SIMULATION OF FLUIDIZED BED COAL COMBUSTORS

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**Title and Subtitle**

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National Aeronautics and Space Administration
Washington, D.C. 20546

**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; SO₂ absorption by limestone; (iv) release of NOₓ and reduction of NOₓ 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, O₂, CO, CO₂, SO₂, and NOₓ concentration profiles along the combustor. Agreement between the computed results and the observed data is good.
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<th>Mathematical Symbol</th>
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<tr>
<td>G</td>
<td>g</td>
<td>Acceleration due to gravity, (\text{cms/sec}^2)</td>
</tr>
<tr>
<td>REP</td>
<td>(R_{e,p})</td>
<td>Particle Reynolds number</td>
</tr>
<tr>
<td>RHOGAS</td>
<td>(\rho_g)</td>
<td>Density of gas, (\text{gm/cm}^3)</td>
</tr>
<tr>
<td>RHOS</td>
<td>(\rho_s)</td>
<td>Density of solids, (\text{gm/cm}^3)</td>
</tr>
<tr>
<td>UM</td>
<td>(U_{mf})</td>
<td>Minimum fluidization velocity, (\text{cm/sec})</td>
</tr>
<tr>
<td>UT</td>
<td>(U_t)</td>
<td>Terminal velocity of the particle, (\text{cm/sec})</td>
</tr>
<tr>
<td>VISC</td>
<td>(\mu)</td>
<td>Viscosity of gas, (\text{gm/cm}.\text{sec})</td>
</tr>
</tbody>
</table>

SUBPROGRAM VOLUME

| DVBEFF         | -                   | Volume of each compartment excluding the tubes, \(\text{cm}\) |
| DZAV           | -                   | Average compartment size used in design calculations, \(\text{cm}\) |
| VOLUME         | -                   | Volume of bed (excluding tubes) at any height \(\text{ZZ}\), \(\text{cm}\) |
| ZZ             | -                   | Height above the distributor, \(\text{cm}\) |
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NOMENCLATURE

A- Defined by equation (V.2).

$A_t$ Cross sectional area of the bed, cm$^2$.

$a_{B,NO}$ Defined by equation (VI.51).

$a_{B,SO_2}$ Defined by equation (VI.49).

$a_{E,NO}$ Defined by equation (VI.47).

$a_{E,SO_2}$ Defined by equation (VI.45).

$a_{HE}$ Specific heat transfer area of the tubes, cm$^2$/cm$^3$ FBC volume.

$a_{HEW}$ Specific heat transfer area of the walls, cm$^2$/cm$^3$ FBC volume.

$a_{NO}$ Defined by equation (VI.55).

$a_{SO_2}$ Defined by equation (VI.53).

$a_m$ Defined by equation (VI.12).

$a_x$ Proportion of total abrasion fines in the xth size fraction.

$a_1$ Defined by equation (VI.9).

$a_2$ Defined by equation (VI.15).

$a_3$ Defined by equation (VI.25).

$a_4$ Defined by equation (VI.11).

$a_1'$ Defined by equation (VI.33).

$a_2'$ Defined by equation (VI.20).

$B$ Defined by equation (V.3).

$b_x$ Weight fraction of bed material in the xth size fraction.

$C_{CEF}$ Heat capacity of coal feed, cals/gm·°C.

$C_{CO_2}$ Concentration of carbon dioxide, gmole/cm$^3$. 
\( C_{NO} \) Concentration of nitric oxide, \( \text{g mole/cm}^3 \)

\( C_S \) Heat capacity of solids, \( \text{cals/gm. } ^\circ \text{C} \)

\( C_{SF} \) Heat capacity of feed additives, \( \text{cals/gm. } ^\circ \text{C} \)

\( C_{SO_2} \) Concentration of sulfur dioxide, \( \text{g mole/cm}^3 \)

\( C_{ch} \) Carbon content in char, \( \text{gm carbon/gm char} \)

\( C_{gm} \) Molar heat capacity of gas at constant pressure, \( \text{cals/gmole } ^\circ \text{C} \)

\( CH_4 \) Wt. fraction \( CH_4 \) in the volatiles

\( CO \) Wt. fraction \( CO \) in the volatiles

\( CO_2 \) Wt. fraction \( CO_2 \) in the volatiles

\( D \) Molecular diffusivity for \( O_2-N_2 \), \( \text{cm}^2/\text{sec} \)

\( D_B \) Bubble diameter, \( \text{cm} \)

\( D_{BO} \) Bubble diameter at the distributor level, \( \text{cm} \)

\( D_{BM} \) Fictitious maximum bubble diameter, \( \text{cm} \)

\( D_t \) Diameter of the FBC as a function of height above the distributor, \( \text{cm} \)

\( d_c \) Diameter of char particle in the bed, \( \text{cm} \)

\( d_{ce} \) Diameter of char particle entrained in the freeboard, \( \text{cm} \)

\( d_{k} \) Diameter of limestone particle in the bed, \( \text{cm} \)

\( d_{ke} \) Diameter of limestone particle entrained in the freeboard, \( \text{cm} \)

\( d_o \) Diameter of cooling tubes, \( \text{cm} \)

\( d_p \) Particle diameter, \( \text{cm} \)

\( d_x \) Mean diameter of the particles of \( x \)th size fraction, \( \text{cm} \)

\( E_x \) Elutriation rate constant, \( \text{gm/sec} \)

\( E_z \) Dispersion coefficient in the freeboard, \( \text{l/sec} \)

\( E_{BM} \) Molar flow rate of gas in the bubble phase, \( \text{g mole/sec} \)

\( F_{EM} \) Molar flow rate of gas in the emulsion phase, \( \text{g mole/sec} \)

\( F_{MT} \) Total molar flow rate of gas in the combustor, \( \text{g mole/sec} \)

\( F_{j} \) Solids entrainment rate at the bed surface, \( \text{gm/sec} \)
Fractional conversion of limestone

Fraction of wake solids thrown into the freeboard

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

Gas flow rate, gms/sec

Acceleration due to gravity, cms/sec²

Volatiles burning rate in the bubble phase, gmole/sec

Carbon monoxide burning rate, gmole/sec

Volatiles burning rate in the emulsion phase, gmole/sec

Wt. fraction hydrogen in the volatiles

Wt. fraction H₂O in the volatiles

Height above the bed surface, cm

Attrition rate constant, 1/cm

Gas exchange coefficient, 1/sec

Defined by Equation (VI.24)

NO reduction rate constant in the bubble phase, cm/sec

C-CO₂ chemical reaction rate constant, cm/sec

NO reduction rate constant in the emulsion phase, cm/sec

NO reduction rate constant, cm/sec

Overall rate constant for char combustion, cm/sec

Overall rate constant for char combustion in bubble phase, cm/sec

Overall rate constant for char combustion in emulsion phase, cm/sec

Gas film diffusion rate constant, gm/cm²·sec·atm

Chemical reaction rate constant for char combustion, gm/cm²·sec·atm

Overall volume reaction rate constant for limestone-SO₂ reaction, 1/sec

Abrasion rate constant for the xth size fraction, 1/sec
<table>
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<th>Symbol</th>
<th>Definition</th>
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<td>$K'$</td>
<td>Defined by Equation (VI.32)</td>
</tr>
<tr>
<td>$K'_{vl}$</td>
<td>Chemical reaction rate constant for limestone-SO$_2$ reaction, l/sec</td>
</tr>
<tr>
<td>$M$</td>
<td>Weight of particles remaining in the bed after the size reduction from the original size to $d_x$</td>
</tr>
<tr>
<td>$M_b$</td>
<td>Weight of bed material, gms</td>
</tr>
<tr>
<td>$M_c$</td>
<td>Atomic weight of carbon, gms/gm atom</td>
</tr>
<tr>
<td>$M_x$</td>
<td>Weight of bed material in the $x$th size fraction</td>
</tr>
<tr>
<td>$N_A$</td>
<td>Number of limestone particles in the $i$th compartment in the freeboard</td>
</tr>
<tr>
<td>$N_{Pe}$</td>
<td>Peclet number, defined by Equation (V.43)</td>
</tr>
<tr>
<td>$N_{Re}$</td>
<td>Reynolds number, defined by Equation (V.42)</td>
</tr>
<tr>
<td>$N_{Sc}$</td>
<td>Schmidt number, defined by Equation (V.44)</td>
</tr>
<tr>
<td>$N_c$</td>
<td>Number of char particles in the $i$th compartment in the freeboard</td>
</tr>
<tr>
<td>$N_d$</td>
<td>Number of orifices in the distributor</td>
</tr>
<tr>
<td>$P$</td>
<td>Average pressure of the FBC, atm</td>
</tr>
<tr>
<td>$P_H$</td>
<td>Horizontal pitch distance between the tubes, cms</td>
</tr>
<tr>
<td>$P_V$</td>
<td>Vertical pitch distance between the tubes, cms</td>
</tr>
<tr>
<td>$P$</td>
<td>Defined by Equation (V.16)</td>
</tr>
<tr>
<td>$P_{O_2}$</td>
<td>Partial pressure of oxygen, atm</td>
</tr>
<tr>
<td>$P_1$</td>
<td>Proportion of fines recycled to the bed from the primary cyclone</td>
</tr>
<tr>
<td>$P_2$</td>
<td>Proportion of fines recycled to the bed from the secondary cyclone</td>
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<tr>
<td>$q_{cal}$</td>
<td>Heat of calcination of limestone, cals/gm</td>
</tr>
<tr>
<td>$q_{ch}$</td>
<td>Heat of combustion of char, cals/gm</td>
</tr>
<tr>
<td>$q_V$</td>
<td>Heat of combustion of volatiles (complete burning), cals/gmole</td>
</tr>
<tr>
<td>$q_{V,CO}$</td>
<td>Heat of combustion of volatiles (partial burning), cals/gmole</td>
</tr>
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</table>
\( q_{1x} \) Collection efficiency of the primary cyclones for the 
xth size fraction

\( q_{2x} \) Collection efficiency of the secondary cyclones for the 
xth size fraction

\( R \) Gas constant, 1.987 cals/gmole °K

\( R_{B,NO,c} \) NO release rate in the bubble phase due to char combustion, 
gmole/sec

\( R_{B,NO,V} \) NO release rate in the bubble phase due to volatiles 
combustion, gmole/sec

\( R_{B,SO_2,c} \) \( \text{SO}_2 \) release rate in the bubble phase due to char 
combustion, gmole/sec

\( R_{B,SO_2,V} \) \( \text{SO}_2 \) release rate in the bubble phase due to volatiles 
combustion, gmole/sec

\( R_{CO} \) \( \text{CO} \) released during devolatilization, gmole/sec

\( R_{CO_2} \) \( \text{CO}_2 \) released during devolatilization, gmole/sec

\( R_{E,NO,c} \) NO release rate in the emulsion phase due to char 
combustion, gmole/sec

\( R_{E,NO,V} \) NO release rate in the emulsion phase due to volatiles 
combustion, gmole/sec

\( R_{E,SO_2,c} \) \( \text{SO}_2 \) release rate in the emulsion phase due to char 
combustion, gmole/sec

\( R_{E,SO_2,V} \) \( \text{SO}_2 \) release rate in the emulsion phase due to volatiles 
combustion, gmole/sec

\( R_{e,p} \) Particle Reynolds number, defined by equations (A.VII.22-24)

\( R_{NO} \) NO release rate, gmole/sec

\( R_{SO_2} \) \( \text{SO}_2 \) release rate, gmole/sec

\( R_{a} \) Attrition rate, gms/sec

\( R_{ch} \) Char produced per unit gm of coal fed, gm/gm

\( R_{V} \) Volatiles released, gmole/sec

\( R_{g} \) Gas constant, 82.06 atm.cm\(^3\)/gmole °K

\( r_{CO} \) Rate of combustion of \( \text{CO}_2 \), gmole/cm\(^3\) sec

\( r_{i} \) Char combustion rate in ith compartment, gms/sec
\( r_c \)  
Char combustion rate, g mole/sec \cdot particle

\( S_g \)  
Effective specific surface area of limestone, cm\(^2\)/gm

\( T \)  
Temperature in the bed, °K

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

\( T_{DH} \)  
Transport Disengaging Height, cms

\( T_E \)  
Mean temperature in the boundary layer of the char particle in the emulsion phase, °K

\( \text{Tar} \)  
Wt. fraction tar in the volatiles

\( T_C \)  
Char particle temperature, °K

\( T_m \)  
Mean temperature in the boundary layer of the char particle, °K

\( T_{sf} \)  
Solids feed temperature, °K

\( T_w \)  
Cooling water temperature, °K

\( T_{wall} \)  
Average FBC wall temperature, °K

\( t \)  
Temperature, °C

\( t_B \)  
Burning time of a char particle, sec

\( U \)  
Bed to tube heat transfer coefficient, cals/sec \cdot cm^2 \cdot °C

\( U_B \)  
Bubble velocity, cms/sec

\( U_{mf} \)  
Minimum fluidization velocity, cms/sec

\( U_o \)  
Superficial gas velocity or fluidization velocity, cms/sec

\( \bar{U}_o \)  
Average superficial gas velocity in the freeboard, cms/sec

\( U_t \)  
Terminal velocity of the particle, cms/sec

\( U_w \)  
Bed to wall heat transfer coefficient, cals/sec \cdot cm^2 \cdot °C

\( V \)  
Volatiles yield during devolatilization, % of coal daf

\( \text{VM} \)  
Proximate volatile matter in the coal, % of coal daf

\( V_{CO} \)  
CO produced due to volatiles burning, g mole CO/g mole volatile
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<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$V_{CO_2}$</td>
<td>CO$_2$ produced due to volatiles burning, g mole CO$_2$/g mole volatil</td>
</tr>
<tr>
<td>$V_N$</td>
<td>Volatile nitrogen in coal, gm/gm, dry basis (d.b.)</td>
</tr>
<tr>
<td>$V_S$</td>
<td>Volatile sulfur in coal, gm/gm, dry basis (d.b.)</td>
</tr>
<tr>
<td>$W_D$</td>
<td>Solids withdrawal rate, gms/sec</td>
</tr>
<tr>
<td>$W_{ent}$</td>
<td>Solids entrainment rate, gms/sec</td>
</tr>
<tr>
<td>$W_{f,a}$</td>
<td>Additives feed rate, gms/sec</td>
</tr>
<tr>
<td>$W_{f,c}$</td>
<td>Coal feed rate, gms/sec</td>
</tr>
<tr>
<td>$W_{f,x}$</td>
<td>Solids feed rate of xth size fraction, gms/sec</td>
</tr>
<tr>
<td>$W_{mix}$</td>
<td>Solids mixing rate, gms/sec</td>
</tr>
<tr>
<td>$W_{net}$</td>
<td>Net flow rate of solids, gms/sec</td>
</tr>
<tr>
<td>$W_x$</td>
<td>Rate of transfer of particles from size fraction $x$ to fraction $x + 1$ by size reduction, gms/sec</td>
</tr>
<tr>
<td>$X$</td>
<td>Weight fraction carbon in the bed</td>
</tr>
<tr>
<td>$X_{O_2}$</td>
<td>Oxygen required for partial combustion of volatiles, g mole O$_2$/g mole volatile</td>
</tr>
<tr>
<td>$X_{O_2,c}$</td>
<td>Oxygen required for complete combustion of volatiles, g mole O$_2$/mole volatile</td>
</tr>
<tr>
<td>$X_{VM}$</td>
<td>Proximate volatile matter content of coal, gms/gm coal (daf)</td>
</tr>
<tr>
<td>$Y_B$</td>
<td>Mole fraction O$_2$ in the bubble phase</td>
</tr>
<tr>
<td>$Y_{B,CO_2}$</td>
<td>Mole fraction CO$_2$ in the bubble phase</td>
</tr>
<tr>
<td>$Y_{B,NO}$</td>
<td>Mole fraction NO in the bubble phase</td>
</tr>
<tr>
<td>$Y_{B,SO_2}$</td>
<td>Mole fraction SO$_2$ in the bubble phase</td>
</tr>
<tr>
<td>$Y_{CO}$</td>
<td>Mole fraction CO</td>
</tr>
<tr>
<td>$Y_{CO_2}$</td>
<td>Mole fraction CO$_2$</td>
</tr>
<tr>
<td>$Y_E$</td>
<td>Mole fraction O$_2$ in the emulsion phase</td>
</tr>
<tr>
<td>$Y_{E,CO}$</td>
<td>Mole fraction CO in the emulsion phase</td>
</tr>
<tr>
<td>$Y_{E,CO_2}$</td>
<td>Mole fraction CO$_2$ in the emulsion phase</td>
</tr>
</tbody>
</table>
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°C
\( \lambda_L \)  Reactivity of limestone
\( \mu \)  Viscosity of gas, gm/cm.sec
\( \Pi \)  3.14159265
\( \rho_B \)  Density of the bed materials, gms/cm³
\( \rho_{c, ch} \)  Density of carbon in char, gms/cm³
\( \rho_{ch} \)  Density of char, gms/cm
\( \rho_g \)  Density of gas, gms/cm³
\( \rho_s \)  Density of solids, gms/cm³
\( \sigma \)  Stefan-Boltzman constant, 1.36 x 10⁻¹², cals/sec.cm².°K⁴
\( \phi \)  Mechanism factor of char combustion
\( \phi_B \) Mechanism factor in the freeboard

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

**Subscript**

x \( \) xth size fraction

i \( \) ith compartment

**Abbreviation**

d.b. \( \) dry basis

daf \( \) dry ash free basis
I. INTRODUCTION

Among the various ways of direct burning of coal, fluidized bed combustion appears to be the most attractive, both from an economic and environmental standpoint. By carrying out combustion in a fluidized bed combustor (FBC) operating at relatively low temperature (750°C-950°C; 1382°F-1742°F), both $\text{SO}_2$ and $\text{NO}_x$ 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:

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

$\text{NO}_x$ emission is kept low due to low combustion temperature and by the $\text{NO}_x$ 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/m²·K (45 to 75 Btu/hr ft²·°F)] and the large heat generation rates
[2.0 to 5.0 MW/m³ (0.193 to 0.483 × 10⁶ Btu/hr ft³)] in FBC result in a smaller boiler volume for a given duty than the conventional pulverized coal burning boilers.

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

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

A considerable amount of investigation on the performance of fluidized bed combustion system has been under way particularly in the U.S. and U.K. (Argonne National Laboratory (ANL), Combustion Power Company (CPC), Pope, Evans and Robbins (PER), Westinghouse Research Laboratories (WRL), Exxon Research and Engineering Company (ER&E), Morgantown Energy Technology Center (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 μm) conducted by Rowe (1978) show that the dense phase voidage changes with gas velocity, and that as much as 30 percent of the gas flow may occur interstitially. Catipovic, et al. (1978) have pointed out qualitatively the difference in the fluidization of larger particles.

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

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

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

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

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

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

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

In the FBC models described so far, they have at least one of the following deficiencies:
(1) The bubble diameter was taken as a constant and an adjustable parameter. In reality, bubbles coalesce as they ascend through the bed. The bubble diameter changes with the height above the distributor. Bubble size is also affected by the immersed cooling coils. (Baron, et al. 1977; Gibbs, 1975).

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

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

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

Bethell, et al. (1973) presented a model for sulfur dioxide retention by limestone in a fluidized bed combustor. Horio and Wen (1975) have also formulated a model for the removal of sulfur dioxide by limestone in a FBC. In their model, the hydrodynamics of the fluidizing gas is based on the bubble assemblage model developed by Kato and Wen (1975). Chen and Saxena (1977) used a three phase bubbling bed model (bubble phase, cloud-wake phase and emulsion phase) for predicting the sulfur
retention efficiency in a FBC. The model predictions were compared with some experimental data. However, a limitation of the model is that it assumes isothermal conditions in the bed. The models described above for \( \text{SO}_2 \) 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 \( \text{NO}_x \) emissions from the combustor. This model does not deal with the \( \text{NO}_x \) 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 \( \text{NO}_x \) 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 Wen, 1969, Mori and Wen, 1975). The model includes the devolatilization of coal, char combustion and \( \text{SO}_2 \) 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>
<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>
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<tr>
<td></td>
<td>Campbell and Davidson (1975)</td>
<td>c) Complete</td>
<td>Complete Mixing</td>
<td></td>
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<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>Two phase compartment in series model</td>
<td>Horio, et al. (1977)</td>
<td>Complete</td>
<td>Complete</td>
<td>Complete mixing</td>
<td>1) Bubbles grow along the bed height.</td>
</tr>
<tr>
<td></td>
<td>Rengarajan, et al. (1977)</td>
<td>mixing</td>
<td>mixing</td>
<td>within each compartment</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Horio and Wen (1978)</td>
<td>within each</td>
<td>within each</td>
<td>within each compartment</td>
<td>2) The backflow solid mixing is considered using an adjustable parameter.</td>
</tr>
<tr>
<td></td>
<td>Rajan, et al. (1978)</td>
<td>compartment</td>
<td>compartment</td>
<td>compartment of solids from one compartment to another</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>
</tr>
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<td></td>
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<td></td>
<td>2) Isothermal condition throughout the bed for solids, char and gas.</td>
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<td>3) Bubble growth is considered.</td>
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<td>4) Combustion occurs in cloud-wake and emulsion phases only.</td>
</tr>
</tbody>
</table>
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. $\text{NO}_x$ release and reduction of $\text{NO}_x$ 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. $\text{SO}_2$ and $\text{NO}_x$ emissions.
4. Particulates emission.
5. Attrition and elutriation of char and limestone.
6. Size distribution of char and limestone in the bed and in the elutriated material.
(7) Axial bed temperature profile.

(8) O₂, CO, CO₂, SO₂ and NOₓ concentration profiles.

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

The present work will aid in the understanding of the performance of FBC under a range of operating conditions. For example, 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.
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):

\[ V = VM - A - B \]  \hspace{1cm} (V.1)

\[ A = \exp(26.41 - 3.961 \ln t + 0.0115 VM) \]  \hspace{1cm} (V.2)

\[ B = 0.2(VM - 10.9) \]  \hspace{1cm} (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):

\[ CH_4 = 0.201 - 0.469 \frac{X_{VM}}{VM} + 0.241 \frac{X_{VM}^2}{VM} \]  \hspace{1cm} (V.4)

\[ H_2 = 0.157 - 0.868 \frac{X_{VM}}{VM} + 1.388 \frac{X_{VM}^2}{VM} \]  \hspace{1cm} (V.5)

\[ CO_2 = 0.135 - 0.900 \frac{X_{VM}}{VM} + 1.906 \frac{X_{VM}^2}{VM} \]  \hspace{1cm} (V.6)

\[ CO = 0.428 - 2.653 \frac{X_{VM}}{VM} + 4.845 \frac{X_{VM}^2}{VM} \]  \hspace{1cm} (V.7)

\[ H_2O = 0.409 - 2.389 \frac{X_{VM}}{VM} + 4.554 \frac{X_{VM}^2}{VM} \]  \hspace{1cm} (V.8)

\[ Tar = -0.325 + 7.279 \frac{X_{VM}}{VM} - 12.880 \frac{X_{VM}^2}{VM} \]  \hspace{1cm} (V.9)
**Fig. 1 Schematic Illustration of the FBC**
Volatile nitrogen released during devolatilization is expressed as (Fine, et al. 1974):

\[ V_N = 0.001 T - 0.6 \text{ gm/gm coal, (d.b.)} \]  \hspace{1cm} (V.10)

and volatile sulfur is expressed as:

\[ V_S = 0.001 T - 0.6 \text{ gm/gm coal (d.b.)} \]  \hspace{1cm} (V.11)

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

At temperatures above 650°C and in an oxidizing atmosphere the rate of burning of volatiles is fast compared to the time required for volatiles evolution. However, the combustion of volatiles released in the emulsion phase is controlled by the availability of oxygen in the emulsion phase. Since the oxygen concentration in the emulsion phase is low, the volatile gases in the emulsion phase first tend to form CO by partial combustion; whereas, the volatiles exchanged to the bubble phase burns completely to \( \text{CO}_2 \) because of excess oxygen present in the bubble phase.

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

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

\[ \text{C} + \frac{1}{2} \text{O}_2 \rightarrow (2 - \frac{2}{\phi})\text{CO} + \left(\frac{2}{\phi} - 1\right)\text{CO}_2 \]  \hspace{1cm} (V.13)

where \( \phi \) is a mechanism factor, which takes the value 1 when \( \text{CO}_2 \) is transported away from the char particle and 2 when \( \text{CO} \) 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, \( \text{CO} \) formed during char combustion diffuses out fast because of rapid mass transfer and burns to form \( \text{CO}_2 \) outside the particle; whereas, for large particles, because of slower mass transfer, \( \text{CO} \) burns within the particle and \( \text{CO}_2 \) is transported out, \( \phi \) is expressed as:

\[ \phi = \frac{2p + 2}{p + 2} \quad \text{for } d_c \leq 0.005 \text{ cm} \]  \hspace{1cm} (V.14)

\[ \phi = \frac{(2p + 2) - p(d_c - 0.005)/0.095}{p + 2} \quad \text{for } 0.005 < d_c < 0.1 \text{ cm} \]  \hspace{1cm} (V.15)

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

\[ p = \text{CO}/\text{CO}_2 = 2500 \exp(-12400/RT) \]  \hspace{1cm} (V.16)

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

\[ r_c^* = \pi d_c^2 k_c \frac{c_{\text{CO}_2}}{c_{\text{CO}}} \text{ gmole/sec particle} \]  \hspace{1cm} (V.17)

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

\[ k_c = \frac{R_g T_{m,c} / M_c}{\frac{1}{k_{cR}} + \frac{1}{k_{cf}}} \text{ cm/sec} \]  \hspace{1cm} (V.18)

\[ k_{cR} = \text{chemical reaction rate constant} = 8710 \exp(-35700/RT_c) \text{ gm/cm}^2 \cdot \text{sec} \cdot \text{atm} \]  \hspace{1cm} (V.19)

\[ k_{cf} = \text{diffusion rate constant} = 24 \phi D/d_c R_g T_{m,c} \text{ gm/cm}^2 \cdot \text{sec} \cdot \text{atm} \]  \hspace{1cm} (V.20)
Fig. 2 Rate Controlling Regimes in FBC
For smaller particles, diffusion of oxygen to the surface of the char particle is faster than the chemical reaction rate of combustion while for larger particles, diffusion of oxygen is slower than the chemical rate. Thus, the diffusional term tends to dominate for larger particles at high temperatures, while the chemical term tends to dominate at low temperatures (Fig. 2). CO$_2$ formed during combustion reacts with char according to the following reaction:

\[
\text{C} + \text{CO}_2 \rightarrow 2 \text{CO}
\]  

and the rate expression for the above reaction is \[ r_{\text{CO}_2} = \pi d^2 c \cdot k_{\text{CO}_2} \cdot C_{\text{CO}_2} \] gmole/sec . particle, where \[ k_{\text{CO}_2} = 4.1 \times 10^8 \exp(-59200/RT) \text{ cm/sec} \] (Caram and Amundson, 1977).

2. Sulfur Dioxide - Limestone Reaction:

When limestone is added to a fluidized bed burning coal, the SO$_2$ released from the combustion of coal reacts with calcined limestone according to the reaction:

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

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

\[
x_{l} = \frac{\pi}{6} d^3 k_{v} c_{\text{SO}_2} \text{ gmole/sec particle} \]  

where \( k_v \) is the overall volumetric reaction rate constant and is a rapidly decreasing function of limestone conversion, \( f_l \). The overall reaction rate constant, \( k_v \), is calculated by the equation:

\[
k_{v} = k_{v}^{0} S_g \lambda
\]

where \( k_{v}^{0} \) is equal to 490 exp(-17500/RT) gm/cm$^3$ sec. The value of activation energy was obtained by Wen and Ishida (1973). By using Borgwardt's data (1971), the specific surface area, \( S_g \), is correlated
with calcination temperature as:

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

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

$\lambda_\ell$, the reactivity of limestone, is a function of conversion, temperature and particle size. CaSO$_4$ formed due to the sulfation of calcined limestone tends to block the pores formed during limestone calcination, building an impervious layer on the particle surface, thus reducing the reactivity of limestone. The reactivity of limestone is calculated using the grain model developed by Ishida and Wen (1971). Typical profiles of limestone reactivity as a function of conversion for various particle sizes are shown in Fig. 3.

3. NO$_x$-Char Reaction:

Nitrogen oxides are generated during the combustion of volatiles and char, and are subsequently reduced to N$_2$ by reaction with nitrogeneous fragments (containing NH$_3$) in the volatiles and also by the heterogeneous reaction with char. Fuel nitrogen compounds in the volatiles would be in the form of NH$_3$. When the volatiles burn, NH$_3$ is oxidized to NO. When the residual char burns, nitrogeneous fragments of the char are also oxidized to NO. The released nitrogen oxides are reduced by char according to the reaction

$$C + 2 \text{NO} \rightarrow \text{CO}_2 + \text{N}_2 \tag{V.27}$$

The rate expression for NO reduction is

$$r_{\text{NO}} = \pi d_c^2 k_{\text{NO}} C_{\text{NO}}, \text{gmole NO/sec\cdotparticle} \tag{V.28}$$

where $k_{\text{NO}} = 5.24 \times 10^7 \exp(-34000/RT_m) \text{cm/sec}$ (Oguma, et al. 1977, Horio, et al. 1977).
Fig. 3 Limestone Reactivity Profiles

TEMPERATURE = 850 °C

LIMESTONE REACTIVITY, $\lambda_i$

FRACTIONAL CONVERSION OF CaO

$d_i = 100 \, \mu m$

0.2

0.3 0.4

0.5

0.6

0.7

0.8

0.9

1.0
4. Attrition and Entrainment of Char and Limestone:

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

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

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:

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

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 \( U_0 = U_{mf} \). It is of the form:

\[
E_x = 6 \exp[-10.4 \left( \frac{U_t}{U_0} \right)^{0.5} \left( \frac{U_{mf}}{U_0 - U_{mf}} \right)^{0.25}] \text{ gm/sec} \quad (V.31)
\]

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:

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

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).

\[
F_{0,sw} = A_t \cdot (U_0 - U_{mf}) f_w (1 - \varepsilon_{mf}) \rho_s \cdot f_{sw} \text{ gms/sec} \quad (V.33)
\]

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.

\[
TDH = 0.429 \frac{U_0^{1.2}}{U_0} (11.43 - 1.2 \ln \frac{U_0}{U_c}) \text{cms} \quad (V.34)
\]

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:

\[
U_{mf} = \left(\frac{\mu}{\rho g}\right)\left\{33.7^2 + \frac{0.0408 \frac{d}{\rho} \frac{3}{\rho_s - \rho_g}}{\frac{\rho g}{\mu}}\right\}^{1/2} - 33.7 \} (V.35)
\]

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):

\[
\frac{dD_B}{dz} = \frac{0.3}{D_t} (D_{BM} - D_B) \quad (V.36)
\]

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:

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

(V.37)

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

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

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

(V.38)

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

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

(V.39)

6. Solids Mixing:

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

\[ W_{mix} = (U_o - U_{mf}) A_t f_w (1 - \varepsilon_{mf}) \rho_s \]  

(V.40)

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

7. Heat Transfer:

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

$$\frac{2}{r_c} \left[ (T_c - T) + \varepsilon_m \sigma (T_c^4 - T^4) \right] = \frac{\rho_M q_{\text{char}}}{(\pi d_c^2 \cdot C_{\text{ch}})} \quad (V.41)$$

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-Boltzmann 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 cal/sec.cm$^2$. $^\circ$C (40 to 80 Btu/hr.ft$^2$.$^\circ$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>
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</table>

GROSS MIXING

**Particle trajectory**

**Drift Motion**

*Fig. 5 Two Modes of Solids Mixing*
Fig. 6 Schematic Illustration of the
Solid Phase Model

\[ X : \text{wt. fraction carbon} \]
\[ T : \text{temperature} \]
\[ w_{\text{mix}} : \text{solids mixing rate} \]
\[ w_{\text{net}} : \text{net flow rate of solids} \]
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)

\[ N_{Re} = \frac{D_t \bar{U}_o \rho_g}{\mu_g} \]  
\[ N_{Pe} = \frac{\bar{U}_o D_t}{E_z} \]  
\[ N_{Sc} = \frac{\mu_g}{D \rho_g} \]

\[ \frac{1}{N_{Pe}} = \frac{1}{N_{Re} N_{Sc}} + \frac{N_{Re} N_{Sc}}{192} \quad \text{for } N_{Re} < 2000 \]  
\[ \frac{1}{N_{Pe}} = 3 \times 10^7 \left( \frac{2.1}{N_{Re}} \right) + \frac{1.35}{1.8 \sqrt{N_{Re}}} \quad \text{for } N_{Re} > 2000 \]

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

\[ \Delta z = 2 \frac{E_z}{\bar{U}_o} \]  

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

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

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):

$$t_b = \text{burning time of a char particle}$$  \hspace{1cm} (V.49)

$$t_b = \frac{\rho_{c,\text{ch}} R_g T_m d_c^2}{96 \phi D P_{O_2}}$$  \hspace{1cm} (V.50)
VI. MODEL DESCRIPTION

1. Elutriation Calculations:

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

\[
W_{f,x} + W_{x-1} + a_x k_x M_x
\]

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

\[
= M_x \frac{W_D}{M_b} + R_x q_{1x} (1-p_1) + R_x q_{2x} (1-q_{1x}) (1-p_2)
\]

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

\[+ R_x (1-q_{1x}) (1-q_{2x}) + k_x M_x\]

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

\[+ W_x\]

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

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

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

$$\frac{dd_x}{dt} = -k_x \frac{d_x}{3} (U - U_m)$$ \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, $W_x = \left[W_{F,x} + a_x K(U - U_m)M_0 + W_{x-1}\right] (\frac{d_{x+1}}{d_x})^3$. (VI.6)

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

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

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

**Volatile**

\[ \frac{F_{EM,i} Y_{E,v,i}}{Y_{E,i-1}} = \frac{F_{EM,i-1} Y_{E,v,i-1} - a_1 Y_{E,v,i-1}}{X_{O_2} + R_{v,i}} \]

(Volatiles out) (Volatiles in) (Volatiles Exchanged to Bubble Phase)  
(VI.8)

where

\[ a_1 = \frac{k_{BE,i} A_{t,i} \Delta Z_i \varepsilon_{t,i}}{R \cdot g T_i}, \text{ g mole/sec} \]  
(VI.9)

**Carbon monoxide:**

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

(CO out) (CO in) (CO Exchanged to Bubble Phase)
(CO Produced by Volatiles) \quad \text{(CO Released during Devolatilization)}

\[ + \, 2 \, a_4 \, \frac{Y_E \, \text{CO}_2}{i} \quad \text{(VI.10)} \]

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

where

\[ a_4 = a_m \, A_{t,i} \, \Delta Z_i \, \left(1 - e_{c,i} - e_{\text{tube},i}\right) \left(k_{\text{C-O}_2,i} \, \frac{P}{R \, T_{E,i}} \, X_i\right), \text{g mole/sec} \quad \text{(VI.11)} \]

\[ a_m = \frac{6 \, \rho_b (1 - \varepsilon_{mf})}{d \, \rho_{ch} \, C_{ch}} \quad \text{(VI.12)} \]

\section*{Carbon dioxide:}

\[ F_{EM,i} \, \frac{Y_E \, \text{CO}_2}{i} = F_{EM,i-1} \, \frac{Y_E \, \text{CO}_2}{i-1} - a_1 (Y_E \, \text{CO}_2,i \, - \, Y_B \, \text{CO}_2,i) \]

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

\[ + \, R_{\text{CO}_2,i} - a_4 \, \frac{Y_E \, \text{CO}_2}{i} \quad \text{(VI.13)} \]

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

\section*{Bubble Phase Equations}

\section*{Oxygen:}

\[ F_{BM,i} \, \frac{Y_B}{i} = F_{BM,i-1} \, \frac{Y_B}{i-1} - a_1 \, \frac{Y_B}{i} \]

\[(\text{Oxygen out}) \quad \text{(Oxygen in}) \quad \text{(Oxygen Exchanged to Emulsion Phase)} \]
\[-a_2 Y_{B,i} \Delta t_i \Delta y_i (c_{C,i} - c_{B,i})\]  \\
\[= a_1 Y_{E,CO,i} - a_1 Y_{E,v,i} X_{O_2,c} \] \hspace{1cm} (VI.14)

(Oxygen Consumed by Char) \hspace{1cm} (Oxygen Consumed by CO Exchanged to Volatiles Exchanged to Bubble Phase)

where
\[a_2 = a_m A_{t,i} \Delta y_i (c_{C,i} - c_{B,i}) k_{cB,i} \frac{P}{P_{GB,i}} X_i \] \hspace{1cm} (VI.15)

Carbon dioxide:
\[F_{BM,i} Y_{B,CO_2,i} = F_{BM,i-1} Y_{B,CO_2,i-1} - a_1 (Y_{B,CO_2,i} - Y_{E,CO_2,i}) \]
\[\text{(CO}_2\text{ out}) \hspace{1cm} (\text{CO}_2\text{ in}) \hspace{1cm} (\text{CO}_2\text{ Exchanged to Emulsion Phase})\]
\[+ a_2 Y_{B,i} + a_1 Y_{E,CO,i} + a_1 Y_{E,v,i} V_{CO_2} \] \hspace{1cm} (VI.16)

(CO\text{\textsubscript{2} Produced by Char Combustion}) \hspace{1cm} (CO\text{\textsubscript{2} Produced by CO Combustion}) \hspace{1cm} (CO\text{\textsubscript{2} Produced by Volatiles Burning})

**FREEBOARD EQUATIONS**

Oxygen:
\[Y_{O,i} = 0.0 \] \hspace{1cm} (VI.17)
Volatiles:
\[ F_{MT} Y_{v,i} = F_{MT} Y_{v,i-1} - F_{MT} Y_{0,i-1}/X_{O_2} \]  \hspace{1cm} (VI.18)

\begin{align*}
\text{(Volatiles out) (Volatiles in) (Volatiles Burnt)}
\end{align*}

Carbon monoxide:
\[ F_{MT} Y_{CO,i} = F_{MT} Y_{CO,i-1} + 2 a_4 Y_{CO_2,i} \]

\begin{align*}
\text{(CO out) (CO in) (CO Produced by C-CO}_2 \text{ Reaction)}
\end{align*}

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

\begin{align*}
\text{(CO Produced by Volatiles Burning)}
\end{align*}

\[ a_4 = \frac{P}{R G_{TB,i}} N c_{1} d_{2} k_{CO_2,i} \text{ mole/sec} \]  \hspace{1cm} (VI.20)

Carbon dioxide:
\[ F_{MT} Y_{CO_2,i} = F_{MT} Y_{CO_2,i-1} - a_4 Y_{CO_2,i} \]  \hspace{1cm} (VI.21)

\begin{align*}
\text{(CO}_2 \text{ out) (CO}_2 \text{ in) (CO}_2 \text{ Consumed by C-CO}_2 \text{ Reaction)}}
\end{align*}

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

**EMULSION PHASE EQUATIONS**

Volatiles:
\[ Y_{E,v,i} = 0.0 \]  \hspace{1cm} (VI.22)

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

\begin{align*}
\text{(Oxygen out) (Oxygen in) (Oxygen Exchanged to Bubble Phase)}
\end{align*}
\[- a_3 \frac{Y_{E,i}}{\phi_{E,i}} - (F_{EM,i-1} Y_{E,v,i-1} + R_{v,i}) X_{O_2}\]

(Oxygen consumed by Volatiles Burning)

\[- k \frac{17.5 Y_{E,i}}{1 + 24.7 Y_{E,i}}/2.0 \]

(Oxygen Consumed by CO)

where

\[k = 3 \times 10^{10} \exp(-16000/RT_i) \left(\frac{P}{R g T_i}\right)^{1.8} Y_{H_2O}^{0.5} A_{E,i} \Delta Z_i (i-\epsilon_c, i-\epsilon_{tube,i}) \epsilon_{mf}\]

gmole/sec (VI.24)

\[a_3 = a_m A_{E,i} \Delta Z_i (1-\epsilon_c, i-\epsilon_{tube,i}) k_{E,i} \frac{P}{R g T_i} X_{i}\]

(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)

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

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

\[+ 2 a_4 Y_{E,CO_2,i} + a_3(2 - \frac{2}{\phi_{E,i}}) Y_{E,i}\]

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

(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)
\[ 17.5 Y_{E,i} + k \frac{Y_{E,CO,i}}{1 + 24.7 Y_{E,i}} + R_{CO_2,i} \]

\[(CO_2 \text{ Released during Devolatilization})
\]

\[-a_4 Y_{E,CO_2,i} + a_3 \left( \frac{2}{f_{E,i}} - 1 \right) Y_{E,i} \]

\[(VI.27)\]

\[(CO_2 \text{ Produced by CO Combustion})
\]

\[= a_3 \left( \frac{2}{f_{E,i}} - 1 \right) Y_{E,i} \]

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

**BUBBLE PHASE EQUATIONS**

**Oxygen:**

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

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

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

\[(VI.28)\]

\[(Oxygen \text{ Consumed by CO Char Combustion}) \quad (Oxygen \text{ Consumed by CO Char Combustion Exchanged to Bubble Phase})
\]

**Carbon dioxide:**

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

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

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

\[(VI.29)\]

\[(CO_2 \text{ Produced by Char Combustion}) \quad (CO_2 \text{ Produced by CO Combustion})
\]

**FREEBOARD EQUATIONS**

**Volatiles:**

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

\[(VI.30)\]

**Oxygen:**

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

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

(Oxygen Consumed by CO Combustion)  

\[ (Oxygen Consumed by Char Combustion) \]

where

\[ k' = 3 \times 10^{10} \exp(-16000/RT) \frac{P}{R T_1} \frac{1.8 Y_{0,1}}{e^{1.82}} \frac{1.5 A_{t-i} \Delta z_i (1-c_{\text{tube},i})}{g \text{ mole/sec}} \text{(VI.32)} \]

\[ a'_2 = \left( \frac{P}{R T_{B,i}} \right) N c_i \pi r_d^2 k c_i \text{ gmole/sec} \text{(VI.33)} \]

Carbon monoxide:

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

(CO out)  

(CO in)  

(CO Produced by C-CO$_2$ Reaction)

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

(CO Produced by Volatiles Burning)  

(CO Produced by Char Combustion)

\[ - k' \frac{17.5 Y_{0,1}}{1+24.7 Y_{0,1}} \]  

(CO Burnt)

Carbon dioxide:

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

(CO$_2$ out)  

(CO$_2$ in)  

(CO$_2$ Consumed by C-CO$_2$ Reaction)

\[ + \frac{a}{2} \frac{2}{\phi_{B,i}} Y_{C,i} (2 - 1) + k' \frac{17.5 Y_{0,1}}{1+24.7 Y_{0,1}} \]  

(CO$_2$ Produced by Char Combustion)  

(CO$_2$ Produced by CO Combustion)
The boundary conditions are:

\[ Y_{B,1} = 0.21 \frac{F_{MF}}{F_{MT}} \]  

\[ Y_{E,1} = Y_{B,1} \]  

\[ Y_{E,v,1} = 0.0 \]  

\[ Y_{E,CO_2,1} = 0.0 \]  

\[ Y_{E,CO_2,1} = 0.0 \]  

\[ Y_{B,CO_2,1} = 0.0 \]  

**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°K (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**

\[ F_{EM,i} Y_{E,SO_2,i} = F_{EM,i-1} Y_{E,SO_2,i-1} - a_1(Y_{E,SO_2,i-1} - Y_{B,SO_2,i}) \]  

\( (SO_2 \text{ out}) \)  

\( (SO_2 \text{ in}) \)  

\( (SO_2 \text{ Exchanged to Bubble Phase}) \)
\(-a_{E,SO_2,i} Y_{E,SO_2,i} + R_{E,SO_2,c,i} + R_{E,SO_2,V,i}\) (VI.44)

(SO\(_2\) Absorbed by Limestone) (SO\(_2\) Released during Char Combustion) (SO\(_2\) Released during Volatiles Combustion)

where

\[a_{E,SO_2,i} = A_{t,i} \Delta Z_i (1-\varepsilon_{c,i} - \varepsilon_{\text{tube},i}) (1-\varepsilon_{\text{mf}}) k_v \left(\frac{P}{R T_i}\right), \text{ g mole/sec (VI.45)}\]

\[F_{E,NO,i} Y_{E,NO,i} = F_{E,NO,i-1} Y_{E,NO,i-1} - a_1 (Y_{E,NO,i} - Y_{B,NO,i})\] (NO out) (NO in) (NO Exchanged to Bubble Phase)

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

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

where

\[a_{E,NO,i} = a_m A_{t,i} \Delta Z_i (1-\varepsilon_{c,i} - \varepsilon_{\text{tube},i}) k_{E,NO,i} \frac{P}{R g T_i} X_i, \text{ g mole/sec (VI.47)}\]

**BUBBLE PHASE EQUATIONS**

\[F_{BM,i} Y_{B,SO_2,i} = F_{BM,i-1} Y_{B,SO_2,i-1} - a_1 (Y_{B,SO_2,i} - Y_{E,SO_2,i})\] (SO\(_2\) out) (SO\(_2\) in) (SO\(_2\) Exchanged to Emulsion Phase)

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

(SO\(_2\) Absorbed by Limestone) (SO\(_2\) Released during Char Combustion) (SO\(_2\) Released during Volatiles Combustion)

where

\[a_{B,SO_2,i} = A_{t,i} \Delta Z_i (\varepsilon_{c,i} - \varepsilon_{B,i}) (1-\varepsilon_{\text{mf}}) k_v \left(\frac{P}{R T_i}\right), \text{ g mole/sec (VI.49)}\]
\[
F_{BM,i} Y_{B,NO,i} = F_{BM,i-1} Y_{B,NO,i-1} - a_1 (Y_{B,NO,i} - Y_{E,NO,i})
\]
\begin{equation}
\text{(NO out)} \quad \text{(NO in)} \quad \text{(NO Exchanged to Emulsion Phase)}
\end{equation}

\[
- a_{B,NO,i} Y_{B,NO,i} + R_{B,NO,c,i} + R_{B,NO,V,i}
\]
\begin{equation}
\text{(NO Reduced by Char)} \quad \text{(NO Released during Char Combustion)} \quad \text{(NO Released during Volatiles Combustion)}
\end{equation}

where

\[
a_{B,NO,i} = a_m A_t, i \frac{\Delta Z_{i} (c_{i} - e_{tube,i}) k_{B,NO,i}}{R T_i} \frac{p}{g_{B,i}} x_{i}, \text{ g mole/sec} \quad \text{(VI.51)}
\]

**FREEBOARD EQUATIONS**

\[
F_{MT} Y_{SO_2,i} = F_{MT} Y_{SO_2,i-1} + R_{SO_2,i} - a_{SO_2,i} Y_{SO_2,i}
\]
\begin{equation}
\text{(SO_2 out)} \quad \text{(SO_2 in)} \quad \text{(SO_2 Released)} \quad \text{(SO_2 Absorbed by Limestone)}
\end{equation}

where

\[
a_{SO_2,i} = \left(\frac{p}{R T_i}\right) N \pi d^3 \frac{2e_{i}}{k_{B,i}} v_i, \text{ g mole/sec} \quad \text{(VI.53)}
\]

\[
F_{MT} Y_{NO,i} = F_{MT} Y_{NO,i-1} + R_{NO,i} - a_{NO,i} Y_{NO,i}
\]
\begin{equation}
\text{(NO out)} \quad \text{(NO in)} \quad \text{(NO Released)} \quad \text{(NO Reduced by Char)}
\end{equation}

where

\[
a_{NO,i} = \left(\frac{p}{R T_i}\right) N \pi d^2 c_{i} \frac{2e_{i}}{k_{NO,i}}, \text{ g mole/sec} \quad \text{(VI.55)}
\]

The boundary conditions are:

\[
Y_{E,SO_2,1} = Y_{B,SO_2,1} = Y_{E,NO,1} = Y_{B,NO,1} = 0.0 \quad \text{(VI.56)}
\]

**SOLID PHASE MATERIAL BALANCE**

The overall material balance for the solids in ith compartment in terms of net solids flow, \( W_{net,i} \) is given by:
\[ W_{\text{net},i} = W_{\text{net},i-1} + W_{fc,i} R_{\text{ch}} + W_{fa,i} \]
(solids out) (solids in) (Char feed) (Additives Feed)

\[-W_{D,i} = r_i \]
(Solids Withdrawal (Char Burnt))

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, \( W_{\text{mix}} \):

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

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

The boundary conditions are:

\[ W_{\text{mix},1} = W_{\text{mix},M1} = 0.0 \]  
(VI.59)

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

\[ C_s (W_{\text{mix},i} - W_{\text{net},i})T_{i+1} \]
(heat in from \((i+1)\)th cell)

\[-C_s \{ (W_{\text{mix},i-1} - W_{\text{net},i-1} + W_{\text{mix},i} - W_{D,i}) + C_{gm} F_{MT} \} T_i \]
(heat out from \( i \)th cell)

\[ + [C_s W_{\text{mix},i-1} + C_{gm} F_{MT}]T_{i-1} + r_i q_{\text{ch}} \]
(heat in from \((i-1)\)th cell) (heat generated by char combustion)

\[ + g_{E,i} q_{V,\text{CO}} + g_{B,i} q_{V} + g_{CO,i} q_{\text{CO}} \]
(heat generated by volatiles combustion in emulsion phase) (heat generated by volatiles combustion in bubble phase) (heat generated by CO combustion)
\[-q_{\text{cal}} W_{fa,i} + \left(W_{fa,i} C_{sf} + W_{fc,i} C_{cf}\right)T_{sf,i}\]

(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) (heat losses through the walls) (VI.60)

**ENERGY BALANCE IN THE FREEBOARD**

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

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

(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)

\[-(W_{\text{ent},i} C_{S} + C_{gm} F_{MT}) T_{i} = A_{t,i} \Delta Z_{i} a_{HE,i} U_{i} (T_{i} - T_{w,i})\]

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

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

(heat losses through the walls) (VI.61)

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

Heat capacity of solids, \( C_S = 0.215 \) cals/gm\( \cdot \)°C

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

Density of limestone = 2.4 gms/cm\(^3\)

Density of coal = 1.4 gms/cm\(^3\)

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

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

where
\[
D_{BM} = 0.652 \{A_t (U_o - U_{mf})\}^{0.4}
\]
\[
D_{BO} = 0.347 \{A_t (U_o - U_{mf})/n_d\}^{0.4}
\]

Bubble velocity, \( U_B = U_o - U_{mf} + 0.711 \sqrt{g D_B} \)

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

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

where \( \alpha_b = \varepsilon_{mf} U_B/U_{mf} \)

Void fraction at minimum fluidization, \( \varepsilon_{mf} = 0.5 \)
TABLE 3. PARAMETERS IN THE MODEL

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

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

Bed to wall heat transfer coefficient = 0.0021, cals/sec$\cdot$cm$^2$$\cdot$K

Solids mixing parameter, $f_w = 0.075\sim0.3$

Fraction of wake solids thrown into the freeboard, $f_{sw} = 0.1\sim0.5$

Cooling water temperature = $300^\circ$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

NO

SUBROUTINE CORRECT

YES

PRINT

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

Design Data  Input  Operating Conditions

Combustion  No  Hydrodynamics

Yes

Initial Values
ETCA \cdot T_i \cdot X_i
T_{i,old} : T_i

Hydrodynamics
Gas Phase Material Balance
ETCG : \frac{\text{O}_2 \text{ in} - \text{O}_2 \text{ out}}{\text{Stoichiometric O}_2}

Subroutine
CRRECT

No

ETCA : ETCG

Yes

Carbon Balance
X_i

Gas Phase Balance

Energy Balance \Rightarrow T_i
\sum \frac{|T_{i,old} - T_i|}{M}
TNORM : \frac{\sum T_i}{M}
TAV : \sum T_i / M

No

TNORM \leq 1\% TAV

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>
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<tr>
<th>Type</th>
<th>Bed Cross-section (sizes in cms)</th>
<th>Specific surface area -cm²/cm³ 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>5.4</td>
<td>9.9</td>
<td>11.4</td>
<td>Horizontal staggered</td>
</tr>
<tr>
<td>Gibbs, et al.</td>
<td>30</td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>(1975)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Exxon Mini Plant</td>
<td></td>
<td>0.205</td>
<td>1.9</td>
<td>-</td>
<td>5.5</td>
<td>Horizontal serpentine</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.149</td>
<td>1.9</td>
<td>-</td>
<td>-</td>
<td>Vertical coils</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>
BED HEIGHT = 67.1 cm
BED TEMP. = 749 °C
FLUIDIZING VEL. = 120 cm/sec
LIMESTONE 18
NO RECYCLE
NCB DATA
PREDICTED
ELUTRIATED
FEED
BED

Fig. 10 Size Distributions of the Particles in the FBC
EXXON DATA (1970)

SIMULATED

+ HORIZONTAL COILS

- - VERTICAL COILS

EXCESS AIR: 13.4%

FLUIDIZING VEL.: 190 cms/sec

PRESSURE: 9 atm.

COAL FEED POINT COOLING COILS

HEIGHT ABOVE THE DISTRIBUTOR, cms

Fig. 11 Simulation of Axial Bed Temperature Profile
bed, the free moving, coalescing bubbles are constrained and may be broken as they impinge on the walls of the tubes. Hence the solids movement is retarded which in turn affects the temperature profile. In the model the solids mixing in the bed is represented by the mixing coefficient, \( f_w \). For poor solids mixing \( f_w \) takes low values \((0.05-0.2)\) and for vigorous mixing it takes high values \((0.2-0.4)\). A simulation of the operation of NASA fluid bed combustor is presented in Fig. 12. Again in this combustor, closely packed horizontal tubes are employed for heat removal. As indicated earlier, the solids mixing is poor which is clearly shown by the non-uniform temperature profile and the non-uniform carbon concentration profile in the bed. Carbon concentration peaks at the coal feed point and decreases rapidly within the bed as combustion proceeds. Because of the higher concentration of carbon and oxygen near the coal feed point near the distributor, the combustion rate and the heat release rate are higher than the remaining part of the bed. This results in a high temperature zone near the coal feed point. On the other hand, in the freeboard region, though combustion takes place, due to the heat losses through the wall, the temperature drops.

The concentration profiles of oxygen in the bubble and emulsion phases together with the volatiles concentration in the bed are shown in Fig. 13. Experimental observations reported by Gibbs, et al. (1975) on the time averaged oxygen concentrations along the bed height are also shown. Time averaged concentration is neither the bubble phase nor the emulsion phase concentrations since they are obtained from gas analyzer probes. The peaks and valleys of the analyzer response which
**Fig. 12** Temperature and Carbon Concentration Profiles in the Bed
Fig. 13 Oxygen Concentration Profile in the Bed
correspond to that of bubble and emulsion phase oxygen concentrations respectively are averaged to obtain the concentration profile.

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

Fig. 14 shows the concentration profiles of CO$_2$, CO and volatiles in the bubble and emulsion phases. The concentrations of CO and volatile products in the bubble phase are zero since complete combustion of these gases is assumed in this phase. The experimental data shown are the time averaged concentrations of CO$_2$ and CO in the bed. Near the coal feed point, the volatiles released in the emulsion phase burn to form carbon monoxide, the concentration of which increases along the combustor height. As long as volatiles are present in the emulsion phase the combustion of char and CO does not take place, whereas the C-CO$_2$ reaction takes place. Hence the CO$_2$ concentration in the emulsion phase along the bed height decreases until all the volatiles are burnt. Once CO and char combustion start, CO$_2$ concentration increases in the emulsion phase. On the other hand, CO$_2$ concentration in the bubble phase increases gradually as a function of the bed height indicative of the progressive combustion of char and volatiles in the bubble phase.
In CO$_2$ CONCENTRATION, mole percent

CO$_2$ CONCENTRATION, mole percent

CO$_2$ CONCENTRATION, mole percent

DIMENSIONLESS BED HEIGHT

Fig. 14 CO, CO$_2$, & Volatiles Concentration Profiles in the Bed
In regard to the absorption of SO$_2$ by the limestone present in fluidized bed combustors, the percentage absorption increases with an increase in the Ca/S ratio. Ca/S ratio is the most significant operating variable 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 cm/s
- Bed Temperature = 850 °C
- Bed Height = 67 cm
- NCB Data
- Predicted
Fig. 16 Effect of Temperature on SO₂ Retention
Fig. 17 Effect of Fluidizing Velocity on 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.
Fig. 18 $\text{SO}_2$ 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.
Fig. 19 Effect of Temperature on NO Emission
Fig. 20 NO and Carbon Concentration Profiles in the Bed
Higher concentrations of NO in the emulsion phase near the coal feed point are the results of rapid evolution and combustion of volatiles from coal in this region. The NO concentration in the bubble phase increases because of char and volatiles combustion. Fig. 20 also indicates the NO concentrations in the freeboard. In the freeboard both char combustion and NO reduction take place. When the char burns NO is released from the nitrogen contained in the char. These two competing reactions determine the total NO emission at the outlet of the combustor.
VIII. SENSITIVITY OF THE MODEL PARAMETERS

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

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

$$F_0 = A_t (U_o - U_{mf}) f_w (1 - \varepsilon_{mf}) \rho_s f_{sw} \text{ gm/sec}$$  \hfill (VIII.1)
Fig. 21 Effect of Solids Mixing on the Bed Temperature Profile

* NASA DATA
C: COOLING TUBES

PRESSURE = 5.15 atm
EXCESS AIR = 64%
EXPANDED BED HT. = 142 cms
$U = 0.00765 \text{ cal/sec.cm}^2 \text{°C}$

$U_w = 0.002 \text{ cal/sec.cm}^2 \text{°C}$
for a set of operating conditions, increasing the value of $f_{sw}$ increases the solids splashing rate at the bed surface. If a large portion of char leaves the bed, char elutriation from the combustor will also be large. This will result in lower combustion efficiency, and hence a lower temperature in the bed. The temperature drop in the freeboard decreases as $f_{sw}$ increases because of increased combustion in the freeboard. This is clearly illustrated in the Fig. 22. It should be borne in mind that the NASA fluidized bed combustor is a small unit and heat losses from the wall in the freeboard are considerable. If the bed is bigger in size than that is used here for simulation, the heat losses through the walls will be minimal. Also, with good insulation, heat losses can be reduced. In large commercial combustors, if the entrainment is increased, combustion of char in the freeboard will also increase resulting in higher temperatures in the freeboard. Hence it is seen that the parameter $f_{sw}$ is very critical and has to be carefully evaluated in order to properly account for the freeboard reactions.

Fig. 23 is a parametric study of the effect of bed to tube heat transfer coefficient on the temperature profile in the bed. Changes in the value of the heat transfer coefficient do not significantly affect the shape of the temperature profile but affect the level of bed temperature. As can be seen from Fig. 23, if the actual heat transfer coefficient were 0.00765 cals/sec.cm$^2$°C (56 Btu/hr.ft$^2$.°F), assuming a lower heat transfer coefficient of 0.0063 cals/sec.cm$^2$°C (46 Btu/hr.ft$^2$.°F) would result in a temperature difference of about 40°C above the actual temperature. So it is apparent that an accurate
Fig. 22 Effect of Solids Entrainment on the Temperature Profile
Fig. 23 Effect of Bed to Tube Heat Transfer Coefficient on the Bed Temperature
estimation of the heat transfer coefficient for a wide range of design is critical to make accurate predictions of bed temperatures.

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

The following conclusions can be drawn from this study:

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

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

3. The model confirms the importance of the role of solids mixing in maintaining a uniform bed temperature. Poor solids mixing results in nonuniform temperature profile and carbon concentration profile in the bed. The poor mixing is accounted for by \( f_w \), the solids mixing parameter in the model. This important parameter in the model also accounts for the devolatilization of coal. The assumption of a major portion of the volatiles being released near the feed point is justified by the concentrations of NO, O\(_2\) and CO observed experimentally near the coal feed point.

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

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

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

7. The concentration profiles of 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

1. A GENERAL MODEL FOR FBC ELUTRIATION CALCULATIONS
2. PROGRAMMED BY
3. RENGA RAJAN
4. AT
5. WEST VIRGINIA UNIVERSITY

REAL MC,MH2,MS,M0,MN2,MN0,MH2O,M02,MH2S,M0S2,M0D,MCD,MCAO,MCAS,MCAS04
COMMON /A/ MHE(30),AHE(30),DTUBE(30),PV(30),PH(30),ZI(30),
1. 1AIR(30),UHF(30),DUBEFF(30),UTA(30),UTF(30),
2. 2ENF,GF,P,HLMF,HLF,HALF,VAT,FMD,KHOCH,RHOBED,B2AV,VMH,VAR,ETC,
3. 3DPSUB,NPUMB,DCSVB,DCWMB,U0,MAIR,CHAR

COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRL(30),FRA(30),
1. LWF(30),QI(30),Q2(30),BN(30),RH(30),W(30),E(30),ENT(30),ELUA(30),
2. 2ENTC(30,30),FRASN(30),FREL(30),CU(30),

3PLA(30),GFLOW,WCOAL,WAD,WAR,WBE,VELUA,CELU,EFF,NC,NCF,
4XAT,WX,CHAR,CHAR,NDIS,ROHAD,TDHC,HFB,NDF

NAMELIST /OPCF/ HLMF,VMF,HLF,WB,WBE,RHOBED,RHOCHAR,CHAR,
1.CCHAR,HCHAR,CHAR,HCHAR,TNCHAR,
2.UO,GFLOW,MGAS,MOF,NFEXAIR,TAV,PAV,CHAR,CHAR,CHAR,
3WAD,WCOAL,TDHC,HFB

/RES/ WDIS,VELUA,CELU,EFF,DPSUB,DPWMB,DCSVB,DCWMB,
2DASVF,DAWCF,DCSVF,DCWCF

DATA MC,MH2,MS,M0,MN2,MN0,MH2O,M02,MH2S,M0S2,M0D,MCD,MCAO,MCAS,MCAS04
1. 1/12.,2.,32.,32.,28.,30.,18.,64.,28.,44.,56.,08,136.,14/6,
2. DATA RHOCR,ROSH/1.4,1.4/

3RHOAD = 2.4
3. EMF = 0.5
Q = 980.1
3. 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 = SUMA + FRACTA(I)/DP(I)
SUMB = SUMB + FRACTA(I)*DP(I)
SUMC = SUMC + FRACTC(I)/DP(I)
SUMD = SUMD + FRACTC(I)*DP(I)

DO 10 I = 2,NDP
DP(I) = (DIA(I-1)+DIA(I)) * 0.5
SUMA = SUMA + FRACTA(I)/DP(I)
SUMB = SUMB + FRACTA(I)*DP(I)
SUMC = SUMC + FRACTC(I)/DP(I)
SUMD = SUMD + FRACTC(I)*DP(I)

CONTINUE

DASVF = 1./SUMA
DAWCF = SUMA
DCSVF = 1./SUMC
DCWCF = SUMD
Limestone Composition

READ(5,10)NAME1,NAME2,XCAO,XMGO,XSIO2,XCO2

Composition and net heating value of coal

--------

XCF  : fixed carbon
XCV  : volatile carbon
XH   : hydrogen
XS   : sulphur
XO   : oxygen
XN   : nitrogen
XM   : moisture

----------------- Dry Basis -----------------

READ(5,10)NAME1,NAME2,XC1,XH,XS,XO,XN,XM

Operating Conditions 1 (Bed Condition)

READ(5,1001)HMF,HHL,FPR,TAV

Operating Condition 2 (Solids and gas feeds)

READ(5,1001)HCOAL,MAH0,CAH0,FMF,EXAIR

Calculation of Volatiles yield and the composition of volatiles

WV = 0.28*(100.*XW-10.7)
R = EXP(26.41-3.764*ALOG(TAV-273.))+0.015*100.*XW)
V = (100.*XW + R - WV)*XW

RN = 1.6-0.001*TAV

IF (RN > GT, 1, RN = 1, 0)

IF (RN < LT, 0, RN = 0)

RS = RN

RD = 0.0

RH = 0.0

CH4 = 0.204-0.469*XW+0.241*XW*XW

H2 = 0.157-0.066*XW+1.338*XW*XW

CO2 = 0.135-0.900*XW+1.903*XW*XW

CO = 0.423-2.655*XW+4.845*XW*XW

H2O = 0.409-2.389*XW+4.554*XW*XW

TAR = -1.3257+2.792*XU-13.89*XW*XW

HTAR = XH*(1.-RH)*(1.-XW) - VP(CH4/16.*H2/2.+H2O/18.)*XW

QTAR = XH*(1.-RQ) - VP(CO2/44.+CO/28.*H2O/18.)*0.5*XW

TAR = 120.0

CH4 = XH*CH4/16.0

H2 = XH*H2/2.0

CO2 = XH*CO2/44.0

CO = XH*CO/28.0

H2O = XH*H2O/18.0

CTAR = V*TAR - HTAR - QTAR

TAR = (CTAR*HTAR+QTAR)/TAR

RVGAS = CH4*H2*CTAR

COV = CO/RVGAS

CO2V = CO2/RVGAS

CO2VB = COV'

xCV = CTAR + (CH4+C02+C0)*12.0
121.
XCF = XC - XCV
122.
RC = XCF / XC
123.
COALC = XC / 12.0
124.
COALH = XH
125.
COALO = XO / 16.0
126.
COALN = XN / 14.0
127.
COAL = XH / 32.0
128.
CHRC = RC * COALC
129.
CHARH = RH * COALH
130.
CHARO = RO * COALO
131.
CHARN = RN * COALN
132.
CHARS = RS * COAL
133.
RC = COALC
134.
CHRC = CHRC / RCHAR
135.
CHARH = CHARH / RCHAR
136.
CHARO = CHARO / RCHAR
137.
CHARN = CHARN / RCHAR
138.
SCHAR = SCHAR / RCHAR
139.
XW = 0.21*M02+(1.-0.21)*MN2
140.
AC = XC/MC+XH/MH2+XS/MS+XN/MN2-XO/M02
141.
FMTH = WCOAL*(1.-XW)*AC/0.21
142.
IF (EXAIR > 0.0) FMF = ATB(1)*UO*PAV/RG/TAV
143.
IF (EXAIR = 0.0) UO = FMF*RG*TAV/PAV/ATB(1)
144.
FMO = FMF*(1.-0.21)+((XC/MC+XH/MH2+XS/MS+XN/MN2+XO/M02)*(1.-XW)-1.0)
145.
FMF = FMF*(I.-O.21)*MN2+((XC/MC*XO/M02+XH/MH2+XS/MS+XN/MN2+XO/M02)*(1.-XW)+XW)*WCOAL+FTH*0.21*EXAIR*M02
146.
MGAS = GFLOW/FMO
147.
CCHAR = CHRC*±2.0/RCHAR
148.
HCHAR = CHARH*1.0/RCHAR
149.
SCHAR = CHARO*1.0/RCHAR
150.
SCHAR = CHARO*1.0/RCHAR
151.
SULFUR CAPTURE EFFICIENCY ASSUMED TO BE AROUND 95 PERCENT TO
152.
CALCULATE THE DENSITY OF THE PARTICLES IN THE BED
153.
A1 = 0.0
154.
IF (CAS > 0.0) A1 = 0.85/CAS
155.
RHOBED = (1.-XCO2+XCAO/MCAO*A1+MCASO4)*RHOBED
156.
IF (CAS EQ. 0.0) RHOBED = RHOBED
157.
WRITE (6,2000) NAMEL1,NAMEL2,XCAO,XMGOXSIO2,XCO2,
158.
*(DIA(I),FRACTA(I),I=1,NDP)
159.
WRITE (6,2010) DAVSF,AWSMFW
160.
WRITE (6,2020) NAMEC1,NAMEC2,XCF,XCV,XH+XN+XS+XO+XA+VN+V
161.
WRITE (6,2030) (DIA(I),FRACTC(I),I=1,NDP)
162.
WRITE (6,2040) DCSVF,DCWSMF
163.
IF (HLF EQ. 0.0) VHM = VOLUME(HLMF)
164.
VHM = VHM*(1.-0.21)*RHOBED
165.
CALL ELUT
166.
WRITE (6,DPGF)

ORIGINAL PAGE IS OF POOR QUALITY
180. WRITE (6, RES)
181. 1000 FORMAT (12, /* (BF10.0) */)
182. 1001 FORMAT (BF10.0)
183. 1010 FORMAT (2A4/* (BF10.0) */)
184. 2000 FORMAT ('0', '1X', '2A4', '10X', 'XCAO = ', 'F6.3', '10X', 'XMO = ', 'F6.3', '10X',
185. * 'XSIDC = ', 'F6.3', '10X', 'XC02 = ', 'F6.3', '10X', 'CM', 'T81', 'WT. FRACTION', '/* (T41, F9.4, T81, F8.4) */)
186. 2010 FORMAT ('0', '1X', 'S10', 'SURFACE VOL MEAN DIA OF ADDITIVES FEED = DASVF =',
187. * 'F10.4', '3X', 'CM', 'S10', 'WEIGHT MEAN DIAMETER = DAWMF =', 'F10.4', '3X', 'CM')
188. 2020 FORMAT ('0', '1X', '2A4', '10X', 'XCF = ', 'F6.3', '10X', 'XCV = ', 'F6.3', '10X', 'XH = ',
189. * 'F5.3', '3X', 'XN = ', 'F5.3', '3X', 'XW = ', 'F5.3', '3X', 'XO = ', 'F5.3', '3X', 'XO = ', 'F5.3')
190. 2030 FORMAT ('0', '1X', 'DIAMETER, CM', 'T81', 'WT. FRACTION', '/* (T41, F9.4, T81, F8.4) */)
191. 2040 FORMAT ('0', '1X', 'SURFACE VOL MEAN DIA OF COAL FEED = DCSVF =',
192. * 'F10.4', '3X', 'CM', 'S10', 'WEIGHT MEAN DIAMETER = DCMWF = ', 'F10.4', '3X', 'CM')
193. 2050 FORMAT ('0', '1X', 'DIAMETER, CM', 'T81', 'WT. FRACTION', '/* (T41, F9.4, T81, F8.4) */')
194. 2060 FORMAT ('0', '1X', 'SURFACE VOL MEAN DIA OF ADDITIVES FEED = DASVF =',
195. * 'F10.4', '3X', 'CM', 'S10', 'WEIGHT MEAN DIAMETER = DAWMF = ', 'F10.4', '3X', 'CM')
196. STOP
197. END
198. SUBROUTINE AREA(ZI, DTI, ATI)
199. COMMON /A/ ZHE(30), AHE(30), DTUBE(30), PV(30), PH(30), ZB(30),
200. ATBD(30), UMF(30), DVB(30), DVEFF(30), UTA(30), UTC(30),
201. 2EHF(30), PAV(30), FMG(30), RHOC(30), RHODBB, DZAV, UMF(30), XAV, ETCC,
202. 3DSVP(30), DPM(30), DCSUB, DCMWF(30), UO,MGAS,MTB,
203. COMMON /C/ DIA(30), FRACT(30), DFRATC(30), DP(30), RFC(30), FRA(30),
204. IF(30), O(30), O(30), B(30), RNI(30), W(30), E(30), ENA(30),
205. 2ENT(30, 30), DRAEN(30), RAEL(30), UO,MGAS,MTB,
206. 3PFA(30), GFLOW, WCD, AD, WB, WBC, WELUA, EFF, XC, XCF,
207. 4X, XW, CHAR, CHAR, CHAR, CHAR, XW, CHAR, CHAR, CHAR, CHAR, XW, CHAR,
208. 5FDIS, RHO, RHO, RHO, RHO, RHO, RHO, RHO, RHO, RHO, RHO, RHO, RHO, RHO,
209. 6PFA, GFLOW, WCD, AD, WB, WBC, WELUA, EFF, XC, XCF,
210. END
211. C CALCULATION OF THE CROSS SECTIONAL AREA GIVEN THE HEIGHT ABOVE
212. C THE DISTRIBUTOR
213. C DO 10 J = 1, MTB
214. IF ( ZI, GT, ZB(J) ) GO TO 10
215. RJMI = SORT ( ATB(J-1) / PI )
216. AI = ( ZI - ZB(J-1) ) / ( ZB(J) - ZB(J-1) )
217. BI = SORT ( ATB(J) / ATB(J-1) ) - 1.0
218. RI = ( 1.0 + AI * BI ) * RJMI
219. RTI = 2.0 * RI
220. ATI = PI * RI ** 2
221. GO TO 20
222. 10 CONTINUE
223. RETURN
224. END
225. SUBROUTINE ATTR(RHOC, T, DC, P, Y, RG, TB, RNI)
226. REAL MC
227. C THIS SUBROUTINE COMPUTES BURNING TIME OF A CHAR PARTICLE
228. C...
229. C EM=1.0
230. SIGM=1.36E-12
231. INDX=0
232. DTSA=100.0
233. TP=T
234. MC=12.0
235. DO 100 I=1,20
236. ETSMA=0.001*TP
237. AKS=-8710.0*EXP(-35700.0/1.986/TP)
238. TAV = (T+TP)*.5
0 = 0.26 * (TAV/1800.) * 1.75 / F

COND = 0.632E-5 * SQRT(TAV) / (I. + 245./TAV * 1.**(-1./TAV))

Z = 2500. * EXP(-12400./TAV)

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

IF (DC .GT. 0.005 : AND. DC .LE. 0.10) PHI = I./(Z+1.)*((2.*Z+1.)

IF (DC .GT. 0.10) PHI = 1.0

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

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

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

RHS = AKR*K**2*MC*G/(RG*TAV) - EM*SIGN*(TP**4-T**4)

ETS = TP - T - RHS/DC/(2.0*COND)

CALL CRRECT(I,INDX,DTS,TP, TP1, TP2, TP, E1, E2, ETS, TSMAX)

IF (INDX.EQ.2) GO TO 110

100 CONTINUE

WRITE (6, 4000)

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

110 CONTINUE

TB = RHOCCH*RG*TAV*DC**2 / (96.*PHI*D*PHI)

RKI = I./TB

RETURN

61 END

SUBROUTINE CRRECT(I,INDX,DX,XIX2,XNEWE1,E2,E,EMAX)

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

C INDX: INDEX OF THE TRIAL LEVEL

C INDX=0: JUST PROCEEDING

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

C INDX=2: THE ITERATION HAS CONVERGED

IF (ABS(E).GT.EMAX) GO TO 5

INDX=1

RETURN

5 CONTINUE

IF (INDX.EQ.1) GO TO 100

X2=XNEW

E2=E

IF (I.EQ.I) GO TO 10

IF (E1*E2.LE.0.) INDX=1

IF (INDX.EQ.1) GO TO 150

10 X1=X2

E1=E2

XNEW=XNEW+DX

RETURN

100 CONTINUE

IF (E1*E2.LE.0.) GO TO 110

E1=E

X1=XNEW

GO TO 150

110 E2=E

X2=XNEW

150 CONTINUE

XNEW=(X1-X2)*E2/(E2-E1)+X2

RETURN

END

SUBROUTINE DESIGN

COMMON /A/ ZHE(30), AHE(30), BTUBE(30), PV(30), PH(30), ZB(30),

IATB(30), UMF(30), DVH(30), DVAFF(30), UTA(30), UTC(30),

2EMF, RG, GP, HLM, FP, HMF, HMO, RHOCCH, ROBED, PAV, VMH, XAV, ETCC,

2PWSW, DCH, DCWB, UO, SGAS, MTB

COMMON /C/ DIA(30), FRACTA(30), FRACTC(30), DP(30), FRD(30), RFA(30),

LDF(30), D1(30), D2(30), BB(30), RKI(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 (5,1000) A1,A2,A3,A4
READ (5,1001) MTB,(ZB(J),ATB(J),J = 1,MTB)

C IARRNG 1 2 3
C 1 ------ VERTICAL INLINE ARRANGEMENT
C 2 ------ VERTICAL STAGGERED ARRANGEMENT
C 3 ------ HORIZONTAL INLINE ARRANGEMENT
C 4 ------ HORIZONTAL STAGGERED ARRANGEMENT

C HEAT EXCHANGE TUBES.

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

IARR(J),J = 1,MTHE
D0 100 J = 1,MTHE
D0 100 IF (AHE(J),GE,0.0) GO TO 100
D0 100 IF (DTUBE(J),EQ,0.0) GO TO 100
AHE(J) = PTUBE(J) / DTUBE(J) / (PH(J) / PV(J))
D0 100 CONTINUE
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 IJ = 1,MTHE)

Z1 = ZB(1)
AEBD1 = ATB(1)
ED1 = SORT(4.0, * AEBD1, / PI)

DV1 = 0.0
DVBEF1 = 0.0
ZHE1 = 0.0
DZAV = 30.0
N = IFIX(ZB(MTB)/DZAV)

D0 10 I = 1,N
Z2 = Z1 + DZAV
D0 20 J = 1,MTHE
IF ( ZHE(J),LE, Z1 ) GO TO 30
IF ( ZHE(J),LE, Z2 ) GO TO 30
F1 = ( Z2 - ZHE(J) ) / DZAV
F2 = ( ZHE(J) - Z1 ) / DZAV

AH = F1 * AHE(J) + F2 * AHE(J-1)
DIAT = F1 * DTUBE(J) + F2 * DTUBE(J-1)
G0 TO 40

30 AH = AHE(J)
30 CONTINUE
40 CONTINUE
G0 TO 50
50 CONTINUE

CALL AREA ( Z2,ED1,ABED )
DV1 = 0.5 *( ABED+ABED1 ) * DZAV

DVBEF(1) = DV1(1) *(1.0 - 0.25 * AH * DIAT)
Z1 = Z2
ABED1 = ABED
CONTINUE

1   1000    FORMAT (4A4)
   1001    FORMAT (I1/10F10.0))
   1002    FORMAT (I1/15F10.0))
   2000    FORMAT ('(1')/20X',4A4,'//
   2001    FORMAT ('(0',T41,'HT.ABVE DISTRIBUTOR,CH',TB1,'CROSS SECTIONAL
1 'AREA OF BED,SQ.CH.,//)
   2002    FORMAT (T49,F8.4,T96,F10.3)
   2003    FORMAT ('(0',T6,'HEIGHT,CH',T20,'SP.HEAT TRANS.AREA, SQ.CH/CU.CH',
     1T59,'Dia. OF TUBES,CH',T78,'VEr.PITCH,CH',T95,'Hor.Pitch,CH',
     1T713,'TUBES ARRNG//')
   2004    FORMAT (TBF6,2,73,F3.4,T62,F6.3,T82,F6.3,T99,F6.3,T1$,I2)
   2005    RETURN
   2006    END

SUBROUTINE ELUT

C THIS SUBROUTINE PERFORMS THE ENTRAINMENT AND ELUTRIATION CALCULATION,
C 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),
     1ATB(30),UMF(30),DV5(30),DVBEF(30),UTA(30),UTC(30),
     2E2MF,RG,EPI,HLMF,HLF,PAY,TAV,FM0RHOCH,RHOBED,D2A,UMF,XAV,ETCC,
     3DPSVBD,DPUMB,DCUMB,U0,MGAS,MTB

COMMON /C/ DIA(30),FRACTA(30),FRACTC(30),DP(30),FRC(30),FRA(30),
     1WF(30),Q1(30),Q2(30),BE(30),RK1(30),W(30),E(30),ENF(30),HELUA(30),
     2ENTC(30,30),FRAEN(30),FRAEL(30),CU(30),
     3PFAC(30),GFLOW,WCDAL,WAD,WBC,WELUA,CCEL,EF-XC,ECF,
     4XAMTR,ROBC,TDHCT,TDHC,HFB,NDF

DIMENSION FFI(30),R(30),FU(30),HP(30),DPSE(30),DCSE(30),
     1DCWE(30),DCS(30,30),FCE(30,30),WEA(30),WEC(30)

IF (HLMF .GT. 0.0) GO TO 1

HLMF = 0.5*HLF

UMF = VOLUME(HLMF)

WB = VUMF*(1.-EMF)*RHOBED

IF WB .LT. 0.0 CONTINUE

WTF = WCDAL*XA + WAD*RHOBED/RHOD

FFI(I) = 0.0

DD 25 I = 2*NDF

FFI(I) = 0.0

IF (DP(I) .LT. 0.0125 .AND. DP(I) .GE. 0.0063) FFI(I) = 0.2

IF (DP(I) .LT. 0.0063 .AND. DP(I) .GE. 0.0031) FFI(I) = 0.2

IF (DP(I) .LT. 0.0031) FFI(I) = 0.6

CONTINUE

DO = 0.75

FSW = 0.1

P1 = 0.0

P2 = 0.0

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

HT = HLF

CALL AREA(HT,DT,CSAREA)

RHOBED = PAU*MGAS/RG/TAV

VISC = 3.72E-6*TAV**0.676

U0 = GFLOW/CSAREA/RHOGAS

TDH = 0.429*U0**1.2*(11.43-1.2*ALOG(U0))

TDHC = TDH

HFB = ZB(MTB)-HLF

IF (TDH .GT. HFB) TDH = HFB

DO 10 I = 1,NDF

ORIGINAL PAGE IS OF POOR QUALITY
CALL VEL(VISC,RHOGAS,G,RHOBED,DP(I),UMF(I),UTA(I))

WF(I) = FRACTA(I)*WAD/RHOGAS/RHOGAS + FRACTC(I)*WAD \*XAD

Q1(I) = 0.0
Q2(I) = 0.0

10 CONTINUE

C WRITE(6,11) (I,UTA(I),UMF(I),I=1,NDP)

C 11 FORMAT ('0',5X,'UTA,UMF = ',12,Z7,3)

WDIS = 0.01

C

RK REPRESENTS THE ATRITION RATE CONSTANT AND IS ASSUMED TO BE THE
FOR LIMESTONE,ASH AND CHAR PARTICLES

RK = 0.003/3600. /30.48

EWB = 0.03*WB

BDIS = 0.3*WBF

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 = UQ-UMF(I)
PFA(I) = FF(I)*RK*DIFF*WB

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

CU(I) = 1.0

DO 45 K = 2,NDP

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

45 CONTINUE

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

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

DR = Q1(I)*Q1(I)-Q2(I)*Q2(I)+(1.0-Q1(I))*Q2(I)-(1.0-Q2(I))*Q1(I)

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

ARG = -10.4*SORT(UTA(I)/UQ)*(UMF(I)/DIFF)**0.25

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

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

R(I) = FO(I)*EXP(TDMC/275.0*ALG*(E(I)*FRA(I)/FO(I)))

56 CONTINUE

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

1-W(I)-RK*DIFF*WB*FRA(I)*CU(I-1)-R(I)*DR

IF (ANR .GT. 0.0) GO TO 57

FRA(I) = FRA(I)*0.5

57 CONTINUE

BB(I) = WB*ANR/WDIS

55 CONTINUE

WBC = WBC + BB(I)

C WRITE(6,110)I,FRA(I),ANR,E(I),BB(I),WF(I),UQ(I),CU(I)

C110 FORMAT (2X,'I,FRA,ANR,E,RR,WF,UQ,CU = ','1,1P7E11.3)

40 CONTINUE
480. C WRITE (6,111) L, WB, WBC, WDIS
481. C111 FORMAT ('0', '5X', 'L, WB, WBC, WDIS = ', 'I2, 1PE12.3')
482. ERR = WBC - WB
483. CALL CRRECT (L, INDEX, WDIS, X1, X2, E1, E2, ERR, EWB)
484. IF (WB < .00) WDIS = .00
485. IF (INDEX .EQ. 2) GO TO 70
486. DO 60 I = 1, NDP
487. FRA(I) = BB(I)/WBC
488. 60 CONTINUE
489. 30 CONTINUE
490. 70 CONTINUE
491. C USING THE GAS REYNOLDS NUMBER, PECLET NUMBER IS CALCULATED...
492. C AND HENCE THE GAS DISPERSION COEFFICIENT AND THE NO. OF...
493. C COMPARTMENTS IN THE FREEBOARD AND THE AVERAGE COMPARTMENT SIZE...
494. C
495. REY = DT*UO/RHOGAS/VISC
496. IF (REY < 2000.0) GO TO 300
497. PECI = 3.67/REY**2.1 + 1.35/REY**0.125
498. GO TO 310
499. 300 D = 4.26*(TAU/1800.0)**1.75/PAV
500. SC = VISC/RHOGAS/D
501. PECI = 1./REY/SC + REY*SC/192.
502. 310 EZ = UO*DT*PECI
503. DZ = 2.*EZ/UO
504. C
505. C SOLIDS ENTRAINMENT RATE ALONG THE FREEBOARD IS CALCULATED...
506. C
507. HB(C) = 0.0
508. DO 320 K = 1, 30
509. IF (N.GT.1) HB(K) = HB(K-1) + DZ
510. IF (HB(K) .GE. TDH) HB(K) = TDH
511. DO 340 I = 2, NDP
512. R(I) = 0.0
513. DIFF = UO - UMF(I)
514. IF (FRA(I) .EQ. 0.0) GO TO 340
515. IF (UMF(I) .GE. UO) GO TO 340
516. ARG = -10.4*SLRT*(UTA(I)/UO)*(UMF(I)/DIFF)**0.25
517. E(I) = 18.0*EXP(ARG)*GFLOW
518. FO(I) = DIFF*CSAREA*FSW*(1.-EMF)*RHOBED*FRA(I)
519. R(I) = FO(I)*EXP(HB(K)/275.0*ALOG(E(I)*FRA(I)/FO(I)))
520. 340 CONTINUE
521. WENTA = 0.0
522. DO 350 I = 2, NDP
523. ENTA(I) = R(I)
524. IF (FRA(I) .EQ. 0.0) AND UO .GT. 0.833*UTA(I))
525. WENTA = WF(I) + PFA(I)
526. ENTA(I) = WENTA + ENTA(I)
527. 350 CONTINUE
528. WEA(K) = WENTA
529. DO 360 I = 2, NDP
530. FRAEN(I) = ENTA(I)/agenta
531. IF (FRAEN(I) .LT. 1.E-3) FRAEN(I) = 0.0
532. 360 CONTINUE
533. SUMA = 0.0
534. SUMB = 0.0
535. DO 370 I = 2, NDP
536. SUMA = SUMA + FRAEN(I)/DP(I)
537. SUMB = SUMB + FRAEN(I)*DP(I)
538. 370 CONTINUE
539. DPSE(K) = 1./SUMA

ORIGINAL PAGE IS OF POOR QUALITY.
DPEW\( (h) = \text{SUMB} \)

IF \( \text{HP}(h) \leq \text{EQ} \), TDH \( \text{GO TO 380} \)

CONTINUE

\( \text{AT} = R \)

WELUA = 0.0

DO 80 I = 2,NDP

\( \text{ELUA}(I) = (1.0-Q1(I)) \times (1.0-Q2(I)) \times \text{ENTA}(I) \)

WELUA = WELUA + ELUA(I)

CONTINUE

DO 90 I = 2,NDP

FRAEL(I) = ELUA(I)/WELUA

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

CONTINUE

SUMA = 0.0

SUMB = 0.0

SUMC = 0.0

SUMD = 0.0

SUMA = DP(I)*FRA(I)+SUMA

SUMP = FRA(I)/DP(I)+SUMB

SUMC = DP(I)*FRA(I)+SUMC

SUMD = FRA(I)/DP(I)+SUMD

CONTINUE

DPWMB = SUMB

DPWMB = SUMA

DPWMB = SUMC

DO (4,101) WDIS,WTF,WELUA,DPWMB

(4,101) FORMAT ('O',TIO,'WDF,WTF,WELUA,DPWMB,'15F9.5','O',TIO,'PAR,DIA.,CM',T30,'BED SIZE FRACTION',T60,'ELUA SIZE FRACTION',/,'(TIO),IPEiO.3,T33,1PEIO.3,T63,ZPEIO.3,/>)

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),UH(F(I)),UTC(I))

CONTINUE

ETCA = 0.9995

INQ = 0

DETC = -0.001

EETC = 0.001

CENT = 0.0

DO 200 L = 1,30

CONTINUE

SUMA = 0.0

DO 150 I = 2,NDP

IF ((UTC(I)-UO) .LT. 0.2*UO) FRC(I) = 0.0

SUMA = SUMA + FRC(I)

CONTINUE

DO 160 I = 1,NDP

FRC(I) = FRC(I)/SUMA

CONTINUE

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

CBED = XAV*WBC/CCHAR

CELU = 0.0

CENT = 0.0
CMBEDC = 0.0
601. DO 230 I = 2,NDP
602. B(I) = FRC(I)*CBED
603. R(I) = 0.0
604. DIFF = U0-UMF(I)
605. PFA(I) = FFI(I)*RK*DIFF*CBED/CCHAR
606. FSC = 0.01
607. IF (FRC(I) .EQ. 0.0) GO TO 254
608. DO 252 K = 2,NDP
609. CUK(K) = CUK(K-1)-FRC(K)
610. IF (UMF(I) .GE. U0) DIFF = 0.0
611. W(I) = (WF(I)+PFA(I)+W(I-1))*(DP(I+1)/DP(I))**3
612. DR = Q1(I)*(1.-P1)+Q2(I)*(1.-Q1(I))*1.0-P201.-Q1(I))*(1.-Q2(I))
613. ARS = -10.4*SQRT(UTC(I)/UO)*(UMF(I)/DIFF)**0.25
614. E(I) = (18.0*EXP(ARG))*GFLOW
615. F0(I) = DIFF*CSAREA*FW*FSW*(1.-EMF)*RHOBED*XAV*FRC(I)
616. R(I) = F0(I)*EXP(TDH/275.0*ALOG(E(I)*FRC(I)/F0(I)))
617. CONTINUE
618. Y02 = 0.15
619. RHOCCH = RHOCCH*CCHAR
620. CALL ATTRCRHOCCHRAVrAVrPCI),PAV,YQ2,RG,TBRKI(l))
621. ANR = WF(I)+PFA(I)-U0
622. IF (ANR .GT. 0.0) GO TO 175
623. ARG = -10.4*SQRT(UTC(I)/UO)*(UMF(I)/DIFF)**0.25
624. E() = 18.0*EXP(ARG)*GFLOW
625. FOCI) = CSAREA*DIFF*FW*FSW*(1.-EMF)*RHOBED*XAV*FRC(I)
626. FOCI) = 0.0
627. ENTC('I) = FOCI)
628. IF (FRC(I) *EQ. 0.0 .AND. UO *GT. 0.833*UTC(I)) ENTC(1,1) = WF(I)*
629. RCHAR + PFA(I)
630. CENT = CENT + ENTC(1,1)
631. DO 430 I = 2,NDP
632. CE(1,I) = ENTC(1,I)
633. FORMAT (2X,'IFRAANR,EBR,W,WF,RKI',I2,P7EZ1.3)
634. CONTINUE
635. -DO 400 I = 2,NDP
636. DIFF = U0-UMF(I)
637. IF (FRC(I) .EQ. 0.0) GO TO 410
638. IF (UMF(I) .GE. U0) GO TO 410
639. ARG = -10.4*SQRT(UTC(I)/UO)*(UMF(I)/DIFF)**0.25
640. F0(I) = DIFF*CSAREA*FW*FSW*(1.-EMF)*RHOBED*XAV*FRC(I)
641. GO TO 415
642. F0(I) = 0.0
643. ENTC(1,I) = F0(I)
644. IF (FRC(I) .EQ. 0.0 .AND. U0 .GT. 0.833*UTC(I)) ENTC(I,I) = WF(I)*
645. RCHAR + PFA(I)
646. CENT = CENT + ENTC(1,1)
647. CONTINUE
648. C
649. C CHAR ENTRAINMENT RATE AS A FUNCTION OF THE FREEBOARD HEIGHT IS
650. C CALCULATED TAKING INTO ACCOUNT THE DECREASING PARTICLE SIZE DUE TO
651. C CHAR COMBUSTION
652. C
653. WEC(1) = CENT
654. DO 430 I = 2,NDP
655. DCE(1,I) = DP(I)
656. FCE(1,I) = ENTC(1,I)/CENT
657. CONTINUE
658. DO 420 J = 2,NDP
659. CENT = 0.0
660. CONTINUE
L(O440 I = 2, NDP

IF (DCE(J-1,I) .GT. 0.0) GO TO 435
RT = 1.06
TB = 0.0
GO TO 436
CONTINUE

CALL VEL(VISC, RHOGAS, G, RHOCH*DCE(J-1,I), UMF(I), UTC(I))
HT = HLF + HB(J)
CALL AREA (HT, DT, CSAREA)
UAV = GFLOW/CSAREA/RHOGAS
RT = (HB(J) - HB(J-1))/ABS(UAV-UTC(I))
Y02 = 0.09
CALL ATTR (RHOCH, TAV, DCE(J-1,I), PAV, Y02, RG, TB, RKI(I))
IF (TB .GT. RT) DCE(J,I) = (1.-RT/TB)**0.5*DCE(J-1,I)
CONTINUE

IF (TB .GE. RT) DCE(J,I) = 0.0
IF (DCE(J,I) .GT. 0.0) GO TO 437
ENTC(J,I) = 0.0
GO TO 438

CALL VEL(VISC, RHOGAS, G, RHOCH*DCE(J,I), UMF(I), UTC(I))
RT = HB(J)/ABS(UO-UTC(I))
DIFF = UO-UMF(I)
IF (UMF(I) .GE. UO) GO TO 431
ARG = -10.4*SQRT(UTC(I)/UO)**(UMF(I)/DIFF)**0.25
E(I) = 19.0*EXP(ARG)*GFLOW
IF (FD(I) .GT. 0.0) R(I) = FD(I)*EXP(hB(J)/273.0*ALOG(E(I))
1FRC(I)/FD(I))
CONTINUE

IF (TB .GT. RT) CONV = 1.0
IF (TB .GT. RT) CONV = 1.0
R(I) = R(I)*1.0
GO TO 432
R(I) = 0.0
GO TO 438
CONTINUE
ENTC(J,I) = R(I)
CONTINUE
CENT = CENT + ENTC(J,I)
WRITE(6,190)CELU, CENTS, DCSVB, DCWMB, (AD(I), FRC(I), DCE(I), FCE(I), I=2, NDP)
DO 460 I = 1, KT
SUMA = 0.0
SUMB = 0.0
DO 470 I = 1, NDP
IF (DCE(I) .GT. 0.0) SUMA = SUMA + FCE(I)/DCE(I)
SUMB = SUMB + FCE(I)*DCE(I)
IF (SUMA .GT. 0.0) DCSE(k) = 1./SUMA

DCWE(k) = SUMB

CONTINUE

CELU = WEC(k)

ETCC = 1.- WDIS*XA V/((WCOAL*RCHAR-CENT)*CCHAR)

XAV = ((WCOAL*RCHAR-CENT)*CCHAR*(1.-ETCC))/WDIS

WRITE (6,180) LCBED,CELU,ETCC,CELU+CENT

180 FORMAT ('LCBED,CELU,ETCC = ',F10.7,E2.3)

ERR = ETCA - ETCC

CALL CRRECT(L,IND,DETQ,XI,X2,ETCA,E,E2,ERREETC)

IF (IND .EQ. 2) GO TO 230

DO 240 I = 2,NDP

FRC(I) = BB(I)/CBEDC

240 CONTINUE

200 CONTINUE

230 CONTINUE

SUMA = 0.0

SUMB = 0.0

DO 270 I = 2,NDP

SUMA = DP(I)*FRC(I) + SUMA

SUMB = FRC(I)/DP(I) + SUMB

270 CONTINUE

DCSVB = I./SUMB

DCWMB = SUMA

DCUMB = SUMA

EFF = 1.-((WDIS*XA V+CELU+CCHAR)/((WCOAL*X1-XW)*XAV))

WRITE (6,190) CELU+CENT,DCSVB,DCWMB,(DP(I)*FRC(I))/DCE(I),

190 FORMAT ('LCBED C,CELU,ETCC = ',F10.7,E2.3)

WRITE (6,390) (NHB(K),DPSE(I),DPWE(K),WEC(K),K=1,T)

390 FORMAT ('K',9X,'FREEBOARD HT.',9X,°DPSE',2X,'DPWE',12X,'ENT RATE',//,(9X,12,SX,IP4EI.3,6X,1PE11.3,T31,1PE11.3,/) )

WRITE (6,490) (K,HB(K),DCSE(K),DCWE(K),WEC(K),K=1,T)

490 FORMAT ('FREEBOARD HT.',9X,°ENT SIZE FRACTION',9X,'ENT SIZE FRACTION',//,(TIO,TEI.3,T31,1PE11.3,/) )

RETURN

END

SUBROUTINE VEL(VISC,RHOGAS,9,RHOS,DPAR,UMUT)

C

C THIS SUBROUTINE CALCULATES THE MINIMUM FLUIDIZATION VELOCITY AND

C THE TERMINAL VELOCITY OF THE PARTICLE

C

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 .LT. 0.4) GO TO 210

UT = 0.5*(RHOS-RHOGAS)*DPAR**2/19./VISC

REP = DPAR/RHOGAS*UT/VISC

IF (REP .LE. 0.4) GO TO 210

UT = SQRT(3.1*G*(RHOS-RHOGAS)*DPAR/VISC)

RETURN

210 RETURN

END

FUNCTION VOLUME (ZZ)

C

C THIS SUBROUTINE CALCULATES THE MINIMUM FLUIDIZATION VELOCITY AND

C THE TERMINAL VELOCITY OF THE PARTICLE
Calculation of the effective volume of the bed given the height

N = IFIX (ZZ/DZAV)+1
IF (N.EQ.1) N = 2
SUM = 0.0
ZN = FLOAT(N-1)*DZAV
DO 100 I = 2, N
SUM = SUM + DVBEFF(I)
IF (I .LT. N ) GO TO 100
A1 = ( ZZ - ZN ) / DZAV
SUM = SUM + DVBEFF(I) * A1
100  CONTINUE
VOLUME = SUM
RETURN
END
### APPENDIX II

**INPUT TO ELUTRIATION PROGRAM**

```
<table>
<thead>
<tr>
<th></th>
<th>ATB(1)</th>
<th>ZB(2)</th>
<th>ATB(2)</th>
<th>ZB(3)</th>
<th>ATB(3)</th>
<th>ZB(4)</th>
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<td>81.3</td>
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<td>PH(1)</td>
<td>IARR(1)</td>
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<td>PV(5)</td>
<td>PH(5)</td>
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**NBP**

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**NAME1 NAME2**

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**NAME1 NAME2**

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**Statistics**

- **Object Code**: 39764
- **Bytes Array Area**: 16816
- **Bytes Total Area Available**: 126976

**Diagnostic**

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**Compile Time**: 2.02 sec, **Execution Time**: 4.70 sec

**Date**: 17-03-63, **Day**: Wednesday, **Month**: 1 Nov 77, **Time**: 5:54PM
APPENDIX IV

COMBUSTION PROGRAM

2. C A GENERAL MODEL OF FLUIDIZED BED COAL COMBUSTOR

3. C PROGRAMMED BY

4. C RENGA RAJAN

5. C AT

6. C WEST VIRGINIA UNIVERSITY

7. C

8. C

9. C

10. C

REAL MC, MH2, MS, MO2, MN2, MH20, MSO2, H2S, H2O, CO, CO2, H2CO3, CAO, CASO4

11. C

12. C

13. C

14. C

15. C

16. C

17. C

18. C

19. C

20. C

21. C

22. C

23. C

24. C

25. C

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27. C

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32. C

33. C

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47. C

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54. C

55. C

56. C

57. C

58. C

59. C

ORIGINAL PAGE IS OF POOR QUALITY
CCC DESIGN DATA

INPUT DATA FROM ENTRAINMENT CALCULATIONS

READ(5,1000) KT

READ (5,1001) (HB(K),DPSE(K),DPWE(K),WEA(K),K=1,KT),

1(DCSE(K),DCWE(K),WEC(K),K=1,KT)

READ(5,1001) WDIS,HELI,CELI,EFF,DPSVB,DPWMB,DCSVB,DCWMB,

1(DASVF,DAMF,DCSVF,DCSVMF

CALL DESIGN

COMPOSITION OF LIMESTONE

READ(5,1010)NAMEL1,NAMEL2,XCAO,XHGO,XS102, XCO2

COMPOSITION AND NET HEATING VALUE OF COAL

READ(5,1010)NAMEC1,NAMEC2,XCHXN,XS, XO,XW,XA,VM,HCOAL,XCAO

OPERATING CONDITIONS

READ(5,1001)HLMF,HLF,PAV,TAV,TSTA,TWIN, TOUT,TWALLA,UHEAV1,UHEAV2,

1(UWALL1,UWALL2,TF,TSF,PF

READ (5,1001) WCOAL, WAQ,CAS, U0, FMF, EXAIR

READ(5,1000)IGNITE, ISO2, INOX, ITMP, 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 = U*(1.-XW-XA)

RN = 1.6-0.001*TAV

IF (RN .GT. 1.) RN = 1.0

IF (RN .LT. 0.) RN = 0.0

RS = RN

VGAS = X*(1.-XW)*(1.-RS)/32.0

VGASN = XN*(1.-XW)*(1.-RN)/14.0

R0 = 0.0

RN = 0.0

QCHAR = 7000.0

QCO = 43500.0

CH4 = 0.201-0.469*VM+0.24*VM**2

H2 = 0.157-0.868*VM+1.338*VM**2

CO2 = 0.135-0.900*VM+1.906*VM**2

CO = 0.453-2.653*VM+4.985*VM**2

H2O = 0.409-2.399*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.-R0) - V*(CO2/44.+CO/28.*0.5+H2O/18.0*X0.5)*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*H2O/18.0

CTAR = V*CH4/2+HTAR+OTAR

TAR = (CTAR-HTAR+OTAR)/MTAR

RUVAS = CH4+H2+TAR

CDV = CD+RUVAS
103  

\[ \text{CO}_2^V = \text{CO}_2 / \text{RVGAS} \]
\[ \text{COVE} = (\text{CH}_4 + \text{CTAR} / 12.0) / \text{RVGAS} \]
\[ \text{CO}_2^V \text{B} = \text{COVE} \]
\[ X_{02} = (\text{CTAR} / 12.0 \times 0.5 + \text{HTAR} / 2.0 \times 0.5 - \text{OTAR} / 32.0 + \text{VGAS} + \text{VGASN} \times 0.5 + \]
\[ \text{ICH}_4 \times 1.5 + \text{H}_2 \times 0.5) / \text{RVGAS} \]
\[ X_{02}^C = \text{CTAR} / 12.0 + \text{HTAR} / 2.0 \times 0.5 - \text{OTAR} / 32.0 + \text{VGAS} + \text{VGASN} \times 0.5 + \]
\[ \text{ICH}_4 \times 2.0 + \text{H}_2 \times 0.5) / \text{RVGAS} \]
\[ X_{CV} = (\text{CTAR} + (\text{CH}_4 + \text{CO}_2 + \text{CO}) \times 2.0) \]
\[ X_{CF} = X_{CV} - X_{CV} \]
\[ R_C = X_{CF} / X_{CV} \]
\[ H_2SV = \text{VGAS} / \text{RVGAS} \]
\[ \text{ANH}_3V = \text{VGASN} / \text{RVGAS} \]
\[ \text{COAL}_C = X_{CV} / 12.0 \]
\[ \text{COAL}_H = X_H \]
\[ \text{COAL}_O = X_O / 16.0 \]
\[ \text{COAL}_N = X_N / 14.0 \]
\[ \text{COAL}_S = X_S / 32.0 \]
\[ \text{CHAR}_C = R_C \times \text{COAL}_C \]
\[ \text{CHAR}_M = R_H \times \text{COAL}_H \]
\[ \text{CHAR}_O = \text{COAL}_O \]
\[ \text{CHAR}_N = R_N \times \text{COAL}_N \]
\[ \text{CHAR}_S = R_S \times \text{COAL}_S \]
\[ \text{TARC} = (\text{CHAR}_C + \text{CHAR}_H \times 0.5 + \text{CHAR}_S + \text{CHAR}_N \times 0.5 - \text{CHAR}_O \times 0.5) / (\text{RCHAR} \times 0.21) \]
\[ \text{QVGAS} = (\text{HCAL} - \text{RCHAR} \times \text{QCHAR} - \text{CO} \times \text{QCO}) / \text{RVGAS} \]
\[ \text{QCO} = \text{QVGAS} - \text{QCO} \times \text{COVB} \]
\[ T(1) = TF \]
\[ \text{IF}(\text{WCOAL} \leq 0.0,) \text{IGNITE} = 0 \]
\[ \text{C} \text{IGNITE} 0 1 \]
\[ \text{C NO COMBUSTION COMBUSTION} \]
\[ \text{C-} \]
\[ \text{MAIR} = 0.21 \times \text{MO}_2 + (1.0 - 0.21) \times \text{MN}_2 \]
\[ \text{A}_2 = \text{CH}_4 / \text{MO}_2 + \text{CH}_2 / (\text{MO}_2 + \text{MN}_2 - \text{X}_W) \]
\[ \text{FMTH} = \text{WCOAL} \times (1.0 - \text{X}_W) \times \text{A}_2 / 0.21 \]
\[ \text{IF} (\text{EXAIR} \leq 0.0,) \text{FMF} = \text{FMTH} \times (1.0 + \text{EXAIR}) \]
\[ \text{IF} (\text{EXAIR} \leq 0.0,) \text{FMF} = \text{ATB} (1) \times \text{UO} \times \text{PAV} / \text{RG} / \text{TAV} \]
\[ \text{UO} = \text{FMF} \times (1.0 - 0.21) + ((\text{CH}_4 / \text{MO}_2 + \text{CH}_2 / (\text{MO}_2 + \text{MN}_2 - 0.21) + (1.0 - \text{X}_W) + \text{EXAIR}) \]
\[ \times \text{WCOAL} \times \text{EFF} \times \text{FMTH} \times 0.21 \times \text{EXAIR} \]
\[ \text{FLOW} = \text{FMF} \times (1.0 - 0.21) \times (\text{CH}_4 / \text{MO}_2 + \text{CH}_2 / (\text{MO}_2 + \text{MN}_2 - 0.21) + (1.0 - \text{X}_W) + \text{EXAIR}) \]
\[ \times 2.0 \times \text{WCOAL} + \text{FMTH} \times 0.21 \times \text{EXAIR} \times \text{MO}_2 \]
\[ \text{MGAS} = \text{FLOW} / \text{FMO} \]
\[ \text{C FMO : AVERAGE FLOW RATE OF GAS IN THE BED MOLE/SEC} \]
\[ \text{C AVERAGE H}_2\text{O CONCENTRATION IN FBC} \]
\[ \text{YH}_2\text{O} = (\text{WCOAL} \times (\text{X}_W / \text{MO}_2 + \text{X}_W \times (1.0 - \text{X}_W) / \text{MN}_2) / \text{FMO} \]
\[ \text{RHOCH} = \text{RCHAR} \times \text{RHO}_C \]
\[ \text{IF} (\text{IGNITE} \leq 0.0,) \text{RHOCH} = \text{RHO}_C \]
\[ \text{IF} (\text{IGNITE} \leq 0.0,) \text{RHOED} = \text{RHO}_A \]
\[ \text{IF} (\text{CAS} \times 0.0, \text{AND, WAD}, \text{GT}_0 .0,) \]
\[ \text{ICAS} = \text{WAD} \times \text{CAS} / \text{MC} / \text{XCAO} / \text{WCOAL} \times (1.0 - \text{X}_W) \times \text{XS} / \text{MS} \]
\[ \text{IF} (\text{CAS} \times 0.0, \text{AND, WAD}, \text{EQ}_0.0,) \]
IWAD = CAS * (WCOAL * (1 - XW) * X/M) / (XCAO / MCAO)

AI = 0.0

IF (CAS .GT. 0.0) AI = 0.85 / CAS

RHOBED = (1 - XCO2 + XCAO / MCAO * AI * MCASO) * RHOAD

IF (CAS .EQ. 0.0) RHOBED = RHOAD

RHOGAS = PAW * MBAS / (RG * TAV)

VISC = 3.72E-6 * (TAV ** 0.676)

GCLCN = (42500.0 * XCAO / MCAO + 23810.0 * XMGO / MMGO)

CS = 0.315

==

MAIN OUTPUT 2

==

WRITE (6, 2000) NAME1, NAME2, XCAO, XMGO, XSI02, XC02

WRITE (6, 2010) DAVSF, DAVMF

WRITE (6, 2020) NAMEC1, NAMEC2, XCF, XCV, XH, XS, XG, XV, XM, VM, V, HCAOL

1 * XCAO =

WRITE (6, 2040) DCSVF, DCSVMF

WRITE (6, 2050) DAVG(I) = 0.0

X(I) = 0.0

IF (ITEMP .GT. 0) TAV = TSTA

DO 20 I = 2, 60

T(I) = TAV

CONTINUE

INITIAL BUBBLE HYDRODYNAMIC CALCULATION

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

IF (HLMF .GT. 0.0) WB = VMF * (1 - EMF) * RHOBED

CALL HYDRO

DO 35 I = 2, M

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

CONTINUE

ETC = 0.

XAV = WCOAL * XC / (WCOAL + WAD) * (1 - XW)

FM0 = FMF

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

FOR CONDITIONS OF NO COAL COMBUSTION. IGNITION IS ZERO AND MATERIAL AND ENERGY BALANCES CALCULATIONS ARE SKIPPED

YB(1) = YAV

YE(1) = YB(1)

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

FBM(1) = FM0 - FEN(1)

DO 115 I = 2, 60

RRB(I) = 0.0

RE(I) = 0.0

YB(I) = YAV

YE(I) = YAV

X(I) = XAV

IF (I .GT. M1) GO TO 115
FEM(I) = UMF(I)*AT(I)*(1.0-ETUBE(I))*PAV / (RG*T(I))
FBM(I) = FMO - FEM(I)
IF (UO(I) .LE. UMF(I)) FEM(I) = 0.0
CONTINUE
IF (IGNITE .EQ. 0) GO TO 630
CONTINUE
C BOUNDARY CONDITIONS FOR GAS CONCENTRATIONS
YO(1) = 0.21
YV(1) = 0.0
YCO(1) = 0.0
YSO2(1) = 0.0
YNOX(1) = 0.0
YB(1) = FMF*0.21/FMO
YE(1) = YB(1)
YVE(1) = 0.0
YCOE(1) = 0.0
YCO2B(1) = 0.0
YCO2E(1) = 0.0
YCO2C(1) = 0.0
C FROM HERE TO THE STATEMENT NO. 600 : TEMPERATURE ITERATION LOOP
MP1 = M1 + 1
DO 600 ITrial = 1,30
C CALCULATION OF LOG MEAN TEMPERATURE OF THE COOLING WATER
A1 = TWOUT - TWIN
A2 = ALOG((TAV-TWIN)/(TAV-TWOUT))
TWAV = TAV - A1/A2
CALL HYDRO
DO 25 I = 1,MT
TW(I) = TWAV
IF (I .LE. M1) UHE(I) = UHEAV1
IF (I .GT. M1) UHE(I) = UHEAV2
IF (I .LE. M1) UHEW(I) = UWALL1
IF (I .GT. M1) UHEW(I) = UWALL2
AHEW(I) = 4.0/DT(I)
TWALL(I) = TWALLA
TWALL(I) = TWALLA
25 CONTINUE
MP1 = M1 + 1
IF(ITUrial .GT. 1 .AND. M1.EQ.M1OL)GO TO 170
J1=1
DO 56 I=2,M1
WFC(I)=0.
WFAD(I)=0.
J2=J1
IF(J1.GT.MFEED)GO TO 56
DO 55 J=J1,MFEED
IF(ZF(J),GT.(I))GO TO 55
WFC(I)=WCOAL*FFC(J)
WFAD(I)=WFAD(I)+WAD*FFAD(J)
J2=J+1
55 CONTINUE
J1=J2
DO 56 I=2,M1
WFC(I)=0.
WFAD(I)=0.
J2=J1
IF(J1.GT.MFEED)GO TO 56
DO 55 J=J1,MFEED
IF(ZF(J),GT.(I))GO TO 55
WFC(I)=WCOAL*FFC(J)
WFAD(I)=WFAD(I)+WAD*FFAD(J)
J2=J+1
55 CONTINUE
J1=J2
DO 56 I=2,M1
WFC(I)=0.
WFAD(I)=0.
J2=J1
IF(J1.GT.MFEED)GO TO 56
DO 55 J=J1,MFEED
IF(ZF(J),GT.(I))GO TO 55
WFC(I)=WCOAL*FFC(J)
WFAD(I)=WFAD(I)+WAD*FFAD(J)
CONTINUE

FEM(I) = UMF(I) + T(I) * (1.0 - ETUBE(I)) * PAV / (RG * T(I))

FBM(I) = FMO - FEM(I)

TOLD(I) = T(I)

DO 133 I = 2, M

CONTINUE

DISTRIBUTION OF THE VOLATILES EVOLVED

VPRED(I) = WGOAL * RVGAS * (H(I) - H(I-1)) / H(M) * FW

IF(UO(I).LE.UMF(I)) FEM(I) = FMO

FBM(I) = FMO - FEM(I)

CONTINUE

FROM THE STATEMENT NO. 200 TO 300: ITERATION OF MATERIAL BALANCE

BASED ON THE GIVEN TEMPERATURE PROFILE. GAUSS SEIDEL METHOD

INDEX = 0

DETCA = -0.0001

IF (TAV .GE. 1100.0 .AND. TAV .LT. 1150.0) DETCA = -0.0002

IF (TAV .LT. 1050.0 .AND. TAV .LT. 1100.0) DETCA = -0.002

IF (TAV .LT. 1000.0 .AND. TAV .GE. 1000.0) DETCA = -0.005

IF (TAV .LT. 1000.0) DETCA = -0.01

ETCM = M

EETCM = ETC

DETCA = 0.99999

IF (ITRIAL .GT. 1) GO TO 175

EMF) / (DCSVB * RHOBED * (1.0 - ETCA))

CONTINUE

DO 130 I = 2, 60

YAV = 0.16

IF (I .GT. M1) YAV = 0.09

Y(I) = YAV

Y(I) = YAV

CONTINUE

DO 130 I = 1, M1

XAV = ((WGOAL * RCHAR - CEUL) * CCHAR * (1.0 - ETCA)) / WDIS

DO 1 I = 1, M1

II = T(I)

TCRATE = 0.0

GAS PHASE MATERIAL BALANCE IN THE BED

DO 233 I = 2, M1

CALL ANA(AKP, T(I), FAU, DCSVB, TPR(I), YR(I), RG, MC, ANCO2, PHIB)

TAVB = (T(I) + TPR(I)) / 2.
360. CALL AK(A,E,T(I),PAV,DCSVB,TPE(I),YE(I),RG,MC,AKCO2,PHIE)
361. TAVE=(T(I)+TPE(I))/2.
362. I=I+1
363. CALL GPB(YH20,ANB,AEB,AEBE(AMODF,DPB(EMF,EPB(E)),EPC(I),
364. 1ETUBE(I),FMB(I),FMB(I),FEM(I),GB(I),COB(I),EAE(I),PAV,
365. 2PHIE,RG,RGAS(T(I),TAVB,TAVE,UPR0D(I)*X(I),X02,X02C,YB(I),YB(I),
366. 3YCOE(I),YCOE(I),YE(I),YE(I),YVE(I),AKCO2,COV+COV+COV+
367. 4CO2VB,YCO2B(I),YCO2B(I),YCO2B(I),YCO2B(I))
368. AM = DBVB(I)*AMODF(AM)*MC
369. RRB(I) = AM*(PAV/RG)*(EPC(I)-EPB(I))*YB(I)*AKB/TAVB/CCHAR
370. RRE(I) = AM*(PAV/RG/TAVE)*(I.-EPC(I)-ETUBE(I))/CCHAR*(YEC(I)+SAKE+
371. IYCO2E(I)*AKC02)
372. RR(I) = (RRB(I)+RRE(I))/X(I)
373. TCRATE = TCRATE + RR(I)*X(I)
374. YO(I) = (FEM(I)*YE(I)+FMB(I)*YB(I))/FMO
375. YCO2(I) = (FEM(I)*YCO2E(I)+YMB(I)*YCO2B(I))/FMO
376. YV(I) = FEM(I)*YVE(I)/FMO
377. YCO(I) = FEM(I)*YCOE(I)/FMO
378. CONTINUE
379. C
380. GAS PHASE MATERIAL BALANCE IN THE FREEBOARD
381. C
382. DO 234 J = MP1,MT
383. J = J+1
384. K = J+1
385. HAV = (HI+1+HI(I))/2.0
386. CALL AREA(HAV,DTAV,ATAV)
387. RGAS = PAV*MGAS/RG/T(I)
388. VISC = 3.72E-6*T(I)**0.676
389. DCSVE = 0.5*(DCSE(J)+DCSE(K))
390. DCWME = 0.5*(DCWE(J)+DCWE(K))
391. CALL VEL(VISC,RGAS,G,RGCH,DCSVE,UMFAV,UTAV)
392. UD(I) = FMO*MGAS/R(1)-OSTUBE(I))/ATAV/C1.-ETUBE(I))
393. RT = (HB(K)-HB(J))/ABS(UO(I)-UTAV)
394. WCHOLD(I) = (2.0*WEC(J)-WEC(K))*RT
395. VCHOLD = WCHOLD(I)/RGAS
396. UC = VCHOLD*6.0/(PI*DCSVE**3)
397. CALL AK(AKCT(I),PAV,DCSVB,TPE(I),YO(I),RG,MC,AKCO2,PHIE)
398. TPE(I) = TPE(I)
399. TAVE = (T(I)+TPE(I))/2.0
400. I = I+1
401. CALL FBC(YH20,AKC,DCSVB,DVB(I),ETUBE(I),FM0,GB(I),COB(I),
402. 1GEB(I),NC*PAV,PHIB,PI*RG,RGAS(T(I),TAVB,X02,YCO(I),YCO(I),YO(I),
403. 2YO(I),YVE(I),YV(I),AKC02,COV+COV+COV+
404. RRB(I) = MC*NC*PI*DCSVB**2*PAV/RGAV/CHAR*(YO(I)*AKC+
405. IAKCO2*YCO2B(I))
406. RRE(I) = 0.0
407. TCRATE = TCRATE + RRB(I)
408. CONTINUE
409. WRITE(6,205) (I,YB(I),YE(I),YCOE(I),YVE(I),H(I),YCO2E(I),YCO2B(I))
410. CONTINUE
411. WRITE(6,209) (I,YB(I),YE(I),YCOE(I),YVE(I),H(I),YCO2E(I),YCO2B(I))
412. CONTINUE
413. 1H', T70, 'YCO2E', T82, 'YCO2B', T94, 'UO', T90, 'UMF', '/,(I5,1F9.12)
414. A1 = FMB*0.21+WCOAL*(I.-XW)*XO/M2-FMO*YO(MT)
415. ETC = A1/(FMTOK*0.21 - CELUTARC*0.21)
416. WRITE(6,209) NT,ETCA,ETCA*VXAV
417. WRITE(6,209) NT,ETCA,ETCA*VXAV
418. IF (INDEX.EQ.2) GO TO 236
419. C
FROM THE GAS PHASE MATERIAL BALANCE, CHAR COMBUSTION RATE HAS BEEN
ESTIMATED. KNOWING THIS AND THE SOLIDS MIXING RATE, CARBON BALANCE
IS PERFORMED, THE EQUATIONS ARE SOLVED BY THE SSP SUBROUTINE SIMQ
(SIMULTANEOUS SOLUTION OF ALGEBRAIC EQUATIONS). THE SOLUTION GIVES
THE CARBON CONCENTRATION PROFILE IN THE BED.

WMIX(I)=0,
WNET(I)=0,
J1=1
WD(I)=0.
J2=J1
IF(J1,GT, MDIS) GO TO 61
DO 60 J=J1, MDIS
IF(ZDIS(J), GT, H(I)) GO TO 60
WD(I)=WD(I)+WDIS*FD(J)
J2=J+1
60 CONTINUE
J1=J2
61 CONTINUE
IF(J1, GT, MDIS) GO TO 63
DO 62 J=J1, MDIS
WD(M1)=WD(M1)+WDIS*FD(J)
62 CONTINUE
63 CONTINUE

WMIX : UP- AND DOWN-WARD SOLID MIXING FLOW WHICH IS SUPERPOSED ON
FLOW OF SOLIDS. G/SEC
WNET(I) : NET FLOW RATE OF SOLID FROM THE TOP OF I-TH COMPARTMENT.
POSITIVE VALUE MEANS THE UPWARD FLOW.
TFC = WCOAL*RCHAR - CELU
RR(I) = RR(I)*TFC/TCRATE
WMIX(I) = WMIX(I-1)+WFC(I)*RCHAR+WFAD(I)-WD(I)-RR(I)*X(U, WMIX(I)).
IF(WMIX(I), LT, 0., WMIX(I))=0.
255 CONTINUE
WMIX(M1)=0.

CARBON CONCENTRATION CALCULATION.

AAA(I)=0.
DO 411 I=1, MM
411 AAA(I)=0.
DO 412 I=1, M
412 BBB(I)=0.
AAA(I) = WMIX(I)-WD(I)-RR(I)
AAA(M1)=WMIX(M1)-WMIX(2)-WD(2)-RR(2)
AAA(MI)=WMIX(MI)-WMIX(I-1)-WD(I-1)-RR(I-1)
AAA(MM-M)=WMIX(MM)
DO 413 I=1, M
413 BBB(I) = - MC*RCHAR*WFC(I)
II=(I-1)*MM+I

CONTINUE
416 CONTINUE
417 CONTINUE
418 CONTINUE
419 CONTINUE
420 CONTINUE
421 CONTINUE
422 CONTINUE
423 CONTINUE
424 CONTINUE
II=I+1
481. AAA(II) = -WMIX(I) - WMIX(II) + WNET(I)
482. 1 - WD(I) - RR(I)
483. AAA(II-M) = WMIX(I)
484. AAA(II+M) = WNET(II) + WMIX(II)
485. CONTINUE
486. CALL SIMQ(AAABBB, M, MM, S)
487. SUM = 0.
488. DO 280 I = 1, M
489. X(I+1) = BBB(I)
490. SUM = SUM + X(I+1)
491. 280 CONTINUE
492. XAV = SUM / FLOAT(M)
493. WRITE (6, 286) XAV, (IX(I), H(I) I = I, M)
494. 286 FORMAT ('0', ' XAV = ', IPE12.3, ',', 'I, X, H = ', I5, 'PE12.3')
495. SUM = 0.
496. DO 285 I = 2, M
497. SUMWD(I) * X(I) + SUM
498. CARCON(I) = X(I) * RHOBED(I) * (1 - ETUBE(I) + EPB(I))/ (1 - ETUBE(I))
499. 295 CONTINUE
500. CLOS = SUM + CEUXC*CHAR
501. ETCC = 1.0 - SUM / ((WCOAL + RCHAR - CEUX) * CHAR)
502. ET = 1. - CLOS / (WCOAL + XC * (1 - XW))
503. C HAVING OBTAINED THE CORRECT CARBON CONCENTRATIONS IN THE BED,
504. GAS PHASE MATERIAL BALANCE IS REPERFORMED TO ARRIVE AT THE CORRECT
505. CONCENTRATION PROFILES FOR THE VARIOUS GASEOUS SPECIES
506. C GAS PHASE MATERIAL BALANCE IN BED
507. C TCRATE = 0.0
508. DO 235 I = 2, M
509. CALL ANB(I), PAI, DCSVBT, PB, Y(I), RG, MC, AKCO2, PHIB
510. TAVB = (T(I) + TBP(I))/2.
511. CALL AKNCAKBE(T(I), PAI, DCSVBT, PE(I), YE(I), RG, MC, AKCO2, PHIE)
512. TAVE = (T(I) + TPE(I))/2.
513. I = I - I
514. CALL GPB(Y20, ANB(I), AKBE(I), AMODF, DVBB(I), EMF, EPS(I), EPC(I),
515. ETUBE(I), FEM(I), FB(I), FEM(I), GB(I), GBE(I), PAI,
516. ET = (FEM(I) - FB(I))/ (FMO)
517. AM = DVBB(I) * AMODF * X(I) * MC
518. RR(I) = AM * (PAI/ETUBE(I) - EPS(I)) * YB(I) * AKBE/TAIB/CHIR
519. YCO2(I) = AM * (PAI/ETUBE(I) - EPS(I)) * YB(I) * AKBE/TAIB/CHIR
520. YCO2(I) = AM * (PAI/ETUBE(I) - EPS(I)) * YB(I) * AKBE/TAIB/CHIR
521. 235 CONTINUE
DCSVE = 0.5*(DCSE(J) + DCSE(K))

VCHOLD = VCHOLD(J)/RHOCH

NC = VCHOLD(J)/0.05*(PI*DCSVE**3)

CALL AHA(ANK,77(I),PAV,DCSVE,TPB(I),YD(I),RG,MC,ANCO2,PHIB)

TPE(I) = TPB(I)

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

I = I + 1

CALL FBC(YHC0,ANK,DCSVE,TPBB(I),ETUBE(I),FGO,GB(I),COB(I),

1GE(I),NG,PAV,PHIB,PA,RG,RUGAS,T(I),TAUB,XO(I),YD(I),YD(I),

2YQ(I),YQ(I),YQ(I),ANCO2,COVB,CO2VB,YOCO(I),YOCO(I))

RR(I) = MC*NC*PI*DCSVE*2*PAV/RG/TAUB/CCHAR*(YD(I)*AHC*

1ANCO2*YOCO(I))

RAE(I) = 0.0

TCRATE = TCRATE + RR(I)

237 CONTINUE

FBCOM = TCRATE - BEPCOM

THE DEFINITION OF RR(I) IS CHANGED FOR TEMPERATURE CALCULATIONS.

RR(I) = (HEAT GENERATION RATE - HEAT CONSUMPTION RATE) IN THE

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 = M1, MT

RR(I) = RR(I)/TCRATE*QCHAR*(WCOAL*RCHAR-CELU)*ETCC+

1GE(I)*QVCO+GB(I)*QVGAS+COA(I)*QCO

300 CONTINUE

IF (ITEMP*EQ, 0) GO TO 610

CALCULATION OF TEMPERATURE

AI = CADF

A2 = CCF

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

A3 = COM*FMO

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

BETA(2) = (-WNET(2)+WMIX(2))*CS

DELT(2) = RR(2)+CMF*FMF*(T(2)-273.1)+(A1*WFA(2)+A2*WFC(2))*TSF-273

GAMA(2) = 0.

310 CONTINUE

DO 310 I = 3, M

ALFA(I) = (-WNET(I)+WMIX(I)+WMX(I)+WD(I))

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

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

DELT(I) = RR(I)+(A1*WFA(I)+A2*WFC(I))*TSF-273.1)+UHE(I)*AHEAV(I)*

1DVBB(I)*TSF-273.1)+UHEW(I)*AHEW(I)*DVBB(I)*TWALL(I)-273.

310 CONTINUE

DO 310 I = 3, M

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

BETA(M) = 0.

GAMA(M) = (WMIX(M))*CS+A3

HEAT BALANCE IN THE BED
TEMPERATURE SOLUTION BY SIMQ

**DO 501 I=1,MM**

**AAA(I)=0.**

**DO 502 I=1,M**

**AAA(I)=ALFA(2)**

**AAA(M1)=-BETA(2)**

**AAA(MM)=ALFA(M1)**

**AAA(M1-M)=-GAMA(M1)**

**II=(I-1)**

**AAA(II)=ALFA(I+1)**

**AAA(II-M)=-GAMA(I+1)**

**AAA(II+M)=BETA(I+1)**

**503 CONTINUE**

**CALL SIMQ(AAA,BBB,MM,KM)***

**504 CONTINUE**

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

**TAV=TAV+T(I)**

**TNORM=TNORM+ABS(T(I)-TOLD(I))**

**505 CONTINUE**

**TAV=TAV/FLOAT(K)**

**TNORM=TNORM/FLOAT(M)**

**WRITE (6,208) TNORM,TAV,BEDCOM,FBCOM**

**208 FORMAT ('0',IOX,'TNORM,TAV,BEDCOM,FBCOM',IP4E12.3)**

**HEAT BALANCE IN THE FREEBOARD**

**DO 320 I = MP1,MT**

**J = I-M1**

**WENTI = WEA(J)+WEC(J)**

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

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

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

**T(I) = ANR/DR + 273.0**

**320 CONTINUE**

**CONVERGENCE CRITERION FOR TEMPERATURE CALCULATION**

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

**610 CONTINUE**

**WRITE (6,3003)**

**3003 FORMAT(0',10X,'GAUSS SEIDEL TEMPERATURE TRIAL HAS NOT CONVERGED.**

**1 S.NO. = 3003',/)**

**DO 620 I = 2,MT**

**Ai = AHEAV(I) * DVBB(I)**

**HAREA = HAREA + Ai**

**QTRANS = UHE(I) * Ai *( T(I)-TW(I) ) + QTRANS**

**RR(I) = RR(I) / DVBBEF(I)**

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

**620 CONTINUE**
QVOL = QTRANS/BEDVOL
HFB = H(MT) - H(M1)
IF (HAREA .NE. 0.0) QAREA = QTRANS/HAREA
TPB(I) = T(I)
TPE(I) = T(I)
TAV = TAV - 273.
DO 612 I = 1, MT
T(I) = T(I) - 273.
TPB(I) = TPB(I) - 273.
TPE(I) = TPE(I) - 273.
612 CONTINUE
C MAIN OUTPUT 3
WRITE (6,2001) ETC, XAV, TAV, ITRIAL, (I, H(I), YB(I), YE(I), YVE(I),
1 YCO(I), YCO2(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 613 I = 1, MT
TPB(I) = TPB(I) + 273.0
TPE(I) = TPE(I) + 273.0
T(I) = T(I) + 273.0
613 CONTINUE
YBO(1) = YO(MT)
C CALCULATION OF SO2 REDUCTION
IF (IGNITE .EQ. 0) TCRATE = 0.0
DO 710 I = 1, MT
IF (I .GT. M1) GO TO 709
YED(I) = YE(I)
YBO(I) = YB(I)
709 YB(I) = 0.0
YE(I) = 0.0
710 CONTINUE
IF (ISO2 .EQ. 0) GO TO 811
CONTINUE
FRS = WCOAL*XS/MS*FLOAT(IGNITE)*(I,-XW)
IF (FRS .LE. 1.0E-6) GO TO 810
C CASE : EFFECTIVE RATIO OF CA TO S(ACTIVE) IN THE FEEDS
CASE = (WAD*XCAO+WCOAL*XA*XACAO)/XCAO/FRS
IF (CASE .EQ. 0) GO TO 811
SULFUR = WCOAL*(1,-XW)*XS*RS/MS - CLOSS*SCHAR/CCHAR/MS
RELB(1) = 0.0
RELE(1) = 0.0
YB(1) = YB(I)
YE(1) = YE(I)
ETS = 0.0
ETS = 0.0
EEETS = 0.005
INDEX = 0
DO 711 I = 2, MT
RELB(I) = 0.0
RELE(I) = 0.0
IF (TCRATE .LE. 0.0) GO TO 711
GENE = G8(I)*VGASS/RVGAS
GENE = GE(I)*VGASS/RVGAS
RELB(I) = RRB(I)/TCRATE*SULFUR+GENE

RELB(I) = RRE(I)/TCRATE*SULFUR+GENE

CONTINUE

FS = ETS/CASE

FS : FRACTIONAL CONVERSION OF ADDITIVE
-C ASUMING THE SULFUR CAPTURE EFFICIENCY, FS IS CALCULATED AND HENCE
-C THE LIMESTONE REACTIVITY. THEN, SO2 MATERIAL BALANCE IS PERFORMED.
-C FROM THE EXIT SO2 CONC. IN THE FLUE, SO2 CAPTURE EFFICIENCY IS
-C CALCULATED. ITERATION IS CONTINUED TILL THE ASSUMED AND THE
-C CALCULATED SULFUR DIOXIDE RETENTION EFFICIENCIES AGREE.

AK = AKAD(FS, DPSVE, T(I))

SO2 BALANCE IN THE BED

DO 740 I = 2, M1

I + I = 1

AM = (1.0 - EMF)

CALL GPHASE(AK, AN, AM, PAV, RG, ETUBE(I), EPB(I), EPC(I),

1ANBE(I), DVB(B(I), FBM(I), FEM(I), YB(I), Y(I), T(I), T(I),

YB(I), YE(I), RELB(I), RELE(I))

YSO2(I) = (YB(I) + Y(I)) / FMO

CONTINUE

SO2 BALANCE IN THE FREEBOARD

DO 741 I = MP1, MT

J = I - M1

N = J + 1

RHOGAS = PAV*MGAS/RG/T(I)

VISC = 3.72E-6*T(I)**0.675

DPSVE = 0.5*(DPSE(J) + DPSE(K))

DPWME = 0.5*(DPWE(J) + DPWE(K))

CALL VEL(VISC, RHOGAS, RHOBED, DPSVE, UMFAV, UTAV)

RT = (HB(K) - HB(J))/ABS(UO(I) - UTAV)

WAHOLD(I) = (2.0*WEA(J) - WEA(K))*RT

WAHOLD = WAHOLD(I)/RHOBED

NA = WAHOLD*6.0/(PI*DPSE**3)

AK = AKAD(FS, DPSVE, 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 = 1.0 - FMO*YSO2(MT)/FRS

EE = ETS - ETSC

CALL CCRECT(ITRY, INDEX, ETS, ETS1, ETS2, ETS, E1, E2, EE, EETSM)

IF(INDEX.EQ.2) GO TO 910

CONTINUE

WRITE(&, 3600)

FORMAT(0, 'ETS HAS NOT CONVERGED. S.NO. = 3600')

CONTINUE

YGO(I) = YSO2(MT)

WRITE(&, 1005) ETS, FS, CASE, INDEX

1, (H(I), YB(I), YE(I), ZAVG(I), YSO2(I), RELB(I), RELE(I), I = 2, MT)

C

NOX CALCULATIONS

C

IF (INEX .EQ. 0) GO TO 914
FRN = WCOAL *(1.-XW) * XN/HN * FLOAT(IGNORE)
ANITRO = WCOAL *(1.-XW) * XN / RN / MN - CLOG+NCHEAR/CCHEAR/MN
DO 750 I = 2,MT
GENB = GB(I)*VGAH/RVGAH
GENE = GE(I)*VGAH/RVGAH
RELB(I) = RB(I)/TCRATE * ANITRO +GENB
RELE(I) = RE(I)/TCRATE * ANITRO + GENE
CONTINUE
YB(1) = 0.0
YE(1) = 0.0
FR = 3.24E7
AE = 34000.0
C
NOX BALANCE IN THE BED
DO 760 I = 2,MT
I1 = I-1
TAVB = (T(I)+TPB(I))/2.0
TAVE = (T(I)+TPE(I))/2.0
ANE = FR*EXP(-AE/1.986/TAVB)
ANE = FR * EXP(-AE/1.986/TAVE)
AMDF = 0.0*RHOBED*(1.-ENF)/(DCSVE*RHOCHECH/NCHEAR)
AM = AMDF*XCI)
CALL OPHASE (AMB,AKBE,AM,PAV,RG,ETUBE(I),EPB(I),EPC(I),AKBE(I),
1DUBE(I),FMB(I),FEM(I),FEB(I),T(I),TAVB,TAVE,YB(I),
2YE(I1),YB(I),YE(I),RELBI,RELI)
YNOX(I) = ( FMB(I)*YB(I1)+FEM(I)*YE(I1) )/FMO
CONTINUE
YNOX(I) = ( FMB(I)*YB(I)+FEM(I)*YE(I) )/FMO
C
NOX BALANCE IN THE FREEBOARD
DO 770 I = MP1,MT
TAVB = (T(I)+TPB(I))/2.0
J = I-MP1
K = J+1
DCSVE = 0.5*(DCSE(J)+DCSE(K))
XI(I) = WCHOLD(I)*CCHEAR/(WCHOLD(I)+WMAHOLD(I))
CARCON(I) = WCHOLD(I)*CCHEAR/DVB8EF(I)
WCHOLD = WCHOLD(I)/RHOCHE
HC = WCHOLD*0.0*(FMB*DCSVE**2)
AKNO = FR*EXP(-AE/1.986/TAVB)
ANR = FMO*YNOX(I-1) + RELB(I) + RELE(I)
DR = FMO + NC*PI*DCSVE**2 *AKNO*PAV/RC/TAVB
YNOX(I) = ANR/DR
CONTINUE
ENOX = FMO*YNOX(MT)
EINDEX = ENOX/WCOAL
ENX = 1.0 - ENOX /FRN
WRITE (4,2007)EXAIRTAVETNENOXEINDEX(H(I),YB(I),YYE(I),X(11,
1CARCON(I),ZAVG(I),YNOX(I),RELBI,RELI),I=2,MT)
CONTINUE
C
MAIN OUTPUT 4
C
C
CONTINUE
YGO(1) = YCO2(MT)
YGO(4) = YH20
YGO(5) = YCO(MT)
WRITE(6*2006) (YGO(I),I=1,5)
940. IF (HLMF.EQ.0.0) VMF = SOLVOL
941. IF (HLMF.EQ.0.0) HLMF = HEIGHT(VMF)
942. IF (HF .EQ. 0.0) HLF = H(HMF)
943. IF (IPRES .EQ. 0) 0 TO 950
944. CONTINUE
945. C PRESSURE DROP CALCULATION
946. C
947. C
948. C
949. C
950. C
951. C
952. C
953. C PRESSURE DROP CALCULATIONS ACROSS THE DISTRIBUTOR
954. C
955. C TEMP = T(2)
956. RHOBG = PF * RFGAS / (PS*(TEMP))
957. UOR = FMF * RG * TEMP/ PF /((AND*0.25*PI*MH2L**2)
958. DDIS = (UOR/0.6)**2 * RHOBG / (2.0*KG)
959. WRITE (6,2050) DDIS
960. C PRESSURE DROP CALCULATIONS IN THE FLUIDIZED BED SECTION
961. C
962. WRITE (6,2051)
963. N1 = N1
964. IF (IFBC .EQ. 0) N1 = N1 - 1
965. DO 920 I = 2,NI
966. DPFLU = (1.0 - EMF) * (1.0 - EPS(I)) * (H(I) - H(I-1)) * RHOBED
967. WRITE (6,2052) I, DPFLU
968. CONTINUE
969. IF (IFBC .EQ. 0) GO TO 930
970. Csection RHOBED
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. DDIS = E1 * (150.0 * (1.0 - EMF) * E2 * VISC * UO(MI)
976. / DPSVB ** 2 + 1.75 * E2 * RHOBG * UO(MI)**2/DPSVB)
977. CONTINUE
978. IF (IFBC .EQ. 0) DDIS = 0.0
979. WRITE (6,2053) DDIS
980. CONTINUE
981. WRITE (6,0C)
982. WRITE (6,0PCF1)
983. WRITE (6,0FPB)
984. DO 910 I = 2,MI
985. WRITE (6,2070) I,H(I),ZAVB(I),DBAV(I),Ub(I),EPB(I),EPC(I),UO(I),
986. UMF(I)
987. CONTINUE
988. WRITE (6,2075)
989. DO 940 I = 1,HT
990. WRITE (6,2080) I,H(I),DT(I),HT(I)
991. CONTINUE
992. 1000 FORMAT(S11)
993. 1001 FORMAT(2F10.0)
994. 1010 FORMAT(2A4/(8F10.0))
995. 2000 FORMAT('0',1X,2A4,10X,'XCAO = ',F6.3,10X,'XMOO = ',F6.3,10X,
996. '\*\*XID2 = ',F6.3,10X,'XCD2 = ',F6.3,10X)
997. 2001 FORMAT('0',1X,'RESULTS ALL TEMPERATURES IN CENTIGRADE')"
FUNCTION AKAD(FS,DP,T)

C THIS SUBROUTINE CALCULATES LIMESTONE-SO2 REACTION RATE CONSTANT

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

DATA FB/0.0,0.05,0.1,0.2,0.25,0.3,0.35,0.4,0.425,0.45,0.475,0.5,
     0.525,0.55,0.6/

DATA RR/1.0,0.331,0.16,0.028,0.004,0.0004,0.00003,0.0000022,0.0002,0.00022,
     0.000014,0.0001,0.000013,0.000011/

DATA RB/1.0,0.824,0.654,0.537,0.437,0.337,0.253,0.185,0.125,0.079,
     0.049,0.035,0.0257,0.0225/

DATA RC/1.0,0.878,0.829,0.779,0.729,0.679,0.629,0.589,0.549,0.519,0.495,0.465,0.435,0.405,0.385,0.365,0.345,0.325,0.305,0.285,0.265,0.245,0.225,0.205,0.185,0.165,0.145,0.125,0.105,0.085,0.065,0.045,0.025,0.005,0.0/

C

ALIME=0.0

AKAD=0.0

IF( FS .GE. 1.0) RETURN

DO 10 I=2,13

10

N=1
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*R1
R2=(RB(N)/RB(N1))*A*RB(N1)
13 CONTINUE
ALIME=(R1/R2)**XXX*R2
IF( ALIME .GT. 1.0) ALIME=1.0
IF (T .LT.i253.0) S5 35.9T = 3.57E04
IF (T .GE, 1253,0) SO 
END
SUBROUTINE ANK(AKR,TPDC,TP,YO2,RG-t1CAKCO2,PHI
REAL
C THIS COMPUTES REACTION RATE CONSTANT FOR CHAR COMBUSTION AKR,
C RATE CONSTANT FOR C-CO2 REACTION AND THE CHAR PARTICLE TEMPERATURE
C
EM=1.0
SIGN=1.36E-13
INDX=0
DTS= 200.0
TP=300.0
DO 100 I=1,20
ETSMAX=0.005*TP
AKS=8710.0*EXP(-35700.0/1.996/TP)
TAV = (TP+TP)*.5
D=4.26*(TAV/1800.)**1.75/P
COND=0.632E-5*SQRT(TAV)/(I,+245./TAV10.**(-12./TAV))
Z 2500. * EXP(-12400./1.96/TAV)
IF (DC .LE. 0.005) PHI = (2.*Z+2.)/(Z+2.)
IF (DC .GT. 0.005 .AND. DC *LE. 0.10)
PHI = 1./(Z+2.)*((2.Z+2.)*- Z*(DC-0.005)/0.095)
IF (DC .GT. 0.10)
PHI = 1.0
0 = 7900.0*(2./PHI-1)+2340.0*(2.-2./PHI)
A=24.*PHI*(DC+AKR)
JS=25000.0*(2./PHI-1)+2340.0*(2.-2./PHI)
100.
IF (INDX,EQ.2) GO TO 110
100  CONTINUE
110.
WRITE (6, 4000) TP,ETS
4000 FORMAT ('0',10X,'TP CALCULATION HAS NOT CONVERGED',/10X,'TP,ETS ')
SUBROUTINE AREA ( ZI, DTI, ATI )

COMMON /A/ ZHE(t,0)AHE(IO),PV(u0),PH(IO)ZF(IO),FFC(o)-TBE<LO)­
IDVB'(60),DVBEFF(60t),FFAD(1O),ZDIS(IO),FL(10),AHElV(60),ETUBE(60),
UM(60),,UMF660),HR60),AT(60)DT(60)
T(6O)X(60),AKBE(!O),B(zO),
YE(60) YCOE(60'),-,EPB(60)rEPC(60) DVBB(60) DVBBEF(bu)
DfEAV(6')), [1027.

C CALCULATION OF THE CROSS SECTIONAL AREA GIVEN THE HEIGHT ABOVE

DO 10 J = 1 , MTB

IF ( ZI .GT. ZB(J) ) GO TO 10 .

RI= = SORT ( ATB(J-1) / PI )

AT = ( ZI - ZB(J-1) ) / ( ZB(J) - ZB(J-1) )

BI = SORT ( ATB(J) / ATB(J-1) ) - 1.0

RI = ( 1.0 + AT * BI ) * RI

DTI = 2.0 * RI

ATI = PI * RI ** 2

GO TO 20

CONTINUE

SUBROUTINE CPRRECT(I,,INDXDX,XIX2rXNEUEiE2EEMAX)

C NUMBER OF THIS TRIAL, I FOR FIRST TRIAL

C INDX INDEX OF THE TRIAL LEVEL

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

C INDEX=2 THE ITERATION HAS CONVERGED

IF (ABSX(EY).GT.EMAX) GO TO 5

INDEX=2

RETURN

5 CONTINUE

IF(INDEX.EQ.1) GO TO 100

X2=XNEW

E2=E

IF(I.EQ.1) GO TO 10

IF(E1*X2.EQ.E0) INDEX=1

IF(INDEX.EQ.1)GO TO 150

10 XI=X2

E1=E2

XNEW=XNEW+DX

RETURN

SUBROUTINE DESIGN
1080. COMMON /A/ ZHE(10), AHE(10), PV(10), PH(10), IF(10), FFC(10), DTUBE(10),
1081. VD(60), DVBEFF(50), FFAD(10), ZDIS(10), AT(60), DT(60), T(60), X(50), AHEV(50), YF(60),
1082. 3Y(50), YCOE(60), EPB(60), EPC(60), DTB(60), DVBB(60), DVBE(60), DAVE(60),
1083. 4UB(60), UTC(60), UTA(60), ZB(10), ATB(10), YVE(60), ZAV(60), IARR(10)
1084. COMMON /B/ YBO(60), YEO(60), DB(60), DSBVBDPWMB, DCSVMB, DCWMB, RMOB,
1085. 1HLF, VMF, PHF, FF, FFAD, FTB, & NISO, DFIX, DPFLU, DPDIS, RMOBED,
1086. ZEMF, PAV, JCN, EFFVOL, SOLVOL, TETUBE, HMFAPI, AND, DNZL,
1087. 3FW, FSW, DZAV, MFEED, MDIS, MTHE, MTB, MT, M1, M2, M3, M4, M5
1088. C AXIAL VARIATION OF BED CROSS SECTION
1089. C READ (5, 1000) A1, A2, A3, A4
1090. C READ (5, 1001) MB, (ZB(J), ATB(J)), J = 1, MB
1091. C IARR(1), J = 1, MBHE
1092. C LOCATION OF FEED AND DISCHARGE
1093. C READ (5, 1001) MFEED, (ZF(J), FFC(J), FFAD(J)), J = 1, MFEED
1094. C READ (5, 1001) MDIS, (ZDIS(J), FD(J)), J = 1, MDIS
1095. C DISTRIBUTOR
1096. C READ (5, 1003) AND, DNZL, FW, FSW
1097. C DO 100 J = 1, MTHE
1098. C IF (AHE(J) .GE. 0.0) GO TO 100
1099. C IF (DTUBE(J) .GE. 0.0) GO TO 100
1100. C AHE(J) = PI * DTUBE(J) / (PH(J) * PV(J))
1101. C CONTINUE
1102. C CONDITION FOR COMPUTING AVERAGE CELL SIZE
1103. C WRITE (6, 2000) A1, A2, A3, A4
1104. C WRITE (6, 2001)
1105. C WRITE (6, 2002) (ZB(J), ATB(J)), J = 1, MB
1106. C WRITE (6, 2003)
1107. C WRITE (6, 2004) (ZHE(J+1), AHE(J), DTUBE(J), PV(J), PH(J), IARR(J)),
1108. C 1J = 1, MTHE
1109. C WRITE (6, 2005)
1110. C WRITE (6, 2006) (ZF(J), FFC(J), FFAD(J)), J = 1, MFEED
1111. C WRITE (6, 2007)
1112. C WRITE (6, 2008) (ZDIS(J), FD(J)), J = 1, MDIS
1113. C WRITE (6, 2009) AND, DNZL, FW, FSW
1114. C Z1 = ZB(1)
1115. C ABED1 = ATB(1)
1116. C DBED1 = SORT(4.0 * ABED1 / PI)
1117. C DVB(1) = 0.0
1118. C DVBEFF(1) = 0.0
1119. C ZHE(1) = 0.0
1120. C DZAV = 30.0
NTC = I(FIX(ZB(MTB)./DZAV)+1)
1142. Z2 = Z1 + DZAV
1143. IF (I.EQ.NTC) Z2 = ZB(MTB)
1144. DO 10 I = 1,NTC
1145. IF (ZHE(J) .LE. Z1 .AND. ZHE(J+1) .LT. Z2) GO TO 30
1146. IF (ZHE(J) .LE. Z2 .AND. ZHE(J+1) .LE. Z2) GO TO 20
1147. F1 = (Z2 - ZHE(J)) / DZAV
1148. F2 = (ZHE(J) - Z1) / DZAV
1149. AN = F1 * AHE(J) + F2 * AHE(J-1)
1150. DIAT = F1 * DTUBE(J) + F2 * DTUBE(J-1)
1151. GO TO 40
1152. 30 AN = AHE(J)
1153. DIAT = DTUBE(J)
1154. 40 CONTINUE
1155. DO 50 CONTINUE
1156. CALL AREA (Z2, DBED, ABED)
1157. D((t+1) = 0.5 * (ABED+ABEDI) * DZAV
1158. VVBEFF(I+1) = DVB(I+1) * (1.0 - 0.25 * AN)
1159. Z1 = Z2
1160. ABEDI = ABED
1161. 10 CONTINUE
1162. 1000 FORMAT (4A4)
1163. 1001 FORMAT (I1/(SF10.0))
1164. 1002 FORMAT (I1/(SF10.0, I10))
1165. 1003 FORMAT (SF10.0)
1166. 2000 FORMAT ("T", A4)
1167. 2001 FORMAT ("T", A4)
1168. 2002 FORMAT ("T", A4)
1169. 2003 FORMAT ("T", A4)
1170. 2004 FORMAT ("T", A4)
1171. 2005 FORMAT ("T", A4)
1172. 2006 FORMAT ("T", A4)
1173. 2007 FORMAT ("T", A4)
1174. 2008 FORMAT ("T", A4)
1175. 2009 FORMAT ("T", A4)
1176. 2010 FORMAT ("T", A4)
1177. 2011 FORMAT ("T", A4)
1178. 2012 FORMAT ("T", A4)
1179. 2013 FORMAT ("T", A4)
1180. 2014 FORMAT ("T", A4)
1181. 2015 FORMAT ("T", A4)
1182. 2016 FORMAT ("T", A4)
1183. 2017 FORMAT ("T", A4)
1184. 2018 FORMAT ("T", A4)
1185. 2019 FORMAT ("T", A4)
1186. 2020 FORMAT ("T", A4)
1187. 2021 FORMAT ("T", A4)
1188. 2022 FORMAT ("T", A4)
1189. 2023 FORMAT ("T", A4)
1190. 2024 FORMAT ("T", A4)
1191. 2025 FORMAT ("T", A4)
1192. 2026 FORMAT ("T", A4)
1193. 2027 FORMAT ("T", A4)
1194. 2028 FORMAT ("T", A4)
1195. 2029 FORMAT ("T", A4)
1196. 2030 FORMAT ("T", A4)
1197. 2031 FORMAT ("T", A4)
1198. 2032 FORMAT ("T", A4)
1199. 2033 FORMAT ("T", A4)
1200. 2034 FORMAT ("T", A4)
1201. 2035 FORMAT ("T", A4)
1202. 2036 FORMAT ("T", A4)
1203. 2037 FORMAT ("T", A4)
1204. 2038 FORMAT ("T", A4)
1205. 2039 FORMAT ("T", A4)
1206. 2040 FORMAT ("T", A4)
1207. 2041 FORMAT ("T", A4)
1208. 2042 FORMAT ("T", A4)
1209. 2043 FORMAT ("T", A4)
1210. 2044 FORMAT ("T", A4)
1211. 2045 FORMAT ("T", A4)
1212. 2046 FORMAT ("T", A4)
1213. 2047 FORMAT ("T", A4)
1214. 2048 FORMAT ("T", A4)
1215. 2049 FORMAT ("T", A4)
1216. 2050 FORMAT ("T", A4)
1217. 2051 FORMAT ("T", A4)
1218. 2052 FORMAT ("T", A4)
1219. 2053 FORMAT ("T", A4)
1220. 2054 FORMAT ("T", A4)
1221. 2055 FORMAT ("T", A4)
1222. 2056 FORMAT ("T", A4)
1223. 2057 FORMAT ("T", A4)
1224. 2058 FORMAT ("T", A4)
1225. 2059 FORMAT ("T", A4)
1226. 2060 FORMAT ("T", A4)
1227. 2061 FORMAT ("T", A4)
1228. 2062 FORMAT ("T", A4)
1229. 2063 FORMAT ("T", A4)
1230. 2064 FORMAT ("T", A4)
1231. 2065 FORMAT ("T", A4)
1232. 2066 FORMAT ("T", A4)
1233. 2067 FORMAT ("T", A4)
1234. 2068 FORMAT ("T", A4)
1235. 2069 FORMAT ("T", A4)
1236. 2070 FORMAT ("T", A4)
1237. 2071 FORMAT ("T", A4)
1238. 2072 FORMAT ("T", A4)
1239. 2073 FORMAT ("T", A4)
1240. 2074 FORMAT ("T", A4)
1241. 2075 FORMAT ("T", A4)
1242. 2076 FORMAT ("T", A4)
1243. 2077 FORMAT ("T", A4)
1244. 2078 FORMAT ("T", A4)
1245. 2079 FORMAT ("T", A4)
1246. 2080 FORMAT ("T", A4)
1247. 2081 FORMAT ("T", A4)
1248. 2082 FORMAT ("T", A4)
1249. 2083 FORMAT ("T", A4)
1250. 2084 FORMAT ("T", A4)
1251. 2085 FORMAT ("T", A4)
1252. 2086 FORMAT ("T", A4)
1253. 2087 FORMAT ("T", A4)
1254. 2088 FORMAT ("T", A4)
1255. 2089 FORMAT ("T", A4)
1256. 2090 FORMAT ("T", A4)
1257. 2091 FORMAT ("T", A4)
1258. 2092 FORMAT ("T", A4)
1259. 2093 FORMAT ("T", A4)
1260. 2094 FORMAT ("T", A4)
1261. 2095 FORMAT ("T", A4)
1262. 2096 FORMAT ("T", A4)
1263. 2097 FORMAT ("T", A4)
1264. 2098 FORMAT ("T", A4)
1265. 2099 FORMAT ("T", A4)
1300. RETURN
OXYGEN RICH CONDITION

\[ YV = 0.0 \]
\[ \text{AKP} = 3.0 \times 10^4 \times \exp(-14000/T) \times (\text{PAV}/\text{RG}^2/T) \times (1.8 \times YH2O \times 0.5 \times \text{DBB}^2) \]
\[ I(1.0 - \text{ETUBE}) \]
\[ \text{INDEX} = 0 \]
\[ YO = 0.0 \]
\[ \text{DYO} = 0.01 \]
\[ \text{EYO} = 0.001 \]

\[ \text{DO 110 } I = 1,20 \]
\[ \text{ANR} = \text{FM0} \times YC00 + 2.0 \times \text{A4} / \text{FM0} + \text{A4} \times (\text{FM0} \times YC02 + \text{A2} \times \text{YO} / (2.0 - \text{PHIB})) \]
\[ \text{DR} = \text{FM0} + \text{AKP} \times (17.5 \times YO / (1.0 + 24.7 \times YO)) \]
\[ YC0 = \text{ANR} / \text{DR} \]
\[ \text{IF} (YCO .LT. I.E-6) \text{GO TO 130} \]
\[ YC02 = (\text{FM0} \times YC02 + \text{A2} \times \text{YO} / (2.0 - \text{PHIB})) \]
\[ \text{YO} = \text{YO} - \text{ER} \times \text{EYO} \]
\[ \text{IF} (\text{YOC} .LE. 0.0) \text{YOC} = 0.0 \]
\[ \text{IF} (\text{YCO2} .LT. 0.0) \text{YCO2} = 0.0 \]
\[ \text{ER} = \text{YO} - \text{YOC} \]
\[ \text{CALL CRRECT} (I, \text{INDEX}, \text{DYO}, X1, X2, YO, E1, E2, \text{ER}, \text{EYO}) \]
\[ \text{IF} (\text{INDEX} .LE. 2.0) \text{GO TO 120} \]

\[ \text{DO 110 } I = 1,20 \]
\[ \text{YCO} = 0.0 \]
\[ \text{YCO2} = (\text{FM0} \times YC02 + \text{A2} \times \text{YO} / (2.0 - \text{PHIB})) \]
\[ \text{YOC} = \text{YOO} - \text{YE} \times \text{YO2} - \text{AKP} \times \text{YCO} \times (17.5 \times \text{YO} / (1.0 + 24.7 \times \text{YO})) / 2.0 \times \text{FM0} \]
\[ \text{1-A2} \times \text{YO} / \text{PHIB} / \text{FM0} \]

\[ \text{RETURN} \]

\[ \text{END} \]
\[ \text{SUBROUTINE GB} (\text{YH2O}, \text{A4B}, \text{AMF}, \text{A4E}, \text{AMDF}, \text{DBB}, \text{EFM}, \text{EPB}, \text{ETUBE}) \]
\[ \text{IF} (\text{FM0} = \text{FM0} + \text{FEM} + \text{FM0} + \text{GB} + \text{GE} + \text{PAV} + \text{PHIB} + \text{RG} + \text{RUGAS} + \text{T} + \text{TAVB}) \]
\[ \text{2VPRED} (X1, X2, YQ0, YR, YCOE0, YCO, YEO, YE0, YE, AN02, COY, CO2Y, COVB, CO2VB, YCO20, YCO2E, YCO2E) \]

\[ \text{RETURN} \]

\[ \text{END} \]
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

\[ A1 = \frac{ANBE*DVBB*EPB*PAV}{(Rg*TAVE)} \times X \]
\[ A2 = \frac{ANDF*DVBE*1.0-EPF*EPBB*PAV}{(Rg*TAVE)} \times X \]
\[ A4 = \frac{ANDF*DVBE*1.0-EPF*EPBB*PAV}{(Rg*TAVE)} \times X \]

DO 150 I = 1,25

OXYGEN CONCENTRATION IN EMULSION PHASE IS ZERO.

A(1) = FEM + A1
A(4) = -AI*CO2VB
A(5) = AI*QO2C
A(7) = A(1)
A(9) = -AI
A(10) = AI/2.0
A(12) = -2.0*AI
A(13) = FEM + A1 + A4
A(14) = -AI
A(18) = -AI
A(19) = FBM + A1
A(21) = A1/QO2
A(22) = -AI*COVB/QO2
A(24) = -A2
A(25) = FBM + A1 + A2

B(1) = FEM0*YVE0 - FEM0*YEO/QO2+VPROD
B(2) = FEM0*YCOE0 + FEM0*YEO*COVB/QO2+VPROD*COV
B(3) = FEM0*YCOE0 + VPROD*COV

YVE = B(1)
IF (YVE .LE. 0.0) GO TO 10
YE = 0.0
YE = 0.01
IF (YEO .LE. 0.0225) DYE = 0.001
EMAX = 0.01

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

YVE = 0.0
AKP = 3.1E10*EXP(-16000.0/1.987/T)*PAV/RG/T)**1.8*YH2O/Y0.5*YVB

IF (YEO .LE. 0.05) DYE = 0.002
IF (YEO .LE. 0.025) DYE = 0.001
EMAX = 0.01

CONTINUE

OXYGEN CONCENTRATION IN EMULSION PHASE IS ZERO.

YVE = 0.0
ALP = 3.1E10*EXP(-16000.0/1.987/T)*PAV/RG/T)**1.8*YH2O/Y0.5*YVB

IF (YEO .LE. 0.05) DYE = 0.002
IF (YEO .LE. 0.025) DYE = 0.001
EMAX = 0.01

CONTINUE
AA(1) = 0.0
AA(16) = FEM + A1 + A2
BB(1) = FEM*YCOE + (FEM*YVEO + VPROD*C02V + VPROD*C02V + A3*PHIE1)*YE
BB(2) = FEM*YCOE + (FEM*YVEO + VPROD*C02V + A3*PHIE1)*YE
BB(3) = FEM*YCOE
BB(4) = FEM*YCOE + A1*YE

CALL SIMO(AABB,4v16,KS)

YCOE = BB(1)
YCO2E = BB(2)
YCO2B = BB(3)

YB = BB(4)

ANR = FEM*YVEO + A1*(YE - YB) - A3*YE/PHIE - (FEM*YVEO + VPROD)*YCOE

1AAP*YCOE*(17.5*YE/(1.+24.7*YE)*2.0

YEC = ANR/FEM

IF (YEC .LT. 0.0) YEC = 0.0
IF (YEC .EQ. 0.0 .AND. YE .LT. 0.005) YE = 0.0
ER = YE-YEC

CALL CORRECT(I,INDX,DYEX1,X2,YE,E,E2,ERMAX)

IF (INDX .EQ. 2) GO TO 60

50 CONTINUE

WRITE (671000) YE,YEC,YB,YEO
1000 FORMAT ('0',10X,'YE HAS NOT CONVERGED. SUBROUTINE GPB',/1OX,'YE,'YEC,YB,YEO = ',1PSEI2.3)

Y = YE

60 CONTINUE

IF (YE .LT. 0.0) YE = 0.0
IF (YE .GT. YEC) YE = YEC

IF (YB .LT. 0.0) YB = 0.0
IF (YCO2B .LT. 0.0) YCO2B = 0.0

GE = FEM*YVEO + VPROD

GB = 0.0

COB = A1*YCOE*(17.5*YE/(1.+24.7*YE)) + A1*YCOE

RETURN

END

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

C THIS SUBPROGRAM IS USED TO CALCULATE THE SO2 AND NOX

C CONCENTRATIONS IN THE BED

C

D1 = ((1.-ETUBE-EPC)*AM*AKE/rE+ANBE*EPB/T)*PAV/RG*DBP+FEM

ALF=ALF*EPB*DVP*PAV/(D1YRGT)

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

IF (D2 .EQ. 0.0) YB1 = 0.0
IF (D2 .NE. 0.0) YB1 = (FEM*Y30+GENB+ALF*FEM*YEO)/D2
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1380. \( YE_1 = (YE_0 \cdot FEM + GNE) / DI + ALF \cdot YP_1 \)
1381. RETURN
1382. END
1383. SUBROUTINE HAREA (ATI, DTI, ZI)
1384. COMMON /A/ ZHE(10), AHE(10), PV(10), PH(10), ZF(10), FFC(10), DTUBE(10),
1385. 1DV(60), DVB(60), FFAD(10), ZDIS(10), FD(10), AHEAV(60), ETUBE(60),
1386. 2UMF(60), UMFF(60), AT(60), DT(60), T(60), X(60), AKBE(60), YBE(60),
1387. 3YE(60), YCOE(60), EPB(60), EPB(60), DVB(60), DVB(60), DVB(60), DVB(60),
1388. 4UB(60), UTC(60), UTB(60), ZB(10), ATB(10), YVE(60), ZAVB(60), TARR(10),
1389. COMMON /B/ YB(60), YE(60), DB(60), DPSVB, DPWMB, DCSVB, DCWMB, DHCM,
1390. 1HMF, VMF, FMF, UF, PF, TF, RG, MGAS, DPFIX, DPFIX, DPFIX, DPFIX, DPFIX,
1391. ZSMF, PAV, HCR, BEDVOL, EFFVOL, SOLVOL, TETUBE, HLMF, PI, AND, DNZL,
1392. 3FW, FSW, DZAV, MFEDE, MDIG, MTHE, NHE, NTB, MT, M1, H, ICR, IFBC, HTC
1393. C
1394. C
1395. C
1396. C
1397. RI = SQRT (ATI / PI)
1398. DTI = 2.0 * RI
1399. IF (ATI .GT. ATB(J)) GO TO 10
1400. A1 = SORT (ATI / ATB(J-1)) - 1.0
1401. B1 = SORT (ATB(J) / ATB(J-1)) - 1.0
1402. C = ZB(J) - ZB(J-1)
1403. ZI = ZB(J-1) + A1 * C / B1
1404. GO TO 20
1405. CONTINUE
1406. 20 CONTINUE
1407. RETURN
1408. END
1409. FUNCTION HEIGHT(VV)
1410. COMMON /A/ ZHE(10), AHE(10), PV(10), PH(10), ZF(10), FFC(10), DTUBE(10),
1411. 1DV(60), DVB(60), FFAD(10), ZDIS(10), FD(10), AHEAV(60), ETUBE(60),
1412. 2UMF(60), UMFF(60), AT(60), DT(60), T(60), X(60), AKBE(60), YBE(60),
1413. 3YE(60), YCOE(60), EPB(60), EPB(60), DVB(60), DVB(60), DVB(60), DVB(60),
1414. 4UB(60), UTC(60), UTB(60), ZB(10), ATB(10), YVE(60), ZAVB(60), TARR(10),
1415. COMMON /B/ YB(60), YE(60), DB(60), DPSVB, DPWMB, DCSVB, DCWMB, RHCM,
1416. 1HMF, VMF, FMF, UF, PF, TF, RG, MGAS, DPFIX, DPFIX, DPFIX, DPFIX, DPFIX,
1417. ZSMF, PAV, HCR, BEDVOL, EFFVOL, SOLVOL, TETUBE, HLMF, PI, AND, DNZL,
1418. 3FW, FSW, DZAV, MFEDE, MDIG, MTHE, NHE, NTB, MT, M1, H, ICR, IFBC, HTC
1419. C
1420. C
1421. C
1422. C
1423. HT = 0.0
1424. SUM = 0.0
1425. DO 100 I = 2, NTC
1426. SUM = SUM + DVB(60)
1427. HT = HT + DZAV
1428. IF (SUM .LT. VV) GO TO 100
1429. HT = (VV - SUM) * DZAV / DVB(60) + HT
1430. GO TO 110
1431. 100 CONTINUE
1432. 110 CONTINUE
1433. CONTINUE
1434. RETURN
1435. END
1436. SUBROUTINE HYDRO
1437. REAL MGAS
1438. COMMON /A/ ZHE(10), AHE(10), PV(10), PH(10), ZF(10), FFC(10), DTUBE(10),
1439. 1DV(60), DVB(60), FFAD(10), ZDIS(10), FD(10), AHEAV(60), ETUBE(60),

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1440. C
1441. C
1442. C
1443. C
1444. C
1445. C
1446. C
1447. C
CALCULATION OF BUBBLE HYDRODYNAMICS

LAST = 0
SUM = 0.0
SUMEFF = 0.0
BEDVOL = 0.0
SWM = 0.0
ICR = 0
MCR = 0.0
IFBC = 0

DIMENSION DTUBEI(60), PHI(60), PV(I(60), IARRNG(60)

RHOGAS = PAVMGAS/(RG*T(2))
VISC = 3.72E-6*T(2)**0.676
AI = 33.7**2+0.040*DPSVB**3*G*(RHOBED-RHOGAS)*RHOGAS/UISC**2
UMF(2) = VISC/(DPSVB*RHOGAS) * (SORT(1) - 33.7)
UMF(1) = UMF(2)
UMF(2) = FMF*MGAS/RHOGAS/(AT(1)*ETUBE(2))
DBO = 0.347*(AT(1)*ETUBE(2)*UO(2)-UMF(2))/AND**0.4
DBA = DBO
H(2) = DBA

DO 200 I = 2,100

IF (I .EQ. 2) GO TO 16
DDB = 5.0
INDEX = 0
EMAX = 0.1
DBA = H(I-1)-H(I-2)

DO 250 I = 1,30

IF (I .LE. MI) GO TO 5

T(I) = T(M1)
X(I) = X(M1)
YB(I) = YB(M1)
YE(I) = YE(M1)
CONTINUE

H(I) = H(I-1)+DBA

C

IDENTIFICATION OF COOLING TUBES IN THE COMPARTMENT

DO 210 J = 1, MTHE

IF (ZH(J) .LE. H(I) .AND. ZHE(J+1) .LT. H(I)) GO TO 210

IF (ZH(J) .LE. H(I-1) .AND. ZHE(J+1) .GE. H(I)) GO TO 220

FI = (H(I)-ZH(J))/DBA

F2 = (ZH(J-H(I-1))/DBA

AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)

DTUBE(I) = FI*DTUBE(J)+F2*DTUBE(J-1)

GO TO 230

AHEAV(I) = AHE(J)

DTUBE(I) = DTUBE(J)

GO TO 240

CONTINUE

CALL AREA(H(I);DT(I);AT(I))

HAV = 0.5*(H(I-1)+H(I))

CALL AREA(HAV;DTAV;ATAV)

DVBB(I) = 0.5*(AT(I)-AT(I-1))DBBA

DVBBEF(I) = DVBB(I)*AT(I)-0.5*AHEAV(I)*DTUBE(I))

ETUBE(I) = 1.0 - DVBBEF(I)/DVBB(I)

IF (I .EQ. 2) GO TO 240

RHOGAS = FAV*MGAS/CR0K(T(I))

VISC = 3.72E-6*X(I)*7.26

A(1) = 33.7**2+0.048**2*X(I)**2X(RHOBED-RHOGAS)*RHOGAS/VISC**2

UMF(I) = VISC/DVBB*RHOGAS**SORT(A(1)-33.7)

UO(I) = FMO*MGAS/RHOGAS/(ATAV(1,-ETUBE(I))

IF (IFBC .GT. 0) GO TO 125

IF (ABS(UO(I)-UMF(I))/(UO(I)-UMF(I)) .LE. 0.01*UMF(I)) GO TO 18

IF (UO(I) .LT. UMF(I)) GO TO 10

GO TO 17

ICR = 1

DBMAX = 0.652*(ATAV(I)-ETUBE(I))*ABS(UO(I)-UMF(I))**0.4

DBC = DBMAX - (DBMAX-DBCC)*EXP(-0.1*HAV/DTAV)

IF (IARRNG(I) .GT. 2 .AND. PHI(I).GE.DBAV(I-1) .AND. DBC.GE.

DBAV(I)) DBO = PHI(I)

IF (LAST .GT. 0) GO TO 260

ER = DBC - DBA

IF (n .EQ. 1 .AND. DBC .LT. DBC) DD = -DD/2.0

CALL CRRECT(+INDEX;DBX;X;DBA;E1;E2;ER;EMAX)

IF (INDEX .EQ. 2) GO TO 260

CONTINUE

DBAV(I) = DBA

ANBE(I) = 1.0/DBAV(I)

C CALCULATIONS FOR UBR --- BUBBLE RISING VEL. AT MIN. FLUIDIZATION,

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) = ( UO(I)-UMF(I) ) / UO(I)*(1.0-ETUBE(I))
1560. ALFB = EMF * UBR / UMF(I)
1561. EPC(I) = EPB(I) * ALFB / (ALFB - 1.0)
1562. IF (EPB(I) .GT. 0.7) EPB(I) = 0.7
1563. IF (EPC(I) .GT. 0.99 - ETUBE(I)) EPC(I) = 0.99 - ETUBE(I)
1564. IF ((EPC(I) - EPB(I)) .GT. 0.01) EPC(I) = EPB(I) + 0.01
1565. BEDVOL = BEDVOL + DVBB(I)
1566. SUMV = SUMV + DVBBF(I)
1567. SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)
1568. SUMEFF = SUMEFF + SOLVOL
1569. SUM = SUM + SOLVOL / (0.5 * (AT(I) + AT(I-1))
1570. IF (ICR .GT. 0) GO TO 35
1571. IF (LAST .GT. 0) GO TO 125
1572. IF (HLF .NE. 0.0) GO TO 20
1573. C TEST FOR CONVERGENCY
1574. C IF (ABS(SUMEFF-U) .LT. 0.01*VMF) GO TO 125
1575. C IF (SUMEFF .LT. VMF) GO TO 20
1576. VOL = SUMV - (SUMEFF-U) * (1.0 - ETUBE(I)) / (1.0 - EPB(I) - ETUBE(I))
1577. H(I) = HEIGHT(VOL)
1578. CALL AREA (H(I), DT(I), AT(I))
1579. BREVOL = BIRDVOL - DVBB(I)
1580. SUMV = SUMV + DVBBF(I)
1581. SUMEFF = SUMEFF - SOLVOL
1582. SUM = SUM - SOLVOL / (0.5 * (AT(I) + AT(I-1)))
1583. LAST = 1
1584. DBA = H(I) - H(I-1)
1585. GO TO 16.
1586. 20 CONTINUE
1587. 10 UO(I) = UOM(I)
1588. 16 GO TO 16.
1589. 10 DBAV(I) = 0.0
1590. C TEST FOR CONVERGENCY
1591. IF (ABS(H(I)-HLF) .LE. 1.0E-3*HLF) GO TO 125
1592. IF (ABS(H(I)) .LT. 0.5 * (H(I)-H(I-1))) GO TO 50
1593. H(I) = HLF
1594. CALL AREA (H(I), DT(I), AT(I))
1595. BREVOL = BIRDVOL - DVBB(I)
1596. SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)
1597. SUMEFF = SUMEFF - SOLVOL
1598. SUM = SUM - SOLVOL / (0.5 * (AT(I) + AT(I-1)))
1599. CALL AREA (H(I), DT(I), AT(I))
1600. LAST = 1
1601. DBA = H(I) - H(I-1)
1602. GO TO 16.
1603. 10 UO(I) = UOM(I)
1604. 16 GO TO 16.
1605. 10 DBAV(I) = 0.0
1606. 16 GO TO 16.
1607. 10 DBAV(I) = 0.0
1608. 16 GO TO 16.
1609. 10 DBAV(I) = 0.0
1610. 16 CONTINUE
1611. 200 CONTINUE
\texttt{\begin{verbatim}128 \textbf{1620.} \text{AHEB(I) = 1000.0} \\
1621. \text{EPB(I) = 0.0} \\
1622. \text{EPC(I) = 0.0} \\
1623. \text{IF (VMF .EQ. 0.0) GO TO 45} \\
1624. \text{C} \\
1625. \text{C \text{FIXED BED CONDITIONS}} \\
1626. \text{C} \\
1627. \text{VOL} = \text{SUMV} + (\text{VMF - SUMEFF}) \\
1628. \text{H(I) = HEIGHT(VOL)} \\
1629. \text{CONTINUE} \\
1630. \text{IF (VMF .EQ. 0.0) H(I) = HLF} \\
1631. \text{IF (I .LE. M1) GO TO 6} \\
1632. \text{T(I) = T(M1)} \\
1633. \text{X(I) = X(M1)} \\
1634. \text{YB(I) = YB(M1)} \\
1635. \text{YE(I) = YE(M1)} \\
1636. \text{CONTINUE} \\
1637. \text{GO TO 310} \\
1638. \text{J = 1,MTHE} \\
1639. \text{IF (ZHE(J) .LE. H(I) .AND. ZHE(J+1) .LT. H(I)) GO TO 310} \\
1640. \text{F1 = (H(I)-ZHE(J))/(H(I)-H(I-1))} \\
1641. \text{F2 = (ZHE(J)-H(I-1))/(H(I)-H(I-1))} \\
1642. \text{AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)} \\
1643. \text{DTUBEI(I) = F1*DTUBE(J)+F2*DTUBE(J-1)} \\
1644. \text{PVII(I) = F1*PV(J)+F2*PV(J-1)} \\
1645. \text{PHII(I) = F1*PH(J)+F2*PH(J-1)} \\
1646. \text{GO TO 330} \\
1647. \text{AHEAV(I) = AHE(.}} \\
1648. \text{DTUBEI(I) = DTUBE(J)} \\
1649. \text{PVII(I) = PV(J)} \\
1650. \text{PHII(I) = PH(J)} \\
1651. \text{GO TO 340} \\
1652. \text{CONTINUE} \\
1653. \text{DO 340 J = 1,MTHE} \\
1654. \text{AHEAV(I) = F1*AHE(J)+F2*AHE(J-1)} \\
1655. \text{DTUBEI(I) = F1*DTUBE(J)+F2*DTUBE(J-1)} \\
1656. \text{PVII(I) = F1*PV(J)+F2*PV(J-1)} \\
1657. \text{PHII(I) = F1*PH(J)+F2*PH(J-1)} \\
1658. \text{GO TO 350} \\
1659. \text{CALL AREA(H(I),DT(I),AT(I))} \\
1660. \text{DVBB(I) = 0.5*(AT(I-1)+AT(I))*(H(I)-H(I-1))} \\
1661. \text{DVBBEF(I) = DVBB(I)*0.05*AHEAV(I)*DTUBEI(I))} \\
1662. \text{ETUBEI(I) = 1.0 - DVBBEF(I)/DVBB(I)} \\
1663. \text{RHOGAS = PAV*MGAS/(RG*T(I))} \\
1664. \text{VISC = 3.72E-6*T(I)**0.676} \\
1665. \text{A1 = 33.7*x*0.040*DPSVB**3*G*(RHOBE-RHOGAS)*RHOGAS/VISC**2} \\
1666. \text{UMF(I) = VISC/(DPSVB*RHOGAS)*(SQRT(A1)-33.7)} \\
1667. \text{HAV = 0.5*(H(I)-H(I-1))} \\
1668. \text{CALL AREA(HAV,DTAV,ATAV)} \\
1669. \text{UGI(I) = F1*MGAS/RHOGAS/(ATAV*(1.-ETUBE(I)))} \\
1670. \text{BEDVOL = BEDVOL + DVBB(I)} \\
1671. \text{SUMV = SUM + DVBBEF(I)} \\
1672. \text{SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)} \\
1673. \text{SOLVOL = SUMEFF + SOLVOL} \\
1674. \text{SUM = SUM + SOLVOL < 0.5 * (AT(I)+AT(I-1))} \\
1675. \text{IFBC = 1} \\
1676. \text{M1 = I} \\
1677. \text{DO 410 K = 2,KT} \\
1678. \text{I = I + 1} \\
1679. \text{H(I) = H(M1)+HB(K)} \end{verbatim}}
IF (ZHE(J) .LE. H(I) .AND. ZHE(J+1) .GT. H(I)) GO TO 410
IF (ZHE(J) .LE. H(I-1) .AND. ZHE(J+1) .GE. H(I)) GO TO 420
F1 = (H(I)-ZHE(J))/(H(I)-H(I-1))
F2 = (ZHE(J)-H(I-1))/(H(I)-H(I-1))
AHEAT(I) = F1*H(J)+F2*AHEAT(J-1)
DTUBE(I) = F1*DTUBE(J)+F2*DTube(J-1)
PVI(I) = F1*PV(J)+F2*PV(J-1)
PHI(I) = F1*PH(J)+F2*PH(J-1)
GO TO 430

IF (ZHE(J) .LE. H(C-I) .AND. ZHE(J+1) .GE. H(I)) GO TO 420

Fl = (H(I)-ZHE(J))/(H(U)-H(I-I))
F2 = (ZHE(J)-H(I-1))/(H(J)-H(J-1))
AHEAT(I) = F1*AHEAT(J)+F2*AHEAT(J-1)
DTUBE(I) = F1*DTUBE(J)+F2*DTUBE(J-1)
PVI(I) = F1*PV(J)+F2*PV(J-1)
PHI(I) = F1*PH(J)+F2*PH(J-1)
GO TO 440

AHEAT(I) = AHEAT(J)
DTUBE(I) = DTUBE(J)
PVI(I) = PVI(J)
PHI(I) = PHI(J)
IARR(I) = IARR(J)
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))
DVBBF(I) = DVBB(I) * (1.-0.25*AHEAT(I)*DTUBE(I))
ETUBE(I) = 1. - DVBBF(I)/DVBB(I)

SUBROUTINE SIMQ(A, B, N, NN, KS)
DIMENSION A(NN), B(N)
C FORWARD SOLUTION
TOL=0.0
KS=0
JJ=-N
DO 65 J=1,N
JY=J+1
JJ=JJ+N+1
BIGA=0.
C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
I=IT+1
IF (ABS(BIGA) .GE. ABS(A(IJ))) 20,30,30
BIGA=A(IJ)
IMAX=I
CONTINUE
20
BIGA=A(IJ)
IMAX=I
CONTINUE
30
C TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
ON
IF (ABS(BIGA) - TOL) 35,35,40
KS=I
WRITE(6,100) KS
100 FORMAT(/' NO SOLUTION', ' KS=',12)
STOP

I=J+N*(J-2)
IMAX=I
C INTERCHANGE ROWS IF NECESSARY
C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
I=IT+1
IF (ABS(BIGA) - ABS(A(IJ))) 20,30,30
BIGA=A(IJ)
IMAX=I
CONTINUE
30
C TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
35
KS=I
WRITE(6,100) KS
100 FORMAT(/' NO SOLUTION', ' KS=',12)
STOP

I=J+N*(J-2)
IMAX=I
C INTERCHANGE ROWS IF NECESSARY
C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
I=IT+1
IF (ABS(BIGA) - ABS(A(IJ))) 20,30,30
BIGA=A(IJ)
IMAX=I
CONTINUE
30
C TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
35
KS=I
WRITE(6,100) KS
100 FORMAT(/' NO SOLUTION', ' KS=',12)
STOP

I=J+N*(J-2)
IMAX=I
C INTERCHANGE ROWS IF NECESSARY
C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
I=IT+1
IF (ABS(BIGA) - ABS(A(IJ))) 20,30,30
BIGA=A(IJ)
IMAX=I
CONTINUE
30
C TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
35
KS=I
WRITE(6,100) KS
100 FORMAT(/' NO SOLUTION', ' KS=',12)
STOP

I=J+N*(J-2)
IMAX=I
C INTERCHANGE ROWS IF NECESSARY
C SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN
I=IT+1
IF (ABS(BIGA) - ABS(A(IJ))) 20,30,30
BIGA=A(IJ)
IMAX=I
CONTINUE
30
C TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )
35
KS=I
WRITE(6,100) KS
100 FORMAT(/' NO SOLUTION', ' KS=',12)
STOP

I=J+N*(J-2)
IMAX=I
DO 50 K=J,N

II=II+1
I2=I2+1
SAVE=A(I1)
A(I1)=A(I2)
A(I2)=SAVE

C DIVIDE EQUATION BY LEADING COEFFICIENT
C
50 A(I1)=A(I1)/BIGA
SAVE=B(IMAX)
B(IMAX)=B(J)
B(J)=SAVE/BIGA
C
C ELIMINATE NEXT VARIABLE
C
IF( J - N) .LE. 70, 75
55 IRS=N*(J-1)
DO 65 IX=JY,N
65 IXJ=IOS+IX
IT=J-IX
DO 60 JX=4YN
IXJX=N*JX-1)+IX
JJX=IXJX+IT
60 A(IXJX)=A(IXJX)-((IXJ)*A(JJX))
55

RETURN
END

SUBROUTINE VELYISCRHOGASG,RHOS,PARUM,UT)

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

A1=33.7**2+0.0409*DPAR*3.0*(RHOS-RHOGAS)*RHOGAS/VISC**2
UM=VISC/(DPAR*RHOGAS)*(SQR(A1)-33.7)
UT=(4.0*(RHOS-RHOGAS)**2**2/225.0/RHOGAS/VISC)**(1./3.)*DPAR
REP=DPAR*RHOGAS*UT/VISC
IF(REP.LT.0.4) GO TO 210
UT=5*(RHOS-RHOGAS)*DPAR**2/18./VISC
REP=DPAR*RHOGAS*UT/VISC
IF(REP.LT.0.4) GO TO 210
UT=SQR(3.1*G*(RHOS-RHOGAS)*DPAR/RHOGAS)

RETURN
210
END

FUNCTION VOLUME (Z)

COMMON /A/, ZHE(10), AHE(10), PV(10), PH(10), ZF(10), FFC(10), DTUBE(10),
DVB(60), DVBEFF(60), FFAD(10), ZDIS(10),FD(10), AHEAV(60), ETUBE(60)
COMMON

YB(60), YE(60), DB(60), DPSV, DMSV, DCW, DCM, RHO

C

CALCULATION 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) GOTO 100

A1 = (ZZ - ZN) / DZAV

SUM = SUM + DVBEFF(I) * A1

CONTINUE

100

VOLUME = SUM

RETURN

END
## APPENDIX V

### INPUT TO COMBUSTION PROGRAM

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<tr>
<th>Input</th>
<th>Value</th>
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### Notes
- The table above summarizes the inputs to the combustion program.
- Each input is associated with a specific value or parameter.
- The values range from 132 to 1.2.
- The program likely uses these inputs to simulate or model combustion processes.
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**Outlet Gas Concentration**

- CO2: 0.0766-01
- CO: 0.0806-01
- H2: 0.051E-03
- H2O: 0.0797E-01

**Pressure Drop Across the Distributor**

7.3566E-02

**Pressure Drop in the Bed**

- 1.0492E-09
- 5.386E-09
- 5.386E-09
- 1.301E-09
- 1.301E-09
- 2.010E-09

**Pressure Drop in the Fixed Bed Section**

0.8
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<td>Minimum Fluid Vel.</td>
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<tr>
<td>Maximum Fluid Vel.</td>
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APPENDIX VII

MANUAL FOR THE COMPUTER PROGRAMS

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

1. Elutriation Main Program

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

2. Combustion Main Program

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

The combustion of coal is specified by the indicator IGNITE. If IGNITE equals to zero, there is no combustion, and bubble hydrodynamics alone is calculated. Otherwise, the combustion calculations are started from CN 248. First the boundary conditions are specified.
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 \( T_{i,\text{OLD}} \) 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

$$k_{vl} = k_{vl} \cdot S_g \cdot \frac{\lambda_l}{1/\sec}$$  \hspace{1cm} (A.VII.3)

where $k_{vl}$ is defined as:

$$k_{vl} = 490 \exp(-17500/RT) \hspace{0.1cm} \text{gm/cm}^3\cdot\text{sec}$$  \hspace{1cm} (A.VII.4)

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

$$S_g = 35.9 \cdot T - 3.67 \cdot 10^4 \text{ cm}^2/\text{gm} \hspace{0.1cm}, \hspace{0.1cm} T < 1253 \hspace{0.1cm} ^\circ\text{K}$$  \hspace{1cm} (A.VII.5)

$$= -38.43 \cdot T + 5.64 \cdot 10^4 \text{ cm}^2/\text{gm} \hspace{0.1cm}, \hspace{0.1cm} T > 1253 \hspace{0.1cm} ^\circ\text{K}$$  \hspace{1cm} (A.VII.6)

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

$$\lambda_{la} = \left(\frac{\lambda_{la2}}{\lambda_{la1}}\right) \left(\frac{f_2 - f_1}{f_2 - f_1}\right) \cdot \lambda_{la1}$$  \hspace{1cm} (A.VII.7)
\[ \lambda_{lb} = \left( \frac{b_{lb}}{\lambda_{lb1}} \right)^{\frac{f_{lb} - f_{l1}}{f_{2} - f_{1}}} \lambda_{lb1} \quad (A.VII.8) \]

\[ \lambda_{lb} = \left( \frac{\ln(d_{lb}/d_{lb})}{\ln(d_{la}/d_{lb})} \right) \lambda_{lb} \quad (A.VII.9) \]

where \( \lambda_{lb} \) is the reactivity of limestone, \( f_{lb} \) is the fractional conversion of limestone and \( d_{lb} \) 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**, \( \lambda = 6.32 \times 10^{-6} \ T_m^{0.5} / \left\{ 1 + \frac{245 \times 10^{(-12/T_m)}}{T_m} \right\} \text{ cals/sec.cm}^{\circ} \text{C} \quad (A.VII.10) \)
- **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 $A_{t,j}, j = 1$-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

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

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

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

$$r_{j-1} = (A_{t,j-1}/\pi)^{1/2}$$  \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-Boltzmann constant, $\sigma = 1.36 \times 10^{-12}$, cals/sec.cm$^2$°K$^4$
- Thermal conductivity of the surrounding gas, and the diffusivity
of $O_2-N_2$ are calculated by Equations (A.VII.10) and (A.VII.11) respectively. Char size reduction rate constant is equal to $(1/t_b)$.

7. **Subprogram CRRECT**

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

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

Period 2: the root is found in the interval ($INDX = 1$)

as shown in Fig. 26.

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

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

1) Initial assumption for the unknown variable, $X$

2) Value of increment, $DX$

3) Tolerance limit for error, $EMAX$

4) Difference between the assumed and calculated values for the variable, $E$

5) Initial value for $INDX$, $INDX = 0$

6) **DO loop for iteration**

7) A statement to get off the **DO loop** when $INDX = 2$
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),

\[
A_{HE} = \frac{\text{Heat transfer area}}{\text{Volume of bed}}
\]

\[
= \frac{\left(\frac{1}{2}\right) \pi d_o \Delta Z}{\left(\frac{1}{2}\right) \left(P_H P_V \Delta Z\right)} = \frac{\pi d_o}{P_H P_V}
\]

\( (A.VII.16) \)
Fig. 27 Arrangement of Cooling Tubes
For the rectangular arrangement (Fig. 27),
\[ a_{HE} = \frac{\pi d_o \Delta Z}{P H P V \Delta Z} = \frac{\pi d_o}{P H V} \]  
(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): \( \frac{1}{2} \pi d_o^2 \Delta Z = \frac{d_o}{4} a_{HE} \)  
(A.VII.18)

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

Volume fraction of tubes is then equal to
\[ \varepsilon_{\text{tube}} = 1 - \text{effective volume/total volume} \]  
(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 program considers the freeboard char combustion and solves the material balance equations for oxygen in the freeboard. There will be two cases in the calculations: (i) oxygen rich or excess air conditions and (ii) oxygen starved conditions. For the oxygen rich case, Regula Falsi method is applied to calculate the oxygen concentration since the calculations involve a trial and error procedure.

11. **Subprogram GPB**

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

12. **Subprogram GPHASE**

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

13. **Subprogram HAREA**

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

\[
Z = Z_{j-1} + \frac{(A_t/A_{j-1})^{1/2} - 1}{(A_j/A_{j-1})^{1/2} - 1} (Z_j - Z_{j-1})
\]  

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

14. 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

As before, computations are performed till \( U_0 \) becomes smaller
than \( U_{mf} \). In the fixed bed section, the bubble fraction is zero.
Fixed bed is equivalent to the condition of minimum fluidization. Total
volume of the bed is the sum of the effective volume of solids in the
fluidized bed section and the difference in the minimum fluidization
volume and the volume of solids in the fluidized section. Total height
of the bed is computed from the total volume of the bed.

16. **Subprogram SIMQ**

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

17. **Subprogram VEL**

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

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

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

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

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

SUBROUTINE SING

Purpose

SOLUTION OF A SET OF LINEAR EQUATIONS

Calling Sequence

CALL SING(A,B,N)

Input Parameters

A - A set of linear equations, size N x N

B - Right-hand side vector, size N

N - Size of the matrix

Output Parameters

B - Solution vector, size N

Notes

1. The solution is obtained using the Gaussian elimination method.
2. If the determinant of the coefficient matrix is zero, a solution may not be available.
3. The routine can be modified by adjusting the pivot strategy.

Examples

Example 1:

A = [[1, 2, 3], [4, 5, 6], [7, 8, 9]]
B = [10, 20, 30]
N = 3

Solution:

B = [4, -8, 6]

Example 2:

A = [[1, 2, 3], [4, 5, 6], [7, 8, 9]]
B = [10, 20, 30]
N = 3

Solution:

No solution exists due to the singular nature of the matrix.

Subroutines and Function Subprograms Required

None

References

1. Numerical Recipes, Cambridge University Press

Modification History

1990: Revised

15.3
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&lt;sub&gt;HE&lt;/sub&gt;</td>
<td>Specific heat transfer area of the tubes, cm&lt;sup&gt;2&lt;/sup&gt;/cm&lt;sup&gt;3&lt;/sup&gt; FBC volume</td>
</tr>
<tr>
<td>AH EW</td>
<td>a&lt;sub&gt;HEW&lt;/sub&gt;</td>
<td>Specific heat transfer area of the walls, cm&lt;sup&gt;2&lt;/sup&gt;/cm&lt;sup&gt;3&lt;/sup&gt; FBC volume</td>
</tr>
<tr>
<td>AK</td>
<td>k&lt;sub&gt;v1&lt;/sub&gt;</td>
<td>Overall volume reaction rate constant for limestone - SO&lt;sub&gt;2&lt;/sub&gt; reaction, l/sec</td>
</tr>
<tr>
<td>AKB</td>
<td>k&lt;sub&gt;c,B&lt;/sub&gt;</td>
<td>Overall rate constant for char combustion in bubble phase, cm/sec</td>
</tr>
<tr>
<td>AKBE</td>
<td>K&lt;sub&gt;BE&lt;/sub&gt;</td>
<td>Gas exchange coefficient, l/sec</td>
</tr>
<tr>
<td>AKC</td>
<td>k&lt;sub&gt;c&lt;/sub&gt;</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&lt;sub&gt;2&lt;/sub&gt; reaction, cm/sec</td>
</tr>
<tr>
<td>AKE</td>
<td>k&lt;sub&gt;c,E&lt;/sub&gt;</td>
<td>Overall rate constant for char combustion in emulsion phase, cm/sec</td>
</tr>
<tr>
<td>AKNO</td>
<td>k&lt;sub&gt;NO&lt;/sub&gt;</td>
<td>NO reduction rate constant, cm/sec</td>
</tr>
<tr>
<td>ALFA</td>
<td>-</td>
<td>Temperature matrix coefficients</td>
</tr>
<tr>
<td>AMODF</td>
<td>a&lt;sub&gt;m&lt;/sub&gt;</td>
<td>Defined by Equation (VI.12)</td>
</tr>
<tr>
<td>AND</td>
<td>n&lt;sub&gt;d&lt;/sub&gt;</td>
<td>Number of orifices in the distributor</td>
</tr>
<tr>
<td>ANH3V</td>
<td>-</td>
<td>NH&lt;sub&gt;3&lt;/sub&gt; content in the volatiles, gmole NH&lt;sub&gt;3&lt;/sub&gt;/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&lt;sub&gt;t&lt;/sub&gt;</td>
<td>Cross sectional area of the bed, cm&lt;sup&gt;2&lt;/sup&gt;</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>ATB</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>BBB</td>
<td></td>
<td>Matrix coefficients</td>
</tr>
<tr>
<td>BEDCOM</td>
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<td>Char combustion rate in the bed, gm/sec</td>
</tr>
<tr>
<td>BEDVOL</td>
<td></td>
<td>Total bed volume, cm³</td>
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<tr>
<td>BETA</td>
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<td>Temperature matrix coefficients</td>
</tr>
<tr>
<td>CADF</td>
<td>C&lt;sub&gt;Sf&lt;/sub&gt;</td>
<td>Heat capacity of feed additives, cals/gm.°C</td>
</tr>
<tr>
<td>CARCON</td>
<td></td>
<td>Carbon concentration, gm carbon/cm³ bed volume (including tubes)</td>
</tr>
<tr>
<td>CAS</td>
<td></td>
<td>Ca/S molar ratio in feed solids</td>
</tr>
<tr>
<td>CASE</td>
<td></td>
<td>Effective Ca/S molar ratio (including Ca in ash)</td>
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<tr>
<td>CCF</td>
<td>C&lt;sub&gt;cf&lt;/sub&gt;</td>
<td>Heat capacity of coal feed, cals/gm.°C</td>
</tr>
<tr>
<td>CCHAR</td>
<td>C&lt;sub&gt;ch&lt;/sub&gt;</td>
<td>Carbon content in char, gm carbon/gm char</td>
</tr>
<tr>
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<td>Char elutriated from the combustor, gms/sec</td>
</tr>
<tr>
<td>CGM</td>
<td>C&lt;sub&gt;gm&lt;/sub&gt;</td>
<td>Molar heat capacity of gas, cals/gmole °C</td>
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<td>CGMF</td>
<td></td>
<td>Molar heat capacity of feed gas, cals/gmole °C</td>
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<td>Carbon content in char, gmole carbon/gm coal</td>
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<tr>
<td>CHARNH</td>
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<td>Hydrogen content in char, gatom hydrogen/gm coal</td>
</tr>
<tr>
<td>CHARN</td>
<td></td>
<td>Nitrogen content in char, gatom nitrogen/gm coal</td>
</tr>
<tr>
<td>CHARO</td>
<td></td>
<td>Oxygen content in char, gatom oxygen/gm coal</td>
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<td>CHARS</td>
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<td>Sulfur content in char, gatom sulfur/gm coal</td>
</tr>
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<td>CH4</td>
<td>CH&lt;sub&gt;4&lt;/sub&gt;</td>
<td>Wt. fraction CH&lt;sub&gt;4&lt;/sub&gt; in the volatiles; CH&lt;sub&gt;4&lt;/sub&gt; released during devolatilization, gmole CH&lt;sub&gt;4&lt;/sub&gt;/gm coal</td>
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<tr>
<td>CLOSS</td>
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<td>Total carbon loss (elutriated + withdrawn), gm/sec</td>
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<td>CO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Wt. fraction CO&lt;sub&gt;2&lt;/sub&gt; in the volatiles; CO released during devolatilization, gmole CO/gm coal</td>
</tr>
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<td>COALC</td>
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<td>Carbon content in coal, gatom carbon/gm coal (d.b.)</td>
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<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
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<tr>
<td>COALH</td>
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<td>Hydrogen content in coal, gatom hydrogen/gm coal (d.b.)</td>
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<td>Nitrogen content in coal, gatom nitrogen/gm coal (d.b.)</td>
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<td>Sulfur content in coal, gatom sulfur/gm coal (d.b.)</td>
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<td>Carbon monoxide burnt in each compartment, gmole/sec</td>
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<td>CO released during devolatilization per mole of volatiles released, gmole CO/gmole volatiles</td>
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<td>COVB</td>
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<td>CO produced during volatiles combustion, gmole CO/gmole volatiles</td>
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<td>Wt. fraction CO₂ in the volatiles; CO₂ released during devolatilization, gmole CO₂/gm coal</td>
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<td>CO₂ released during devolatilization per mole of volatiles released, gmole CO₂/gmole volatiles</td>
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<td>CO2VB</td>
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<td>CO₂ produced during volatiles combustion, gmole CO₂/gmole volatiles</td>
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<td>CS</td>
<td>C_S</td>
<td>Heat capacity of solids, cals/gm °C</td>
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<td>CTAR</td>
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<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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<td>Weight mean particle diameter of additives in the feed, cm</td>
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<td>Bubble diameter in each compartment, cm</td>
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<td>d_co</td>
<td>Surface volume mean diameter of char particles in the freeboard, cm</td>
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<td>d_c</td>
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<td>Surface volume mean diameter of coal particles in the feed, cm</td>
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<td>DCWE</td>
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<td>Weight mean diameter of char particles in the freeboard, cm</td>
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<tr>
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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>Increment in combustion efficiency</td>
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<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>Pressure drop across the fixed bed section, cm H₂O</td>
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<tr>
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<td>Pressure drop across the fluid bed section, cm H₂O</td>
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<td>dₜₑ</td>
<td>Surface volume mean particle diameter of additives entrained in the freeboard, cm</td>
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<td>dₛₑ</td>
<td>Surface volume mean particle diameter of additives in the bed, cm</td>
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<td>Weight mean particle diameter of additives entrained in the freeboard, cm</td>
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<td>Weight mean particle diameter of additives in the bed, cm</td>
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<td>DTUBE</td>
<td>(SEE DESIGN)</td>
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<td>DVBB</td>
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<td>Volume of each compartment, cm³</td>
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<td>Mathematical Symbol</td>
<td>Description</td>
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<td>DT</td>
<td>$D_t$</td>
<td>Diameter of the combustor, cm</td>
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<tr>
<td>EETCM</td>
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<td>Tolerance limit for combustion efficiency convergency</td>
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<tr>
<td>EETSM</td>
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<td>Tolerance limit for sulfur dioxide retention efficiency convergency</td>
</tr>
<tr>
<td>EFF</td>
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<td>Combustion efficiency calculated from elutriation calculations</td>
</tr>
<tr>
<td>EFFVOL</td>
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<td>Volume of bed (excluding tubes), cm$^3$</td>
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<tr>
<td>EINDEX</td>
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<td>Nitric oxide emission index, gmole NO/gm coal burnt</td>
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<tr>
<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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<tr>
<td>EPB</td>
<td>$\varepsilon_{B}$</td>
<td>Bubble fraction</td>
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<tr>
<td>EPC</td>
<td>$\varepsilon_{c}$</td>
<td>Cloud fraction including bubble</td>
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<tr>
<td>ETC</td>
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<td>Carbon combustion efficiency</td>
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<td>Assumed carbon combustion efficiency</td>
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<td>Carbon combustion efficiency based on carbon balance</td>
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<td>Carbon combustion efficiency based on oxygen balance</td>
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<td>$NO_x$ emission efficiency</td>
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<td>Sulfur dioxide retention efficiency</td>
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<tr>
<td>ETSC</td>
<td></td>
<td>Calculated sulfur dioxide retention efficiency</td>
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<tr>
<td>ETUBE</td>
<td>$\varepsilon_{tube}$</td>
<td>Volume fraction of tubes in each compartment</td>
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<td></td>
<td>Excess air, fraction</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<tr>
<td>FBCOM</td>
<td>-</td>
<td>Char combustion rate in the freeboard, gm/sec</td>
</tr>
<tr>
<td>FBM</td>
<td>F&lt;sub&gt;BM&lt;/sub&gt;</td>
<td>Molar flow rate of gas in the bubble phase, gmole/sec</td>
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<td>FD</td>
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<td>Fraction of solids withdrawn from the bed at each location</td>
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<tr>
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<td>F&lt;sub&gt;EM&lt;/sub&gt;</td>
<td>Molar flow rate of gas in the emulsion phase, gmole/sec</td>
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<td>FPAD</td>
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<td>Fraction of total additives fed at each location</td>
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<tr>
<td>FFC</td>
<td>-</td>
<td>Fraction of total coal fed at each location</td>
</tr>
<tr>
<td>FMF</td>
<td>-</td>
<td>Molar feed rate of fluidizing air, gmole/sec</td>
</tr>
<tr>
<td>FMTH</td>
<td>-</td>
<td>Stoichiometric air feed rate, gmole/sec</td>
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<tr>
<td>FMO</td>
<td>F&lt;sub&gt;MT&lt;/sub&gt;</td>
<td>Total molar flow rate of gas in the combustor, gmole/sec</td>
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<tr>
<td>FR</td>
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<td>Frequency factor for char-NO reaction, cm/sec</td>
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<tr>
<td>FRN</td>
<td>-</td>
<td>Feed rate of fuel nitrogen, gatom/sec</td>
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<tr>
<td>FRS</td>
<td>-</td>
<td>Feed rate of fuel sulfur, gatom/sec</td>
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<tr>
<td>FS</td>
<td>f&lt;sub&gt;S&lt;/sub&gt;</td>
<td>Fractional conversion of limestone</td>
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<td>FSW</td>
<td>(SEE DESIGN)</td>
<td></td>
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<tr>
<td>FW</td>
<td>f&lt;sub&gt;W&lt;/sub&gt;</td>
<td>Solids mixing parameter, ratio of wake volume to the bubble volume including the wakes</td>
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<tr>
<td>G</td>
<td>g</td>
<td>Acceleration due to gravity, cm/sec²</td>
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<tr>
<td>GAMA</td>
<td>-</td>
<td>Temperature matrix coefficients</td>
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<tr>
<td>GB</td>
<td>g&lt;sub&gt;B&lt;/sub&gt;</td>
<td>Volatiles burning rate in the bubble phase, gmole/sec</td>
</tr>
<tr>
<td>GE</td>
<td>g&lt;sub&gt;E&lt;/sub&gt;</td>
<td>Volatiles burning rate in the emulsion phase, gmole/sec</td>
</tr>
<tr>
<td>GENB</td>
<td>-</td>
<td>SO&lt;sub&gt;2&lt;/sub&gt; or NO&lt;sub&gt;X&lt;/sub&gt; release rate in the bubble phase or in the freeboard due to volatiles combustion, gmole/sec</td>
</tr>
</tbody>
</table>
FORTRAN Symbol | Mathematical Symbol | Description
--- | --- | ---
GENE | - | SO\textsubscript{2} or NO\textsubscript{x} release rate in the emulsion phase or in the freeboard due to volatiles combustion, gmole/sec
GFLOW | G | Gas flow rate, gms/sec
H | - | Height above the distributor, cms
HB | h | Height above the bed surface, cms
HAREA | - | Total heat transfer area of cooling tubes (based on outside diameter of tube), cm\textsuperscript{2}
HCHAR | - | Hydrogen content in char, gm hydrogen/gm char
HCOAL | - | Lower heating value of coal, cals/gm
HCR | - | Critical bed height above which there is a fixed bed section, cm
HFB | - | Freeboard height, cm
HLF | - | Expanded bed height, cm
HLMF | - | Bed height at minimum fluidization, cm
HTAR | - | Hydrogen content in tar, gm hydrogen/gm coal fed
H2 | H\textsubscript{2} | Wt. fraction H\textsubscript{2} in the volatiles; H\textsubscript{2} released during devolatilization, gmole H\textsubscript{2}/gm coal
H2O | H\textsubscript{2}O | Wt. fraction H\textsubscript{2}O in the volatiles; H\textsubscript{2}O released during devolatilization, gmole H\textsubscript{2}O/gm coal
H2SV | - | H\textsubscript{2}S content in the volatiles, gmole H\textsubscript{2}S/gmole volatiles
IARR | (SEE DESIGN) | Indicator for critical bed height
FCR | - | Indicator for fixed bed section
IFBC | - | Indicator for combustion calculations
IGNITE | - | Indicator for NO\textsubscript{x} calculations
INOX | - | Indicator for pressure drop calculations
<table>
<thead>
<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
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<td>Indicator for SO₂ calculations</td>
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<td>ITEMP</td>
<td>-</td>
<td>Indicator for temperature calculations</td>
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<tr>
<td>ITRIAL</td>
<td>-</td>
<td>Number of trials made in the combustion calculations</td>
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<td>KT</td>
<td>-</td>
<td>Number of compartments in freeboard</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>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>-</td>
<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>MFEED</td>
<td>-</td>
<td>No. of solids feed locations</td>
</tr>
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<td>Molecular weight of combustion gases, gms/gmole</td>
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<td>-</td>
<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>-</td>
<td>Molecular weight of magnesium oxide, gms/gmole</td>
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<td>Atomic weight of nitrogen, gms/gatom</td>
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<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<tr>
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<td>Molecular weight of nitric oxide, gms/gmole</td>
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<td>Molecular weight of nitrogen, gms/gmole</td>
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<td>Molecular weight of oxygen, gms/gmole</td>
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<td>Atomic weight of sulfur, gms/gatom</td>
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<td>MSO2</td>
<td>-</td>
<td>Molecular weight of sulfur dioxide, gms/gmole</td>
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<tr>
<td>MTAR</td>
<td>-</td>
<td>Average molecular weight of tar in the volatiles, gms/gmole</td>
</tr>
<tr>
<td>MTB</td>
<td>(SEE DESIGN)</td>
<td></td>
</tr>
<tr>
<td>MTHE</td>
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</tr>
<tr>
<td>M1</td>
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<td>No. of compartments in the bed + 1</td>
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<tr>
<td>NA</td>
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<td>No. of additive particles in the freeboard</td>
</tr>
<tr>
<td>NAMEC1</td>
<td>-</td>
<td>Name of coal</td>
</tr>
<tr>
<td>NAMEC2</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>NAMEL1</td>
<td>-</td>
<td>Name of limestone</td>
</tr>
<tr>
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<td>-</td>
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</tr>
<tr>
<td>NC</td>
<td>-</td>
<td>No. of char particles in the freeboard</td>
</tr>
<tr>
<td>NCHAR</td>
<td>-</td>
<td>Nitrogen content in char, gm nitrogen/gm char</td>
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<tr>
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<td>-</td>
<td>Total number of compartments in the combustor using DZAV + 1</td>
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<tr>
<td>OCHAR</td>
<td>-</td>
<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>
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<tr>
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<td>-</td>
<td>Pressure of fluidizing air at the inlet to the distributor, atm</td>
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<td>(SEE DESIGN)</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>
<tr>
<td>QAREA</td>
<td>-</td>
<td>Heat transfer rate to the tubes per unit heat transfer area of tubes, cals/cm²·sec</td>
</tr>
<tr>
<td>QCHAR</td>
<td>-</td>
<td>Heat of combustion of char, cals/gm</td>
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<td>QCLCN</td>
<td>-</td>
<td>Heat of calcination of limestone, cals/gm</td>
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<tr>
<td>QCO</td>
<td>-</td>
<td>Heat of combustion of carbon monoxide, cals/gmole</td>
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<tr>
<td>QTRANS</td>
<td>-</td>
<td>Total heat transferred to the cooling medium, cals/sec</td>
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<td>-</td>
<td>Heat of partial combustion of volatiles, cals/gmole</td>
</tr>
<tr>
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<td>-</td>
<td>Heat of combustion of volatiles, cals/gmole</td>
</tr>
<tr>
<td>QVOL</td>
<td>-</td>
<td>Heat transfer rate per unit volume of bed, cals/cm³</td>
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<tr>
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<td>A</td>
<td>Defined by Equation (V.2)</td>
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<td>Fraction of carbon remaining in char after devolatilization, gm carbon/gm carbon in coal</td>
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<td>RCHAR</td>
<td>_ch</td>
<td>Char produced per unit gm of coal fed, gm/gm</td>
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<td>Total release rate of SO₂ or NOₓ in the bubble phase, gmole/sec²</td>
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<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>-</td>
<td>Fraction of hydrogen remaining in char after devolatilization, gm hydrogen/gm hydrogen in coal</td>
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<td>RHOAD</td>
<td>-</td>
<td>Density of additives, gms/cm³</td>
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<td>RHOASH</td>
<td>-</td>
<td>Density of ash, gms/cm³</td>
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<td>_b</td>
<td>Density of the bed materials, gms/cm³</td>
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<tr>
<td>RHOC</td>
<td>-</td>
<td>Density of coal, gms/cm³</td>
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<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<tr>
<td>RHOCH</td>
<td>( \rho_{ch} )</td>
<td>Density of char, gms/cm(^3)</td>
</tr>
<tr>
<td>RHOGAS</td>
<td>( \rho_g )</td>
<td>Density of gas, gms/cm(^3)</td>
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<td>RHOFG</td>
<td>-</td>
<td>Density of the fluidizing air at the inlet to the distributor, gms/cm(^3)</td>
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<td>Fraction of nitrogen remaining in char after devolatilization, gm nitrogen/gm nitrogen in coal</td>
</tr>
<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>
</tr>
<tr>
<td>RRB</td>
<td>-</td>
<td>Rate of combustion of char in the bubble phase, gms/sec</td>
</tr>
<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, gmoles volatiles/gm coal</td>
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<tr>
<td>SCHAR</td>
<td>-</td>
<td>Sulfur content in char, gm sulfur/gm char</td>
</tr>
<tr>
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<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>
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<td>SULFUR</td>
<td>-</td>
<td>Sulfur released during char combustion, gatom/sec</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>Temperature, °K</td>
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<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>
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<tr>
<td>TARC</td>
<td>-</td>
<td>Stoichiometric air required per unit gm of char, gmoles/gm char</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
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<tr>
<td>TAV</td>
<td>Mean bed temperature, °K</td>
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<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>
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<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>
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<td>Total char combustion rate, gm/sec</td>
</tr>
<tr>
<td>TETUBE</td>
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<td>Total volume fraction of tubes in the bed</td>
</tr>
<tr>
<td>TF</td>
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<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>
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<td>Temperature criterion for convergency</td>
</tr>
<tr>
<td>TOLD</td>
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<td>Bed temperature in the previous iteration, °K</td>
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<tr>
<td>TPB</td>
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<td>Char particle temperature in the bubble phase, °K; also in the freeboard, °K</td>
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<tr>
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<td></td>
<td>Char particle temperature in the emulsion phase, °K</td>
</tr>
<tr>
<td>TSF</td>
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<td>Temperature of feed solids, °K</td>
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<tr>
<td>TSTA</td>
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<td>Starting temperature (assumed) for iteration, °K</td>
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<tr>
<td>TW</td>
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<td>Cooling water temperature, °K</td>
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<td>TWALL</td>
<td></td>
<td>Wall temperature, °K</td>
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<td>Average wall temperature used for heat losses, °K</td>
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<td>Log mean temperature of the cooling water</td>
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<td>Inlet water temperature, °K</td>
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<td>Outlet water temperature, °K</td>
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<td>FORTRAN Symbol</td>
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<tr>
<td>UB</td>
<td>$U_B$</td>
<td>Bubble velocity, cm/sec</td>
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<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>
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<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>
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<tr>
<td>UT</td>
<td>$U_t$</td>
<td>Terminal velocity of the particle, cm/sec</td>
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<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>
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<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>
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<tr>
<td>VAHOLD</td>
<td>-</td>
<td>Volumetric additives holdup in the freeboard; cm$^3$ solid volume</td>
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<tr>
<td>VCHOLD</td>
<td>-</td>
<td>Volumetric char hold-up in the freeboard, cm$^3$ solid volume</td>
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<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>
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<tr>
<td>VISC</td>
<td>$\mu$</td>
<td>Viscosity of gas, gm/cm·sec</td>
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<tr>
<td>VM</td>
<td>-</td>
<td>Proximate volatile matter in coal, gm/gm coal (daf)</td>
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<td>-</td>
<td>Bed volume at minimum fluidization (excluding the internals), cm³</td>
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<td>VPROD</td>
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<td>Volatiles released in each compartment, gmole/sec</td>
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<tr>
<td>WAD</td>
<td>$W_{f,a}$</td>
<td>Additives feed rate, gms/sec</td>
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<td>-</td>
<td>Additives hold-up in the freeboard, gms</td>
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<td>WB</td>
<td>$M_b$</td>
<td>Weight of bed materials, gms</td>
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<td>-</td>
<td>Char hold-up in the freeboard, gms</td>
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<tr>
<td>WCOAL</td>
<td>-</td>
<td>Coal feed rate as received basis, gms/sec</td>
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<tr>
<td>WD</td>
<td>-</td>
<td>Solids withdrawal rate at each location, gms/sec</td>
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<tr>
<td>WDIS</td>
<td>$W_D$</td>
<td>Solids withdrawal rate, gms/sec</td>
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<td>WEA</td>
<td>-</td>
<td>Additives entrainment rate in the freeboard, gms/sec</td>
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<td>WEC</td>
<td>-</td>
<td>Char entrainment rate in the freeboard, gms/sec</td>
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<td>-</td>
<td>Solids (excluding char) elutriation rate from the combustor, gms/sec</td>
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<td>WFAD</td>
<td>$W_{f,a}$</td>
<td>Additives feed rate in each compartment, gms/sec</td>
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<td>WFC</td>
<td>$W_{f,c}$</td>
<td>Coal feed rate in each compartment, gms/sec</td>
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<tr>
<td>WMIX</td>
<td>$W_{\text{mix}}$</td>
<td>Solids mixing rate, gms/sec</td>
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<td>WNET</td>
<td>$W_{\text{net}}$</td>
<td>Net flow rate of solids, gms/sec</td>
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<td>B</td>
<td>Defined by Equation (V.3)</td>
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<td>X</td>
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<td>Weight fraction carbon in the bed</td>
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<td>Ash content in coal as received basis, gm ash/gm coal</td>
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<td>Calcium oxide content in ash, gm CaO/gm ash</td>
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<td>Carbon content in coal, gm carbon/gm coal (d.b.)</td>
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<td>Calcium oxide content in limestone, gm CaO/gm limestone</td>
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<td>Fixed carbon content in coal, gm carbon/gm coal (d.b.)</td>
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<td>Carbon dioxide content in limestone, gm CO2/gm limestone</td>
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<td>Volatile carbon content in coal, gm carbon/gm coal (d.b.)</td>
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<td>-</td>
<td>Hydrogen content in coal, gm hydrogen/gm coal (d.b.)</td>
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<td>Magnesium oxide content in limestone, gm MgO/gm limestone</td>
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<td>Nitrogen content in coal, gm nitrogen/gm coal (d.b.)</td>
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<td>Oxygen content in coal, gm oxygen/gm coal (d.b.)</td>
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<td>X02</td>
<td>X_{O_2}</td>
<td>Oxygen required for partial combustion of volatiles, gmole O_2/gmole volatile</td>
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<tr>
<td>X02C</td>
<td>X_{O_2,c}</td>
<td>Oxygen required for complete combustion of volatiles, gmole O_2/gmole volatile</td>
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<td>XS</td>
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<td>Sulfur content in coal, gm sulfur/gm coal (d.b.)</td>
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<td>XS102</td>
<td>-</td>
<td>Silicon dioxide content in limestone, gm SiO_2/gm limestone</td>
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<td>Moisture content in coal as received basis, gm H_2O/gm coal</td>
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<td>Average O_2 concentration (assumed) for iteration, mole fraction</td>
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<td>Mole fraction O_2 or SO_2 or NO in the bubble phase</td>
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<td>Mole fraction CO</td>
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<td>Y_E,CO</td>
<td>Mole fraction CO in the emulsion phase</td>
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<td>Y_CO2</td>
<td>Mole fraction CO$_2$</td>
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<td>Y_B,CO$_2$</td>
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<td>Mole fraction $O_2$ or SO$_2$ or NO in the emulsion phase</td>
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<td>Y_E</td>
<td>Mole fraction $O_2$ in the emulsion phase</td>
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<td>Gaseous species concentrations at the exit, mole fraction</td>
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<td>Y_H$_2$O</td>
<td>Mole fraction H$_2$O</td>
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<td>YNOX</td>
<td>Y_NO</td>
<td>Mole fraction NO</td>
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<td>Y_O</td>
<td>Mole fraction $O_2$</td>
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<td>YSO2</td>
<td>Y_SO$_2$</td>
<td>Mole fraction SO$_2$</td>
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<tr>
<td>YV</td>
<td>Y_V</td>
<td>Mole fraction volatiles</td>
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<td>Y_E,V</td>
<td>Mole fraction volatiles in the emulsion phase</td>
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<td>ZAVG</td>
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<td>Average height of each compartment above the distributor, cm</td>
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<tr>
<td>ZF</td>
<td>-</td>
<td>Locations of solids feed ports, cms</td>
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<td>ZHE</td>
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</tr>
<tr>
<td>ZDIS</td>
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### MAIN PROGRAM ELUTRIATION

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<tbody>
<tr>
<td>AHE</td>
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<td>Cross sectional area of the bed, cm$^2$</td>
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<tr>
<td>ATB</td>
<td>$A_t$</td>
<td>Ca/S molar ratio in feed solids</td>
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<td>Carbon content in char, gm carbon/gm char</td>
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<tr>
<td>CCHAR</td>
<td>$C_{ch}$</td>
<td>Char elutriated from the combustor, gms/sec</td>
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<tr>
<td>CELU</td>
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<td>Carbon content in char, gm mole carbon/gm coal</td>
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<tr>
<td>CHARC</td>
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<td>Hydrogen content in char, gatom hydrogen/gm coal</td>
</tr>
<tr>
<td>CHARN</td>
<td></td>
<td>Nitrogen content in char, gatom nitrogen/gm coal</td>
</tr>
<tr>
<td>CHARO</td>
<td></td>
<td>Oxygen content in char, gatom oxygen/gm coal</td>
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<tr>
<td>CHARS</td>
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<td>Sulfur content in char, gatom sulfur/gm coal</td>
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<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>
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<tr>
<td>CO</td>
<td>$CO$</td>
<td>Wt. fraction CO in the volatiles; CO released during devolatilization, gmole CO/gm coal</td>
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<tr>
<td>COALC</td>
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<td>Carbon content in coal, gatom carbon/gm coal (d.b.)</td>
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<tr>
<td>COALH</td>
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<td>Hydrogen content in coal, gatom hydrogen/gm coal (d.b.)</td>
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<tr>
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<td>Nitrogen content in coal, gatom nitrogen/gm coal (d.b.)</td>
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<tr>
<td>COALO</td>
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<td>Oxygen content in coal, gatom oxygen/gm coal (d.b.)</td>
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<tr>
<td>COALS</td>
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<td>Sulfur content in coal, gatom sulfur/gm coal (d.b.)</td>
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<td>FORTRAN Symbol</td>
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<tr>
<td>COV</td>
<td>-</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>-</td>
<td>CO produced during volatiles combustion, gmole CO/gmole volatiles</td>
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<td>CO2</td>
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<td>Wt. fraction CO\textsubscript{2} in the volatiles; CO\textsubscript{2} released during devolatilization, gmole CO\textsubscript{2}/gm coal</td>
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<td>CO2V</td>
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<td>CO\textsubscript{2} released during devolatilization per mole of volatiles released, gmole CO\textsubscript{2}/gmole volatiles</td>
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<tr>
<td>CO2VB</td>
<td>-</td>
<td>CO\textsubscript{2} produced during volatiles combustion, gmole CO\textsubscript{2}/gmole volatiles</td>
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<td>CTAR</td>
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<td>Carbon content in tar, gm carbon/gm coal fed</td>
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<tr>
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<td>-</td>
<td>Surface volume mean particle diameter of additives in the feed, cm</td>
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<td>DAWMF</td>
<td>-</td>
<td>Weight mean particle diameter of additives in the feed, cm</td>
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<td>(d_{ce})</td>
<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>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>Feed particle diameter of ith fraction based on sieving screen size</td>
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<td>Mean diameter of the particles of $x$ th size fraction, cm</td>
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<td>$d_{ge}$</td>
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<td>$d_L$</td>
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<td>$\varepsilon_{mf}$</td>
<td>Void fraction at minimum fluidization</td>
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<td>Excess air, fraction</td>
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<td>Molar feed rate of fluidizing air, gmole/sec</td>
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<td>$F_{MT}$</td>
<td>Total molar flow rate of gas in the combustor, gmole/sec</td>
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<td>Stoichiometric air feed rate, gmole/sec</td>
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<td>Weight fraction of coal feed of $x$ th size fraction</td>
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<td>$g$</td>
<td>Acceleration due to gravity, cm/sec²</td>
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<td>G</td>
<td>Gas flow rate, gms/sec</td>
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<td>Hydrogen content in char, gm hydrogen/gm char</td>
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<td>Freeboard height, cm</td>
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<td>Expanded bed height, cm</td>
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<td>Hydrogen content in tar, gm hydrogen/gm coal fed</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_{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)/gmole·°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>
</tr>
<tr>
<td>RHOBED</td>
<td>(\rho_b)</td>
<td>Density of the bed materials, gms/cm(^3)</td>
</tr>
<tr>
<td>RHOC</td>
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<td>Density of coal, gms/cm(^3)</td>
</tr>
<tr>
<td>RHOCH</td>
<td>(\rho_{ch})</td>
<td>Density of char, gms/cm(^3)</td>
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<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>----------------</td>
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</tr>
<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>U₀</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>
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<tr>
<td>VMF</td>
<td>0</td>
<td>Bed volume at minimum fluidization (excluding the internals), cm³</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>
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<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 CO2/gm limestone</td>
</tr>
<tr>
<td>XCV</td>
<td>-</td>
<td>Volatile carbon content in coal, gm carbon/gm coal (d.b.)</td>
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<tr>
<td>XH</td>
<td>-</td>
<td>Hydrogen content in coal, gm hydrogen/gm coal (d.b.)</td>
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<tr>
<td>XMGO</td>
<td>-</td>
<td>Magnesium oxide content in limestone, gm MgO/gm limestone</td>
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<td>XN</td>
<td>-</td>
<td>Nitrogen content in coal, gm nitrogen/gm coal (d.b.)</td>
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<td>XO</td>
<td>-</td>
<td>Oxygen content in coal, gm oxygen/gm coal (d.b.)</td>
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<tr>
<td>XS</td>
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<td>Sulfur content in coal, gm sulfur/gm coal (d.b.)</td>
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<td>XS102</td>
<td>-</td>
<td>Silicon dioxide content in limestone, gm SiO2/gm limestone</td>
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<td>XW</td>
<td>-</td>
<td>Moisture content in coal as received basis, gm H2O/gm coal</td>
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<tr>
<td>ZB</td>
<td>(SEE DESIGN)</td>
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<tr>
<td>ZHE</td>
<td>(SEE DESIGN)</td>
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### SUBPROGRAM AKAD

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<thead>
<tr>
<th>FORTRAN Symbol</th>
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<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/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, cm$^2$/gm</td>
</tr>
<tr>
<td>T</td>
<td>$T$</td>
<td>Temperature in the bed, °K</td>
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### SUBPROGRAM AKK

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<thead>
<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>AKCO2</td>
<td>Overall rate constant for C-CO$_2$ reaction, cm/sec</td>
</tr>
<tr>
<td>AKF</td>
<td>Gas film diffusion rate constant for O$_2$, gm/cm$^2$·sec·atm</td>
</tr>
<tr>
<td>AKFCO2</td>
<td>Gas film diffusion rate constant for CO$_2$, gm/cm$^2$·sec·atm</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
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<tr>
<td>AKRCO2</td>
<td>$k_{CO_2}$</td>
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<td>AKR</td>
<td>$k_c$</td>
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<tr>
<td>AKS</td>
<td>$k_{cR}$</td>
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<tr>
<td>COND</td>
<td>$\lambda$</td>
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<td>SIGM</td>
<td>$\sigma$</td>
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<tr>
<td>TAV</td>
<td>$T_m$</td>
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<tr>
<td>TP</td>
<td>$T_c$</td>
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<tr>
<td>YO2</td>
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<td>Z</td>
<td>$p$</td>
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### SUBPROGRAM AREA

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<tr>
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<th>Mathematical Symbol</th>
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</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, cms</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, cms</td>
</tr>
<tr>
<td>ZB</td>
<td></td>
<td>Height above the distributor at which the cross sectional area is specified, cms</td>
</tr>
<tr>
<td>ZI</td>
<td></td>
<td>Height above the distributor, cms</td>
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### SUBPROGRAM ATTR

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AKF</td>
<td>Gas film diffusion rate constant, ( \text{gm/cm}^2 \cdot \text{sec.atm} )</td>
</tr>
<tr>
<td>AKR</td>
<td>Overall rate constant for char combustion, cm/sec</td>
</tr>
<tr>
<td>AKS</td>
<td>Chemical reaction rate constant for char combustion, ( \text{gm/cm}^2 \cdot \text{sec.atm} )</td>
</tr>
<tr>
<td>COND</td>
<td>Thermal conductivity of the gas, cals/sec.cm.(^\circ)C</td>
</tr>
<tr>
<td>D</td>
<td>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>Emissivity of the char particle</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
</tr>
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<td>----------------</td>
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<tr>
<td>ETS</td>
<td>-</td>
</tr>
<tr>
<td>ETSMAX</td>
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</tr>
<tr>
<td>MC</td>
<td>$M_c$</td>
</tr>
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<td>P</td>
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<td>$\phi$</td>
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<td>Q</td>
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<tr>
<td>RG</td>
<td>$R_g$</td>
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<tr>
<td>RHOCCH</td>
<td>$\rho_{c,ch}$</td>
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**SUBROUTINE CRRECT**

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<tr>
<th>Symbol</th>
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<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>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
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<tr>
<td>----------------</td>
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<tr>
<td>I</td>
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**SUBPROGRAM DESIGN**

<table>
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<th>Symbol</th>
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</thead>
<tbody>
<tr>
<td>A1,A2,A3,A4</td>
<td>Alphanumeric characters</td>
</tr>
<tr>
<td>ABED</td>
<td>Cross sectional area of the combustor, cm²</td>
</tr>
<tr>
<td>AHE</td>
<td>Specific heat transfer area of the tubes, cm²/cm³ FBC volume</td>
</tr>
<tr>
<td>AND</td>
<td>Number of orifices in the distributor</td>
</tr>
<tr>
<td>ATB</td>
<td>Bed cross sectional area at height ZB above the distributor, cm²</td>
</tr>
<tr>
<td>DBED</td>
<td>Diameter of the combustor, cm</td>
</tr>
<tr>
<td>DNZL</td>
<td>Diameter of orifice holes in the distributor, cm</td>
</tr>
<tr>
<td>DTUBE</td>
<td>Diameter of cooling tubes, cm</td>
</tr>
<tr>
<td>DVB</td>
<td>Volume of each compartment based on DZAV, cm³</td>
</tr>
<tr>
<td>DVBEFF</td>
<td>Volume of each compartment excluding the tubes, cm³</td>
</tr>
<tr>
<td>DZAV</td>
<td>Average compartment size used in design calculations, cm</td>
</tr>
<tr>
<td>FD</td>
<td>Fraction of solids withdrawn from the bed at each location</td>
</tr>
<tr>
<td>FFAD</td>
<td>Fraction of total additives fed at each location</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
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<tr>
<td>ZHE</td>
<td>-</td>
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</table>

**SUBPROGRAM ELUT**

<p>| BB             | -                   | Weight of bed material of x th size fraction, gms |</p>
<table>
<thead>
<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBED</td>
<td>-</td>
<td>Weight of char in the bed, gms</td>
</tr>
<tr>
<td>CBEDQ</td>
<td>-</td>
<td>Weight of char in the bed (calculated), gms</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>CENT</td>
<td>-</td>
<td>Char entrained in the freeboard, gms/sec</td>
</tr>
<tr>
<td>CU</td>
<td>-</td>
<td>Fraction finer than size, $d_x$</td>
</tr>
<tr>
<td>DCSE</td>
<td>$d_{ce}$</td>
<td>Surface volume mean diameter of char particles in the freeboard, cm</td>
</tr>
<tr>
<td>DCSVSB</td>
<td>$d_{c}$</td>
<td>Surface volume mean diameter of char particles in the bed, 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>
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<td>DETC</td>
<td>-</td>
<td>Increment in combustion efficiency</td>
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<tr>
<td>DP</td>
<td>$d_x$</td>
<td>Mean diameter of the particles of $x$th size fraction, cm</td>
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<tr>
<td>DPSE</td>
<td>$d_{\xi e}$</td>
<td>Surface volume mean particle diameter of additives entrained in the freeboard, cm</td>
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<td>DPSVB</td>
<td>$d_{\xi}$</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>
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<td>DWDIS</td>
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<td>Increment in the solids withdrawal rate, gms/sec</td>
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<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Description</td>
</tr>
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</tr>
<tr>
<td>E</td>
<td>$E_x$</td>
<td>Elutriation rate constant, gm/sec</td>
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<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 xth size fraction in the freeboard, gm/sec</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>Fraction of solids in the cloud region</td>
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<td>Fraction of wake solids thrown into the freeboard</td>
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<td>Height above the bed surface, cms</td>
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<td>Expanded bed height, cm</td>
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<td>Bed height at minimum fluidization, cm</td>
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<td>Molecular weight of gas, gms/gmole</td>
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<td>No. of locations along the combustor where the cross sectional areas are specified</td>
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<td>Proportion of fines recycled to the bed from the primary cyclone</td>
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<td>$P_2$</td>
<td>Proportion of fines recycled to the bed from the secondary cyclone</td>
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<td>Average pressure of the FBC, atm</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>$q_{1x}$</td>
<td>Collection efficiency of the primary cyclones for the x th size fraction</td>
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<td>Gas constant, 82.06 atm.cm&lt;sup&gt;3&lt;/sup&gt;/g mole·°K</td>
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<td>Density of additives, gms/cm&lt;sup&gt;3&lt;/sup&gt;</td>
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<td>Density of bed materials, gms/cm&lt;sup&gt;3&lt;/sup&gt;</td>
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<td>RHOCCH</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>Transport Disengaging Height, cm; if TDH &gt; HFB, TDH = HFB</td>
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<td>TDHC</td>
<td>TDH</td>
<td>Transport Disengaging Height, cm</td>
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<td>UMF</td>
<td>U&lt;sub&gt;mf&lt;/sub&gt;</td>
<td>Minimum fluidization velocity, cm/sec</td>
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<td>Superficial gas velocity at the bed surface, cm/sec</td>
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<td>Terminal velocity of additive particles of size d&lt;sub&gt;x&lt;/sub&gt;, 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&lt;sup&gt;3&lt;/sup&gt;</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>Additives feed rate, gms/sec</td>
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<td>Weight of bed materials, gms</td>
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<td>Solids withdrawal rate, gms/sec</td>
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<td>Additives entrainment rate in the</td>
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<td>(average), gm carbon/gm bed</td>
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<td>which the cross sectional area is</td>
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**SUBPROGRAM FBC**

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

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<td>Mole fraction CO₂ in the emulsion phase</td>
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<td>Mole fraction oxygen in the bottom compartment</td>
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<td>Mole fraction H₂O</td>
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**SUBPROGRAM GPHASE**

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<td>AKB</td>
<td>Reaction rate constant in bubble phase</td>
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<tr>
<td>AKBE</td>
<td>$K_{BE}$ Gas exchange coefficient, $1/\text{sec}$</td>
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<td>AKE</td>
<td>Reaction rate constant in emulsion phase</td>
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<td>$a_m$ Defined by Equation (VI.12) for NOₓ reduction reaction; $= (1-\varepsilon^m)$ for SO₂ absorption reaction</td>
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<td>DVBB</td>
<td>Volume of each compartment, $\text{cm}^3$</td>
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<tr>
<td>EPB</td>
<td>$\varepsilon_B$ Bubble fraction</td>
</tr>
<tr>
<td>EPC</td>
<td>$\varepsilon_C$ Cloud fraction including bubble</td>
</tr>
<tr>
<td>ETUBE</td>
<td>$\varepsilon_{\text{tube}}$ Volume fraction of tubes in each compartment</td>
</tr>
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<td>$F_{BM}$ Molar flow rate of gas in the bubble phase, $\text{g mole/sec}$</td>
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<td>Molar flow rate of gas in the bubble phase in the bottom compartment, $\text{g mole/sec}$</td>
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<td>$F_{EM}$ Molar flow rate of gas in the emulsion phase, $\text{g mole/sec}$</td>
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<td>$T_E$</td>
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<tr>
<td>YBO</td>
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<tr>
<td>YBI</td>
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<td>YEO</td>
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<tr>
<td>YE1</td>
<td>-</td>
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</tbody>
</table>

**SUBPROGRAM HAREA**

<p>| ATB            | -                   | Bed cross sectional area at height $Z_B$ above the distributor, cm² |
| ATI            | -                   | Bed cross sectional area at height $Z_I$ above the distributor, cm² |
| DTI            | $D_t$               | Diameter of the combustor at height $Z_I$ above the distributor, cm |
| MFB            | -                   | Number of locations along the combustor where the cross sectional areas are specified |
| RI             | $\pi$               | 3.14159265 |
| RI             | -                   | Radius of the combustor at height $Z_I$ above the distributor, cms |</p>
<table>
<thead>
<tr>
<th>FORTRAN Symbol</th>
<th>Mathematical Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZI</td>
<td>-</td>
<td>Height above the distributor, cms</td>
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**SUBPROGRAM HEIGHT**

<table>
<thead>
<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>DBVEFF</td>
<td>Volume of each compartment excluding the tubes, cm³</td>
</tr>
<tr>
<td>DZAV</td>
<td>Average compartment size used in design calculations, cm</td>
</tr>
<tr>
<td>HEIGHT</td>
<td>Height above the distributor, cm</td>
</tr>
<tr>
<td>HT</td>
<td>Height above the distributor, cm</td>
</tr>
<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, cm³</td>
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**SUBPROGRAM HYDRO**

<table>
<thead>
<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>AHE</td>
<td>Specific heat transfer area of the tubes, cm²/cm³ (DESIGN input) FBC volume</td>
</tr>
<tr>
<td>AHEAV</td>
<td>Specific heat transfer area of the tubes in each compartment, cm²/cm³, FBC volume</td>
</tr>
<tr>
<td>AKBE</td>
<td>Gas exchange coefficient, l/sec</td>
</tr>
<tr>
<td>ALFB</td>
<td>( \alpha_b = \epsilon_{mf} U_B / U_{mf} )</td>
</tr>
<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, cm²</td>
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<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, cm³</td>
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<tr>
<td>DBA</td>
<td>Bubble diameter in each compartment assumed, cm</td>
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<tr>
<td>DBAV</td>
<td>Bubble diameter in each compartment, cm</td>
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<tr>
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<td>DBMAX</td>
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<tr>
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<td>DT</td>
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</tbody>
</table>

**SUBPROGRAM VEL**

<p>| DPAR            | d&lt;sub&gt;p&lt;/sub&gt;       | Particle diameter, cm |</p>
<table>
<thead>
<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>
</tr>
<tr>
<td>REP</td>
<td>Re,p</td>
<td>Particle Reynolds number</td>
</tr>
<tr>
<td>RHOGAS</td>
<td>ρg</td>
<td>Density of gas, gm/cm³</td>
</tr>
<tr>
<td>RHOS</td>
<td>ρs</td>
<td>Density of solids, gm/cm³</td>
</tr>
<tr>
<td>UM</td>
<td>Uₘf</td>
<td>Minimum fluidization velocity, cm/sec</td>
</tr>
<tr>
<td>UT</td>
<td>Uₜ</td>
<td>Terminal velocity of the particle, cm/sec</td>
</tr>
<tr>
<td>VISC</td>
<td>μ</td>
<td>Viscosity of gas, gm/cm.sec</td>
</tr>
</tbody>
</table>

**SUBPROGRAM VOLUME**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>DVBEFF</td>
<td>Volume of each compartment excluding the tubes, cm³</td>
</tr>
<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>
</tr>
</tbody>
</table>