR} \) | \( d_P \) | Particle diameter, cm
<table>
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<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>G</td>
<td>g</td>
<td>Acceleration due to gravity, cms/sec²</td>
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<tr>
<td>REP</td>
<td>Re,p</td>
<td>Particle Reynolds number</td>
</tr>
<tr>
<td>RHOGAS</td>
<td>ρ_g</td>
<td>Density of gas, gm/cm³</td>
</tr>
<tr>
<td>RHOS</td>
<td>ρ_s</td>
<td>Density of solids, gm/cm³</td>
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<tr>
<td>UM</td>
<td>U_{mf}</td>
<td>Minimum fluidization velocity, cm/sec</td>
</tr>
<tr>
<td>UT</td>
<td>U_t</td>
<td>Terminal velocity of the particle, cms/sec</td>
</tr>
<tr>
<td>VISC</td>
<td>μ</td>
<td>Viscosity of gas, gm/cm.sec</td>
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**SUBPROGRAM VOLUME**

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<th>Symbol</th>
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<tbody>
<tr>
<td>DVBEFF</td>
<td>Volume of each compartment excluding the tubes, cm³</td>
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<tr>
<td>DZAV</td>
<td>Average compartment size used in design calculations, cm</td>
</tr>
<tr>
<td>VOLUME</td>
<td>Volume of bed (excluding tubes) at any height ZZ, cm³</td>
</tr>
<tr>
<td>ZZ</td>
<td>Height above the distributor, cms</td>
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