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A MATHEMATICAL MODEL FOR FLUIDIZED BED COAL COMBUSTION

F. Preto

APRIL 1985

Presented to International Energy Agency (IEA) Executive Committee
Paris, May 9, 1985.

ENERGY RESEARCH PROGRAM
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A MATHEMATICAL MODEL FOR
FLUIDIZED BED COAL COMBUSTION

by

F. Preto*

ABSTRACT

Fluidized bed coal combustion is one of the most promising technologies for burning coal in a clean and efficient manner. The development of this technology necessarily includes theoretical studies as well as experimental research. As part of these theoretical studies, mathematical modelling has been carried out at Queen's University at Kingston under a research program partly funded by Energy, Mines and Resources Canada.

In its current form, the mathematical model includes submodels for all the major processes occurring in fluidized bed coal combustion. The model is based on the two phase theory for bubbling fluidization. For each phase mass balances have been written which include terms for the various effluxes occurring within that phase. These include coal combustion, sulphur capture, NO reduction, homogeneous gas phase reactions and interphase transfer. A numerical simulation of the model has been developed, and is presented in this report.

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MODELE MATHEMATIQUE POUR
COMBUSTION DE CHARBON PAR LIT FLUIDISE

par

F. Preto*

ABSTRAIT

La combustion de charbon par lit fluidisé est une des technologies les plus prometteuse pour brûler le charbon de façon propre et efficace. Le développement de cette technologie comprend essentiellement des études théoriques ainsi que des recherches expérimentales. Faisant partie des études théoriques, le modelage mathématique fut accompli à l'Université Queens près de Kingston par l'entremise d'un programme de recherche en partie subventionné par Energie, Mines et Ressources, Canada.

Sous sa forme courante, le modèle mathématique possède des sous-modèles pour les processus majeurs existant dans la combustion de charbon par lit fluidisé. Le modèle est basé sur la théorie à deux phases pour la fluidisation à bulles. Pour chaque phase, un bilan a été rédigé incluant les termes des effusions s'y produisant. Parmi ceux-ci nous retrouvons la combustion de charbon, absorption de soufre, réduction d'oxides nitriques, réactions homogènes en phase gazeuse et transfert d'interphase. Une simulation numérique du modèle a été développée et est présentée dans cet exposé.

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INTRODUCTION

Current research in coal combustion is aimed at developing reliable technologies that utilize coal in an efficient, economical and environmentally sound manner. Fluidized bed combustion of coal (FBC), as an alternative to conventional pulverized coal combustors equipped with flue gas scrubbers, has many advantages for both power generation and process heat production. An abundant amount of FBC research has been done, on both bench scale and pilot-plant scale, and much useful information has been gathered. One ultimate aim of this research is to arrive at a point where experimental results can be generalized, and process analyses and design can be conducted, by means of mathematical models.

Fluidized combustor models, published in the literature, have been reviewed by LaNauze and Jung (1982), Olofsson (1980) and Park, Levenspiel and Fitzgerald (1980). These reviews are essentially point by point comparisons of the various models, rather than critical assessments of the models' predictive capabilities or accessibility.

The available models are in some cases overcomplicated, with the inclusion of irrelevant minutiae, and in other cases too rudimentary, with the exclusion of important factors. In most cases the validity of the models can be questioned. This is usually because some important facets (e.g. sulphur capture, elutriation) of the FBC process have been left out. Comprehensive models have been developed (Louis et. al. 1982, Wells et. al. 1982) which are reasonably accurate, but these are also quite complicated and require significant computing facilities.

The object of studies at Queen's University's FBC laboratory was to develop a model which would include all the significant processes occurring in a fluidized bed combustor and yet not include so much detail that a numerical solution would be either unworkable or too costly. It was recognized that at the current state of understanding a "complete" model was impossible, therefore some approximations were necessary. The desired model should also be amenable to changes, i.e., if a more accurate sulphur capture model were to be developed it should be easily incorporated. With these objectives in mind, the model of

Becker, Beer and Gibbs (1975) was chosen as the basis for the Queen's model, as it outlines a relatively simple framework which lends itself to a modular approach. In this manner, as a greater understanding of each process becomes available, the algorithm for that process can easily be replaced. The full development and numerical solution of the model was part of the doctoral research of the author, and may be found in his thesis (Preto 1985).*

The purpose of this report is threefold. The principal objective is to make the Queen's simulation available to other researchers. To this end the full listings of the current version of the computer programs have been included in Appendix B. The second objective is to provide assistance in running the simulation. To this end the computational scheme is described, and the programs themselves are summarized and documented. The final objective is to outline the development of the mathematical model. To this end the basic assumptions are given, and the major submodels are briefly described. The complete development, testing and evaluation of the model may be found in Preto (1985).

* In this connection, the author would like to express his appreciation to Professor H.A. Becker, Queen's University, for his cooperation and encouragement.

MODEL DEVELOPMENT

The physical and chemical processes occurring in a fluidized bed combustor must be properly understood to develop a useful model. The following sections outline the assumptions and basic principles used in developing the overall model.

Model Basis

The model for fluidized bed combustion of coal proposed by Becker, Beer and Gibbs (1975) has its basis in the two-phase model for bubbling fluidization. This model, proposed by Davidson and Harrison (1963), visualizes a swarm of solids-free bubbles travelling through a particulate "emulsion" phase. The two-phase model assumes that the fluidizing gas in excess of that required for fluidization bypasses the bed in the form of bubbles.

In the development of the fluidized combustion model, the following additional assumptions were made:

- (a) Inert particles constitute the bulk of material in the bed.
- (b) Particle mixing is good so that the emulsion is effectively uniform in temperature.
- (c) The combustor, and therefore the bed, are of uniform cross-sectional shape and area.
- (d) Gas flow is statistically uniform over the combustor cross-section, and mean values of local gas properties in the bubble and emulsion vary only with height above the base of the bed.

Within the limitations imposed by these assumptions, the various transfer streams can be estimated (Figure 1) and the relevant material and energy balances developed.

Mass balances for each molecular species can be estimated by consideration of each of the various efflux processes described above. The summation of the mass balances over all molecular species gives the total mass balances.

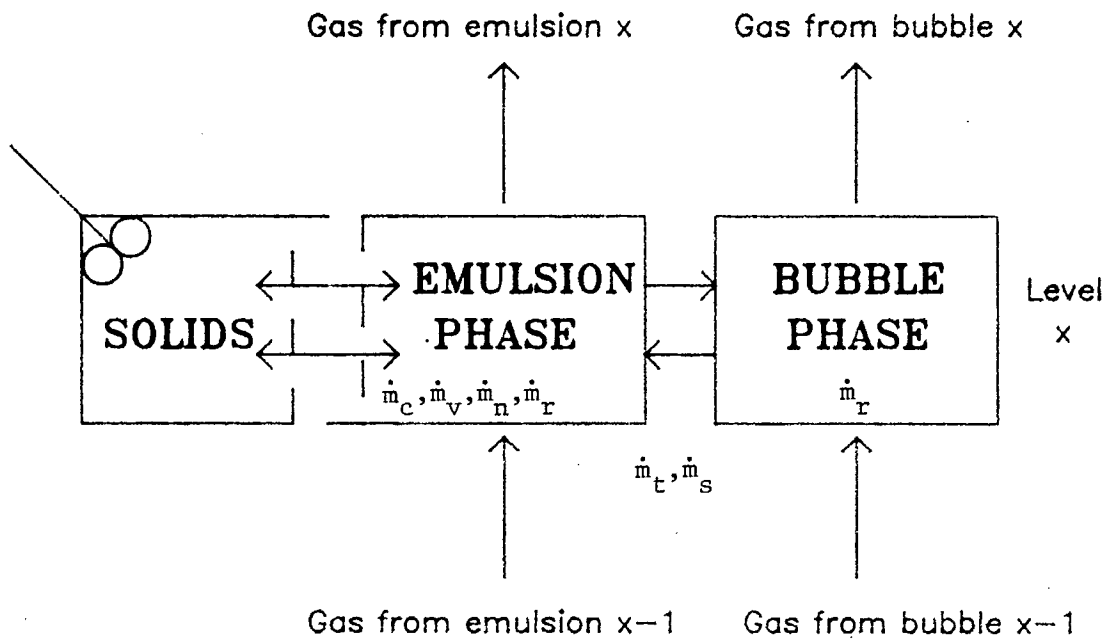


Figure 1. Schematic diagram of a level in the FBC model
(Notation is defined on pp. 28, 29)

For the emulsion phase

$$\frac{d\dot{m}_1}{dx} = \dot{m}_{t,0} - \dot{m}_{s,1} - \dot{m}_{v,1} - \dot{m}_{c,1} - \dot{m}_{n,1} \quad (1)$$

$$r_{i\text{mir},1} = 0 \quad (2)$$

For the bubble phase

$$\frac{d\dot{m}_0}{dx} = \dot{m}_{s,1} - \dot{m}_{t,0} \quad (3)$$

$$\Sigma_i \dot{m}_{i\text{mir},0} = 0 \quad (4)$$

At the top of the bed, the freeboard conditions are estimated by solving only the emulsion balances. In the freeboard, particle composition and temperature are uniform over the combustor cross-section, and mean local properties vary only with height above the top of the bed.

In order to satisfy the assumptions made in adopting a two-phase model with constant emulsion gas velocity, any excess gas generated in the emulsion due to combustion must be transferred to the bubble phase. This is accomplished by introducing a term in the mass and energy balances known as fluidization saturation flux.

$$\dot{m}_{is,1} = \dot{n}_{s,i} M_i [\delta_s w_{i,1} + (1 - \delta_s) w_{i,0}] \quad (5)$$

The remaining efflux processes are estimated by theoretical and empirical submodels as outlined in the following sections. The detailed development of the submodels is presented in Preto (1985).

Coal Combustion

The combustion of coal takes place in three stages:

1. heating and drying
2. devolatilization
3. char combustion.

Stages two and three, i.e., devolatilization and char combustion, interact; but to an extent which is presently unknown. Large particles have both stages occurring simultaneously. The level of interaction depends on the rank of fuel being fired. In this study, the two stages are treated as though they occur consecutively.

Heating and Drying

The time required to heat and dry coal particles can be estimated from an energy balance around the particle.

For the heating and drying stage, only radiation, convection and evaporation are believed to be significant:

$$m_p C_p \frac{dT_p}{dt} = S_p \sigma_B \epsilon (T_B^4 - T_p^4) + S_p \alpha (T_B - T_p) + (\Delta H_v) \dot{m}_{H_2O} \quad (6)$$

Once the particle is dry ($T > 373$ K) heating continues ($\dot{m}_{H_2O} = 0$) until the particle reaches 700 K (Solomon and Colket 1978) at which point devolatilization begins.

Devolatilization

There is scanty information on the mechanisms by which the devolatilization of coal takes place in fluidized beds. The limited data available at high temperatures are derived from pulverized coal flames and from flow experiments. Anthony and Howard (1976) reviewed the available fundamental information on devolatilization. The mechanisms involved depend on such operating conditions as temperature, pressure, particle size, gas phase concentrations, and the particular coal.

Pillai (1981) has considered devolatilization of coal ($0.1 < D_p < 10$ mm) in a fluidized bed and found the data to fit a power law relationship of the form

$$t_v = z_1 D_p^{z_2} \quad (7)$$

where the constants z_1 and z_2 are dependent on coal type (average $z_1 = 10$, $z_2 = 0.75$ for bed temperature 775°C ; t_v in seconds, and D_p in mm) and bed temperature. Furthermore Pillai (1981) found that all fuels exhibited the relationship

$$z_1 \propto T^{-3.8} \quad (8)$$

For each particle size fed to the bed, the turnover time and devolatilization time can be estimated. This allows formulation of a devolatilization scheme to calculate the distribution of volatiles throughout the bed. Figure 2 presents a scheme whereby the devolatilization pattern for each coal size increment can be estimated. The overall devolatilization pattern can be obtained by summation over all the size increments.

Char Combustion

The combustion of char can be generalized as the reaction of carbon with oxygen to form carbon monoxide and/or carbon dioxide. The following char combustion scheme is proposed:

- (a) Possible heterogeneous reactions:



- (b) Reaction (10) is endothermic, whereas (9) is exothermic. Char particles burn at higher temperatures than the bed, indicating that (9) is more likely to apply.
- (c) Under kinetic control, the atmosphere surrounding a particle will be the same as the emulsion, and CO_2 and O_2 will both be present. The relative rates at 800°C are 1 for reaction (10) and 100,000 for reaction (9).
- (d) Diffusion controls the rate of reaction in large particles (>1 mm) and at high temperatures. Analysis of bed material from a fluidized bed combustor (Preto (1985) shows that very

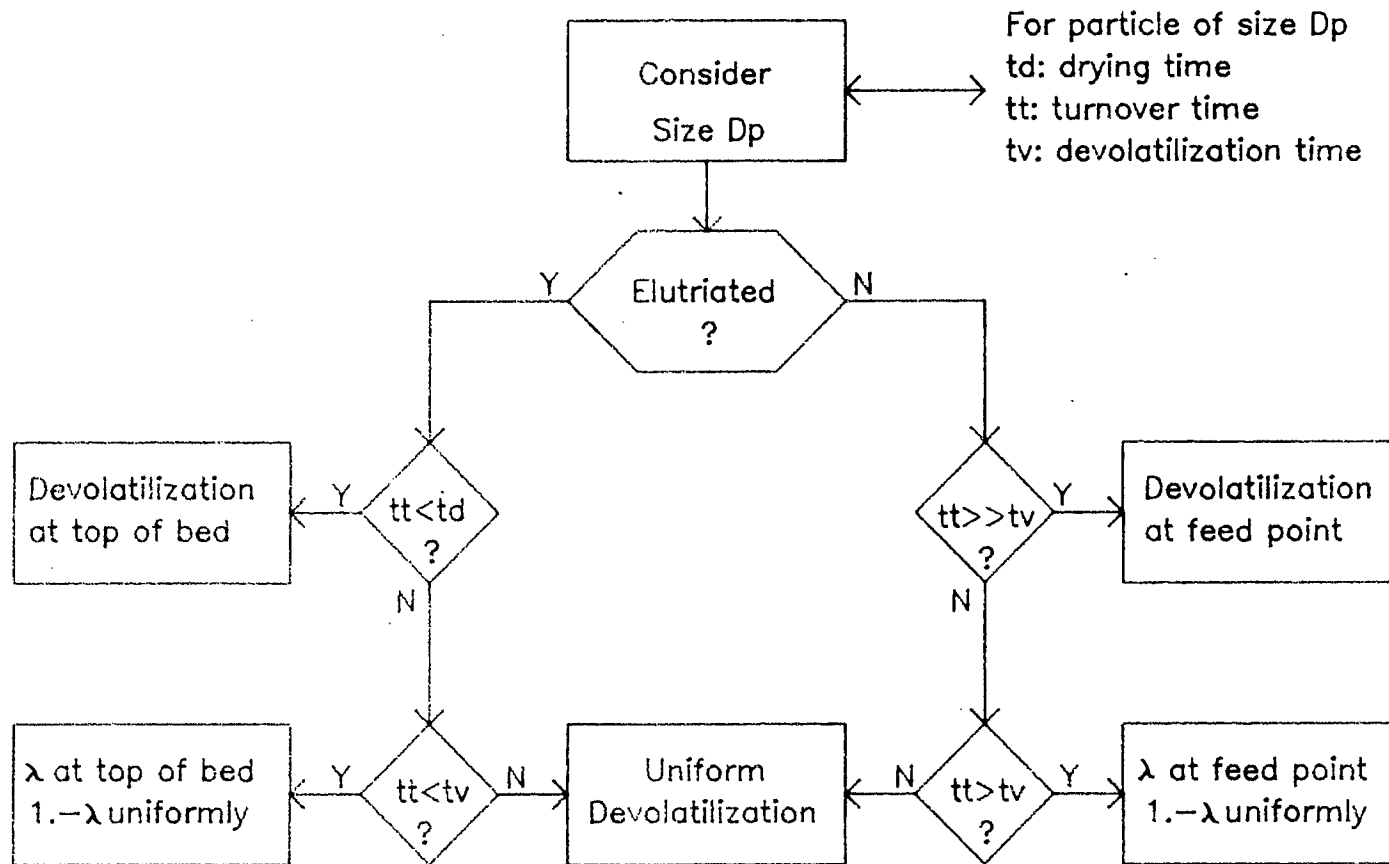


Figure 2. Coal Particle Devolatilization Scheme

few particles survive above the 2 mm size range. Ash resistance and pore diffusion would be significant for large particles, but based on these data, it may be assumed that the ash is scoured away as the particle burns.

- (e) Pore effects and adsorption/desorption contributions are felt to be minor and so are not included.

An adequate model therefore needs only to consider kinetics, diffusion and heat transfer. In developing the model, the following additional assumptions are made:

- (f) The particle is spherical throughout combustion.
- (g) The gas around a burning particle is effectively stagnant; $Re < 1$.
- (h) Char particles are sufficiently separated so that each one burns independently.
- (i) The reaction mechanism is such that oxygen diffuses to the surface where it reacts with the char. Applying these assumptions to a combined diffusion and kinetic model yields the following carbon balance around a single particle:

$$\frac{dm_p}{dt} = \frac{-M_c w_c}{w_c - w_a} \frac{k_d k_r k_s^2 m_p^{2/3}}{k_r k_s m_p^{1/3} + k_d} x_{O_2, l} \quad (11)$$

This equation can be integrated to give the history of a burning char particle.

Homogeneous gas phase reactions

A common approach to modelling gas phase reactions is to assume complete combustion in the presence of excess oxygen. However, if one considers the species known to be present in a combustor,

CO	H ₂	N ₂	SO ₂
CO ₂	H ₂ O	NO	SO ₃
CH ₄	O ₂	NO ₂	

the complete combustion approach is inadequate, and equilibrium calculations are necessary. The two most accessible methods, aside from extensive "number-crunching" to solve nonlinear equations, are both based on minimizing Gibbs free energy:

- (a) equilibrium constant formulation

(b) Gibbs function minimization.

Although (a) is simpler to use, it involves formulating equations based on specific independent reactions, and consequently requires a numerical scheme to solve nonlinear algebraic equations based on these arbitrary reactions. Gibbs function minimization techniques, reviewed by Smith and Missen (1982), offer a much more versatile approach in that no reactions need be considered, and the number of equations necessary is equal to the number of distinct elements plus one. The method chosen for this study is the RAND variation of second-order non-stoichiometric algorithms (Smith and Missen 1982).

Sulphur dioxide capture model

The FBC model framework outlined in equations (1)-(4) is suited to a model which estimates the local SO₂ reaction rate, rather than a separate bubbling bed sulphur capture model. The sulphur capture model developed in this study is based on the assumption that the sorbent is well mixed throughout the emulsion, and that the concentration of SO₂ is constant throughout the compartment at level x. The model is based on the commonly accepted concept that pore plugging leads to an exponential decrease in the surface available for SO₂ capture. The equations developed are based on application of the catalyst deactivation theory of Levenspiel (1972) to model particle sulphation. The rate of reaction of SO₂ is

$$r = \frac{6\tau \dot{m}_n k_n c_{SO_2}}{\omega p_p D_p (1 + k_p \tau)} \left[1 - \exp(-(k_p t_c + t_c/\tau)) \right] \quad (12)$$

The residence time of limestone particles in the bed can be estimated from

$$\tau = \frac{\dot{m}_n}{(Ca/S) \dot{m}_f w_s M_n} \quad (13)$$

where m_n = sorbent weight in the bed

Ca/S = calcium to sulphur ratio

\dot{m}_f = coal feedrate

w_s = fraction of sulphur in coal

M_n = ratio of in-bed sorbent molecular weight to sulphur molecular weight.

Nitric oxide emissions

The level of fuel nitrogen converted to NO is due to a combination of NO forming and reducing processes. NO is generated by combustion of both volatiles and char. NO is reduced by reactions with nitrogenous fragments in the volatiles and by heterogeneous reaction with char. Modelling is broken down into three processes:

1. Evolution of NO during devolatilization, with partial conversion to N_2 .
2. Evolution of NO during char combustion.
3. Reduction of NO due to reaction with char.

Empirical data on the evolution of NO have been published by Ber et. al (1980). The reduction of NO is assumed to be by heterogeneous reaction with the char in the bed. For a first order reaction this can be expressed as

$$r = k_c S_c c_{NO} \quad (14)$$

The surface area of char available for reaction can be calculated from $S_c = 6 m_c / D_p \rho_c$, where D_p is the mean char particle diameter.

Interphase transfer

Assuming that the transfer of material is by concentration gradient, the mass flux can be calculated from

$$\dot{m}_{it,0}''' = \dot{m}_{it,1}''' - K_w a (w_{i,0} - w_{i,1}) \quad (15)$$

where K_w is the overall mass transfer coefficient.

The mass transfer between the phases occurs simultaneously with homogeneous gas-phase reactions. This adds complications in that chemical kinetic submodels are necessary for precise predictions. The gain in accuracy resulting from their addition is expected to be minor (Becker, Beer and Gibbs 1975), therefore it is assumed that in the absence of strong reactions, the binary diffusivities are all equal and the mixture molecular weight is a constant. K_w would then have the same value for all molecular species.

Estimates of K_w can be made by considering exchange to take place due to diffusion across the bubble boundary and due to gas circulation. Diffusion can be estimated by applying the penetration theory to molecular diffusion and dispersion (Becker, Beer and Gibbs 1975).

Experiments by Preto (1985) have shown that FBC behaviour is markedly different from a bubbling bed in that bubbles contain a significant amount of solids and have very ill-defined boundaries. It is likely that interphase transfer is predominantly determined by bubble gas circulation. This circulation can be incorporated into a dimensionless mass transfer group

$$X = \frac{4.5 \times U_{mb} L_{mb}}{\zeta D_b \sqrt{g D_b}} \quad (16)$$

which can be interpreted as the number of mass transfer units, i.e., the number of times a bubble exchanges its own volume (V_b) in passing through the bed.

Freeboard modelling

The freeboard zone extends from the surface of the bed to the top of the combustor. In this region a large number of phenomena occur simultaneously. Significant combustion, heat release, sulphur capture and NO reduction can take place. In order to estimate these the solids loading must be known. Although there has been some research in this area (George and Grace 1978, Horio et. al. 1980), there is no reliable method to estimate entrainment rates and solids loading for fluidized bed combustors. In fact, there is little information on any of the phenomena in the freeboard, and any model of the freeboard is therefore necessarily simplistic.

The submodels already described in this chapter, including sulphur capture and NO reduction, are extended to the freeboard with the following restrictions:

1. The gas phase is in plug flow.
2. The temperature profile is estimated from enthalpy change due to the various reactions.
3. The carbon loading of the freeboard is calculated from recycle considerations.
4. The char combustion rate is based solely on residence time in the freeboard.
5. The char particle size is constant, as set by the elutriation submodel.
6. Devolatilization of elutriated fines is assumed to occur in a plane at the top of the bed.
7. The "splash zone" effects caused by bubbles bursting at the bed surface are ignored.

The freeboard model is thus very primitive, but does provide a starting basis for further improvement as experimental data become available.

Energy balance

An overall energy balance is used to determine the steady state "bed" temperature. The temperature profile in the freeboard is determined as part of the freeboard integration. In solving the bed energy balance the following assumptions are made:

1. The solids in the bed are assumed to be perfectly mixed.
2. All solid streams leaving the bed are at the bed temperature.
3. The gross calorific value of the coal is defined as the enthalpy of combustion such that the products are ash, H₂O (liq.), CO₂ (g), SO₂ (g) and N₂ (g).
4. Heat transfer due to radiation between the bed and freeboard is neglected.
5. Solids splashed into the freeboard return to the bed at the same temperature.
6. Heat transfer to immersed tubes is equal throughout the bed.

Closure

This section has outlined the basic principles and equations which comprise the Queen's model for fluidized bed coal combustion. The discussion has been brief and many of the details in the derivations have been omitted. The complete derivation may be found in Preto (1985). The initial model outline may be found in Becker, Beer, and Gibbs (1975).

In some cases a completely theoretical development was not feasible and the submodel required experimental data. Correlations (Preto, 1985) were used to predict minimum fluidization velocity, bed expansion, and heat transfer to immersed tubes. Experimental data were also used to estimate some model parameters.

FBC MODEL COMPUTER PROGRAM

MODFBC is the main program in the overall simulation of fluidized bed coal combustion. The simulation is based on the submodels and empirical relations detailed in the previous three chapters. The synopses and listings of the computer programs are given in Appendices A and B respectively. In this chapter the general calculation procedure and program organization are described.

Computational algorithm

The modelling of FBC is carried out according to the algorithm summarized in Figure 3. The algorithm is based on finding the coal feedrate required to satisfy the steady state energy balance at a given bed temperature. This procedure can be broken down into five phases:

1. The data input is used to carry out an approximate energy balance, from which the steady state coal feedrate is estimated (generally $\pm 25\%$).
2. The parameters associated with fluidization hydrodynamics are estimated.
3. The energy balance loop is set up. The estimated coal feedrate is used to solve the mass balances. For the given bed temperature, an overall energy balance is used to correct the coal feedrate. This procedure is repeated until the coal feedrate converges.
4. The mass balances, within the energy balance loop, are set up by calculating the fluxes associated with combustion, sulphur capture and NO reduction. The mass balances are then solved by integration from the distributor plate to the top of the bed.
5. The freeboard conditions are calculated by simultaneously integrating the mass and energy balances from the top of the bed to the top of the freeboard.

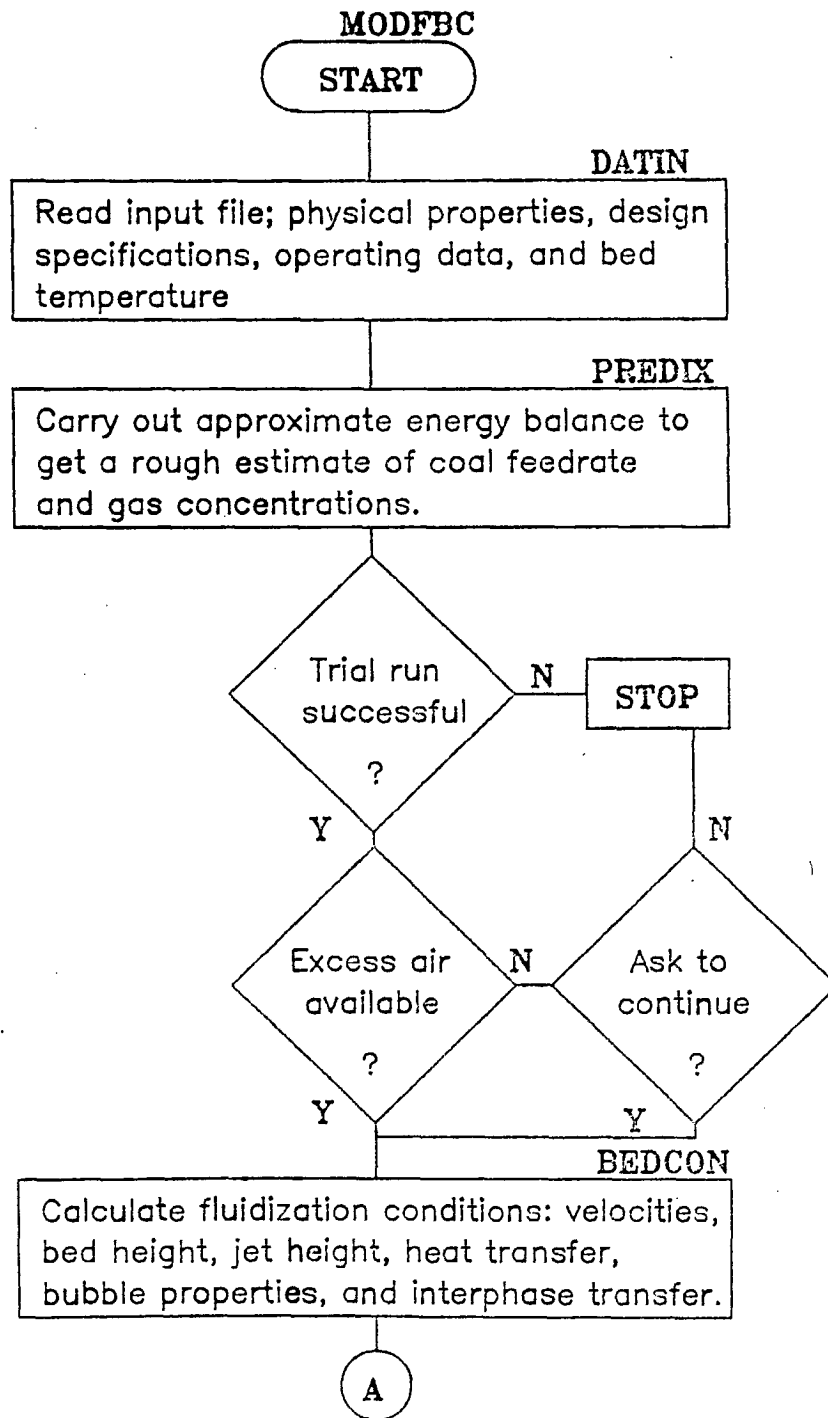


Figure 3(a). Algorithm for computer simulation

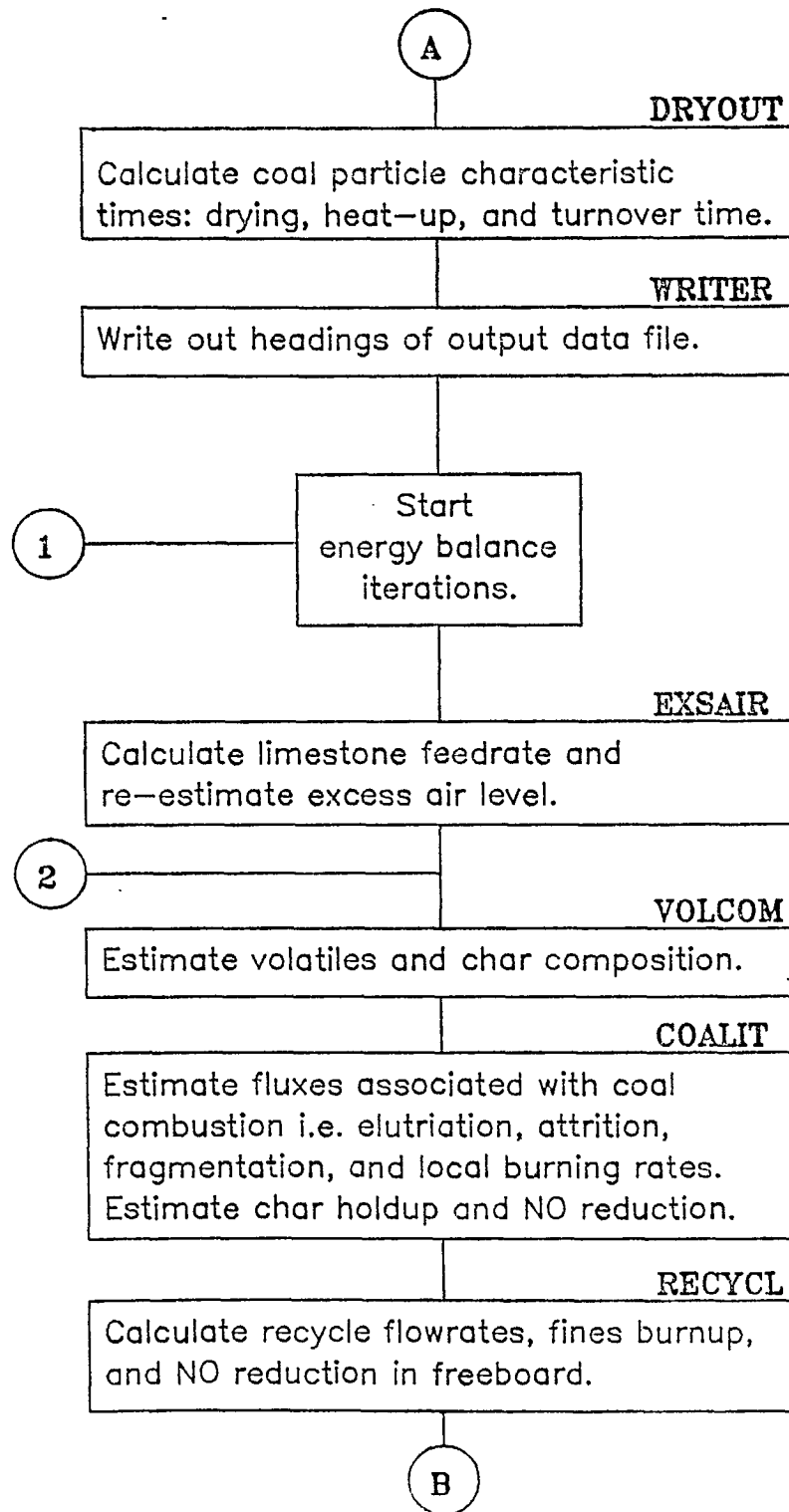


Figure 3(b). Algorithm for computer simulation

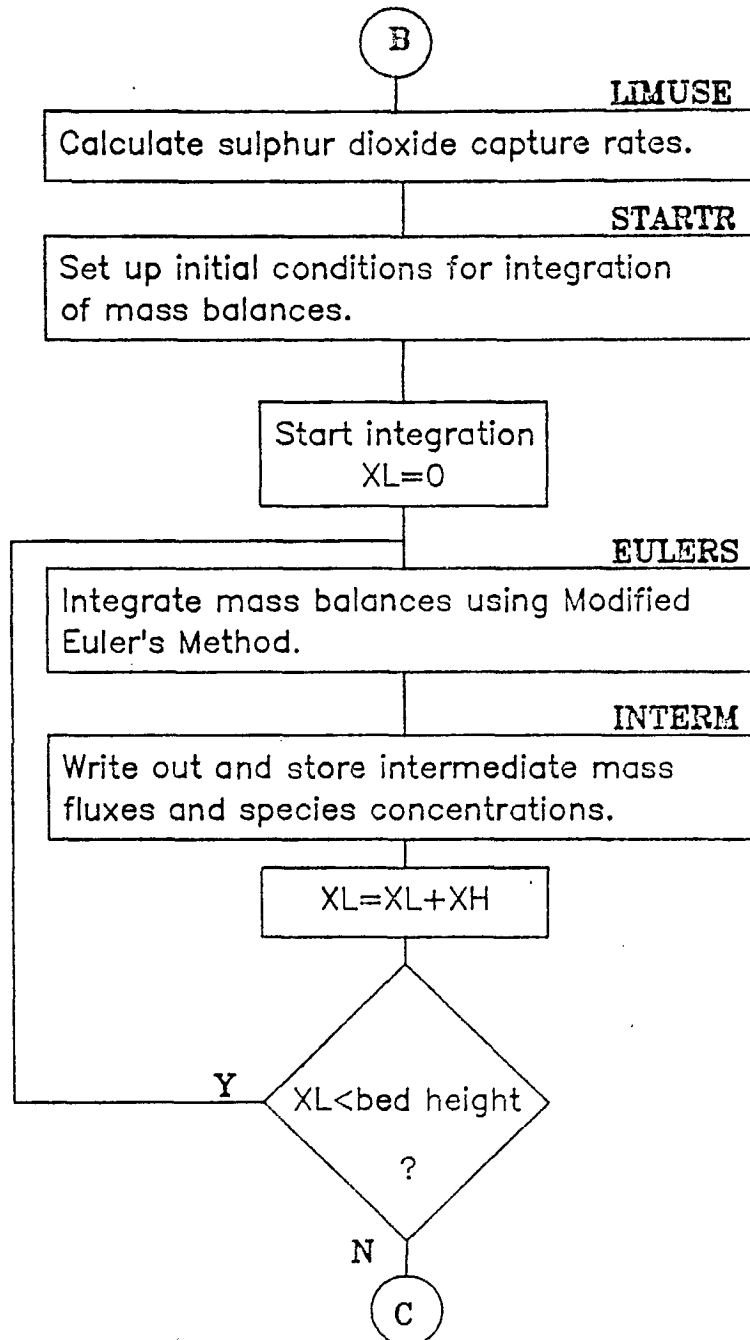


Figure 3(c). Algorithm for computer simulation

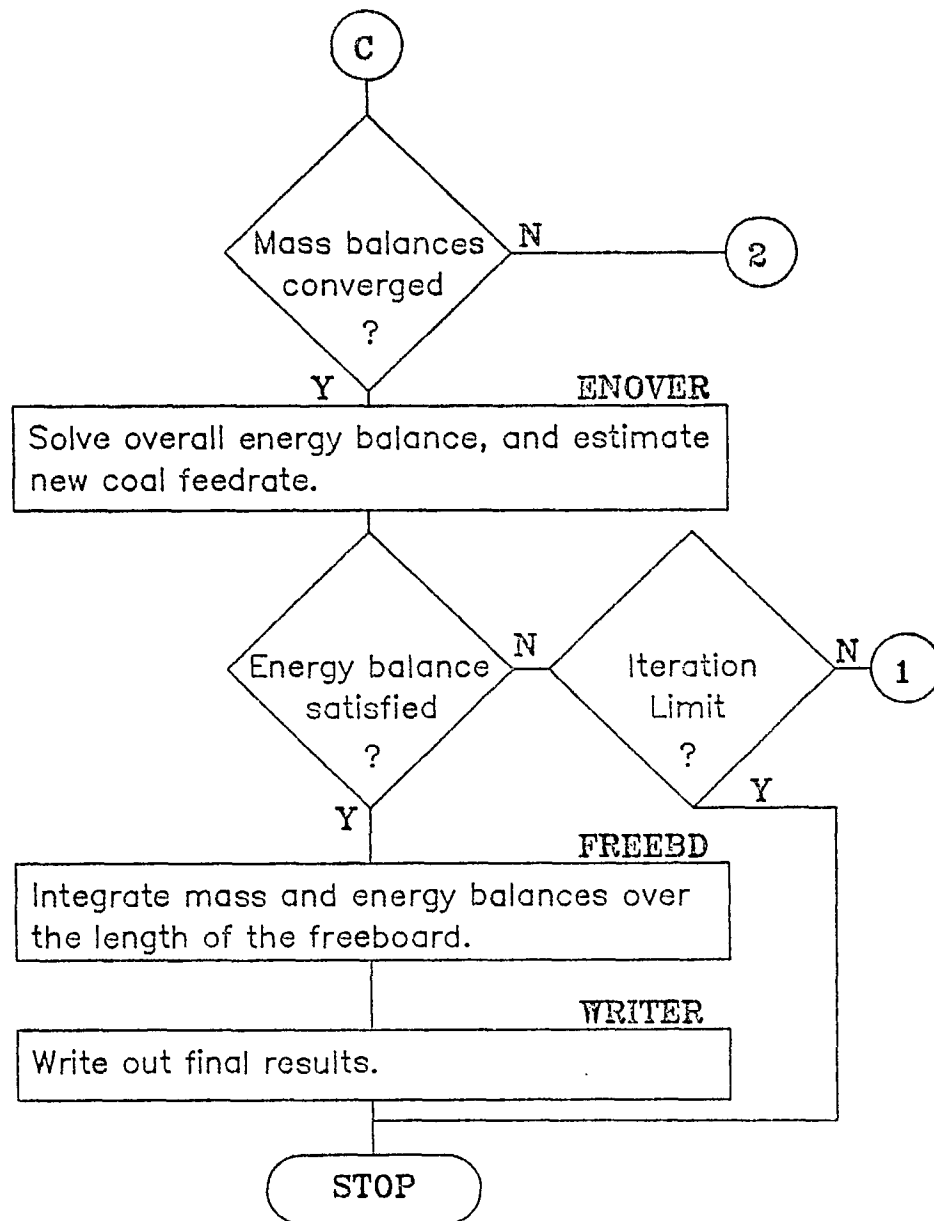


Figure 3(d). Algorithm for computer simulation

The mass fluxes associated with coal combustion are calculated in incremental form, i.e., the various local fluxes (drying, heating, devolatilization, char combustion, fragmentation, attrition and elutriation) are estimated for each feed size increment. The total local combustion flux is then obtained by adding all the incremental fluxes. The local fluxes are estimated using a compartmental approach whereby the bed is split into a number of levels. The coal residence time in each level is estimated from the mixing submodel. The gas composition at each level is stored during each iteration of the mass balance integration, and subsequently used to estimate the local flux. This increases computer memory requirements, however it considerably reduces program running time.

Numerical integration

The ordinary differential equations which define the FBC model can be solved by numerical integration. For reasons of shorter computational time and smaller memory requirements, the Modified Euler Method was chosen:

Predictor step.

$$\bar{y}_{n+1} = y_n + h f(x_n, y_n) \quad (17)$$

Corrector step.

$$y_{n+1} = y_n + \frac{h}{2} [f(x_{n+1}, \bar{y}_{n+1}) + f(x_n, y_n)] \quad (18)$$

where $f(x, y) = dy/dx$. The method is simple and yields modest accuracy. The model is not yet sophisticated or accurate enough to merit a more elaborate method. The program structure is such that more accurate methods can easily be introduced.

Program organization

The FBC model simulation consists of a main program, MODFBC, and 58 subroutines. The computer programs are written in FORTRAN to run on the Queen's University Computing Centre's IBM 3081-G24 computer. The typical CPU time required for solution is 150 seconds, depending on the convergence criteria.

The functions of MODFBC have been described in this chapter. Program synopses for all the subroutines are given in Appendix A. Furthermore, the program listings in Appendix B are extensively documented. The model organization, i.e., the order in which subroutines are called, is illustrated in Figure 4. Five of the subroutines, block P, calculate gas properties: density, viscosity, thermal conductivity and thermo-chemical properties.

Program operation

All input to and output from the model is done through data files, rather than directly to/from the user. The data arrays used throughout the model are defined in the file COMMON which is listed in Appendix B. Examples of the various data files are also given in Appendix B.

Program inputs

The input data is read in from the file FILEIN and then checked for validity. The method by which the data are entered is as a whole array rather than as certain elements within the array. The arrays entered are described in COMMON and identified in FILEIN. The data formats must be followed exactly. The inputs required by the program can be divided into four categories and are listed below along with values typical of the Queen's AFBC pilot plant:

1. Operating Conditions
 - (a) Bed temperature (850°C)
 - (b) Bed slumped height (0.45 m)
 - (c) Bed bulk density (1100 kg/m³)
 - (d) Superficial gas velocity (2.0 m/s)
 - (e) Operating pressure (101,000 Pa)
 - (f) Air inlet temperature (305 K)
 - (g) Solids feed temperature (300 K)
 - (h) Ambient temperature (298 K)
 - (i) Ca/S ratio (2.5)
 - (j) Recycle ratio (fraction) (0.9)
 - (k) Air humidity (1% wt H₂O)

Figure 4(a). FBC Model Program Organization

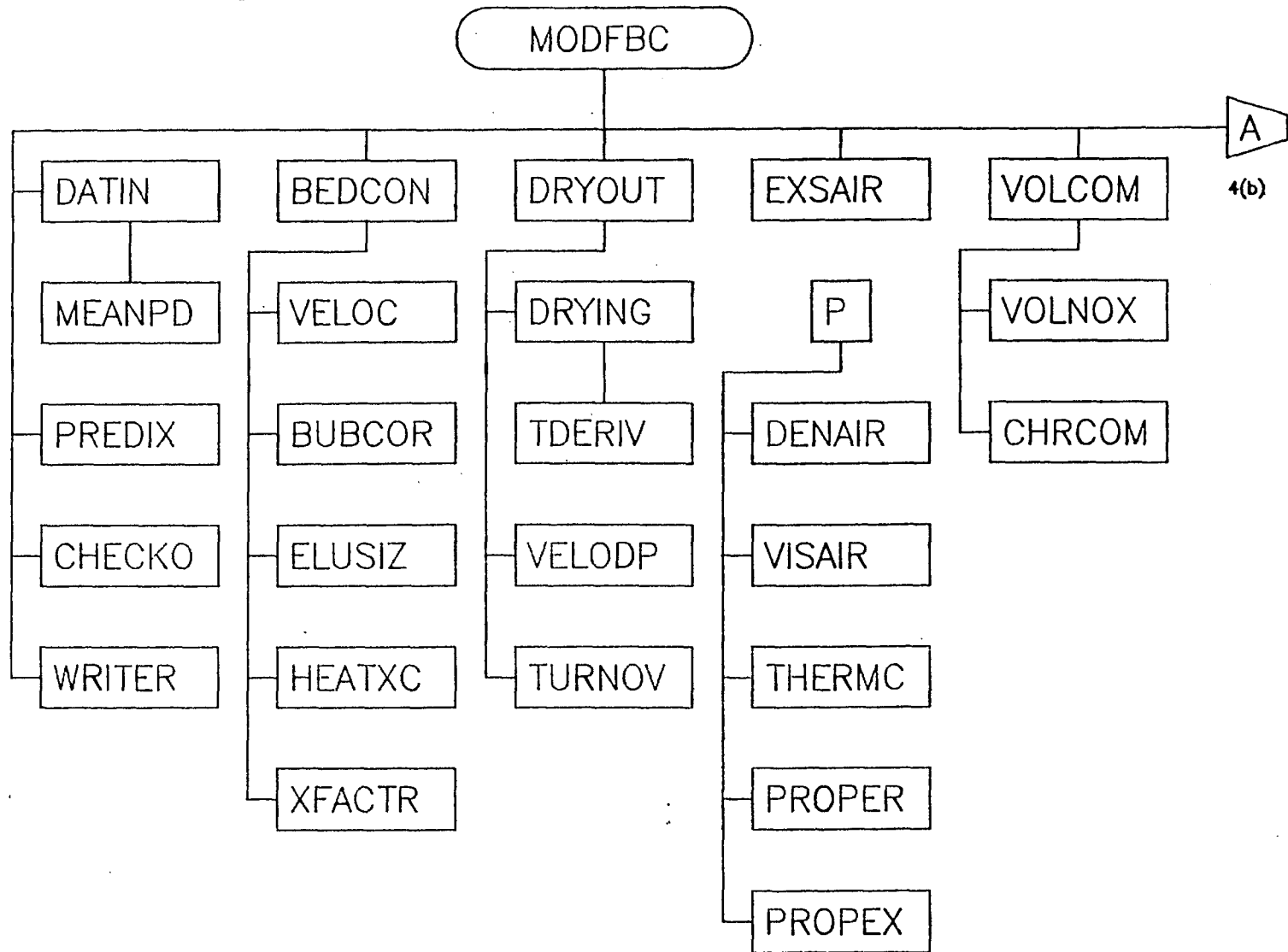
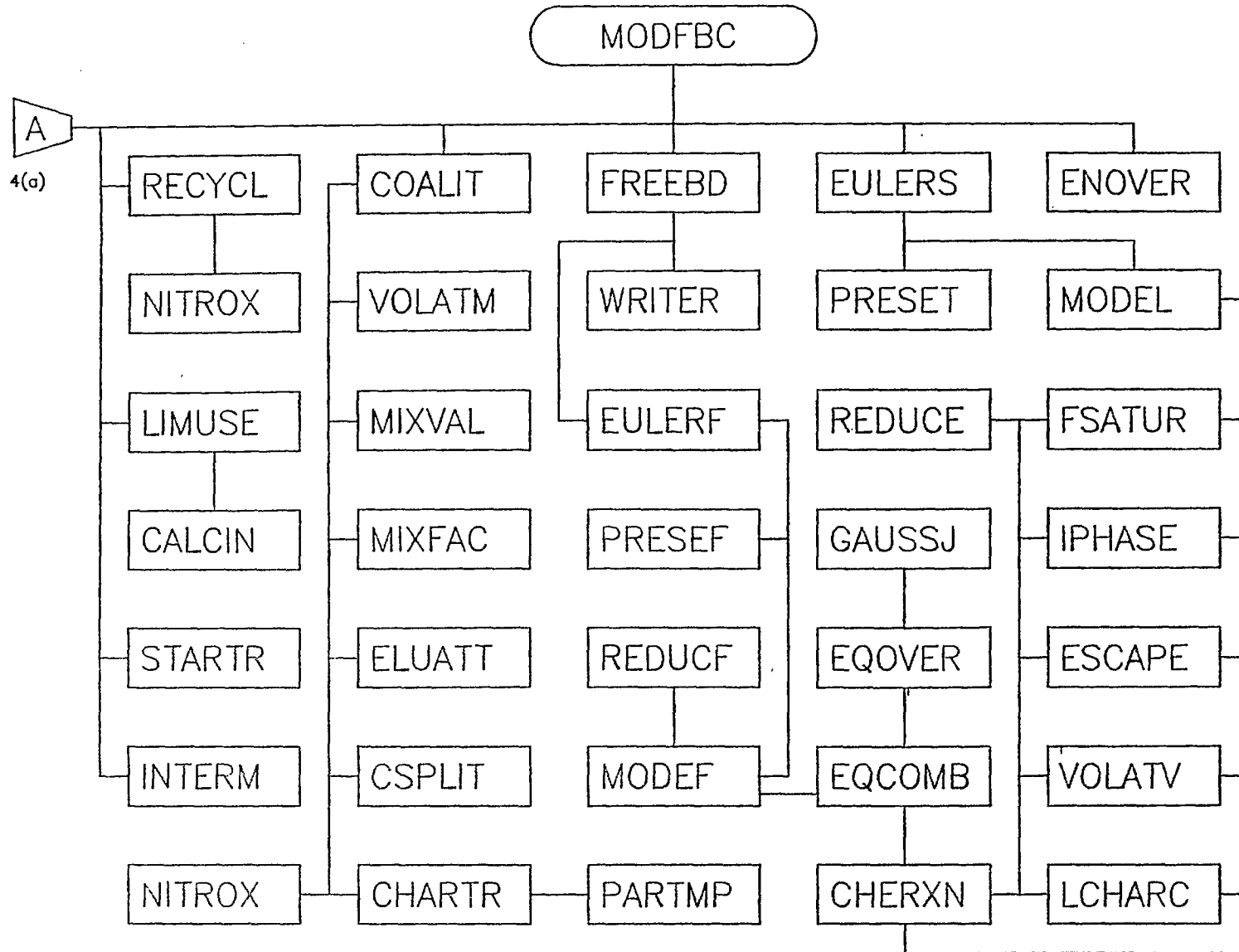


Figure 4(b). FBC Model Program Organization



2. Combustor Description

- (a) Length (0.381 m)
- (b) Width (0.406 m)
- (c) Height (3.34 m)
- (d) Wall thickness (0.2 m)
- (e) Wall thermal conductivity (5.0 J/s m K)
- (f) Feed location (bottom = 1 ... top = 10)
- (g) Number of orifices (400)
- (h) Cyclone efficiency (0.9)

Heat exchanger:

- (i) Number of tubes (12 + 4)
- (j) Tube length (0.38 m)
- (k) Tube diameter (O.D.) (0.0213 m)
- (l) Inlet water temperature (278 K)
- (m) Outlet water temperature (328 K)

3. Solids Properties

- (a) Sieve analysis of coal, limestone and bed material
- (b) Coal composition and calorific value
- (c) Limestone composition (98% CaCO₃)

Coal, bed, limestone:

- (d) Density
- (e) Heat capacity
- (f) Sphericity

4. Model Parameters

- (a) Char combustion kinetics
(A = 9000 kg/m² s k Pa) (E = - 18,000 K)
- (b) Gas diffusivity at char particle (0.0002 m²/s)
- (c) SO₂ capture constants
(k_N = 0.400 m/s) (k_P = 0.004 s⁻¹)
- (d) NO reduction constant (k_C = 0.026 m/s)
- (e) Degree of equilibrium (0.8)
- (f) Coal fragmentation factor (0.5)
- (g) Residence time factor (10.0)
- (h) CHI: Fraction of circulating gas exchanged (0.45)

Program outputs

The program is set up to write out intermediate results during the integration of the mass balances. The results of each energy balance are also recorded. The subroutine CHECKO can be called anywhere in the model to cause the current values of all the data arrays to be printed. This is a diagnostic feature and normally CHECKO is only called at the end of the program. Aside from CHECKO, a summary of the simulation results are written to the file SUMOUT. An example of this printout is shown in Figure 5.

FLUIDIZED BED COMBUSTION OF COAL MODEL
STEADY STATE

TEMPERATURE= .1.224E+03 K
 BED AREA= 1.547E-01 M2 BED HEIGHT= 6.133E-01 M
 OP. PRESSURE= 1.010E+05 PA PRESSURE DROP= 4.854E+03 PA
 MIN. AIR VEL.= 9.322E-01 M/S ACTUAL AIR VEL.= 1.900E+00 M/S
 DP (MM) COAL:STONE:BED = 1.611E+00 1.572E+00 1.572E+00

PARAMETERS:

 INTERPHASE FACTOR X/LMF 9.113E+00 RESIDENCE MULT.= 1.000E+01
 SO2 CAPTURE CONSTANT 3.500E-01 NOX REDUCTION = 7.000E-03
 CHAR KINETICS CONSTS. 9.000E+03 <--A E--> -1.800E+04
 CHAR COMB DIJ 298 2.000E-04 FRAGMENT. FACTOR 5.000E-01

RESULTS:

 COAL FEEDRATE = 2.918E+01 <KG/HR> STONE = 1.461E+01
 % EXCESS AIR = 3.388E+00 CA/S RATIO = 3.000E+00
 BED CHAR FRACTION = 4.979E-03 RECYCLE RATIO= 8.570E-01
 CARBON LOSS STREAMS KG/HR OVERFLOW= 5.090E-02
 RECYCLE PRODUCT = 4.949E-02 BAGHOUSE = 3.845E-02
 COAL ENERGY IN = 2.284E+05 J/S COOLING LOAD= 9.479E+04
 HEAT TRANS. COEFF= 2.530E+02 W/M2.K RADIATION= 9.906E+01

GAS STREAMS TOP OF BED ... COMPOSITION MOLE FRACTION

	EMULSION PHASE	BUBBLE PHASE
CO	1.401E-03	1.459E-05
CO2	1.605E-01	1.387E-01
H2	3.819E-04	3.965E-06
H2O	7.230E-02	5.936E-02
NO	1.421E-03	1.348E-03
NO2	9.502E-07	9.619E-07
N2	7.434E-01	7.525E-01
O2	1.821E-02	4.671E-02
SO2	1.780E-03	1.382E-03
CH4	5.728E-04	5.937E-06

GAS STREAM LEAVING BED ...

	TOP OF BED	TOP OF UNIT
CO	6.660E-04	5.092E-04
CO2	1.489E-01	1.503E-01
H2	1.815E-04	3.832E-05
H2O	6.544E-02	6.635E-02
NO	1.382E-03	1.386E-03
NO2	9.564E-07	9.561E-07
N2	7.462E-01	7.460E-01
O2	3.332E-02	3.168E-02
SO2	1.569E-03	1.584E-03
CH4	2.722E-04	1.325E-04

Figure 5. Summary of simulation results

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NOTATION

Subscripts

0	a property of the bubble gas
l	a property of the emulsion gas
b	bubble
c	char
i	molecular species
n	relating to pollutant reactions
p	particle
r	relating to homogeneous chemical reaction
s	relating to fluidization saturation flux
t	relating to interphase material transfer
v	coal volatile matter

Superscripts

()''	per unit area of a plan at height x in the bed
()'''	per unit volume of the bed at height x
([˙])	per unit time; indicates fluxes, not rate of change with time

Variables

a	mean interfacial area between bubbles and emulsion, per unit volume of bed (m^{-1})
c	molar density of gas (mol/m^3)
C_p	heat capacity ($J/kg K$)
D	diameter (m)
g	acceleration due to gravity (m/s^2)
ν_H	enthalpy change (J/kg)
k_c	NO reaction rate constant
k_d, k_r, k_s	char combustion constants
k_n	limestone reaction rate constant
k_p	limestone surface reduction constant

K_w	overall mass transfer coefficient for material transfer between bubbles and emulsion ($\text{kg}/\text{m}^2 \text{ s}$)
L_{mf}	bed height at point of minimum bubbling (m)
m	mass (kg)
M_i	molecular weight of species i (kg/mol)
n	moles of material (mol)
S_c	surface area of char particle (m^2)
S_p	surface area of particle (m^2)
t	time (s)
t_c	complete sulphation time(s)
T	temperature (K)
U_{mb}	superficial gas velocity at minimum bubbling (m/s)
w_i	mass fraction of species i
x	height above base of bed
x_i	mole fraction of species i
X	dimensionless mass transfer factor
z_1, z_2	devolatilization constants as per Eq. 7
α	convective heat transfer coefficient ($\text{J}/\text{s m}^2 \text{ K}$)
δ_s	saturation flux coefficient
ϵ	emissivity
ζ	bubble velocity coefficient
ρ	density (kg/m^3)
σ_B	Boltzmann's constant
τ	residence time(s)
χ	gas circulation coefficient
ω	limestone surface effectiveness factor

APPENDIX A

COMPUTER PROGRAM SYNOPSES

The computer simulation consists of a main program, MODFBC, and 58 subroutines. MODFBC supervises data input and output, checks for limiting conditions, calls the subroutines which calculate the fluidization and combustion parameters, sets up the model integration, and checks the convergence criteria. The overall program structure has already been outlined. The complete program listings are given in appendix B. In this section the functions of the subroutines will be summarized.

- BEDCON calculates the bed conditions; bed pressure drop, bed height at the minimum fluidization velocity and at the superficial velocity, and proportions of gas in the emulsion and bubble phases at the bottom of the bed.
- BUBCOR calculates a correction factor to be applied to the bubble flowrate as predicted by the two-phase theory of fluidization. Correction is based on bed height and aspect ratio.
- CALCIN calculates the degree of calcination of the limestone based on the approach to the equilibrium partial pressure of carbon dioxide.
- CHARTR calculates the char burning characteristics (burnout time, burning rate, diffusion and kinetics coefficients) for a given size particle.
- CHECKO prints out the current data values in all the defined common blocks to logical unit 3.
- CHERXN sets up the calculations for estimating the homogeneous reaction flux in both the emulsion and bubble phases.

- CHRCOM estimates the composition of the char component of the coal. The resultant analysis is on a wet basis.
ARGUMENTS:
WET - Wet basis coal analysis (COAL)
- COALIT calculates the various fluxes associated with coal combustion. This is done by estimating these fluxes separately for each coal feed size increment. The total combustion flux is then obtained by adding all the incremental fluxes. The local fluxes are estimated from calculations of the degree of coal mixing within the bed. Coal losses due to overflow and elutriation are estimated and used together with combustion rates to estimate char holdup in the bed. The amount of char in the bed is then used to calculate the rate of NO reduction due to reaction with the char.
- CSPLIT calculates the ratio of CO₂/CO formed during char combustion based on particle temperature.
ARGUMENTS:
TX - Temperature at surface of char particle (K)
FC - Fraction of char converted to CO₂
- DATIN reads the input data from logical unit 2.
- DENAIR calculates the density of air at a given temperature and pressure.
ARGUMENTS:
T - Absolute temperature (K)
P - Absolute pressure (Pa)

DRYING calculates the drying and heating up (to 900 K) time for a given size coal particle.

ARGUMENTS:

SI - Particle diameter (m)
WW - Moisture mass fraction
J - Flag : 1 - Coal, 2 - Limestone
TS - Solid temperature at start (K)
TD - Time to heat-up particle to 373 K (s)
TD1 - Time to dry particle (s)
TV - Time until devolatilization starts (900K) (s)
MM - Sieve identifier

DRYOUT sets up procedures for estimating the characteristic times and velocities for the various coal size increments.

ELUATT calculates the attrition and elutriation rates for a given size coal particle.

ARGUMENTS:

EF - The mass fraction of initial particle elutriated
AF - The mass fraction of initial particle attrited

ELUSIZ calculates the particle size corresponding to 50% mass flux fraction elutriated.

ENOVER performs an overall energy balance for the given temperature and feed conditions. If the balance fails a new coal feedrate is established.

ARGUMENTS:

IOK - Flag to identify a successful (1) energy balance

EQCOMB sets up the arrays for calculating homogeneous reaction based on degree of approach to equilibrium. This includes providing initial estimates of equilibrium concentrations and estimating reaction rates should the equilibrium calculations fail.

ARGUMENTS:

SN - Species concentration
B - Element balance
BIO - Initial element balance
Z - Vector identifying species being considered

EQOVER calculates equilibrium composition based on the RAND variation of second order chemical equilibrium algorithms.

ARGUMENTS:

STO - Starting moles of gaseous species
FIN - Final moles of gaseous species
TX - Temperature of reaction (K)

ESCAPE calculates the local fluxes due to sulphur capture and nitric oxide reduction.

EULERF carries out the integration of the model throughout the freeboard, by using the Modified Euler Method.

EULERS carries out the integration of the model throughout the bed, by using the Modified Euler Method.

EXSAIR calculates the excess air factor for given coal and air feedrates.

FREEBD sets up the initial conditions and rate expressions for model integration throughout the freeboard.

FSATUR estimates the fluidization saturation flux by diverting excess gas produced in the emulsion phase to the bubble phase.

GAUSSJ solves a matrix of simultaneous linear equations by Gauss-Jordan elimination.
ARGUMENTS:
EQU - Matrix of simultaneous linear equations

HEATXC estimates the heat transfer coefficients for heat transfer to immersed tubes. The coefficient is estimated for convection, conduction, and radiation mechanisms.

INTERM stores intermediate values during the model integration.
ARGUMENTS:
IB - Current bed level (1-10)

IPHASE calculates the local interphase transfer between bubbles and emulsion. Distinction is made between the bubbling bed and the jet zone near the distributor plate.

LCHARC calculates the local fluxes associated with char combustion.

LIMUSE calculates the fluxes associated with sulphur capture. This is done by estimating these fluxes separately for each limestone feed size increment. The total flux is then obtained by adding all the incremental fluxes.

MEANPD calculates the volume-to-surface mean particle diameters from sieve analyses of the feed materials.

MIXFAC generates a mixing pattern (distribution) given a degree of mixing constant ($M=0$ for complete segregation; $M=1$ for complete mixing).

ARGUMENTS:

M - Degree of mixing

XB - Mass fraction of minor constituent in the bed

MIXVAL estimates the degree of mixing of coal and limestone throughout the bed.

ARGUMENTS:

DP - Particle diameter (minor constituent) (m)

PDEN - Particle density (minor constituent) (kg/m^3)

UMB - Min. fluidization velocity of minor constituent (m/s)

M - Degree of mixing

MODEF sets up the differential equations for the freeboard processes by estimating the local fluxes. The differential equations are then integrated by EULERF.

MODEL sets up the differential equations for the in-bed processes by calling all the subroutines which estimate the local fluxes. The differential equations are then integrated by EULERS.

NITROX estimates the nitric oxide reduction due to reaction with char in the bed and in the freeboard.

ARGUMENTS:

IJ - Flag : 1 for bed, 2 for freeboard calculations

CH - Mass of char (kg)

- PARTMP calculates the temperature at the surface of a burning char particle. This is done by iterating until an energy balance around the particle is satisfied.
- ARGUMENTS
- TPN - Temperature at surface of a burning char particle (K)
- MNM - Flag : 1 for rigorous, 2 for approximate calculations
- PREDIX carries out an approximate energy balance around the bed, from which the steady state coal feedrate is estimated ($\pm 25\%$) This is a quasi-empirical approach to determine if the input data are acceptable. This routine also provides initial estimates of the gas concentrations throughout the bed. The results of the routine are then used as the initial guesses for the detailed simulation.
- ARGUMENTS
- IFLAG - Flag to identify successful (1) preliminary balance
- PRESEF evaluates mole and mass flowrates and fractions at every level of the freeboard integration. The values are checked to ensure they fall within acceptable limits. Unacceptable concentrations (i.e. negative values) cause the simulation to terminate.
- PRESET evaluates mole and mass flowrates and fractions at every level of the bed integration. The same limitations as in PRESEF are imposed.
- PROPER calculates the thermodynamic properties of various chemical species at a given temperature and pressure.
- ARGUMENTS:
- TV - Temperature (K)
- PROPEX assigns the chemical species' physical properties to the appropriate data array.

RECYCL calculates the flowrate of recycle char and estimates subsequent char combustion.

REDUCE estimates the current species concentrations for use in the estimation of local fluxes in the bed.
ARGUMENTS:
IR - Transfer stream identifier (1-6)

REDUCF does the same as REDUCE for the freeboard.
ARGUMENTS:
IR - Transfer stream identifier (1-6)

STARTR sets up the initial gas concentrations and initial conditions for integration, and initializes the energy balance.

TDERIV estimates the temperature/time derivative used in carrying out an energy balance around a particle (DRYING).
ARGUMENTS:
SI - Particle diameter (m)
TP - Particle temperature (K)
J - Flag : 1 - Coal, 2 - Limestone
DR - Temperature derivative
SMP - Particle mass (kg)

THERMC estimates the thermal conductivity of air at a given temperature.
ARGUMENTS:
T - Temperature (K)

TURNOV estimates particle turnover time in the fluidized bed.
ARGUMENTS:
DP - Particle diameter (m)
TT - Particle turnover time (s)

- VELOC calculates the minimum fluidizing, slugging, and terminal velocity, as well as emulsion void fraction for given bed material.
- VELODP calculates the minimum fluidizing velocity and terminal velocity for a given particle size.
ARGUMENTS:
DP - Particle diameter (m)
PDEN - Particle density (kg/m^3)
UMB - Minimum fluidization velocity (m/s)
UTP - Particle terminal velocity (m/s)
- VISAIR calculates the viscosity of air at a given temperature.
ARGUMENTS:
T - Temperature (K)
- VOLATM calculates the devolatilization time for a given coal particle size at a given temperature.
ARGUMENTS:
SI - Particle diameter (m)
TD - Bed temperature (K)
- VOLATV calculates the local volatile emission/combustion fluxes.
- VOLCOM estimates the composition of the volatile component of the coal. The resultant analysis is on a wet basis.
- VOLNOX estimates which portion of the fuel nitrogen is released with the volatiles. The routine then estimates how much of this portion is converted to NO.

WRITER prints out intermediate results at the end of each iteration (logical unit 3), and prints out the final results once a solution is obtained (logical unit 1).

ARGUMENTS:

JK - Location of block to be printed

XFACTR calculates the interphase transfer factor for the orifice region and for the bubbling bed.

APPENDIX B

COMPUTER PROGRAM LISTINGS

```

*****
*****
*
*   THIS FILE CONTAINS DEFINITION OF COMMON STATEMENTS USED IN MODFBC *
*
*****
*****
*

```

ALLOWANCE HAS BEEN MADE FOR 20 CHEMICAL SPECIES AND SIX TRANSFER STREAM

THE CURRENT VERSION OF THE MODEL CONSIDERS 10 SPECIES

- 1 CO
- 2 CO2
- 3 H2
- 4 H2O
- 5 NO
- 6 NO2
- 7 N2
- 8 O2
- 9 SO2
- 10 CH4

NOTE: ANY SPECIES NUMBER MAY BE USED LIMIT SET BY NS <20

THE 6 TRANSFER STREAMS ARE

1 SATURATION FLUX	MASS/VOL.TIME	(KG/M3.S)
2 INTERPHASE FLUX	"	"
3 HOMOGENEOUS REACTION FLUX	"	"
4 VOLATILE COMBUSTION	"	"
5 CHAR COMBUSTION	"	"
6 SO2 CAPTURE & NO REDUCTION	"	"

```

*****
COMMON BLOCKS ARE DEFINED BELOW
*****

```

```

C
COMMON/OERALL/NS ,XH,XL ,TBU(2) ,EMO(2,2,20) ,BUO(2,2,20) ,ENO(2,20)
C

```

```

NS  NUMBER OF SPECIES BEING CONSIDERED
XH  INCREMENT FOR INTEGRATION OF BED
XL  CURRENT LEVEL OF INTEGRATION (M)
FOR THE ARRAYS DEFINED BELOW
I=1 NEW OR CURRENT AND I=2 OLD OR PREVIOUS VALUE
TEMP: TBU(I) BUBBLE PHASE TEMPERATURE
MASS:
EMO & BUO (I,J,20)
WHERE J: 1 MOLE FRACTION
        2 MASS FLOWRATE MASS/AREA.TIME (IN PHASE)
        (KG/M2.S) (PER UNIT AREA)
ENERGY:
ENO(I,20) 1 - COAL FEEDRATE KG/S

```

- 2 - OVERALL ENERGY BALANCE J/S
- 3 - HEAT IN FROM COAL
- 4 - HEAT IN FROM AIR
- 5 - " SULPHATION OF CAO
- 6 -
- 7 - HEAT OUT VAPORIZATION OF WATER
- 8 - " UNBURNT HC&CO
- 9 - " CHAR LOSS
- 10 - " SOLIDS OVERFLOW
- 11 - " FROM CALCINATION OF LIMESTONE
- 12 - " IMMERSSED TUBES
- 13 - " THROUGH WALLS
- 14 - " PRODUCT GASES
- 15 -
- 16 -
- 17 -
- 18 -
- 19 -
- 20 -

C

COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)

C

NS1 NUMBER OF SPECIES BEING CONSIDERED
 EM SPECIES STREAMS IN EMULSION (KG/M3.S)
 BU SPECIES STREAMS IN BUBBLE (KG/M3.S)
 DEM,DBU DIFFERENTIAL EQUATIONS AS PER MASS BALANCES
 (I,20) WHERE I=1 IS NEW, I=2 IS OLD VALUE

C

COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)

C

BED 1 - AREA OF UNIT (M2) (READ IN AS TB IN CELSIUS
 2 - LENGTH OF UNIT (M)
 3 - WIDTH OF UNIT (M)
 4 - HEIGHT OF UNIT (M)
 5 - BED SLUMPED HEIGHT (M)
 6 - BED BULK DENSITY (KG/M3)
 7 - BED HEIGHT AT UMB (M)
 8 - BED HEIGHT AT U (M)
 9 - EMB - VOID FRACTION COEFFICIENT
 10 - ORIFICE JET HEIGHT (M)
 TB CURRENT BED TEMPERATURE (K)
 AIR 1 - VELOCITY (M/S)
 2 - UMB - BED (M/S)
 3 - PRESSURE (PA)
 4 - PRESSURE DROP ACROSS BED (PA)
 5 - TEMPERATURE OF AIR INLET (K)
 6 - EXAIR (FRACTION)
 7 - FRACTION O2 (MOLE)
 8 - " N2
 9 - " H2O
 10 - EMULSION STARTING RATE MOLE/M2.S

COAL 1 - MOISTURE WEIGHT FRACTION
 2 - ASH " (DRY BASIS)
 3 - VOLATILES " "
 4 - FIXED CARBON " "
 5 - CALORIFIC VALUE (J/KG)
 6 - C WEIGHT FRACTION (DRY BASIS)
 7 - H "
 8 - O "
 9 - N "
 10 - S "
 HOT 1 - # OF IN-BED TUBES
 2 - TUBE LENGTH (M)
 3 - TUBE DIAMETER (M)
 4 - TWATER IN (K)
 5 - TWATER OUT (K)
 6 -
 7 - T SOLIDS FEED (K)
 8 - CP WATER (J/KG.K)
 9 - T AMBIENT - ROOM TEMP - (K)
 10 - THICKNESS OF WALLS
 PTX ,1 COAL
 ,2 LIMESTONE
 ,3 BED
 1, PARTICLE SPHERICITY
 2, DENSITY (KG/M3)
 3, HEAT CAPACITY (J/KG.K)
 4, MEAN PARTICLE DIAM (M)
 5, UMB (M/S)
 6, UMS (M/S)
 7, FEEDRATE (KG/S)
 8, DP WHICH HAS UTP=U (M)
 9,
 10, ATTRITION CONSTANT

C
 COMMON/SHAKE/SIV(20,4),CPROP(20,14)
 C

SIV 20 SIEVE TRAY ANALYSIS
 ,1 OPENING MM
 ,2 COAL FRACTION ABOVE
 ,3 LIMESTONE "
 ,4 BED MATERIAL "
 CPROP 20 COAL AND LIME PARTICLE SIZE INCREMENTS (M)
 CORRESPONDING PARTICLE CHARACTERISTICS
 ,1 UMB
 ,2 UTP
 ,3 TD1 - DRYING TIME
 ,4 TV - TIME TO START DEVOL.
 ,5 TO - CHAR PARTICLE BURNOUT TIME
 ,6 TT - PARTICLE TURNOVER TIME
 ,7 RT - CHAR COMBUSTION RATE
 ,8 EF - RATIO ELUTRIATED/FED

,9 AF - RATIO ATTRITED/FED
,10 M - MIXING COEFFICIENT
,11 TD - DEVOLATILIZATION TIME
,12 - LIMESTONE-SO2 CAPTURE RATE
,13
,14 - NO REDUCTION RATE

C
COMMON/GASCON/GASX(11,22),GASB(11,22)
C

GASX(I,J)
CONTAINS MOLE FRACTIONS IN EMULSION AT X LEVELS IN BED
I,1-10 LEVELS IN THE BED PROPER
,11 LEVEL IMMEDIATELY ABOVE BED
J SPECIES AS ALREADY DEFINED WITH THE FOLLOWING EXCEPTIONS
,16 - NO REDUCTION RATE KG/S
,17 - VOLATILE EMISSION RATE KG/S
,18 - CHAR COMBUSTION RATE KG/S
,19 - FRACTION OF CHAR AS CO2 (REST CO)
,20 - SO2 ABSORPTION RATE KG/S
,21 - IS TOTAL MOLES OF EMULSION GAS MOL/M2.S

GASB(I,J):
CONTAINS MOLE FRACTIONS IN BUBBLE AT X LEVELS IN BED
DEFINITIONS AS FOR EMULSION PHASE EXCEPT:

,21 - IS TOTAL MOLES OF BUBBLE GAS MOL/M2.S

GASX AND GASB SPECIAL CASES:

(10,22) - CURRENT MASS RATE KG/M2.S
(11,22) - CURRENT MOLE RATE MOLE/M2.S

BUILDUP OF EXCESS TRANSFER POTENTIAL:

GASB (1,22) - NO REDUCTION
2 - VOLATILE "
3 - CHAR "
5 - SO2 CAPTURE
6 -

TEMPORARY STORAGE LOCATIONS:

4 - FRACTION CO2
7 - SO2 CONCENTRATION KMOL/M3
8 - NO MOLE FRACTION

C
COMMON/BURNS/VCOM(11),CM(5)
C

VCOM(1-10), MASS FRACTION COMPOSITION OF VOLATILES AS PER
SPECIES AT TOP OF THIS FILE
VCOM(11) , O2 NECESSARY FOR ABOVE SPECIES
CM(5), MASS FRACTION C,H,O,N,S IN CHAR
1 2 3 4 5

C
COMMON/EQUIL/NSE,NLM,AES(5,10)
C

NSE - NO. OF SPECIES BEING INCLUDED IN EQUIL. CALCULATION
NLM - NO OF ELEMENTS IN NSE
AES - ATOM MOLE IN ONE MOLE OF EACH SPECIES 1-10

- 1 - C
- 2 - H
- 3 - O
- 4 - N
- 5 - S

C
COMMON/UNITS/IN,IOUT,SPECY(20)

C
IN READ FROM UNIT OR FILE "IN"
IOUT WRITE TO UNIT IOUT
SPECY CONTAINS TITLES FOR SPECIES

C
COMMON/CONST/PP(5,20),GG(50)

C
PP PHYSICAL PROPERTIES OF SPECIES
1, MOL. WT. (KG/MOL)) ENTERED THROUGH
2, HEAT OF FORMATION 298 J/MOL) SUB PROPEX

3, HEAT CAPACITY AT T (J/MOL.K)) ENTERED IN
4, ENTROPY AT T (J/MOL.K)) SUBROUTINE
5, ENTHALPY H-H298 AT T (J/MOL)) PROPER
GG GENERAL PURPOSE ARRAY:
1 NUMBER OF SPECIES BEING CONSIDERED =NSP
2 CA/S RATIO
3 CACO3 WEIGHT FRACTION IN LIMESTONE
4 RECYCLE FRACTION 0 TO 1
5 CYCLONE EFFICIENCY FACTOR 0 TO 1
6 FEED LOCATION : INTEGER 1 TO 10 ;1 BOTTOM;10 TOP
7 RESIDENCE TIME OF ELUTRIABLE PARTICLE
- I.E. FACTOR TO MX TURNOVER TIME BY
8 REFRACTORY THERMAL CONDUCTIVITY J/S.M.K
9 STEFAN-BOLTZMANN CONSTANT
10 NO REDUCTION CONSTANT S-1
11 SO2 CONSTANT -KN
12 SO2 CONSTANT -KP
13 CHAR KINETICS TERM A
14 CHAR KINETICS TERM -E
15 # OF ORIFICES IN DISTRIBUTOR
16 PERFECT MIXING FACTOR I.E. DEGREE OF EQUILIBRIUM
17 INTERPHASE TRANSFER - CHI FRACTION OF CIRCULATING
GAS EXCHANGED
18 DD DIFFUSIVITY AT 298 (CHAR COMBUSTION)
19 CHAR DENSITY KG/M3
20 COAL FRAGMENTATION FACTOR

* NOTE: ABOVE MUST BE READ IN BY SUBROUTINE DATIN *
* BELOW ARE CALCULATED BY VARIOUS SUBROUTINES *

21 DENSITY OF AIR KG/M3
22 VISCOSITY OF AIR KG/M.S
23 LMF M (FROM EMF CORREL. OF BROADHURST&BECKER)

- 24 L EXPANDED M
- 25 VOLUME OF EMULSION PHASE M3
- 26 VOLUME OF BUBBLE PHASE M3
- 27 VOLUMETRIC RATE OF EMULSION PHASE M3/S
- 28 VOLUMETRIC RATE OF BUBBLE PHASE M3/S
- 29 THERMAL CONDUCTIVITY OF AIR J/S.M.K
- 30 DP (M) FOR 50% ELUTRIATION (B.S. XU)
- 31 BUBBLE CORRECTION FACTOR SUB BUBCOR
- 32 FN - FUEL NITROGEN FRACTION IN VOLATILES
- 33 FRN- VOLATILE NITROGEN (NH3>>NO,N2) FRACTION
- 34 MASS FRACTION OF COAL AS VOLATILES
- 35 MASS FRACTION OF COAL AS CHAR
- 36 CHAR HOLDUP - FRACTION OF BED
- 37 BED OVERFLOW KG/S
- 38 FRACTIONAL CALCINATION LEVEL 0-1
- 39 CORRECTED GG(7); RES TIME FACTOR FOR COAL FINES
- 40 RESIDENCE TIME OF LARGE LIMESTONE PARTICLES
- 41 CHAR LEAVING BED KG/S
- 42 CHAR FINES - BURNUP IN BED KG/S
- 43 CHAR LOST AT CYCLONE KG/S
- 44 CHAR LOST AS RECYCLE PRODUCT KG/S
- 45 MEAN BUBBLE DIAMETER M
- 46 BUBBLING THEORY INTERPASE FACTOR X/LMF M-1
- 47 HEAT TRANSFER COEFFICIENT TUBES J/S.M2.K
- 48 H. T. COEFF. OUTSIDE WALL J/S.M
- 49 HEAT TRANSFER TO TUBES - RADIATION J/S.M2.K
- 50 XNO AVERAGE FOR BED

```

*****
*   UNITS: SI   *
*   *   *   *
*   BASE UNITS: *
*   K KELVIN   *
*   M METRE    *
*   S SECOND   *
*   KG KILOGRAM *
*   MOL GMMOLE *
*   DERIVED UNITS: *
*   PRESSURE - PA - PASCAL (KG/M.S2) *
*   ENERGY - J - JOULE (KG.M2/S2) *
*   POWER - W - WATT (KG.M2/S3) *
*****

```

```

C*****
C   MODFBC *
C   THIS IS THE MAIN PROGRAM WHICH RUNS SIMULATION *
C   FOR FLUIDIZED BED COMBUSTION OF COAL *
C *
C*****
COMMON/OERALL/NS ,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/EQUIL/NSE,NLM,AES(5,10)
DIMENSION ATIME(2),ENBAL(2)

C
C*****
C   COMMON BLOCKS HAVE BEEN DEFINED IN COMMON.DAT
C*****
      IP=6
      IOUT=1

C
C   READ IN DATA
C
      CALL DATIN

C
C   CARRY OUT QUICK MASS/ENERGY BALANCE TO ESTIMATE FEEDRATES
C
      CALL PREDIX(IFLAG)
      IF(IFLAG.EQ.1) GOTO 100
      WRITE(6,101)
101  FORMAT(' PREDIX CANNOT SOLVE MASS/ENERGY BALANCES ')
303  STOP
100  CONTINUE

C
C   IF EXCESS AIR IS LESS THAN 0.0 ASK FOR PERMISSION TO CONTINUE
C
      IF(AIR(6).GT.1.0) GOTO 305
      WRITE(6,306)
306  FORMAT(' EXCESS AIR IS BELOW ZERO ',/,
* ' ENTER 29 IF YOU WISH TO CONTINUE ')
      READ(5,307)NSC
307  FORMAT(I2)
      IF(NSC.EQ.29) GOTO 305
      STOP
305  CONTINUE

C
C   ZERO ENERGY BALANCE TERMS AND SET COAL RATE
C
      ENO(1,1)=PTX(7,1)

```

```

      ENO(2,1)=0.0
      ENO(2,2)=0.0
      ENO(1,2)=0.0
C
C      EVALUATE BED CHARACTERISTICS
C
      CALL BEDCON
C
C      ESTIMATE INTEGRATION STEP SIZE IN METERS
C
      XH=XH*BED(8)
      NS1=NS
C
C      CALCULATE PARTICLE DRYING/TURNOVER TIMES
C
      CALL DRYOUT
C
C      WRITE CONDITIONS/HEADINGS IF DESIRED
C
      CALL WRITER(1)
C
C      INTEGRATION LOOP START
C
      ILM=10
      DO 300 ILO=1,ILM
      DO 520 IXOR=1,2
      PTX(7,1)=ENO(1,1)
      WRITE(6,665)ENO(2,2),ENO(1,1),ILO,IXOR
665  FORMAT(' FROM E.BAL=',F7.3,' COAL KG/S=',1PE9.2,
* ' AT ITERATION ',I2,' V. ',I2)
      CALL EXSAIR
C
C      CALCULATE LIMESTONE FEEDRATE BASED ON DESIRED CA/S RATIO
C
      CX=PTX(7,1)*(1.0-COAL(1))
      S=CX*COAL(10)/0.032064
      CA=GG(2)*S
      PTX(7,2)=CA*0.10008*(1.0/GG(3))
C
C      ZERO COMBUSTION ARRAY
C
      DO 108 I=1,11
      DO 108 J=16,20
108  GASX(I,J)=0.0
C
C      EVALUATE LOCAL AND OVERALL COAL COMBUSTION
C
C      VOLATILE / CHAR COMPOSITION FIRST
C
      CALL VOLCOM
      CALL COALIT

```

```

      CALL RECYCL
C
C   EVALUATE LIMESTONE/SO2 LOCAL REACTION RATES
C
      CALL LIMUSE
C
C   START INTEGRATION
C
      CALL STARTR
      ITEM=0
      ITOT=0
201  CONTINUE
C
C   HEIGHT INCREMENT
C
      XL=XL+XH
C
C   INTEGRATION ROUTINE
C
      CALL EULERS
C
C   STORE & WRITE OUT INTERMEDIATE RESULTS
C   AT APPROPRIATE LEVELS:EVERY TENTH OF BED HEIGHT
C
      ITEM=ITEM+1
      ITOT=ITOT+1
      IF(ITEM.LT.10)GOTO 107
      ITEM=0
      IB=INT(FLOAT(ITOT)/10.0)
      CALL INTERM(IB)
      CALL WRITER(2)
C
C   INTEGRATION LIMIT IS BED HEIGHT-BED(8)
C
107  IF(XL.LT.BED(8)) GO TO 201
520  CONTINUE
C
C   ACCOUNT FOR ANY UNBURNT VOLATILES
C
      GASX(11,17)=GASX(11,17)+GASB(2,22)
C
C   CARRY OUT OVERALL ENERGY BALANCE
C
      CALL ENOVER(IOK)
      CALL WRITER(3)
C
C   CHECK FOR CONVERGENCE
C
      IF(IOK.EQ.1.AND.ILO.GT.2) GOTO 102
300  CONTINUE
C

```

```
C    NORMAL EXIT INDICATES LACK OF CONVERGENCE AFTER GG(20) TRIES
C    WRITE OUT FAILURE MESSAGE AND STOP
C
    WRITE(IP,500)
500  FORMAT(' FAILURE TO CONVERGE IN MODFBC - OVERALL ')
C
C    WRITE OUT COMPLETE DATA SET
C
    CALL CHECKO
    STOP
C
C    ENERGY BALANCE IS SATISFIED
C
102  CONTINUE
    WRITE(IP,513)
513  FORMAT(' ENERGY BALANCE SATISFIED ')
C    OPTIONAL COMPLETE PRINTOUT (REMOVE C)
C    CALL CHECKO
C
C    FREEBOARD INTEGRATION
C
    CALL FREEBD
C
C    WRITE OUT STEADY STATE CONDITIONS
C
C    OPTIONAL COMPLETE PRINTOUT (REMOVE C)
C    CALL CHECKO
    CALL WRITER(5)
    STOP
    END
```

```

SUBROUTINE BEDCON
C
C ESTABLISH BED CONDITIONS
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
C
C CALL VELOCITY CALCULATION ROUTINE
C
CALL VELOC
C
C ESTIMATE PRESSURE DROP ACROSS BED
C
AIR(4)=BED(6)*BED(5)*9.80665
C
C ESTIMATE BED HEIGHT AT UMB FROM BROADHURST&BECKER CORRELATIONS
C
V=(BED(6)*BED(5)*BED(1))/((1.0-BED(9))*PTX(2,3))
GG(23)=V/BED(1)
IF(GG(23).LT.BED(5)) GG(23)=BED(5)
BED(7)=GG(23)
C
C ESTIMATE EXPANDED HEIGHT OF BED BASED ON NO EXPANSION AT UMF
C
A=(AIR(1)-AIR(2))*0.738
B=PTX(4,3)**1.006
C=PTX(2,3)**0.376
D=AIR(2)**0.937
E=GG(21)**0.126
AA=1.0+(7.30*A*B*C)/(D*E)
IF(AA.LE.1.01) AA=1.01
BED(7)=BED(5)
GG(24)=AA*BED(5)
BED(8)=GG(24)
GG(25)=BED(5)*BED(1)
IF(GG(24).GE.BED(4)) WRITE(6,101)
101 FORMAT(' WARNING** EXPANDED BED HEIGHT GREATER THAN UNIT HEIGHT')
C
C VOLUME OF BUBBLE PHASE
C
CALL BUBCOR
GG(26)=GG(24)*BED(1)-GG(25)
C
C VOLUMETRIC RATE IN EMULSION
GG(27)=AIR(2)*BED(1)
C
C CORRECT FOR BUBCOR I.E. REDUCED BUBBLE VOLUME
GG(27)=GG(27)/GG(31)
AIR(2)=GG(27)/BED(1)
C
C VOLUMETRIC RATE IN BUBBLE
GG(28)=AIR(1)*BED(1)-GG(27)
C

```



```
C      EMULSION FLOWRATE   (MOLE/M2.S)
C
      AIR(10)=AIR(3)*GG(27)/(8.3147*TB)
      AIR(10)=AIR(10)/BED(1)
C
      ELUTRIATION SIZE
C
      CALL ELUSIZ
C
      HEAT TRANSFER COEFFICIENT FOR IMMersed TUBES
C
      CALL HEATXC
C
      CALCULATE INTERPHASE MASS TRANSFER FACTOR
C
      CALL XFACTR
C
      RETURN
      END
```

```

SUBROUTINE BUBCOR
C
C   CALCULATE CORRECTION FACTOR DELTAF
C   I.E. ACTUAL BUBBLE FLOW/TWO-PHASE THEORY BUBBLE FLOW
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
C
H=BED(8)
D=(4.0*BED(1)/3.141593)**0.5
B=H/D
IF(B.LT.2.0) GOTO 100
HS=2.0*D
DELF=(0.8*HS+1.0*(H-HS))/H
GOTO 200
100 DELF=0.6+0.09*H/D
200 GG(31)=DELF
RETURN
END

```

```

SUBROUTINE CALCIN
C
C   CALCULATE FRACTIONAL LIMESTONE CALCINATION LEVEL
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
COMMON/GASCON/GASX(11,22),GASB(11,22)
C
E=-159000.0
A=12000000.0
PE=3.0*GASX(10,2)
C
C   DEGREE OF CALCINATION BASED ON DEVIATION FROM
C   EQUILIBRIUM TEMPERATURE
C
TE=E/(8.3144*(ALOG(PE/A)))
DT=ABS(TE-TB)
GG(38)=1.0-0.001*DT
IF(GG(38).LT.0.10) GG(38)=0.10
RETURN
END

```

```

SUBROUTINE CHARTR
C
C   CALCULATE CHAR BURNING TIMES AND RATES
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
COMMON/COMB/SI,ON,TO,RT,RTM,TP,RC,NF,RE,PR,DNU,ALPHA,XNO,RNO
C
C*****
C
C   DEFINITION OF COMMON BLOCK /COMB/
C   THIS BLOCK IS USED ONLY IN CHAR BURNING CALCULATIONS
C   /COMB/ SI - PARTICLE DIAMETER M
C           ON - OXYGEN MOLE FRACTION
C           TO - BURNOUT TIME S
C           RT - BURNING RATE OVERALL      KG/S
C           RTM- BURNING RATE MAIN PARTICLE KG/S
C           TP - TEMPERATURE OF PARTICLE K
C           RC - MOLE RATIO OF CO/CO2
C           NF - CONTROLLING MECHANISM 2-DIFF 1-REACTION
C           RE - REYNOLDS NUMBER
C           PR - PRANDTL "
C           DNU- NUSSELT "
C           ALPHA - CONVECTIVE HEAT TRANSFER COEFF.
C           XNO - NO MOLE FRACTION
C           RNO - NO/CHAR REDUCTION
C*****
REAL STX(2)
C
C   GUESS PARTICLE TEMPERATURE - START ITERATION
C
CALL PARTMP(TP,2)
M=1
505 CONTINUE
C
C   CALCULATE CHAR BURNING RATE AND TIMES
C
DO 300 IJ=1,2
C   CONVERT SIZE TO MM
SS=SI*1000.0
C   CO2/CO RATIO
RC=0.0004*EXP(6240.0/TB)
C   STARTING MASS
SMO=3.141592*(SI**3.)*PTX(2,1)/6.0
C   DELTA TO CALCULATE RATE
IF(IJ.EQ.1) SMO=SMO*1.01
C   REACTION RATE COEFFICIENT
RR=GG(13)*AIR(3)*0.001*(EXP(GG(14)/TP))
C   DIFFUSIVITY
DIJ=((TP/298.0)**1.5)*GG(18)
C   DIFFUSION RATE COEFFICIENT

```

```

DR=(2.0+RC)/(1.0+RC)
DR=DR*DIJ*BED(9)*4.0*3.141592*AIR(3)*0.001/(8.288*TP)
C   CALCULATE BURNOUT TIME
    PF=1.0
    D=GG(19)
    SM=SMO
101  CONTINUE
C   SURFACE AREA COEFFICIENT
    SK=(3.0/(4.0*3.141592*D))**(1.0/3.0)
C   BURNING RATES
    FDR=DR
    FRR=RR
C   BP TERM
    BP=12.0*COAL(4)/(COAL(4)-COAL(2))
    BP=BP*2.0*FDR*(SK**2.0)*FRR/3.0
    BPM=(SM*COAL(4))**(1.0/3.0)
    BPO=(SK*FRR*BPM*BPM)+(2.0*FDR*BPM)
    TO=BPO/(BP*ON)
300  STX(IJ)=TO
C   OVERALL RATE BASED ON STARTING MASS
    RT=0.01*SMO/(STX(1)-STX(2))
C   RATE FOR MAIN PARTICLE
    RTM=0.01*SM/(STX(1)-STX(2))
C
C   CHECK PARTICLE TEMPERATURE
C   REPEAT CALCULATIONS IF DIFFERENT
C
    CALL PARTMP(TPN,2)
    ERR=ABS((TP-TPN)/TP)
    IF(ERR.LT.0.002) GOTO 506
    TP=TPN
    M=M+1
    IF(M.LT.99) GOTO 505
506  CONTINUE
    RETURN
    END

```

SUBROUTINE CHECKO

C
C
C

THIS SUBROUTINE PRINTS OUT ALL COMMON BLOCKS TO UNIT 3

COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/EQUIL/NSE,NLM,AES(5,10)

C

IP=3
WRITE(IP,100)XH,TB
100 FORMAT(' XH= ',1PE15.5,' TB= ',1PE15.5)
WRITE(IP,301)
301 FORMAT(' EMO')
DO 401 I=1,20
401 WRITE(IP,302)EMO(1,1,I),EMO(1,2,I),EMO(2,1,I),EMO(2,2,I)
WRITE(IP,303)
303 FORMAT(' BUO')
DO 402 I=1,20
402 WRITE(IP,302)BUO(1,1,I),BUO(1,2,I),BUO(2,1,I),BUO(2,2,I)
302 FORMAT(' ',1P4E15.5)
WRITE(IP,305)
305 FORMAT(' ENO')
DO 501 I=1,20
501 WRITE(IP,302)ENO(1,I),ENO(2,I)
WRITE(IP,304)
304 FORMAT(' TBU')
WRITE(IP,302)TBU(1),TBU(2)
WRITE(IP,502)
502 FORMAT(' EM 1-6,DEM 1')
DO 503 I=1,20
503 WRITE(IP,504)(EM(J,I),J=1,6),DEM(1,I)
WRITE(IP,505)
505 FORMAT(' BU 1-6,DBU 1')
DO 506 I=1,20
506 WRITE(IP,504)(BU(J,I),J=1,6),DBU(1,I)
504 FORMAT(' ',1P7E9.2)
WRITE(IP,306)
306 FORMAT(' BED --- AIR ---- COAL ---- HOT ')
DO 450 I=1,10
450 WRITE(IP,302)BED(I),AIR(I),COAL(I),HOT(I)
DO 451 I=1,10
451 WRITE(IP,307)PTX(I,1),PTX(I,2),PTX(I,3)
307 FORMAT(' PTX',1P3E15.5)
WRITE(IP,310)
310 FORMAT(' SIV')

```

DO 452 I=1,20
452 WRITE(IP,302)(SIV(I,J),J=1,4)
WRITE(IP,320)
320 FORMAT(' CPROP')
DO 321 I=1,20
WRITE(IP,322) SIV(I,1)
WRITE(IP,322)(CPROP(I,J),J=1,5)
WRITE(IP,322)(CPROP(I,J),J=6,10)
321 WRITE(IP,322)(CPROP(I,J),J=11,14)
322 FORMAT(' ',1P6E12.5)
WRITE(IP,325)
325 FORMAT(' GASX')
DO 326 I=1,22
IF(I.LE.NS) WRITE(IP,330)SPECY(I)
IF(I.GT.NS) WRITE(IP,333)I
333 FORMAT(' ',I3)
330 FORMAT(' ',A4)
WRITE(IP,322)(GASX(J,I),J=1,5)
326 WRITE(IP,322)(GASX(J,I),J=6,11)
WRITE(IP,510)
510 FORMAT(' GASB')
DO 511 I=1,22
IF(I.LE.NS) WRITE(IP,330)SPECY(I)
IF(I.GT.NS) WRITE(IP,333)I
WRITE(IP,322)(GASB(J,I),J=1,5)
511 WRITE(IP,322)(GASB(J,I),J=6,11)
WRITE(IP,370)
370 FORMAT(' VCOM')
WRITE(IP,322)(VCOM(I),I=1,5)
WRITE(IP,322)(VCOM(I),I=6,11)
WRITE(IP,371)
371 FORMAT(' CM')
WRITE(IP,322)(CM(I),I=1,5)
WRITE(IP,308)
308 FORMAT(' PP')
DO 453 I=1,20
453 WRITE(IP,409)(PP(J,I),J=1,5)
WRITE(IP,410)
410 FORMAT(///,' GG: ')
WRITE(IP,409)(GG(L),L=1,5)
WRITE(IP,409)(GG(L),L=6,10)
WRITE(IP,409)(GG(L),L=11,15)
WRITE(IP,409)(GG(L),L=16,20)
WRITE(IP,409)(GG(L),L=21,25)
WRITE(IP,409)(GG(L),L=26,30)
WRITE(IP,409)(GG(L),L=31,35)
WRITE(IP,409)(GG(L),L=36,40)
WRITE(IP,409)(GG(L),L=41,45)
WRITE(IP,409)(GG(L),L=46,50)
409 FORMAT(' ',1P5E12.3)
RETURN

```

END

SUBROUTINE CHERXN

C
C
C

ESTIMATE LOCAL HOMOGENEOUS GAS PHASE REACTION

COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/EXIST/AVE(20),AVB(20)
REAL STO(10),FIN(10),SCON(10)

C
C
C

EMULSION

DO 100 I=1,10
STO(I)=GG(16)*AVE(I)/PP(1,I)
100 SCON(I)=STO(I)
CALL EQOVER(STO,FIN,TB)
DO 101 I=1,10
STO(I)=FIN(I)-SCON(I)
101 EM(3,I)=STO(I)*PP(1,I)

C
C
C

BUBBLE

DO 102 I=1,10
STO(I)=GG(16)*AVB(I)/PP(1,I)
102 SCON(I)=STO(I)
CALL EQOVER(STO,FIN,TB)
DO 103 I=1,10
STO(I)=FIN(I)-SCON(I)
103 BU(3,I)=STO(I)*PP(1,I)
CALL REDUCE(3)
RETURN
END

```

SUBROUTINE CHRCOM(WET)
C
C   CALCULATE COMPOSITION OF CHAR
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
REAL WET(10)

C
GG(35)=1.0-(GG(34)+WET(2))
C
C
CM(1)=(VCOM(1)*0.01201/PP(1,1))+(VCOM(2)*0.01201/PP(1,2))
CM(1)=CM(1)+(VCOM(10)*0.01201/PP(1,10))
C
H
CM(2)=VCOM(3)+(VCOM(4)*0.002016/PP(1,4))
CM(2)=CM(2)+(VCOM(10)*0.004032/PP(1,10))
C
O
CM(3)=(VCOM(1)*0.016/PP(1,1))+(VCOM(2)*0.032/PP(1,2))
CM(3)=(VCOM(4)*0.016/PP(1,4))+(VCOM(5)*0.016/PP(1,5))+CM(3)
CM(3)=(VCOM(6)*0.032/PP(1,6))+(VCOM(9)*0.032/PP(1,9))+CM(3)
CM(3)=CM(3)+VCOM(8)+VCOM(11)
C
N
CM(4)=(VCOM(5)*0.014008/PP(1,5))+(VCOM(6)*0.014008/PP(1,6))
CM(4)=CM(4)+VCOM(7)
C
S
CM(5)=VCOM(9)*0.032066/PP(1,9)
C
CHECK BALANCE
SUM=0.0
DO 100 I=1,5
B=WET((I+5))
C
CORRECTION FOR MOISTURE CONTENT
IF(I.EQ.2)B=B+(WET(1)*0.002016/0.018016)
IF(I.EQ.3)B=B+(WET(1)*0.016/0.018016)
CM(I)=(B-CM(I)*GG(34))/GG(35)
IF(CM(I).LT.0.00001) CM(I)=0.0
SUM=SUM+CM(I)
100 CONTINUE
DO 102 I=1,5
102 CM(I)=CM(I)/SUM
RETURN
END

```

```

SUBROUTINE COALIT
C
C CALCULATE FLUXES ASSOCIATED WITH COAL COMBUSTION
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/MXF/X(10),Y(10)
COMMON/COMB/SI,ON,TO,RT,RTM,TP,RC,NF,RE,PR,DNU,ALPHA,XNO,RNO
C /COMB/ IS DEFINED IN SUBROUTINE CHARTR
REAL NRAT(20)
C
C ATTRITION RATE CONSTANT BASED ON ARENA & MASSIMILLA
C
PTX(10,1)=1.0E-08
SIDP=PTX(4,3)
IF(SIDP.LT.PTX(4,2)) SIDP=PTX(4,2)
FTR=26.6*(SIDP*1000.0)-12.0
IF(FTR.LT.3.5) FTR=3.5
IF(FTR.GT.20.0) FTR=20.0
PTX(10,1)=FTR*PTX(10,1)
C
C CALCULATE COAL BURNING RATE FOR EACH PARTICLE SIZE
C
DO 100 I=1,20
IF(SIV(I,2).EQ.0.0) GOTO 200
SI=SIV(I,1)
C DEVOLATILIZATION TIME
CALL VOLATM(SI,CPROP(I,11))
C M - DEGREE OF MIXING
CALL MIXVAL(SI,PTX(2,1),CPROP(I,1),CPROP(I,10))
C ESTIMATE DISTRIBUTION BASED ON M
CALL MIXFAC(CPROP(I,10),0.005)
C O2 LOCAL AVERAGES
XNO=0.0
ON=0.0
DO 109 K=1,10
109 ON=X(K)*GASX(K,8)+ON
C ESTIMATE BURNING TIME/RATE
CALL CHARTR
CPROP(I,5)=TO
CPROP(I,7)=RT
C
C ELUTRIATION / ATTRITION LOSSES
C
CALL ELUATT(CPROP(I,8),CPROP(I,9))
200 CONTINUE
100 CONTINUE
C

```

```

C     ESTIMATE CHAR HOLDUP IN BED
C
      CH=0.0
      DO 500 I=1,20
      IF(SIV(I,1).LT.GG(30))GOTO 500
C
C     FRAGMENTATION FACTOR
C
      BTIME=CPROP(I,5)
      SIDP=SIV(I,1)*1000.0
      IF(SIDP.LE.1.2) GOTO 501
      DN=GG(20)*(SIDP**(2.0/3.0))
      IF(DN.LT.1.0) DN=1.0
C     FIND RANGE & GET TO,EL,AL BY INTERPOLATION
      DX=DN/1000.0
      DO 523 MT=1,11
      LT=MT+1
      IF(DX.LE.SIV(MT,1).AND.DX.GT.SIV(LT,1)) GOTO 520
523  CONTINUE
      GOTO 500
520  FR=(DX-SIV(LT,1))/(SIV(MT,1)-SIV(LT,1))
      BTIME=CPROP(LT,5)+FR*(CPROP(MT,5)-CPROP(LT,5))
      CPROP(I,8)=CPROP(LT,8)+FR*(CPROP(MT,8)-CPROP(LT,8))
      CPROP(I,9)=CPROP(LT,9)+FR*(CPROP(MT,9)-CPROP(LT,9))
501  TOT=CPROP(I,11)+BTIME
      TOT=TOT*SIV(I,2)*PTX(7,1)
      CH=CH+TOT
500  CONTINUE
      GG(36)=CH/(BED(1)*BED(5)*BED(6))
C     IF COAL LOADING IS GREATER THAN 25% GIVE ERROR
      IF(GG(36).LT.0.25) GOTO 502
      WRITE(6,503)GG(36)
503  FORMAT(' CARBON LOADING GREATER THAN 25 % - EXECUTION STOPPED',
* ' C.L.= ',1PE12.3)
      CALL CHECKO
      STOP
502  CONTINUE
C
C     NO REDUCTION RATES
C
      DO 110 I=1,20
      SI=SIV(I,1)
      CALL NITROX(1,CH)
110  CPROP(I,14)=RNO
C
C     ESTIMATE OVERFLOW STREAM
C
C     LIMESTONE MINUS FINES
      SUM=1.0
      DO 510 I=1,20
      IF(SIV(I,1).GT.GG(30)) GOTO 510

```

```

SUM=SUM-SIV(I,3)
510 CONTINUE
SUM=PTX(7,2)*(1.0-SUM)
GG(37)=0.70*PTX(7,2)-SUM
DO 530 K=1,20
NRAT(K)=0.0
IF(SIV(K,1).LE.GG(30)) GOTO 530
NRAT(K)=SIV(K,2)
530 CONTINUE
SUM=0.0
DO 521 K=1,20
521 SUM=SUM+NRAT(K)
DO 522 K=1,20
522 NRAT(K)=NRAT(K)/SUM
C
C ESTIMATE VOLATILE/CHAR DISTRIBUTION THROUGHOUT BED
C
DO 600 I=1,20
IF(SIV(I,2).EQ.0.0) GOTO 600
SI=SIV(I,1)
C FEEDRATE AT THIS SIZE
FDR=PTX(7,1)*SIV(I,2)
C VOLATILES
VFDR=FDR*GG(34)
C CHAR
CFDR=FDR*GG(35)
C PARTICLES ELUTRIATED
IF(SI.GT.GG(30)) GOTO 300
C VOLATILE SPLIT
IF(CPROP(I,6).LT.CPROP(I,3)) GOTO 400
IF(CPROP(I,3).LE.CPROP(I,6).AND.CPROP(I,6).LE.CPROP(I,4))GOTO 401
C TT.GT.TV UNIFORM DISTRIBUTION
XVD=0.1*VFDR
DO 402 K=1,10
402 GASX(K,17)=XVD+GASX(K,17)
GOTO 405
C ALL VOLATILES AT TOP
400 CONTINUE
GASX(11,17)=GASX(11,17)+VFDR
GOTO 405
C VOLATILES SPLIT
401 VS=0.5
GASX(11,17)=VS*VFDR+GASX(11,17)
XVD=((1.0-VS)/10.0)*VFDR
DO 403 K=1,10
403 GASX(K,17)=XVD+GASX(K,17)
C ALL CHAR LOST
405 CONTINUE
GASX(11,18)=GASX(11,18)+CFDR
GOTO 600
C LARGER PARTICLES

```

```

300 CONTINUE
C FEED POINT
MF=INT(GG(6))
IF(MF.LT.1)MF=1
IF(MF.GT.10)MF=10
C VOLATILE DISTRIBUTION
IF(CPROP(I,6).GT.(10.0*CPROP(I,4))) GOTO 301
IF(CPROP(I,6).GT.CPROP(I,4)) GOTO 302
C VOLATILES UNIFORMLY
XVD=0.1*VFDR
DO 303 K=1,10
303 GASX(K,17)=XVD+GASX(K,17)
GOTO 310
C VOLATILES AT FEED POINT
301 GASX(MF,17)=VFDR+GASX(MF,17)
GOTO 310
C VOLATILES SPLIT
302 VS=0.2
GASX(MF,17)=VS*VFDR+GASX(MF,17)
XVD=((1.0-VS)/10.0)*VFDR
DO 304 K=1,10
304 GASX(K,17)=XVD+GASX(K,17)
C
C CHAR DISTRIBUTION
C
310 CONTINUE
C LOSSES TO ELUTRIATION/ATTRITION
EL=CFDR*CPROP(I,8)
AL=CFDR*CPROP(I,9)
GASX(11,18)=GASX(11,18)+EL+AL
C LOSSES IN OVERFLOW
OV=GG(36)*GG(37)
OV=OV*NRAT(I)
C TOTAL LOSSES
ALL=EL+AL+OV
CFDR=CFDR-ALL
C O2 LOCAL FRACTION
Y(1)=GASX(1,8)+GASB(1,8)
Y(1)=Y(1)/2.0
Y(10)=GASX(10,8)+GASB(10,8)
Y(10)=Y(10)/2.0
DF=(Y(1)-Y(10))/9.0
DO 315 K=2,9
315 Y(K)=Y(K-1)-DF
OSUM=0.0
DO 311 K=1,10
311 OSUM=OSUM+Y(K)
DO 312 K=1,10
312 Y(K)=Y(K)/OSUM
C LOCAL CHAR BURNING RATE
DO 313 K=1,10

```

```
TLC=Y(K)*CFDR
GASX(K,18)=GASX(K,18)+TLC
C   CO/CO2 SPLIT
    CALL CSPLIT(TB,FCO2)
    GASX(K,19)=GASX(K,19)+FCO2*NRAT(I)
313 CONTINUE
600 CONTINUE
C   LOCAL NO REDUCTION
    TLN=CPROP(13,14)
    DO 601 I=1,10
601  GASX(I,16)=TLN*0.1
    RETURN
    END
```

```
      SUBROUTINE CSPLIT(TX,FC)
C
C      RATIO OF CO2/CO FORMED BY CHAR COMBUSTION
C
      RC=0.0004*EXP(6240.0/TX)
      RC=RC*44.0/28.0
C      FRACTION CO
      FCO=1.0/(1.0+RC)
C      FRACTION CO2
      FC=1.0-FCO
      RETURN
      END
```



```

SUBROUTINE DATIN
C
C READ INPUT DATA
C
REAL*4 TITLE(2)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/EQUIL/NSE,NLM,AES(5,10)
IOUT=1
IN=2
C
C INTEGRATION STEP SIZE
C
XH=0.01
C
C NS SETS THE NUMBER OF SPECIES INCLUDED IN CURRENT CALCULATIONS
C
NS=10
C
C WRITE OUT TITLE AT TOP OF NEW PAGE
C
WRITE(6,886)
886 FORMAT('1',20X,' FLUIDIZED BED COMBUSTION OF COAL ',
*/,20X,' MATHEMATICAL MODEL RUN ')
READ(IN,100)(TITLE(K),K=1,2)
100 FORMAT(10A4)
READ(IN,100)TITLE
READ(IN,100)(SPECY(I),I=1,10)
101 FORMAT(F10.5)
108 FORMAT(I2)
105 FORMAT(5F10.5)
C READ BEDPAR BLOCK
C*****
C
C IMPORTANT NOTE:
C THE BED TEMPERATURE IS READ IN (CELSIUS) AS BED(1). THIS IS THEN
C CONVERTED TO KELVIN. LATER, THE BED AREA IS CALCULATED FROM THE
C GIVEN DIMENSIONS AND THIS VALUE IS PLACED IN BED(1).
C
C*****
READ(IN,100)TITLE
READ(IN,105)(BED(I),I=1,5)
READ(IN,105)(BED(I),I=6,10)
TB=BED(1)+273.0
CALL PROPER(TB)
CALL PROPEX
READ(IN,100)TITLE
READ(IN,105)(AIR(I),I=1,5)
READ(IN,105)(AIR(I),I=6,10)

```

```

      READ(IN,100)TITLE
      READ(IN,105)(COAL(I),I=1,5)
      READ(IN,105)(COAL(I),I=6,10)
      READ(IN,100)TITLE
      READ(IN,105)(HOT(I),I=1,5)
      READ(IN,105)(HOT(I),I=6,10)
      READ(IN,100)TITLE
      DO 209 I=1,3
209  READ(IN,105)(PTX(I,J),J=1,3)
102  FORMAT(2F15.5)
      READ(IN,100)TITLE
      READ(IN,105)(GG(I),I=1,5)
      READ(IN,105)(GG(I),I=6,10)
      READ(IN,105)(GG(I),I=11,15)
      READ(IN,105)(GG(I),I=16,20)
C    BOLTZMANN'S CONSTANT
      GG(9)=0.0000000567
C    SIEVE RESULTS
      READ(IN,100)TITLE
      DO 210 I=1,20
210  READ(IN,105)(SIV(I,J),J=1,4)
      READ(IN,100)TITLE
C    REACTION SET-UP
      READ(IN,111)NS,NLM
      DO 110 I=1,10
110  READ(IN,112)(AES(J,I),J=1,5)
112  FORMAT(5F3.1)
111  FORMAT(2I2)
      READ(IN,100)TITLE
      WRITE(6,100)TITLE
203  FORMAT(' ',10A4)
C
C    CALCULATE MEAN PARTICLE DIAMETER BASED ON SIEVE ANALYSIS
C
      CALL MEANPD
      RETURN
      END

```

```
FUNCTION DENAIR(T,P)
C
C GIVES ESTIMATE OF DENSITY OF AIR
C
C COMMON/CONST/PP(5,20),GG(50)
C
C T IN K AND P IN PA
C DENAIR=1.29425*273.3*P/(T*101325.0)
C
C DENSITY IN KG/M3
C GG(21)=DENAIR
C RETURN
C END
```

```

SUBROUTINE DRYING(SI,WW,J,TS,TD,TD1,TV,MM)
C
C   CALCULATE DRYING AND HEAT-UP TIME OF A PARTICLE
C
C   SUBROUTINE ARGUMENTS
C   SI - PARTICLE DIAM M
C   WW - WEIGHT FRACTION WATER
C   J - COAL 1, LIME 2 ETC
C   TS - STARTING MATERIAL TEMPERATURE   K
C   TD - TIME TO REACH 373 K
C   TD1- TIME TO DRY OUT
C   TV - TIME TO DEVOL. START I.E. TP=900 K
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
C
C   HEATUP TO 373 K
C
TP=TS
H=SI*FLOAT(MM)
SMP=3.141593*(SI**3.0)*PTX(2,J)/6.0
TD=0.0
TD1=0.0
IF(TS.GE.373.0) GOTO 200
HEAT TO 373
201 CALL TDERIV(SI,TP,J,DR,SMP)
TBAR=TP+H*DR
CALL TDERIV(SI,TBAR,J,DRB,SMP)
TP=TP+(H/2.0)*(DRB+DR)
TD=TD+H
IF(TP.LT.373.0) GOTO 201
C   DRY OUT PARTICLE
RATE=DR*PTX(3,J)*SMP
C   WATER PRESENT
WP=WW*SMP
C   JOULES REQUIRED
WP=WP*2257000.0
C   TIME REQUIRED
TD1=TD+WP/RATE
200 CONTINUE
C   HEAT TO 900K
TV=TD1
202 CALL TDERIV(SI,TP,J,DR,SMP)
TBAR=TP+H*DR
CALL TDERIV(SI,TBAR,J,DRB,SMP)
TP=TP+(H/2.0)*(DRB+DR)
TV=TV+H
IF(TP.LT.900.0) GOTO 202
RETURN
END

```

```

SUBROUTINE DRYOUT
C
C FLUIDIZATION VELOCITIES, TURNOVER, DRYING, AND HEATING TIMES
C FOR COMPLETE RANGE OF PARTICLE SIZES
C
COMMON/BEDPAR/TB, BED(10), AIR(10), COAL(10), HOT(10), PTX(10,3)
COMMON/SHAKE/SIV(20,4), CPROP(20,14)
COMMON/UNITS/IN, IOUT, SPECY(20)
COMMON/CONST/PP(5,20), GG(50)
C
DO 100 I=1,20
IF(SIV(I,2).EQ.0.0) GOTO 100
SI=SIV(I,1)
C
C CALCULATE VELOCITIES
CALL VELODP(SI,PTX(2,1),CPROP(I,1),CPROP(I,2))
C
PARTICLE TURNOVER TIME
CALL TURNOV(SI,CPROP(I,6))
C
DRYING TIME - HEATING TIME
MM=I
CALL DRYING(SI,COAL(1),1,HOT(7),TD,CPROP(I,3),CPROP(I,4),MM)
100 CONTINUE
RETURN
END

```

```

SUBROUTINE ELUATT(EF,AF)
C
C ELUTRIATION AND ATTRITION RATES
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/COMB/SI,ON,TO,RT,RTM,TP,RC,NF,RE,PR,DNU,ALPHA,XNO,RNO
COMMON/CONST/PP(5,20),GG(50)
C
C WEIGHT RATIO ELUTRIATED/FED
C
EF=(GG(30)/SI)**3.0
C
C WEIGHT RATIO ATTRITION/FED
C
AF=3.0*PTX(10,1)*TO*(AIR(1)-AIR(2))/SI
RETURN
END

```

SUBROUTINE ELUSIZ

C

COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)

C

C

C

C

DP (M) OF PARTICLE WITH 50% MASS FLUX FRACTION ELUTRIATED
AS PER XU AND BECKER

GG(30)=AIR(1)/2154.0

GG(30)=GG(30)**1.163

RETURN

END

```

SUBROUTINE ENOVER(IOK)
C
C OVERALL ENERGY BALANCE
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASK(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/EQUIL/NSE,NLM,AES(5,10)
IOK=0
C
C HEAT FROM COAL
ENO(1,3)=COAL(5)*PTX(7,1)
C
C CALCINATION OF LIMESTONE
H298=182600. J/MOL
C
C HEAT OF REACTION AT TB
HR=0.100*PTX(3,2)*(TB-298.0)
HP=0.056*PTX(3,2)*(TB-298.0)+1.0*PP(5,2)
H=182600.0+HP-HR
H=H/0.10008
ENO(1,11)=H*PTX(7,2)*GG(3)
C
C HEAT OUT DUE TO MOISTURE IN FUEL
C
C WATER IN AIR
WI=AIR(9)*AIR(10)*BED(1)*(GG(28)+GG(27))/GG(27)
C
C WATER OUT
WO=GASX(10,4)*GASX(10,21)+GASB(10,4)*GASB(10,21)
WO=WO*BED(1)
C
C WATER FROM FUEL
WO=WO-WI
C
C VAPORIZATION = 44016. J/MOL
ENO(1,7)=WO*44016.
C
C UNREACTED COMBUSTIBLES
C
C CO
H298=PP(2,2)-PP(2,1)
HP=PP(5,2)
HR=PP(5,1)+0.5*PP(5,8)
H1=(H298+HP-HR)*(-1.0)
C
C CH4
H298=(PP(2,2)+2.0*PP(2,4))-PP(2,10)
HP=PP(5,2)+2.0*PP(5,4)
HR=PP(5,10)+2.0*PP(5,8)

```



```

H2=(H298+HP-HR)*(-1.0)
C UNBURNT VOLATILES - APPROXIMATION -
HV=(H1+H2)/4.0
H3=HV*GASX(11,17)/0.025
C TOTAL
CO=(GASX(10,1)*GASX(10,21)+GASB(10,1)*GASB(10,21))*BED(1)
CH=(GASX(10,10)*GASX(10,21)+GASB(10,10)*GASB(10,21))*BED(1)
ENO(1,8)=H1*CO+H2*CH
C
C UNBURNT CHAR LOSS
C
CL=GG(43)+GG(44)+GG(37)*GG(36)+GASX(11,18)
CL=CL/0.012
ENO(1,9)=ABS(PP(2,2))*CL
C
C SOLIDS OVERFLOW
C
ENO(1,10)=GG(37)*PTX(3,3)*(TB-HOT(7))
C
C IMMERSED TUBES
C
TT=ALOG((TB-HOT(4))/(TB-HOT(5)))
TT=(HOT(5)-HOT(4))/TT
A=3.141593*HOT(3)*HOT(2)
ENO(1,12)=GG(47)*A*TT*HOT(1)
C
C THROUGH CONTAINING WALLS
C
ENO(1,13)=GG(48)*BED(8)
C
C COMBUSTION GASES
C
DO 200 I=1,NS
A=(GASX(10,I)*GASX(10,21)+GASB(10,I)*GASB(10,21))*BED(1)
200 ENO(1,14)=A*PP(5,I)+ENO(1,14)
C
C OVERALL BALANCE
C
HIN=ENO(1,3)+ENO(1,4)+ENO(1,5)
HOUT=0.0
DO 201 I=7,14
201 HOUT=HOUT+ENO(1,I)
ENO(1,2)=(HIN-HOUT)/HIN
A=ABS(ENO(1,2))
IF(A.LT.0.005) GOTO 300
C INTERPOLATION
IF(ENO(2,2).NE.0.0) GOTO 301
CN=0.10*ENO(1,1)*A/ENO(1,2)
CN=CN*(-1.0)+ENO(1,1)
GOTO 302
301 CN=(ENO(2,1)-ENO(1,1))/(ENO(2,2)-ENO(1,2))

```

```

        CN=CN*(-ENO(1,2))
        CN=CN+ENO(1,1)
        IF(CN.LE.0.0) CN=0.5*ENO(1,1)
302  DO 303 I=1,14
303  ENO(2,I)=ENO(1,I)
        IF(CN.GT.ENO(1,1).AND.ENO(2,2).LT.0.0) GOTO 304
        IF(CN.LT.ENO(1,1).AND.ENO(2,2).GT.0.0) GOTO 304
        IF(ENO(2,2).LT.0.0)CN=ENO(1,1)*1.05
        IF(ENO(2,2).GT.0.0)CN=0.95*ENO(1,1)
304  CONTINUE
        DIF=ABS(ENO(1,1)-CN)/ENO(1,1)
        IF(DIF.LT.0.005) GOTO 300
        ENO(1,1)=CN
        RETURN
C    SUCCESSFUL BALANCE
300  IOK=1
        DO 305 I=1,14
305  ENO(2,I)=ENO(1,I)
        RETURN
        END

```

```

SUBROUTINE EQCOMB(SN,B,BIO,Z)
C
C EQUILIBRIUM CALCULATIONS INITIAL GUESS
C AND FINAL COMPOSITION IF EQ. CALC. FAIL
C
COMMON/EQUIL/NSE,NLM,AES(5,10)
C
C DIMENSIONS OF FOLLOWING MUST MATCH NSE,NLM
C *****
REAL A(3,3),B(3),H(3),G(3),SG(6),SN(6),SB(6),BIO(3),DEL(7)
INTEGER Z(6)
C
C CHECK ELEMENT BALANCE
DO 650 I=1,NLM
B(I)=0.0
DO 650 K=1,NSE
650 B(I)=B(I)+AES(I,Z(K))*SN(K)
C DIFFERENCE
DO 651 I=1,NLM
651 G(I)=BIO(I)-B(I)
C MAKE SURE ALL DIFFERENCES ARE POSITIVE
656 DO 652 I=1,NLM
652 IF(G(I).LT.0.0) GOTO 653
GOTO 654
653 DO 655 I=1,NLM
655 G(I)=G(I)+BIO(I)*0.1
GOTO 656
654 CONTINUE
C H2 TO H2O OR CH4
C O/H
SX=G(3)/G(2)
IF(SX.GT.0.5) GOTO 670
C C/H
IF(SX.GT.0.25) GOTO 680
SN(3)=SN(3)+G(2)/2.0
GOTO 671
670 SN(4)=SN(4)+G(2)/2.0
G(3)=G(3)-G(2)/2.0
GOTO 671
680 SN(6)=SN(6)+G(2)/4.0
G(1)=G(1)-G(2)/4.0
671 CONTINUE
C OXYGEN/CARBON
M=1
657 SX=G(3)/G(1)
IF(SX.GE.1.0) GOTO 660
C DISSOCIATE SOME CO2 IF NECESSARY
IF(SN(2).LE.0.0) GOTO 681
G(3)=G(3)+SN(2)*2.0*0.20
G(1)=G(1)+0.2*SN(2)
SN(2)=0.8*SN(2)

```

```

M=M+1
IF(M.LT.20) GOTO 657
C SOME METHANE METHINKS
681 EXC=G(1)-G(3)
    WL=SN(4)/2.0
    IF(WL.LT.EXC) EXC=WL
    SN(4)=SN(4)-EXC*2.0
    SN(6)=SN(6)+EXC
    G(1)=G(1)-EXC
    G(3)=G(3)+3.0*EXC
    SX=G(3)/G(1)
    IF(SX.GE.1.0) GOTO 660
    SN(1)=G(1)
    SN(5)=0.0
    RETURN
C O/C
660 IF(SX.GT.2.0) GOTO 662
C SOME CO PRESENT
    SN(1)=SN(1)+2.0*G(1)-G(3)
    SN(2)=SN(2)+G(3)-G(1)
    SN(5)=0.0
    IF(SN(2).EQ.0.0) GOTO 663
    SN(5)=SN(5)+0.05*SN(2)
    SN(1)=SN(1)+0.10*SN(2)
    SN(2)=0.90*SN(2)
    GOTO 663
C CO2
662 SN(2)=SN(2)+G(1)
    SN(5)=SN(5)+(G(3)-G(1))/2.0
663 CONTINUE
    RETURN
    END

```

```

SUBROUTINE EQOVER(STO,FIN,TK)
C
C CALCULATE EQUILIBRIUM COMPOSITION BASED ON RAND VARIATION
C OF 2ND ORDER CHEM. EQUILIBRIUM ALGORITHMS
C
COMMON/CONST/PP(5,20),GG(50)
COMMON/EQUIL/NSE,NLM,AES(5,10)
REAL STO(10),FIN(10)
C
C DIMENSIONS OF FOLLOWING MUST MATCH NSE,NLM
C *****
REAL A(3,3),B(3),H(3),G(3),SG(6),SN(6),SB(6),BIO(3),DEL(7)
REAL RES(4),NM,NK,MAX1,MAX2
DOUBLE PRECISION EQU(4,5)
INTEGER Z(6)
C
NSE=6
NLM=3
NSEX=NSE+1
NLMX=NLM+1
C Z CONTAINS LOCATIONS OF REACTING SPECIES
Z(1)=1
Z(2)=2
Z(3)=3
Z(4)=4
Z(5)=8
Z(6)=10
C PARTIAL PRESSURE OF REACTING SPECIES
PALL=0.0
DO 189 I=1,10
189 PALL=PALL+STO(I)
PR=0.0
DO 187 I=1,NSE
187 PR=PR+STO(Z(I))
PR=PR/PALL
C FEED CONDITIONS
DO 501 K=1,10
501 FIN(K)=STO(K)
C INCREASE SMALLEST MOLES TO ONE
TRY=99999999.99999
DO 502 K=1,NSE
502 IF(STO(Z(K)).LT.TRY) TRY=STO(Z(K))
DO 503 K=1,10
503 STO(K)=STO(K)/TRY
C INERT SPECIES
SNM=0.0
DO 504 K=1,10
DO 505 J=1,NSE
505 IF(Z(J).EQ.K) GOTO 504
SNM=SNM+STO(K)

```

```

504 CONTINUE
C
C ESTIMATE BIO I.E. ATOM BALANCE
C
184 CONTINUE
DO 185 I=1,NLM
BIO(I)=0.0
DO 185 K=1,NSE
185 BIO(I)=BIO(I)+AES(I,Z(K))*STO(Z(K))
C
C ESTIMATE N INITIAL GUESSES - EQUIL
C
DO 650 I=1,NSE
650 SN(I)=0.0
CALL EQCOMB(SN,B,BIO,Z)
DO 651 I=1,NSE
651 SN(I)=ABS(SN(I)+0.25)
C
C RT R=0.0083144 KJ/MOL.K
RT=TX*0.0083144
CALL PROPER(TX)
C
C START LOOP - LIMIT 100 ITERATIONS
C
DO 444 IEQ=1,100
C
NM
NK=0.0
NM=0.0
DO 102 I=1,NSE
102 NK=NK+SN(I)
C
GK
DO 107 I=1,NSE
K=Z(I)
SG(I)=(PP(5,K)+PP(2,K))/1000.0
SG(I)=SG(I)-TX*PP(4,K)/1000.0
107 SG(I)=SG(I)+RT*(ALOG(SN(I)/NK)+ALOG(PR))
C
VARIOUS ARRAYS A,B,G
DO 104 J=1,NLM
DO 105 I=1,NLM
A(I,J)=0.0
DO 105 K=1,NSE
105 A(I,J)=A(I,J)+AES(I,Z(K))*AES(J,Z(K))*SN(K)
B(J)=0.0
G(J)=0.0
DO 106 K=1,NSE
B(J)=B(J)+AES(J,Z(K))*SN(K)
106 G(J)=G(J)+AES(J,Z(K))*SN(K)*SG(K)/RT
104 CONTINUE
C
CONSTANTS HK,GK,GH
GK=0.0
DO 108 K=1,NSE

```

```

108 GK=GK+SN(K)*SG(K)/RT
    DO 112 J=1,NLM
112 SB(J)=BIO(J)-B(J)
C
C   SET UP MATRIX FOR SOLUTION
C
    AZERO=1.0E-30
    DO 200 I=1,NLM
    DO 200 J=1,NLM
    IF(A(J,I).LT.AZERO) A(J,I)=AZERO
200 EQU(I,J)=A(J,I)
    DO 201 J=1,NLM
201 EQU(J,NLMX)=B(J)
    DO 202 I=1,NLM
202 EQU(NLMX,I)=B(I)
    EQU(NLMX,NLMX)=-SNM
C   X VECTOR
    DO 203 J=1,NLM
203 EQU(J,(NLM+2))=SB(J)+G(J)
    EQU((NLM+1),(NLM+2))=GK
C   SOLVE MATRIX
    CALL GAUSSJ(EQU)
C   SOLUTION VECTOR
    DO 300 J=1,NLMX
300 RES(J)=EQU(J,(NLM+2))
C
C   CALCULATE D.NK
C
    DO 301 K=1,NSE
    RHS=0.0
    DO 302 I=1,NLM
302 RHS=RHS+RES(I)*AES(I,Z(K))
    RHS=RHS-SG(K)/RT
    RHS=RHS+RES(NLMX)
301 DEL(K)=RHS*SN(K)
C
C   CALCULATE NEW NK
C
C   RELAXATION FACTOR
    RE=0.8
C   LIMIT INCREASE TO 2.0X
    TRY=-1.0
    DO 343 I=1,NSE
    IF(DEL(I).LT.0.0) GOTO 343
    RAT=DEL(I)/SN(I)
    IF(RAT.LT.TRY) GOTO 343
    NN=I
    TRY=RAT
343 CONTINUE
    RAT=0.8
    IF(TRY.LT.1.5) GOTO 344

```

```

RAT=1.5*SN(NN)/DEL(NN)
C LIMIT ZERO MOLES
344 TRY=1.0
DO 345 I=1,NSE
RIT=SN(I)+DEL(I)
IF(RIT.GT.0.0) GOTO 345
RIT=0.8*SN(I)/ABS(DEL(I))
IF(RIT.GT.TRY) GOTO 345
TRY=RIT
NN=I
345 CONTINUE
RIT=0.8
IF(TRY.GT.0.8) GOTO 346
RIT=0.8*SN(NN)/ABS(DEL(NN))
C DECIDE WHICH FACTOR
346 IF(RAT.LT.RE) RE=RAT
IF(RIT.LT.RE) RE=RIT
DO 128 I=1,NSE
128 SN(I)=SN(I)+RE*DEL(I)
C
C FINISHED - CHECK FOR SOLUTION
C
IF(RE.NE.0.8) GOTO 444
DO 136 I=1,NSE
RAT=ABS(DEL(I))/SN(I)
136 IF(RAT.GT.0.02) GOTO 444
GOTO 445
444 CONTINUE
C
C CANNOT FIND EQUILIBRIUM - CHECK MOLE BALANCES & OUTPUT
C
CALL EQCOMB(SN,B,BIO,Z)
C EQUILIBRIUM SOLUTION
C
445 CONTINUE
C MOLES AT END
SUM=0.0
DO 641 K=1,NSE
641 SUM=SUM+SN(K)
C MOLE FRACTIONS
SE=0.0
DO 642 K=1,NSE
SN(K)=SN(K)/SUM
C M.W.
642 SE=SE+PP(1,Z(K))*SN(K)
C KG AT START
SX=0.0
DO 644 K=1,NSE
644 SX=SX+FIN(Z(K))*PP(1,Z(K))
C MOLES OUT
SA=SX/SE

```



```
DO 645 K=1,NSE
645  FIN(Z(K))=SN(K)*SA
      RETURN
      END
```

```

SUBROUTINE ESCAPE
C
C   CALCULATE SO2 & NOX REACTION FLUXES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/EXIST/AVE(20),AVB(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
REAL NR,NL,NA

C
C   ESTIMATE LOCAL EMISSION
C
IA=INT(10.0*(XL-XH)/BED(8))+1
C   RATE KG/S
C   SO2
SR=GASX(IA,20)*0.1
SR=SR+GASB(5,22)
C   NO
NR=GASX(IA,16)*0.1
NR=NR+GASB(1,22)

C
C   REACTION FLUXES
C
C   NOX
C   CONVERT TO MOLES/M3.S
NR=NR/(BED(1)*XH*PP(1,5))
C   MOLES OF NO AVAILABLE
NA=AVE(5)/PP(1,5)
C   LIMITING REACTANT
NL=NR
IF(NA.LT.NR) NL=NA
C   REACTION NO >> N2 + O2
EM(6,5)=-NL*PP(1,5)
EM(6,8)=0.5*NL*PP(1,8)
EM(6,7)=0.5*NL*PP(1,7)
C   RESERVE CAPACITY
FX=NL/NR
GASB(1,22)=(1.0-FX)*NR*PP(1,5)*BED(1)*XH

C
C   SO2
C   CONVERT TO MOLES/M3.S
SR=SR/(BED(1)*XH*PP(1,9))
C   MOLES OF SO2 AVAILABLE
SA=AVE(9)/PP(1,9)
C   LIMITING REACTANT
SL=SR
IF(SA.LT.SL) SL=SA
C   REACTION

```

```

EM(6,9)=-SL*PP(1,9)
EM(6,8)=EM(6,8)-((SL/2.0)*PP(1,8))
C RESERVE CAPACITY
FX=SL/SR
GASB(5,22)=(1.0-FX)*SR*PP(1,9)*BED(1)*XH
C
C HEAT DUE TO CAO + 1/2O2 + SO2 -> CASO4
C
R=ABS(EM(6,9)*BED(1)*XH)
C H298=484900.0 J/MOL
HR=0.056*PTX(3,2)*(TB-298)
HR=HR+0.5*PP(5,8)
HR=HR+PP(5,9)
HP=0.13606*PTX(3,2)*(TB-298.0)
H=484900.0+HP-HR
H=H/PP(1,9)
ENO(1,5)=ENO(1,5)+H*R
C
C CO2 RELEASED DUE TO CALCINATION OF LIMESTONE
C LOCAL CALCINATION KG/S
CA=PTX(7,2)*GG(3)*GG(38)/100.0
C MOLES/S.M3
CA=CA/(0.100*BED(1)*XH)
C CO2 GENERATED
EM(6,2)=CA*PP(1,2)
CALL REDUCE(6)
RETURN
END

```

```

SUBROUTINE EULERF
C
C THIS ROUTINE HAS MODIFIED EULER EQUATIONS
C CALL MODEF TO EVALUATE DERIVATIVES FOR FREEBOARD FLUXES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
C
C STORE PREVIOUS OVERALL BALANCES IN LOCATION 2
C
DO 100 I=1,NS
DO 100 J=1,2
100 EMO(2,J,I)=EMO(1,J,I)
C
C EVALUATE DERIVATIVES
C
CALL MODEF
C
C APPLY FIRST EQUATION TO EACH SPECIES IN TURN
C
DO 101 I=1,NS
101 EMO(1,2,I)=EMO(2,2,I)+XH*DEM(1,I)
C STORE DERIVATIVES IN LOCATION 2
DO 102 I=1,NS
102 DEM(2,I)=DEM(1,I)
CALL PRESEF
C
C EVALUATE DERIVATIVES WITH NEW CONDITIONS
C
CALL MODEF
C
C APPLY SECOND EQUATION OF MODIFIED EULERS METHOD
C
DO 107 I=1,NS
107 EMO(1,2,I)=EMO(2,2,I)+0.5*XH*(DEM(1,I)+DEM(2,I))
CALL PRESEF
C
C CARRY OUT ENERGY BALANCE TO DETERMINE TEMPERATURE AT THIS LEVEL
C
C CALCULATE NEW ENTHALPY
DO 360 MX=1,4
ENO(1,20)=0.0
DO 363 K=1,NS
363 ENO(1,20)=ENO(1,20)+EMO(1,1,K)*(PP(2,K)+PP(5,K))
ENO(1,20)=ENO(1,20)*GASX(11,22)
C ENTHALPY LOSS I.E. TO WALLS & RADIATION
C ASSUMED EQUAL HERE I.E ADIABATIC SYSTEM
ED=ENO(1,20)-ENO(2,20)

```

```
ET=ABS(ED/ENO(2,20))
IF(ET.LT.0.01) GOTO 370
C HEAT CAPACITY
CP=0.0
DO 364 K=1,NS
364 CP=CP+EMO(1,1,K)*PP(3,K)
C NEW TEMPERATURE
DT=ED/(CP*GASX(11,22))
TN=TB-DT
CALL PROPER(TN)
360 CONTINUE
RETURN
370 TB=TN
ENO(2,20)=ENO(1,20)
RETURN
END
```

```

SUBROUTINE EULERS
C
C THIS ROUTINE HAS MODIFIED EULER EQUATIONS
C CALL MODEL TO EVALUATE DERIVATIVES FOR IN-BED FLUXES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
C
C STORE PREVIOUS OVERALL BALANCES IN LOCATION 2
C
DO 100 I=1,NS
DO 100 J=1,2
EMO(2,J,I)=EMO(1,J,I)
100 BUO(2,J,I)=BUO(1,J,I)
C
C EVALUATE DERIVATIVES
C
CALL MODEL
C
C APPLY FIRST EQUATION TO EACH SPECIES IN TURN
C
DO 101 I=1,NS
EMO(1,2,I)=EMO(2,2,I)+XH*DEM(1,I)
101 BUO(1,2,I)=BUO(2,2,I)+XH*DBU(1,I)
C STORE DERIVATIVES IN LOCATION 2
DO 102 I=1,NS
DEM(2,I)=DEM(1,I)
102 DBU(2,I)=DBU(1,I)
CALL PRESET
C
C EVALUATE DERIVATIVES WITH NEW CONDITIONS
C
CALL MODEL
C
C APPLY SECOND EQUATION OF MODIFIED EULERS METHOD
C
DO 107 I=1,NS
EMO(1,2,I)=EMO(2,2,I)+0.5*XH*(DEM(1,I)+DEM(2,I))
107 BUO(1,2,I)=BUO(2,2,I)+0.5*XH*(DBU(1,I)+DBU(2,I))
CALL PRESET
RETURN
END

```

SUBROUTINE EXSAIR

```
C
C
C   CALCULATE EXCESS AIR FACTOR
C
C   COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
C   COMMON/CONST/PP(5,20),GG(50)
C
C   OXYGEN IN AIR
C   OIN=0.208*AIR(1)*BED(1)*1000.0/(0.08206*TB)
C   OXYGEN IN COAL
C   OIN=OIN+CF*COAL(8)/0.032
C   OXYGEN FOR CARBON
C   CF=PTX(7,1)*(1.0-COAL(1))
C   OC=CF*COAL(6)/0.01201
C   OXYGEN FOR SULPHUR
C   OS=CF*COAL(10)/0.032066
C   OXYGEN FOR HYDROGEN
C   OH=CF*COAL(7)/0.002016
C   FOR NITROGEN
C   ON=CF*COAL(9)/0.028016
C   TOTAL REQUIRED
C   OR=OC+OH+OS+ON
C   EXCESS AIR FACTOR
C   AIR(6)=OIN/OR
C   RETURN
C   END
```

SUBROUTINE FREEBD

C
C
C

FREEBOARD SIMULATION

COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/EQUIL/NSE,NLM,AES(5,10)

C
C
C
C
C

AT START OF INTEGRATION MUST INITIATE INLET GAS CONCENTRATIONS
AS COMBINATION OF BUBBLE AND EMULSION PHASES. RESULT IS STORED
IN ARRAY EMO

NS=10
NS1=10
XH=(BED(4)-BED(8))/100.0
TOT=0.0
DO 450 J=1,NS
EMO(1,2,J)=EMO(1,2,J)+BUO(1,2,J)
450 TOT=EMO(1,2,J)/PP(1,J)
DO 451 K=1,NS
451 EMO(1,1,K)=EMO(1,2,K)/(PP(1,K)*TOT)

C
C
C

SET UP OTHER INITIAL CONDITIONS & DERIVATIVES

DO 453 K=1,20
453 DEM(2,K)=0.0
TBU(1)=TB
TBU(2)=TB

C
C
C

ENTHALPY AT START

CALL PROPER(TB)
ENO(1,20)=0.0
DO 454 K=1,NS
454 ENO(1,20)=ENO(1,20)+EMO(1,1,K)*(PP(2,K)+PP(5,K))
ENO(1,20)=ENO(1,20)*TOT
ENO(2,20)=ENO(1,20)

C
C
C
C
C

HETEROGENEOUS REACTIONS: ASSUME LINEAR IN FREEBOARD
EXCEPT VOLATILES WHICH ARE BURNED AT TOP OF BED ASAP
CALCULATE RATES AS KG/S.M

H=BED(4)-BED(8)
GASX(11,16)=GASX(11,16)/H
GASX(11,18)=GASX(11,18)/H


```
GASX(11,20)=GASX(11,20)/H
C
C   ENTER INTEGRATION LOOP
C
   ITEM=0
   WRITE(3,333)
333  FORMAT('          FREEBOARD  INTEGRATION  ')
801  CONTINUE
C   INCREMENT HEIGHT
   XL=XL+XH
C   INTEGRATION ROUTINE
   CALL EULERF
C   WRITE OUT INTERMEDIATE RESULTS
   ITEM=ITEM+1
   IF(ITEM.LT.10) GOTO 802
   ITEM=0
   CALL WRITER(4)
C   CHECK LEVEL - LIMIT IS UNIT HEIGHT
802  IF(XL.LT.BED(4)) GOTO 801
   RETURN
   END
```

```

SUBROUTINE FSATUR
C
C ESTIMATE FLUIDIZATION SATURATION FLUX
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/CONST/PP(5,20),GG(50)
DO 100 I=1,NS
EM(1,I)=0.0
100 BU(1,I)=0.0
C
C DIRECTION OF TRANSFER
C
DF=0.0
IF(GASX(11,22).GT.AIR(10)) DF=-1.0
IF(GASX(11,22).LT.AIR(10)) DF=1.0
IF(DF.EQ.0.0)GOTO 200
C
C FLUX IN MOLES/M2.S
C
FX=ABS(GASX(11,22)-AIR(10))
IF(DF.EQ.-1.0) GOTO 300
C
TRANSFER INTO EMULSION
DO 101 I=1,NS
101 EM(1,I)=FX*BUO(1,1,I)*DF/XH
GOTO 301
C
TRANSFER FROM EMULSION
300 DO 102 I=1,NS
102 EM(1,I)=FX*EMO(1,1,I)*DF/XH
C
BUBBLE FLOW
301 DO 103 I=1,NS
103 BU(1,I)=-EM(1,I)
C
CONVERT TO KG/M3.S
DO 104 I=1,NS
EM(1,I)=EM(1,I)*PP(1,I)
104 BU(1,I)=BU(1,I)*PP(1,I)
CALL REDUCE(1)
200 RETURN
END

```

```

SUBROUTINE GAUSSJ(EQU)
C
C SOLVE MATRIX OF SIM EQ BY GAUSS-JORDAN ELIMINATION
C
DOUBLE PRECISION EQU(4,5),PE
IX=4
IY=5
C
C MAKE PIVOTAL ELEMENT 1.0
C
DO 601 K=1,IX
IF(EQU(K,K).EQ.0.0)GO TO 603
PE=EQU(K,K)
DO 602 I=1,IY
602 EQU(K,I)=EQU(K,I)/PE
C
C SET OTHER ELEMENTS IN COLUMN K EQUAL TO ZERO
C
DO 601 J=1,IX
IF(J.EQ.K)GO TO 601
PE=EQU(J,K)
DO 604 I=1,IY
604 EQU(J,I)=EQU(J,I)-PE*EQU(K,I)
601 CONTINUE
RETURN
C
C A ZERO PIVOTAL ELEMENT DETECTED WRITE ERR MSG AND HALT
C
603 CONTINUE
WRITE(6,607)
607 FORMAT(10X,'ERROR... ZERO PIVOT ELEMENT IN GAUSSJ')
DO 605 I=1,IX
605 WRITE(6,606)(EQU(I,L),L=1,IY)
606 FORMAT(' ',1P7E10.3,/)
STOP
END

```

```

SUBROUTINE HEATXC
C
C HEAT TRANSFER COEFFICIENT FOR IMMersed TUBES
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/CONST/PP(5,20),GG(50)
C
C HEAT TRANSFER DUE TO CONVECTION AND CONDUCTION
C
C GAS PROPERTIES AT FILM TEMPERATURE
TF=(TB+HOT(5))/2.0
A=DENAIR(TF,AIR(3))
B=VISAIR(TF)
C=THERMC(TF)
C
C HEAT CAPACITY OF GAS AT MIDDLE OF BED
CALL PROPER(TF)
CP=0.0
DO 100 I=1,10
100 CP=CP+GASX(5,I)*PP(3,I)
W=0.0
DO 101 I=1,10
101 W=W+GASX(5,I)*PP(1,I)
CP=CP*W
C
C DENSITY
D=GG(21)*W/0.02885
C
C CORRELATION
COR=PTX(4,3)**3.0
COR=COR*9.80665/((GG(22)/D)**2.0)
COR=COR*(PTX(2,3)-D)/D
COR=0.60*(COR**0.246)
GG(47)=COR*GG(29)/PTX(4,3)
C
C HEAT TRANSFER DUE TO RADIATION
C
TW=HOT(5)
TD=TB-TW
T4=(TB**4.0)-(TW**4.0)
C
C EFFECTIVE EMISSIVITY
EB=0.85
ET=0.80
EE=1.0/((1.0/EB)+(1.0/ET)-1.0)
GG(49)=GG(9)*T4*EE/TD
C
C HEAT TRANSFER THROUGH CONTAINING WALL
C J/SM I.E. PER M OF BED HEIGHT
C
C WALL THICKNESS RATIO
COR=(BED(2)+BED(3)+4.0*HOT(10))/(BED(2)+BED(3))
COR=ALOG(COR)
COR=2.0*3.145193*GG(8)*(TB-HOT(9))/COR

```

```
GG(48)=COR  
A=DENAIR(TB,AIR(3))  
B=VISAIR(TB)  
C=THERMC(TB)  
CALL PROPER(TB)  
RETURN  
END
```

```

SUBROUTINE INTERM(IB)
C
C STORE INTERMEDIATE CONCENTRATIONS & MOLE RATES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/EQUIL/NSE,NLM,AES(5,10)
C
C TOTAL MOLE/M2.S RATE
GASX(IB,21)=GASX(11,22)
GASB(IB,21)=GASB(11,22)
C
C MOLE FRACTIONS
DO 100 I=1,NS
GASX(IB,I)=EMO(1,1,I)
100 GASB(IB,I)=BUO(1,1,I)
RETURN
END

```

```

SUBROUTINE IPHASE
C
C LOCAL INTERPHASE TRANSFER
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/EXIST/AVE(20),AVB(20)
REAL TE(20),TZ(20)

C
C TRANSFER UNITS PER M OF EXPANDED BED
C
FIX=GG(46)*BED(7)/BED(8)

C
C CHECK ORIFICE JET HEIGHT
C
IF(XL.GT.BED(10)) GOTO 104
CE=XL/BED(10)
CE=4.0*EXP(1.0-CE)
FIX=GG(46)*BED(7)*CE/BED(8)
104 CONTINUE

C
C CURRENT MOLES IN BUBBLE PHASE
CE=0.0
CB=0.0
DO 100 I=1,NS
CE=CE+AVE(I)/PP(1,I)
100 CB=CB+AVB(I)/PP(1,I)
DO 101 I=1,NS
TE(I)=AVE(I)/(PP(1,I)*CE)
101 TZ(I)=AVB(I)/(PP(1,I)*CB)

C
EXCHANGE RATE
CB=FIX*XH*CB
IF(CB.GT.CE) CB=CE

C
FLUX IN KG/M3.S
DO 102 I=1,NS
TE(I)=TE(I)*CB*PP(1,I)
102 TZ(I)=TZ(I)*CB*PP(1,I)

C
NET FLUX
DO 103 I=1,NS
EM(2,I)=TZ(I)-TE(I)
103 BU(2,I)=TE(I)-TZ(I)
CALL REDUCE(2)
RETURN
END

```

```

SUBROUTINE LCHARC
C
C   CALCULATE CHAR BURNING FLUX
C
COMMON/OERALL/NS ,XH,XL ,TBU(2) ,EMO(2,2,20) ,BUO(2,2,20) ,ENO(2,20)
COMMON/BEDPAR/TB ,BED(10) ,AIR(10) ,COAL(10) ,HOT(10) ,PTX(10,3)
COMMON/TRANSF/NS1 ,EM(6,20) ,BU(6,20) ,DEM(2,20) ,DBU(2,20)
COMMON/GASCON/GASX(11,22) ,GASB(11,22)
COMMON/EXIST/AVE(20) ,AVB(20)
COMMON/CONST/PP(5,20) ,GG(50)
COMMON/BURNS/VCOM(11) ,CM(5)
REAL CS(5)

C
IA=INT(10.0*(XL-XH)/BED(8))+1
C   RATE KG/S
CR=GASX(IA,18)*0.1
C   CO2 FRACTION
CD=GASX(IA,19)
C   UNBURNT CHAR
CR=CR+GASB(3,22)
C   CONVERT TO KG/M3.S
RF=1.0
103 CR1=CR*RF/(BED(1)*XH)
C   SPLIT ACCORDING TO COMPOSITION
DO 100 I=1,5
100 CS(I)=CR1*CM(I)
C   MOLES OF MOLECULES CREATED
CS(1)=CS(1)/0.01201
CS(2)=CS(2)/0.002016
CS(3)=CS(3)/0.032
CS(4)=CS(4)/0.014008
CS(5)=CS(5)/0.032066
C   ESTIMATE FLUXES FROM CHAR
EM(5,1)=(1.0-CD)*CS(1)
EM(5,2)=CD*CS(1)
EM(5,3)=CS(2)
EM(5,5)=CS(4)
EM(5,8)=CS(3)
EM(5,9)=CS(5)
C   ESTIMATE O2 REQUIRED
OX=EM(5,2)+EM(5,9)+(EM(5,1)+EM(5,5))/2.0
OX=OX-EM(5,8)
C   O2 AVAILABLE
OA=AVE(8)/PP(1,8)
IF(OA.GE.OX) GOTO 101
C   NOT ENOUGH O2
CA=AVE(2)/(PP(1,2)*2.0)
ON=OA+CA
IF(ON.GE.OX) GOTO 102
RF=RF*0.9

```



```

        IF(RF.GT.0.120) GOTO 103
C      NO BURNING AT ALL
        DO 104 I=1,NS
104    EM(5,I)=0.0
        GASB(3,22)=CR*BED(1)*XH
        RETURN
C      PARTIAL BURNING
102    ON1=OX-OA
        EM(5,2)=EM(5,2)-2.0*ON1
        EM(5,1)=EM(5,1)+2.0*ON1
        EM(5,8)=-OA
        GOTO 105
C      COMPLETE BURNING
101    EM(5,8)=-OX
105    CONTINUE
C      CONVERT BACK TO KG
        DO 106 I=1,NS
106    EM(5,I)=EM(5,I)*PP(1,I)
        GASB(3,22)=CR*(1.0-RF)*BED(1)*XH
        CALL REDUCE(5)
        RETURN
        END

```

```

SUBROUTINE LIMUSE
C
C   CALCULATE SO2/LIMESTONE REACTION RATES
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/CONST/PP(5,20),GG(50)
C
C   GET CALCINATION FACTOR
C
CALL CALCIN
C
C   SO2
C   KMOLES OF SPECIES IN 1M3
C   TM=12.186/TB
C   CO=0.002*TM
C   GASB(7,22)=CO
C   RESIDENCE TIME OF LARGE PARTICLES
C   ASH=COAL(2)*(1.0-COAL(1))*PTX(7,1)/PTX(7,2)
C   W=BED(1)*BED(5)*BED(6)*(1.0-ASH)
C   XS=COAL(10)*(1.0-COAL(1))
C   MW RATIO=2.375 ASSUMES 25% CASO4 IN LIME
C   TAU=W/(GG(2)*PTX(7,1)*XS*2.375)
C   GG(40)=TAU
C   SIDP=1000.0*PTX(4,2)
C   REACTION RATE CONSTANTS
C   CKN=GG(11)
C   CKP=GG(12)
C   SURFACE EFFECTIVENESS
C   SA=3.141593*(SIDP**2.0)
C   SA=2.0/(SA+1.0)
C   SA=EXP(SA)
C
C   ACCOUNT FOR PARTICLE SIZE
C
DO 100 I=1,20
IF(SIV(I,3).LE.0.0) GOTO 200
SI=SIV(I,1)
TAR=TAU
C   ELUTRIATED ???
IF(SI.LT.GG(30))GOTO 400
C   LARGE SIZE
401 RATE=6.0*CKN*CO*PTX(7,2)*SIV(I,3)*TAR*GG(3)
A=1.0+CKP*TAR
C   ASSUME COMPLETE REACTION AT TWO HOURS
FAC=A*7200.0/TAR
IF(FAC.GT.10) FAC=10
FAC=1.0-EXP(-FAC)
RATE=RATE*FAC*1000.0/(A*PTX(2,2)*SIDP*SA)
C   CALCINATION FACTOR

```

```

RATE=RATE*GG(38)
C   RATE IS IN KMOL/S  CONVERT TO KG/S
CPROP(I,12)=RATE*1000.0*PP(1,9)
IF(SI.GE.GG(30)) GOTO 402
GF=CPROP(I,12)*TF/TN
GB=CPROP(I,12)-GF
GASX(11,20)=GF
DO 102 K=1,10
102 GASX(K,20)=0.1*GB+GASX(K,20)
GOTO 200
402 DO 101 K=1,10
101 GASX(K,20)=0.1*CPROP(I,12)+GASX(K,20)
GOTO 200
C   ELUTRIABLE SIZE FRACTION
400 CONTINUE
C   CONSIDER RECYCLE RATE
TX=TAU*GG(4)*GG(5)
C   FINES RESIDENCE TIME IN BED
TN=CPROP(I,6)*GG(7)
C   RESIDENCE TIME IN FREEBOARD
TF=(BED(4)-BED(8))/AIR(1)
TN=TN+TF
IF(TX.GT.TN) TN=TX
IF(TN.LT.TAU) TAR=TN
GOTO 401
200 CONTINUE
100 CONTINUE
RETURN
END

```

```

SUBROUTINE MEANPD
C
C   CALCULATE MEAN PARTICLE DIAMETER
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
REAL SV(20,4)
C
C   MAKE SURE TOTAL WEIGHT FRACTION SUM IS 1.0
DO 103 K=2,4
T=0.0
DO 104 I=1,20
104 T=T+SIV(I,K)
DO 105 I=1,20
105 SIV(I,K)=SIV(I,K)/T
103 CONTINUE
C   CONVERT SIEVE OPENINGS TO MEAN DIAMETER IN M
SIV(1,1)=SIV(1,1)/500.0
DO 100 I=2,20

100 SV(I,1)=(SIV(I,1)+SIV(I-1,1))/2000.0
DO 120 I=2,20
120 SIV(I,1)=SV(I,1)
C   CALCULATE DP
DO 102 K=2,4
T=0.0
DO 101 I=1,20
101 T=T+SIV(I,K)/SIV(I,1)
102 PTX(4,K-1)=1.0/T
IF(PTX(4,3).GT.0.0)GOTO 106
PTX(4,3)=PTX(4,2)
DO 107 I=1,20
107 SIV(I,4)=SIV(I,3)
106 CONTINUE
C
C   CHECK BED PARTICLE SIZE
C   SHOULD BE GREATER THAN OR EQUAL TO LIMESTONE FEED SIZES
C
IF(PTX(4,3).GE.PTX(4,2))GOTO 108
PTX(4,3)=PTX(4,2)
108 RETURN
END

```

```

SUBROUTINE MIXFAC(M,XB)
C
C THIS ROUTINE GENERATES A MIXING PATTERN GIVEN M AND XBED
C
COMMON/MXF/X(10),Y(10)
REAL M
C
AK=0.01
AKL=AK/25.0
C
CHECK LIMITS OF M
C
IF(M.LT.0.02) GOTO 200
IF(M.GT.0.98) GOTO 300
C
CALCULATE DISTRIBUTION BASED ON CURVES XY=K
C
DO 500 I=1,10
500 X(I)=1.0-M*(1.0-XB)
DO 501 I=1,10
YSUM=0.0
N=11-I
DO 502 J=1,10
L=((I-1)*10)+(J-1)
YY=1.0-(FLOAT(L))/100.0
X1=((AK/YY)+(XB*M))*M
X2=YY-(XB*(1.0-M))
IF(X2.LT.AKL)GOTO 503
X1=X1+((AK/X2)*(1.0-M))
IF(X1.LT.1.0)GOTO 502
503 X1=1.0
502 YSUM=YSUM+X1
X(N)=YSUM/10.0
IF(X2.LT.AKL)GOTO 504
501 CONTINUE
504 CONTINUE
C TRANSFER TO X - ORDER AND SMOOTH OUT
400 KK=IFIX(M*10.0)+1
DO 600 I=1, KK
DO 601 L=1,10
601 Y(L)=X(L)
X(1)=(Y(1)+Y(2))/2.0
X(10)=(Y(9)+Y(10))/2.0
DO 602 K=2,9
602 X(K)=(Y(K)+Y(K+1)+Y(K-1))/3.0
600 CONTINUE
GOTO 800
C
C COMPLETE SEGREGATION
C
200 CONTINUE

```

```

DO 201 I=1,10
YY=1.0-(FLOAT(I-1))/10.0
L=11-I
X(L)=0.0
IF(YY.LE.XB)X(L)=1.0
201 CONTINUE
GOTO 800

C
C COMPLETE MIXING
C
300 CONTINUE
DO 301 I=1,10
301 X(I)=XB
C
C X TO INDICATE DISTRIBUTION OF JETSAM IN EACH SECTION
C
800 YSUM=0.0
DO 506 I=1,10
506 YSUM=YSUM+X(I)
DO 507 I=1,10
507 X(I)=X(I)/YSUM
NC=0
DO 508 I=1,10
YSUM=(X(I)*XB)/0.1
IF(YSUM.LE.1.0)GOTO 508
X(I)=X(I)/YSUM
NC=1
508 CONTINUE
IF(NC.EQ.1)GOTO 800
RETURN
END

```

```

SUBROUTINE MIXVAL(DP,PDEN,UMB,M)
C
C   CALCULATE DEGREE OF MIXING   M
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
REAL M
C
C   M=1 PERFECT MIXING   ;   M=0 COMPLETE SEGREGATION
C
HS=BED(8)/((4.0*BED(1)/3.141593)**0.5)
HS=(1.0-EXP(-HS))**1.4
C   ASSUME JETSAM CONCENTRATION IS SMALL
FBED=0.10**0.5
DER=(DP/PTX(4,3))**0.7
IF(PDEN.LT.PTX(2,3)) PDEN=1.10*PTX(2,3)
RR=((PDEN/PTX(2,3))-1.0)**1.1
UP=AIR(2)
IF(UP.LT.UMB) UP=UMB
UF=AIR(2)
RATIO=((UP/UF)**0.5)+0.9*RR*DER-2.2*FBED*HS
UTO=RATIO*UF
Z=(AIR(1)-UTO)/(AIR(1)-UF)
RAX=AIR(1)/UTO
IF(RAX.GT.20.0) RAX=20.0
Z=Z*EXP(RAX)
IF(Z.LT.-10.0) Z=-10.0
IF(Z.GT.10.0) Z=10.0
M=1.0/(1.0+EXP(-Z))
C   CHECK THAT M FALLS WITHIN LIMITS 0-1
IF(M.LT.0.0) M=0.0
IF(M.GT.1.0) M=1.0
RETURN
END

```

```

SUBROUTINE MODEF
C
C SET UP DIFFERENTIAL EQUATIONS FOR FREEBOARD FLUXES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/EXIST/AVE(20),AVB(20)
REAL STO(10),FIN(10),SCON(10),NR,NL,NA,CS(5)
C
C MASS BALANCES
C
C INITIALIZE TRANSFER STREAMS
C
DO 102 I=1,NS1
DO 102 J=1,6
102 EM(J,I)=0.0
C EVALUATION OF FLUXES IS BASED ON VALUES IN AVE,AVB
C LACK OF PERFECT MIXING COMPENSATED BY USING
C A PARTIAL AVAILABILITY FACTOR PFM
PFM=0.9
DO 103 I=1,NS1
103 AVE(I)=PFM*EMO(1,2,I)/XH
C
C HOMOGENEOUS GAS PHASE REACTION
C
C REDUCED MIXING IN THE FREEBOARD
C THEREFORE REDUCE APPROACH TO EQUILIBRIUM
XEQ=GG(16)/100.0
DO 100 I=1,10
STO(I)=XEQ*AVE(I)/PP(1,I)
100 SCON(I)=STO(I)
CALL EQOVER(STO,FIN,TB)
DO 101 I=1,10
STO(I)=FIN(I)-SCON(I)
101 EM(3,I)=STO(I)*PP(1,I)
CALL REDUCF(3)
C
C VOLATILE COMBUSTION
C
C RATE TO KG/M3.S
VR=GASX(11,17)/(BED(1)*XH)
IF(VR.LE.0.0) GOTO 804
C OXYGEN REQUIRED
OR=ABS(VR*VCOM(11))/PP(1,8)
OL=OR
C OXYGEN AVAILABLE

```



```

OA=AVE(8)/PP(1,8)
C SET LIMIT IF NOT ENOUGH AVAILABLE
IF(OA.LT.OL) OL=OA
C PARTIAL COMBUSTION
FX=OL/OR
IF(FX.GT.1.0) FX=1.0
GASX(11,17)=GASX(11,17)-FX*VR*BED(1)*XH
IF(GASX(11,17).LT.(1.0E-10)) GASX(11,17)=0.0
VR=FX*VR
DO 106 J=1,10
106 EM(4,J)=VR*VCOM(J)
EM(4,8)=EM(4,8)+VR*VCOM(J)
CALL REDUCF(4)
804 CONTINUE
C
C LOCAL SO2 AND NOX FLUXES
C
C NOX
C RATE IN KG/S.M
NR=GASX(11,16)*EMO(1,1,5)/GG(50)
C CONVERT TO MOLES/M3.S
NR=NR/(BED(1)*PP(1,5))
C MOLES OF NO AVAILABLE
NA=AVE(5)/PP(1,5)
C LIMITING REACTANT
NL=NR
IF(NA.LT.NR) NL=NA
C REACTION NO >> N2 + O2
EM(6,5)=-NL*PP(1,5)
EM(6,8)=0.5*NL*PP(1,8)
EM(6,7)=0.5*NL*PP(1,7)
C
C SO2
C RATE IN KG/S.M
SR=GASX(11,20)
C CONVERT TO MOLES/M3.S
SR=SR/(BED(1)*PP(1,9))
C MOLES OF SO2 AVAILABLE
SA=AVE(9)/PP(1,9)
C MOLES OF OXYGEN AVAILABLE
SO=AVE(8)/PP(1,8)
C LIMITING REACTANT
SL=SR
IF(SA.LT.SL) SL=SA
SO2=SO*2.0
IF(SO2.LT.SL) SL=SO2
C REACTION
EM(6,9)=-SL*PP(1,9)
EM(6,8)=EM(6,8)-((SL/2.0)*PP(1,8))
GG(50)=GG(50)+SL*PP(1,9)*BED(1)*XH

```

```

      CALL REDUCF(6)
C
C   LOCAL CHAR COMBUSTION
C
C   RATE KG/S.M
      CR=GASX(11,18)
C   CO2 FRACTION
      CD=GASX(11,19)
C   CONVERT TO KG/M3.S
      RF=1.0
111  CR1=CR*RF/BED(1)
C   SPLIT ACCORDING TO COMPOSITION
      DO 110 I=1,5
110  CS(I)=CR1*CM(I)
C   MOLES OF MOLECULES CREATED
      CS(1)=CS(1)/0.01201
      CS(2)=CS(2)/0.002016
      CS(3)=CS(3)/0.032
      CS(4)=CS(4)/0.014008
      CS(5)=CS(5)/0.032066
C   ESTIMATE FLUXES FROM CHAR
      EM(5,1)=(1.0-CD)*CS(1)
      EM(5,2)=CD*CS(1)
      EM(5,3)=CS(2)
      EM(5,5)=CS(4)
      EM(5,8)=CS(3)
      EM(5,9)=CS(5)
C   ESTIMATE O2 REQUIRED
      OX=EM(5,2)+EM(5,9)+(EM(5,1)+EM(5,5))/2.0
      OX=OX-EM(5,8)
C   O2 AVAILABLE
      OA=AVE(8)/PP(1,8)
      IF(OA.GE.OX) GOTO 121
C   NOT ENOUGH O2
      CA=AVE(2)/(PP(1,2)*2.0)
      ON=OA+CA
      IF(ON.GE.OX) GOTO 122
      RF=RF*0.9
      IF(RF.GT.0.120) GOTO 111
C   NO BURNING AT ALL
      DO 112 I=1,NS
112  EM(5,I)=0.0
      GOTO 805
C   PARTIAL BURNING
122  ON1=OX-OA
      EM(5,2)=EM(5,2)-2.0*ON1
      EM(5,1)=EM(5,1)+2.0*ON1
      EM(5,8)=-OA
      GOTO 115
C   COMPLETE BURNING
121  EM(5,8)=-OX

```

```

115 CONTINUE
C   CONVERT BACK TO KG
    DO 113 I=1,NS
113  EM(5,I)=EM(5,I)*PP(1,I)
805  CALL REDUCF(5)
C
C   TERMS EVALUATED ABOVE ARE ALREADY NEGATIVE
C   OR POSITIVE DEPENDING ON DIRECTION OF TRANSFER
C   SO ONLY HAVE TO SUM TERMS INTO DEM
C
C   SET UP DERIVATIVES
C
    DO 300 I=1,NS1
    DEM(1,I)=0.0
    SMLE=1.0
    DO 301 J=1,6
    DEM(1,I)=DEM(1,I)+EM(J,I)
    A=ABS(EM(J,I))
    IF(SMLE.GT.A.AND.A.GT.0.0)SMLE=A
301  CONTINUE
    IF(ABS(DEM(1,I)).LT.(0.001*SMLE))DEM(1,I)=0.0
300  CONTINUE
    RETURN
    END

```

```

SUBROUTINE MODEL
C
C   SET UP DIFFERENTIAL EQUATIONS FOR IN-BED FLUXES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/EXIST/AVE(20),AVB(20)
C
C   MASS BALANCES
C
C   INITIALIZE TRANSFER STREAMS
C
DO 102 I=1,NS1
DO 102 J=1,6
EM(J,I)=0.0
102 BU(J,I)=0.0
C
C   EVALUATION OF FLUXES IS BASED ON VALUES IN AVE,AVB
C
C   LACK OF PERFECT MIXING COMPENSATED BY USING
C   A PARTIAL AVAILABILITY FACTOR PFM
PFM=0.9
DO 103 I=1,NS1
AVE(I)=PFM*EMO(1,2,I)/XH
103 AVB(I)=PFM*BUO(1,2,I)/XH
C
C   FLUIDIZATION SATURATION FLUX
C
CALL FSATUR
C
C   INTERPHASE TRANSFER
C
CALL IPHASE
C
C   HOMOGENEOUS GAS PHASE REACTION
C
IF(XL.LT.BED(10)) GOTO 105
CALL CHERXN
105 CONTINUE
C
C   VOLATILE COMBUSTION
C
CALL VOLATV
C
C   LOCAL SULPHUR CAPTURE AND NO REDUCTION
C
CALL ESCAPE
C

```

```

C LOCAL COMBUSTION OF CHAR
C
C CALL LCHARC
C
C TERMS EVALUATED ABOVE ARE ALREADY NEGATIVE
C OR POSITIVE DEPENDING ON DIRECTION OF TRANSFER
C SO ONLY HAVE TO SUM TERMS INTO DEM,DBU
C
C SET UP DERIVATIVES
C
DO 100 I=1,NS1
DEM(1,I)=0.0
DBU(1,I)=0.0
SMLE=1.0
SMLB=1.0
DO 101 J=1,6
DEM(1,I)=DEM(1,I)+EM(J,I)
DBU(1,I)=DBU(1,I)+BU(J,I)
A=ABS(EM(J,I))
IF(SMLE.GT.A.AND.A.GT.0.0)SMLE=A
A=ABS(BU(J,I))
IF(SMLB.GT.A.AND.A.GT.0.0)SMLB=A
101 CONTINUE
IF(ABS(DEM(1,I)).LT.(0.001*SMLE))DEM(1,I)=0.0
IF(ABS(DBU(1,I)).LT.(0.001*SMLB))DBU(1,I)=0.0
100 CONTINUE
RETURN
END

```

```

SUBROUTINE NITROX(IJ,CH)
C
C ESTIMATE NO CONSUMPTION RATE BASED ON CHAR CONTENT OF BED
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/COMB/SI,ON,TO,RT,RTM,TP,RC,NF,RE,PR,DNU,ALPHA,XNO,RNO
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/CONST/PP(5,20),GG(50)
COMMON/GASCON/GASX(11,22),GASB(11,22)
C
GOTO (501,502), IJ
C
C NO REDUCTION IN BED PROPER
C
501 CONTINUE
C EXIT MOLE FRACTION
GG(50)=GASB(10,5)
C GENERATED AMOUNT
TA=12.186/TB
TM=PTX(7,1)*(1.0-COAL(1))*COAL(9)*(1.0-GG(32))/14.008
TM=TM/(GG(27)+GG(28))
CNO=TM/TA
IF(CNO.GT.COAL(9)) CNO=COAL(9)
XNO=(GG(50)+CNO)/2.0
GASB(8,22)=XNO
C CONVERT TO KG/M3
XNO=XNO*298.0*0.030/(0.0224*TB)
C CHAR SURFACE AREA
CSA=6.0*CH/(GG(19)*SI)
RST=BED(8)/AIR(2)
C REACTION RATE KG/S
RNO=GG(10)*CSA*XNO/RST
RETURN
C
C NO REDUCTION IN FREEBOARD
C
502 DO 504 I=1,20
IF(SIV(I,1).LE.GG(30)) GOTO 505
504 CONTINUE
505 CHB=GG(36)*BED(1)*BED(5)*BED(6)
CHB=CHB/(BED(1)*BED(8))
CHF=CH/(BED(1)*AIR(1))
RNO=CHF*CPROP(I,14)/CHB
GASX(11,16)=RNO
C TO GET REDUCTION (KG/S) MX BY (LOCAL XNO/BED XNO)
RETURN
END

```

```

SUBROUTINE PARTMP(TPN,MNM)
C
C   CALCULATE TEMPERATURE OF BURNING CHAR PARTICLE
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
COMMON/COMB/SI,ON,TO,RT,RTM,TP,RC,NF,RE,PR,DNU,ALPHA,XNO,RNO
C
GOTO (701,702), MNM
701 SP=3.141592*(SI**2.0)
C   FRACTION CO2 (PC IS WEIGHT RATIO)
PC=RC*(28.0/44.0)
FCO2=1.0/(1.0+PC)
FCO=1.0-FCO2
C   ENTHALPY OF COMBUSTION
HC=PTX(3,1)*(TP-298.0)*0.012
HRCO=(PP(5,1)-0.333*PP(5,8)-0.666*HC-110541.2)/PP(1,1)
HRC2=(PP(5,2)-0.5*PP(5,8)-0.5*HC-393505.2)/PP(1,2)
HEIN=(HRC2*FCO2)+(HRCO*FCO)
C   TOTAL ENTHALPY
HM=HEIN*RTM
C   REYNOLDS NO.
RE=SI*GG(21)*AIR(2)/GG(22)
C   PRANDTL NO.
PR=PP(3,7)*PP(1,7)*0.8+PP(3,2)*PP(1,2)*0.1+PP(3,8)*PP(1,8)*0.1
PR=PR*GG(22)/GG(29)
C   NUSSELT NO.
DNU=2.0*(1.0+0.3*(RE**0.5)*(PR**0.33333))
C   CONVECTIVE HEAT TRANSFER COEFF.
ALPHA=DNU*GG(29)/SI
C   RADIATION
RX=SP*GG(20)*0.9*((TB**4.0)-(TP**4.0))
C   NEW TEMPERATURE
TPN=TB-((HM-RX)/(SP*ALPHA))
DELTA=(TPN-TP)*0.5
IF(DELTA.GT.20.0) DELTA=20.0
TPN=TP+DELTA
RETURN
C   SUMMARIZED CURVEFIT OF ABOVE PROCEDURE FOR IMM PARTICLES
702 TPN=-12.263
TPN=TPN+1050.0*ON-974.21*(ON**2.0)
TPN=TB+TPN
RETURN
END

```

```

SUBROUTINE PREDIX(IFLAG)
C
C ESTIMATE COAL AND LIMESTONE FEEDRATES AND GAS CONCENTRATIONS
C BY DOING A ROUGH AND READY MASS/ENERGY BALANCE
C
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
REAL COALEN(2,2),GAS(10)
C
C CARBON LOSS CONSIDERING RECYCLE
COVER=0.025*(2.-GG(4))
C COMBUSTION EFFICIENCY
CEFF=0.80
C ENERGY LOSS FACTOR
CLOSS=0.075+COVER
C FRACTION SULFUR ABSORBED
SABS=1.0-0.775*(EXP((GG(2)-1.0)*(-1.135)))
C BED AREA
BED(1)=BED(2)*BED(3)
C HEAT EXCH AREA
HTA=2.0*3.14159*(HOT(3)/2.0)*HOT(2)
HTA=HTA*HOT(1)
C INTIAL COAL GUESS & ENERGY
COALEN(1,1)=516.0*BED(1)
COALEN(2,2)=0.0
C
C CALCULATIONS
C
DO 100 I=1,40
200 CONTINUE
C HEAT IN
HEIN=COALEN(1,1)*COAL(5)*(1.0-CLOSS)
C HEAT TO IMMersed TUBES
TLM=HOT(5)-HOT(4)
TLM=TLM/(LOG((TB-HOT(4))/(TB-HOT(5))))
HT=300.0*HTA*TLM*3600.0
C LIMESTONE FEEDRATE
SIN=COALEN(1,1)*COAL(10)/0.032064
CA=GG(2)*SIN
SLIME=CA*0.100089*(1.0/GG(3))
C ASH RATE
ASH=COAL(2)*COALEN(1,1)
C COAL RATE (UNBURNT)
CCOAL=COVER*COALEN(1,1)*COAL(4)
C HEAT LOSS SOLIDS
HSOL=ASH+SLIME+CCOAL

```



```

HSOL=PTX(3,3)*HSOL*(TB-HOT(7))
C   GAS CONCENTRATIONS
C   C
CM=COALEN(1,1)*COAL(6)/0.012
EXC=CM
CM=(1.-COVER)*CM
C   O2 IN
VOL=BED(1)*AIR(1)*298./TB
VOLM=VOL*160632.0
C   O2 FOR SO2
SOX=SIN*(1.0-SABS)
GAS(9)=SOX
C   & FOR CASO4
SLS=SOX+(SIN*SABS*1.5)
GAS(8)=VOLM*AIR(7)-SLS
C   O2 USED BY H2
GAS(4)=0.98*COALEN(1,1)*COAL(7)/0.002
GAS(8)=GAS(8)-0.5*GAS(4)
GAS(3)=0.01*COALEN(1,1)*COAL(7)/0.002
GAS(10)=GAS(3)*0.5
CM=CM-GAS(10)
C   O2 FOR FUEL NITROGEN
GAS(6)=COALEN(1,1)*COAL(9)*0.5/0.014
GAS(7)=VOLM*AIR(8)+GAS(6)/2.0
GAS(8)=GAS(8)-GAS(6)
C   WATER IN AIR FEED
GAS(4)=GAS(4)+VOLM*AIR(9)
C   NO / NO2 SPLIT
GAS(5)=0.9*GAS(6)
GAS(6)=0.1*GAS(6)
C   O2 IN COAL
GAS(8)=GAS(8)+COALEN(1,1)*COAL(8)/0.032
AIR(6)=100.*(GAS(8)/EXC-1.0)
C   INCOMPLETE COMBUSTION
GAS(1)=0.0
IF(AIR(6).GT.200.0) CEFF=1.0
IF((AIR(6).LT.0.0).OR.(AIR(6).GT.200.0)) GOTO 300
CEFF=0.05+0.05*(3.-AIR(6)/50.0)
GAS(1)=CEFF*CM
CEFF=1.0-CEFF
300 IF(AIR(6).GT.0.0)GOTO 301
GAS(1)=2.*(CM-GAS(8))/CEFF
R=(1.0-CEFF)*CM
IF(GAS(1).LT.R) GAS(1)=R
301 GAS(2)=CM-GAS(1)
C   OXYGEN OUT
GAS(8)=GAS(8)-(GAS(2)+0.5*GAS(1))
IF(GAS(8).LT.0.0) GAS(8)=0.0
C   MOISTURE IN COAL
WAT=COAL(1)*(1066.-(HOT(7)*1.8-460.0)+0.5*(TB*1.8-460.0))
HWAT=WAT*COALEN(1,1)*2324.4

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WAT=COAL(1)*COALEN(1,1)/0.0180
C   TOTAL WATER OUT
GAS(4)=GAS(4)+WAT
C   CO2 FROM LIMESTONE
COL=SLIME*GG(3)/0.10008
GAS(2)=GAS(2)+COL
C   HEAT OF CALCINATION OF LIMESTONE
CALC=COL*43.65*4.184
C   MINUS HEAT OF RXN TO CASO4
R=SIN*SABS*115.9*4.184
CALC=(CALC-R)*1000.0
C   CORRECT FOR CO LOSS
COR=-GAS(1)*4.184*67.63*1000.0
AM=0.0
DO 101 J=1,10
AM=AM+GAS(J)
101 COR=COR+PP(5,J)*GAS(J)
C   SUM IT ALL UP
COALEN(2,1)=HEIN-(HWAT+HSOL+COR+HT+CALC)
A=ABS(COALEN(2,1))
B=0.01*HEIN
IF(A.LT.B)GOTO 302
C   INTERPOLATE
IF(COALEN(2,2).NE.0.0)GOTO 303
CN=100.0*BED(1)
GOTO 304
303 CN=(COALEN(1,2)-COALEN(1,1))/(COALEN(2,2)-COALEN(2,1))
CN=CN*(-COALEN(2,1))
CN=CN+COALEN(1,1)
IF(CN.LE.0.0) CN=0.5*COALEN(1,1)
304 COALEN(1,2)=COALEN(1,1)
COALEN(2,2)=COALEN(2,1)
COALEN(1,1)=CN
100 CONTINUE
WRITE(6,400)
400 FORMAT(' PREDIX CANNOT FIND A PRELIMINARY SOLUTION ')
IFLAG=0
GOTO 105
302 IFLAG=1
105 PTX(7,1)=COALEN(1,1)/3600.0
PTX(7,2)=SLIME/3600.0
AIR(6)=1.0+AIR(6)/100.0
IF(IFLAG.EQ.0)GOTO 110
WRITE(6,111)TB
111 FORMAT(' PRELIMINARY RESULTS: @',F10.2,' K')
WRITE(6,112)COALEN(1,1),SLIME
112 FORMAT(' COAL= ',F10.2,' LIME= ',F10.2,' KG/HR')
WRITE(6,113)AIR(6)
113 FORMAT(' EXCESS AIR FACTOR= ',F10.2)
110 CONTINUE
DO 102 I=1,10

```

```

102  GASX(10,I)=GAS(I)/AM
      GASX(10,8)=GASX(10,8)/4.0
C
C    PREDICT INITIAL GAS CONCENTRATIONS THROUGHOUT BED
C    I.E. ASSUME LINEAR VARIATION
C
      DO 405 I=1,10
405   GASX(1,I)=0.0
      GASX(1,4)=AIR(9)
      GASX(1,7)=AIR(8)
      GASX(1,8)=GAS(8)/AM
      DO 401 I=1,10
      GS=(GASX(10,I)-GASX(1,I))/10.0
      DO 402 J=2,9
402   GASX(J,I)=GASX(J-1,I)+GS
401   CONTINUE
      GASB(1,8)=0.18
      GASB(10,8)=0.03
      GASB(10,9)=GASX(10,9)
      GASB(10,5)=GASX(10,5)
      RETURN
      END

```

```

SUBROUTINE PRESEF
C
C EVALUATE MOLE AND MASS FLOWRATES AND MOLE FRACTIONS
C AT THE CURRENT LEVEL IN THE FREEBOARD
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/CONST/PP(5,20),GG(50)
C
GASX(11,22)=0.0
GASX(10,22)=0.0
C TOTAL MOLES
DO 103 I=1,NS
103 GASX(11,22)=GASX(11,22)+EMO(1,2,I)/PP(1,I)
C MOLE FRACTIONS
DO 104 I=1,NS
104 EMO(1,1,I)=EMO(1,2,I)/(GASX(11,22)*PP(1,I))
C MASS TOTALS
DO 105 I=1,NS
105 GASX(10,22)=GASX(10,22)+EMO(1,2,I)
C
C CHECK FOR NEGATIVE MASS FRACTIONS. IF ANY THEN EXIT
C ANYTHING GREATER THAN 0.98 WILL ALSO CAUSE EXIT
C
DO 106 I=1,NS
IF(EMO(1,1,I).LT.0.0.OR.EMO(1,1,I).GT.0.98)GO TO 107
106 CONTINUE
RETURN
C
C EXIT PROCEDURE
C
107 CONTINUE
WRITE(6,108)XL,I
108 FORMAT(/,' INVALID WEIGHT FRACTION AT LEVEL ',1PE15.5,
*' FOR SPECIES ',I3,/, ' EXECUTION HALTED ',/)
C WRITE OUT COMPLETE DATA SET
CALL CHECKO
STOP
END

```

```

SUBROUTINE PRESET
C
C EVALUATE MOLE AND MASS FLOWRATES AND MOLE FRACTIONS
C AT THE CURRENT LEVEL IN THE BED
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/CONST/PP(5,20),GG(50)
C
GASX(11,22)=0.0
GASB(11,22)=0.0
GASX(10,22)=0.0
GASB(10,22)=0.0
C
TOTAL MOLES
DO 103 I=1,NS
IF(EMO(1,2,I).LT.0.0)GOTO 201
GASX(11,22)=GASX(11,22)+EMO(1,2,I)/PP(1,I)
201 IF(BUO(1,2,I).LT.0.0)GOTO 103
GASB(11,22)=GASB(11,22)+BUO(1,2,I)/PP(1,I)
103 CONTINUE
C
MOLE FRACTIONS
DO 104 I=1,NS
EMO(1,1,I)=EMO(1,2,I)/(GASX(11,22)*PP(1,I))
BUO(1,1,I)=BUO(1,2,I)/(GASB(11,22)*PP(1,I))
C
DO NOT ALLOW ANY SPECIES IN EMULSION BELOW 0.00000001
SL=1.0E-08
IF(ABS(EMO(1,1,I)).GT.SL) GOTO 104
EMO(1,1,I)=SL
EMO(1,2,I)=EMO(1,1,I)*GASX(11,22)*PP(1,I)
104 CONTINUE
C
MASS TOTALS
DO 105 I=1,NS
GASX(10,22)=GASX(10,22)+EMO(1,2,I)
105 GASB(10,22)=GASB(10,22)+BUO(1,2,I)
C
CHECK FOR NEGATIVE MASS FRACTIONS. IF ANY EXIT
C ANYTHING GREATER THAN 0.98 WILL ALSO CAUSE EXIT
C
DO 106 I=1,NS
IF(EMO(1,1,I).GT.0.98.OR.BUO(1,1,I).GT.0.98)GO TO 107
IF(EMO(1,1,I).LT.0.0.OR.BUO(1,1,I).LT.0.0)GO TO 107
106 CONTINUE
RETURN
C
EXIT PROCEDURE
C
107 CONTINUE
WRITE(6,108)XL,I
108 FORMAT(/,' INVALID WEIGHT FRACTION AT LEVEL ',1PE15.5,

```

*' FOR SPECIES ',I3,/, ' EXECUTION HALTED ',/)
C WRITE OUT COMPLETE DATA SET
CALL CHECKO
STOP
END

```

SUBROUTINE PROPER(TV)
C
C THIS FILE CALCULATES SPECIES PROPERTIES AT A GIVEN TEMPERATURE
C
COMMON/CONST/PP(5,20),GG(50)
C
C 3=CP ; HEAT CAPACITY
C 4=S ; ENTROPY
C 5=H ; ENTHALPY
C T MUST BE IN DEGREES K
TX=TV/100.0
TX2=TX*TX
TX3=TX2*TX
C
CH4
PP(3,10)=4.1005+1.4388*TX+0.004201*TX2-0.0017803*TX3
PP(4,10)=36.082+3.1386*TX-0.10471*TX2+0.0021556*TX3
PP(5,10)=0.2737*TX+0.09625*TX2-0.0016183*TX3-1.6187
C
SO2
PP(3,9)=5.9236+1.5003*TX-0.10531*TX2+0.0026419*TX3
PP(4,9)=49.2+4.0019*TX-0.21114*TX2+0.0049779*TX3
PP(5,9)=0.74626*TX+0.044822*TX2-0.0011166*TX3-2.6065
C
O2
PP(3,8)=6.1261+0.31446*TX-0.0093772*TX2-0.0000037879*TX3
PP(4,8)=41.868+2.8851*TX-0.1667*TX2+0.0041699*TX3
PP(5,8)=0.60401*TX+0.016796*TX2-0.00035402*TX3-1.9402
C
N2
PP(3,7)=7.0155-0.10279*TX+0.029194*TX2-0.0011061*TX3
PP(4,7)=38.798+2.8474*TX-0.17166*TX2+0.0044327*TX3
PP(5,7)=0.63096*TX+0.0082485*TX2-0.000056527*TX3-1.9468
C
NO2
PP(3,6)=5.5322+1.3184*TX-0.079589*TX2+0.0017147*TX3
PP(4,6)=48.115+3.6395*TX-0.1861*TX2+0.0043389*TX3
PP(5,6)=0.64435*TX+0.0474*TX2-0.0011384*TX3-2.3202
C
NO
PP(3,5)=6.9301-0.0065059*TX+0.022272*TX2-0.00098397*TX3
PP(4,5)=43.234+2.8944*TX-0.17134*TX2+0.0043631*TX3
PP(5,5)=0.62397*TX+0.012339*TX2-0.00020105*TX3-1.9592
C
H2O
PP(3,4)=7.7246+0.015807*TX+0.029945*TX2-0.0010291*TX3
PP(4,4)=37.04+3.2692*TX-0.19068*TX2+0.0049639*TX3
PP(5,4)=0.71015*TX+0.012826*TX2+0.000055944*TX3-2.228
C
H2
PP(3,3)=6.8475+0.023963*TX-0.00065734*TX2+0.00019814*TX3
PP(4,3)=24.106+2.9244*TX-0.18448*TX2+0.0048345*TX3
PP(5,3)=0.7014*TX-0.001671*TX2+0.0001792*TX3-2.0818
C
CO2
PP(3,2)=5.1859+1.5157*TX-0.096572*TX2+0.0023054*TX3
PP(4,2)=41.614+3.7224*TX-0.18886*TX2+0.0044172*TX3
PP(5,2)=0.6605*TX+0.048568*TX2-0.0010994*TX3-2.383
C
CO
PP(3,1)=6.8632-0.040783*TX+0.024789*TX2-0.0010178*TX3

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```
PP(4,1)=40.24+2.8415*TX-0.1694*TX2+0.004344*TX3
PP(5,1)=0.6189*TX+0.010572*TX2-0.0001317*TX3-1.93
C CONVERT CP TO JOULES/DEGREE MOLE
C CONVERT S TO      "
C CONVERT H TO      JOULES/MOLE
DO 100 I=1,10
PP(3,I)=PP(3,I)*4.184
PP(4,I)=PP(4,I)*4.184
100 PP(5,I)=PP(5,I)*4184.0
RETURN
END
```


SUBROUTINE PROPEX

C
C THIS FILE CONTAINS CONSTANT SPECIES PROPERTIES
C
C COMMON/CONST/PP(5,20),GG(50)
C
C 1 - MOLECULAR WEIGHT (KG/MOL)
C 2 - HEAT OF FORMATION (J/MOL) AT 298 K
C
C CO
C PP(1,1)=0.02801055
C PP(2,1)=-110541.
C
C CO2
C PP(1,2)=0.04400995
C PP(2,2)=-393522.
C
C H2
C PP(1,3)=0.002016
C PP(2,3)=0.0
C
C H2O
C PP(1,4)=0.018016
C PP(2,4)=-241826.
C
C NO
C PP(1,5)=0.030008
C PP(2,5)=90291.
C
C NO2
C PP(1,6)=0.046008
C PP(2,6)=33095.
C
C N2
C PP(1,7)=0.0280134
C PP(2,7)=0.0
C
C O2
C PP(1,8)=0.0319988
C PP(2,8)=0.0
C
C SO2
C PP(1,9)=0.064066
C PP(2,9)=-296842.
C
C CH4
C PP(1,10)=0.016043
C PP(2,10)=-74873.
C
C RETURN
C
C END

```

SUBROUTINE RECYCL
C
C CALCULATE FINES RECYCLE RATE AND SUBSEQUENT COMBUSTION RATE
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/COMB/SI,ON,TO,RT,RTM,TP,RC,NF,RE,PR,DNU,ALPHA,XNO,RNO
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/CONST/PP(5,20),GG(50)
C
C CHAR LEAVING BED
GG(41)=GASX(11,18)
IF(GG(5).EQ.0.0) GG(5)=0.01
C
C CHARACTERISTICS OF ELUTRIATED PARTICLES
C
DO 100 K=1,20
100 IF(SIV(K,1).LT.GG(30)) GOTO 101
101 CONTINUE
C RESIDENCE TIME IN BED
RT=CPROP(K,6)*GG(7)
C RESIDENCE TIME IN FREEBOARD
C BURNING ONLY IN BOTTOM 1/3
RTF=(BED(4)-BED(8))/3.0*AIR(1)
RT=RT+RTF
C HEATUP TIME
HU=CPROP(K,4)-CPROP(K,3)
C COMBUSTION TIME
TC=HU+CPROP(K,5)
C UTILIZATION FACTOR
UF=TC/RT
IF(UF.LT.1.01) GG(39)=(TC/(1.01*CPROP(K,6)))
IF(UF.LT.1.01) UF=1.01
IF(UF.GT.5.6) UF=5.6
UF=EXP(1.0-UF)
C CALCULATE A CONVERSION LEVEL
Y=-1.0
IF(HU.GT.RT) Y=0.01
IF(TC.LE.RT) Y=0.99
IF(Y.EQ.-1.0) Y=UF
C CALCULATE RECYCLE FLOW
DEN=Y*GG(4)+1.0/GG(5)-GG(4)
DEN=DEN*GG(5)
IF(DEN.LE.1.0) GOTO 102
DEN=1.0
102 R=GG(41)/DEN
C CHAR BURNUP IN BED
GG(42)=Y*R*GG(4)*GG(5)
C ESTIMATE CHAR LOSS AT CYCLONE
GG(43)=R*(1.0-GG(5))
C RECYCLE PRODUCT

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```
GG(44)=GG(41)-(GG(42)+GG(43))
C COMBUSTION SPLIT BETWEEN BED AND FREEBOARD
GF=GG(42)*RTF/RT
GB=GG(42)-GF
GASX(11,18)=GF
GASX(11,19)=GASX(10,19)
DO 401 I=1,10
401 GASX(I,18)=0.1*GB+GASX(I,18)
C
C ESTIMATE NO REDUCTION DUE TO FINES CARRYOVER
C
CALL NITROX(2,R)
RETURN
END
```

```
      SUBROUTINE REDUCF(IR)
C
C      AVAILABLE SPECIES FLOWRATES IN FREEBOARD
C
      COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
      COMMON/EXIST/AVE(20),AVB(20)
C
      DO 100 I=1,NS1
100   AVE(I)=AVE(I)+EM(IR,I)
      RETURN
      END
```

```
      SUBROUTINE REDUCE(IR)
C
C      AVAILABLE SPECIES FLOWRATES IN BED
C
      COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
      COMMON/EXIST/AVE(20),AVB(20)
C
      DO 100 I=1,NS1
      AVE(I)=AVE(I)+EM(IR,I)
100   AVB(I)=AVB(I)+BU(IR,I)
      RETURN
      END
```

```

SUBROUTINE STARTR
C
C   SET UP INITIAL CONDITIONS FOR START OF ITERATION LOOP
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/SHAKE/SIV(20,4),CPROP(20,14)
COMMON/UNITS/IN,IOUT,SPECY(20)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
COMMON/EQUIL/NSE,NLM,AES(5,10)
C
C   INITIALIZE INLET GAS CONCENTRATIONS EMO,BUO
C
NS=10
NS1=10
XL=0.0
DO 450 J=1,NS
EMO(1,1,J)=0.000001
450 BUO(1,1,J)=0.000001
EMO(1,1,4)=AIR(9)
EMO(1,1,7)=AIR(8)
EMO(1,1,8)=AIR(7)
BUO(1,1,8)=AIR(7)
BUO(1,1,7)=AIR(8)
BUO(1,1,4)=AIR(9)
BX=AIR(10)*GG(28)/GG(27)
DO 451 K=1,NS
EMO(1,2,K)=EMO(1,1,K)*AIR(10)*PP(1,K)
451 BUO(1,2,K)=BUO(1,1,K)*BX*PP(1,K)
C
C   SET UP OTHER INITIAL CONDITIONS & DERIVATIVES
C
DO 452 K=1,5
452 GASB(K,22)=0.0
GASX(11,22)=AIR(10)
DO 453 K=1,20
DEM(2,K)=0.0
453 DBU(2,K)=0.0
DO 454 K=3,20
454 ENO(1,K)=0.0
C
C   ENTHALPY IN INLET AIR
CALL PROPER(AIR(5))
AR=AIR(10)*BED(1)*(GG(28)+GG(27))/GG(27)
ENO(1,4)=(AIR(9)*PP(5,4)+AIR(7)*PP(5,8)+AIR(8)*PP(5,7))*AR
C   PHYSICAL PROPERTIES AT CURRENT BED TEMPERATURE
CALL PROPER(TB)
RETURN

```

END

```

SUBROUTINE TDERIV(SI,TP,J,DR,SMP)
C
C TEMPERATURE DERIVATIVE OF COAL PARTICLE
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
C
C SURFACE AREA
701 SP=3.141592*(SI**2.0)
C REYNOLDS NO.
RE=SI*GG(21)*AIR(2)/GG(22)
C PRANDTL NO.
PR=PP(3,7)*PP(1,7)*0.8+PP(3,2)*PP(1,2)*0.1+PP(3,8)*PP(1,8)*0.1
PR=PR*GG(22)/GG(29)
C NUSSELT NO.
DNU=2.0*(1.0+0.3*(RE**0.5)*(PR**0.33333))
C CONVECTIVE HEAT TRANSFER COEFF.
ALPHA=DNU*GG(29)/SI
C RADIATION TERM
RX=SP*GG(9)*0.9*((TB**4.0)-(TP**4.0))
C CONVECTIVE TERM
TC=SP*ALPHA*(TB-TP)
C DERIVATIVE
DR=(TC+RX)/(SMP*PTX(3,J))
RETURN
END

```



```
FUNCTION THERMC(T)
C
C ESTIMATE THERMAL CONDUCTIVITY OF AIR
C
COMMON/CONST/PP(5,20),GG(50)
C
C T IN K
C THERMC=0.001*(19.178+0.047567*T)
C
C THERMAL CONDUCTIVITY J/S.M.K
C GG(29)=THERMC
RETURN
END
```

```
      SUBROUTINE TURNOV(DP,TT)
C
C      CALCULATE PARTICLE TURNOVER TIME (S)
C
      COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
      COMMON/CONST/PP(5,20),GG(50)
C
      DELF=GG(31)
      DELD=0.35
      DELW=-0.194
      DELW=DELW-0.1111*(LOG10(DP))
      IF(DELW.LT.0.1) DELW=0.1
      TT=BED(7)/(DELF*(AIR(1)-AIR(2))*(DELW+DELD))
      RETURN
      END
```

```

SUBROUTINE VELOC
C
C ESTIMATE FLUIDIZATION, SLUGGING, AND TERMINAL VELOCITIES
C
COMMON/SHAKE/SIV(20,4),CPROP(20,12),LPROP(20,8)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
C
C PROPERTIES OF AIR
DEN=DENAIR(TB,AIR(3))
VIS=VISAIR(TB)
THC=THERMC(TB)
C
C BOUYANCY
DO 700 IL=1,3
SIG=9.80665*(PTX(2,IL)-DEN)
R1=(VIS**2.0)/(DEN*SIG*PTX(4,IL)**3.0)
R2=PTX(2,IL)/DEN
C
C EVALUATE UMF
C
C
TOS=52400.0*(R1**0.82)*(R2**0.22)+1.65
UMB=((SIG*PTX(4,IL))/(TOS*DEN))**0.5
C
C EVALUATE UMS & EMB USING BROADHURST AND BECKER EQUATIONS
C
C
200 R3=((1.27324*BED(1))**0.5)/(1.5*BED(5))
R1=1.0/R1
R2=1.0/R2
TOS=51.4*(R3**1.79)*(R2**1.09)
TOS=TOS+0.00416*(R1**0.41)*(R2**0.59)
UMS=((TOS*SIG*PTX(4,IL))/DEN)**0.5
C
C EMB
400 EMB=0.586*(PTX(1,IL)**(-0.72))*((1.0/R1)**0.029)*(R2**0.021)
C
C SMALLEST SIZE FOR WHICH THE CURRENT SUPERFICIAL VELOCITY
C IS THE TERMINAL PARTICLE VELOCITY
DO 702 IM=1,20
IK=21-IM
PDP=SIV(IK,1)
600 RE=(PDP*DEN*UMB)/VIS
IF(RE.LT.0.4)UTP=UMB*91.6
IF(RE.GT.1000.0)UTP=UMB*8.72
I=1
605 I=I+1
IF(I.GT.100)GO TO 606
IF(RE.LT.0.4)GO TO 601
IF(RE.LT.500)GO TO 602
IF(RE.LT.200000.0)GO TO 603
606 CONTINUE
GOTO 701
601 UTP=(SIG*PDP**2.0)/(18.0*VIS)
RE=(PDP*DEN*UTP)/VIS

```

```

IF(RE.GT.0.4)GO TO 605
GOTO 701
602 UTP=((SIG**2.0)*4.0)/(225.0*DEN*VIS)
    UTP=(UTP**(1.0/3.0))*PDP
    RE=(PDP*DEN*UTP)/VIS
    IF(RE.LT.0.4.OR.RE.GT.500.0)GO TO 605
    GOTO 701
603 UTP=((3.1*SIG*PDP)/DEN)**0.5
    RE=(PDP*DEN*UTP)/VIS
    IF(RE.LT.500.0.OR.RE.GT.200000.0)GO TO 605
701 CONTINUE
    IF(UTP.GT.AIR(1))GOTO 703
702 CONTINUE
C  ASSIGN VALUES TO PROPER ARRAYS
703 PTX(8,IL)=PDP
    PTX(5,IL)=UMB
    AIR(2)=UMB
    PTX(6,IL)=UMS
    BED(9)=EMB
700 CONTINUE
    RETURN
    END

```

```

SUBROUTINE VELODP(DP,PDEN,UMB,UTP)
C
C ESTIMATE FLUIDIZATION VELOCITIES FOR GIVEN PARTICLE SIZE
C
COMMON/CONST/PP(5,20),GG(50)
COMMON/UNITS/IP
C
DEN=GG(21)
VIS=GG(22)
SIG=9.80665*(PDEN-DEN)
R1=(VIS**2.0)/(DEN*SIG*DP**3.0)
R2=PDEN/DEN
C
C UMF
C
TOS=52400.0*(R1**0.82)*(R2**0.22)+1.65
UMB=((SIG*DP)/(TOS*DEN))**0.5
C
C TERMINAL VELOCITY OF LOWER SIZE LIMIT
C
600 RE=(DP*DEN*UMB)/VIS
IF(RE.LT.0.4)UTP=UMB*91.6
IF(RE.GT.1000.0)UTP=UMB*8.72
I=1
605 I=I+1
IF(I.GT.100)RETURN
IF(RE.LT.0.4)GO TO 601
IF(RE.LT.500)GO TO 602
IF(RE.LT.200000.0)GO TO 603
RETURN
601 UTP=(SIG*DP**2.0)/(18.0*VIS)
RE=(DP*DEN*UTP)/VIS
IF(RE.GT.0.4)GO TO 605
RETURN
602 UTP=((SIG**2.0)*4.0)/(225.0*DEN*VIS)
UTP=(UTP**(1.0/3.0))*DP
RE=(DP*DEN*UTP)/VIS
IF(RE.LT.0.4.OR.RE.GT.500.0)GO TO 605
RETURN
603 UTP=((3.1*SIG*DP)/DEN)**0.5
RE=(DP*DEN*UTP)/VIS
IF(RE.LT.500.0.OR.RE.GT.200000.0)GO TO 605
RETURN
END

```

```
FUNCTION VISAIR(T)
C
C ESTIMATE VISCOSITY OF AIR AT GIVEN TEMPERATURE
C
COMMON/CONST/PP(5,20),GG(50)
C
C T IN K
C VISAIR=6.31E-06+(T*4.18E-08)-((T**2.0)*6.70E-12)
C
C VISCOSITY IN KG/M.S
C GG(22)=VISAIR
RETURN
END
```

```
      SUBROUTINE VOLATM(SI,TD)
C
C      CALCULATE DEVOLATILIZATION TIME FOR A GIVEN PARTICLE SIZE
C
      COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
      COMMON/CONST/PP(5,20),GG(50)
C
C      CONVERT SIZE FROM METERS TO MM
      SS=SI*1000.0
      Y=1048.0/TB
      Z=10.0*(Y**3.8)
      Y=0.75/Y
      TD=Z*(SS**Y)
      RETURN
      END
```

```

SUBROUTINE VOLATV
C
C CALCULATE LOCAL VOLATILE EMISSION AND COMBUSTION FLUXES
C
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/TRANSF/NS1,EM(6,20),BU(6,20),DEM(2,20),DBU(2,20)
COMMON/EXIST/AVE(20),AVB(20)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
C
C LOCAL EMISSION RATE
C
A=10.0*(XL-XH)/BED(8)
IA=INT(A)+1
C LOCAL RATE KG/S
VR=GASX(IA,17)*0.1
C PREVIOUS UNBURNT ??
VR=VR+GASB(2,22)
C CONVERT TO KG/M3.S
VR=VR/(BED(1)*XH)
C COMBUSTION
C OXYGEN REQUIRED
OR=ABS(VR*VCOM(11))/PP(1,8)
OL=OR
C OXYGEN AVAILABLE
OA=AVE(8)/PP(1,8)
C LIMITING SPECIES
IF(OA.LT.OL) OL=OA
C FRACTION COMBUSTED
FX=OL/OR
IF(FX.GE.1.0) GOTO 100
GASB(2,22)=(1.0-FX)*VR*BED(1)*XH
VR=FX*VR
100 CONTINUE
DO 101 J=1,10
101 EM(4,J)=VR*VCOM(J)
EM(4,8)=EM(4,8)+VR*VCOM(11)
CALL REDUCE(4)
RETURN
END

```



```

SUBROUTINE VOLCOM
C
C ESTIMATE VOLATILES COMPOSITION
C
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
COMMON/BURNS/VCOM(11),CM(5)
REAL N,WET(10)
C
C CONVERT ALL TO WET BASIS
C
WET(1)=COAL(1)
DO 102 I=2,10
102 WET(I)=COAL(I)*(1.0-COAL(1))
C
C VOLATILES COMPOSITION
C
DO 400 I=1,11
400 VCOM(I)=0.0
CALL VOLNOX
C=WET(6)-WET(4)
N=GG(32)*WET(9)
H=0.0
O=0.0
S=0.0
T=C+N
IF(T.GT.WET(3)) GOTO 200
IF(T.EQ.WET(3)) GOTO 150
MX=1.0
101 H=WET(7)*MX
O=WET(8)*MX
TN=T+H+O
IF(TN.LE.WET(3)) GOTO 100
MX=MX*0.95
IF(MX.GT.0.006) GOTO 101
H=0.0
O=0.0
100 IF(TN.EQ.WET(3)) GOTO 150
S=WET(3)-TN
IF(S.GT.WET(10)) S=WET(10)
EX=(WET(3)-TN)-WET(10)
C=C+EX
WET(4)=WET(4)-EX
GOTO 150
200 EXT=T-WET(3)
C=C-EXT
WET(4)=WET(4)+EXT
150 CONTINUE
C NOW HAVE C H O N S GOING TO VOLATILES
C ADD MOISTURE TO THIS TOTAL AND CONVERT TO MOLES
C=C/0.01201

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```

N=N/0.014008
S=S/0.032066
O=O/0.016
H=H/0.001008
VCOM(4)=WET(1)/PP(1,4)
C   CONVERT S TO SO2
    RO=S*2.0
    O=O-RO
    VCOM(9)=S
C   N TO NO AND N2
    RO=N*GG(33)
    O=O-RO
    VCOM(5)=RO
    VCOM(7)=(N-RO)/2.0
C   75% OF H TO CH4
    GX=0.75
303  CX=GX*H
302  H=H-CX
    C=C-CX/4.0
    VCOM(10)=CX/4.0
C   REMAINING CARBON TO CO
    O=O-C
    VCOM(1)=C
C   ANY AVAILABLE O TO H2O
    IF(O.LE.0.0) GOTO 304
    IF(O.GT.(H/2.0)) GOTO 305
    H=H-O*2.0
    VCOM(4)=VCOM(4)+O
    O=0.0
    VCOM(8)=0.0
    GOTO 304
305  O=O-H/2.0
    VCOM(8)=O/2.0
    VCOM(4)=VCOM(4)+H/2.0
    H=0.0
304  VCOM(3)=H/2.0
    IF(O.LT.0.0) VCOM(11)=O/2.0
C
C   MASS FRACTION OF COAL LOST DURING DEVOL.
C
    GG(34)=WET(1)+WET(3)
C
C   CONVERT BACK TO MASS FRACTION
C
    SUM=0.0
    DO 306 I=1,10
    VCOM(I)=VCOM(I)*PP(1,I)
306  SUM=SUM+VCOM(I)
    VCOM(11)=VCOM(11)*PP(1,8)
    SUM=SUM+VCOM(11)
    DO 307 I=1,11

```

```
307 VCOM(I)=VCOM(I)/SUM
C
C DO MASS BALANCE TO GET COMPOSITION OF REMAINING CHAR
C
CALL CHRCOM(WET)
RETURN
END
```

SUBROUTINE VOLNOX

C
C
C

CALCULATE FATE OF FUEL NITROGEN

COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/GASCON/GASX(11,22),GASB(11,22)
COMMON/CONST/PP(5,20),GG(50)

C
C
C

FUEL N INTO VOLATILES

FN=1.95*COAL(3)-0.56
IF(FN.LT.0.10) FN=0.10
CN=1.0/(1.0+FN)
GG(32)=1.0-CN

C
C
C

RELATIVE CONVERSION OF NH3 TO NO/N2

FN=(TB**0.5)*EXP(-1510.0/TB)
FN=FN*0.00000003876*GASX(5,8)/GASX(5,5)
CN=1.0/(1.0+FN)
GG(33)=1.0-CN
RETURN
END

```

SUBROUTINE WRITER(JK)
C
C THIS ROUTINE WRITES OUT RESULTS OF SIMULATION
C
COMMON/OERALL/NS ,XH ,XL ,TBU(2) ,EMO(2,2,20) ,BUO(2,2,20) ,ENO(2,20)
COMMON/BEDPAR/TB ,BED(10) ,AIR(10) ,COAL(10) ,HOT(10) ,PTX(10,3)
COMMON/TRANSF/NS1 ,EM(6,20) ,BU(6,20) ,DEM(2,20) ,DBU(2,20)
COMMON/GASCON/GASX(11,22) ,GASB(11,22)
COMMON/SHAKE/SIV(20,4) ,CPROP(20,14)
COMMON/UNITS/IN ,IOUT ,SPECY(20)
COMMON/CONST/PP(5,20) ,GG(50)
COMMON/BURNS/VCOM(11) ,CM(5)
COMMON/EQUIL/NSE ,NLM ,AES(5,10)
C
GOTO (701,702,703,704,705) , JK
RETURN
C
C WRITE OUT FILE HEADING
C
701 DO 800 IT=1,3,2
WRITE(IT,100)
100 FORMAT(20X,' FLUIDIZED BED COMBUSTION OF COAL MODEL ')
C
C WRITE OUT BED CHARACTERISTICS
C
WRITE(IT,101)
101 FORMAT(30X,' STEADY STATE ',/,)
WRITE(IT,102)TB
102 FORMAT(' TEMPERATURE= ',1PE12.3,' K ')
WRITE(IT,103)BED(1) ,BED(8)
103 FORMAT(' BED AREA= ',1PE12.3,' M2 ',
*' BED HEIGHT= ',1PE12.3,' M')
WRITE(IT,104)AIR(3) ,AIR(4)
104 FORMAT(' OP. PRESSURE= ',1PE12.3,' PA ',
*' PRESSURE DROP= ',1PE12.3,' PA')
WRITE(IT,107)AIR(2) ,AIR(1)
107 FORMAT(' MIN. AIR VEL.= ',1PE12.3,' M/S ',
*' ACTUAL AIR VEL.= ',1PE12.3,' M/S ')
DC=PTX(4,1)*1000.0
DL=PTX(4,2)*1000.0
DB=PTX(4,3)*1000.0
WRITE(IT,110)DC ,DL ,DB
110 FORMAT(' DP (MM) COAL:STONE:BED = ',1P3E12.3,/)
IF(IT.EQ.1)GOTO 135
WRITE(IT,108)
108 FORMAT(' ', ' INTERMEDIATE RESULTS: EMULSION/BUBBLE ',/, ' ',
*' BED LEVEL MOLE FRACTIONS MOLE/M2.S')
WRITE(IT,109)
109 FORMAT(' ',4X,'XL',8X,'CO',8X,'O2',7X,'NO',8X,'SO2',7X,'TOTAL')
135 CONTINUE
800 CONTINUE

```

```

      RETURN
C
C      WRITE INTERMEDIATE RESULTS
C
702  WRITE(3,201)XL,EMO(1,1,1),EMO(1,1,8),EMO(1,1,5),
      *EMO(1,1,9),GASX(11,22)
      WRITE(3,202)XL,BUO(1,1,1),BUO(1,1,8),BUO(1,1,5),
      *BUO(1,1,9),GASB(11,22)
201  FORMAT(' ',1P6E10.2)
202  FORMAT(' ',1P6E10.2,/)
      RETURN
C
C      WRITE ENERGY BALANCE
C
703  WRITE(3,302)ENO(2,1),ENO(2,3),ENO(2,2)
302  FORMAT(' ', 'COAL KG/S=' ,1PE10.2, 'J IN=' ,1PE10.2, 'J BAL=' ,1PE10.2)
      WRITE(3,305)ENO(2,3),ENO(2,4),ENO(2,5)
305  FORMAT(' HEAT INPUTS:          COAL - AIR - SULPHATION ',/,
      *' ',1P3E10.2)
      WRITE(3,307)
307  FORMAT(' HEAT OUT: VAP H2O - UNBURNT HC - CHAR LOSS - SOLIDS ')
      WRITE(3,306)ENO(2,7),ENO(2,8),ENO(2,9),ENO(2,10)
      WRITE(3,308)
308  FORMAT(' HEAT OUT: CALCIN - IMMERSSED T - WALL LOSS - GASES ')
      WRITE(3,306)ENO(2,11),ENO(2,12),ENO(2,13),ENO(2,14)
306  FORMAT(' ',1P4E10.2)
      WRITE(3,301)
301  FORMAT(' ',40('*'))
      WRITE(3,303)ENO(1,1)
303  FORMAT(' ', 'NEW COAL FEEDRATE --> KG/S =' ,1PE10.2)
      RETURN
C
C      WRITE INTERMEDIATE RESULTS FOR FREEBOARD
C
704  WRITE(3,402)XL,EMO(1,1,1),EMO(1,1,2),EMO(1,1,8),
      *EMO(1,1,9),GASX(11,22)
402  FORMAT(' ',1P7E9.2)
      RETURN
C
C      WRITE FINAL RESULTS
C
705  CONTINUE
      WRITE(IOUT,502)
502  FORMAT(' ', 'PARAMETERS: ',/, ' -----')
      WRITE(IOUT,503)GG(46),GG(7)
503  FORMAT(' INTERPHASE FACTOR X/LMF',1PE12.3, ' RESIDENCE MULT.= ',
      *1PE12.3)
      WRITE(IOUT,505)GG(11),GG(10)
505  FORMAT(' SO2 CAPTURE CONSTANT ',1PE12.3, ' NOX REDUCTION = ',
      *1PE12.3)
      WRITE(IOUT,506)GG(13),GG(14)

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506 FORMAT(' CHAR KINETICS CONSTS. ',1PE12.3,' <--A      E--> ',
*1PE12.3)
WRITE(IOUT,507)GG(18),GG(20)
507 FORMAT(' CHAR COMB DIJ 298 ',1PE12.3,' FRAGMENT. FACTOR ',
*1PE12.3,/)
WRITE(IOUT,508)
508 FORMAT(' RESULTS: ',/,', '-----')
A=PTX(7,1)*3600.0
B=PTX(7,2)*3600.0
WRITE(IOUT,509)A,B
509 FORMAT(' COAL FEEDRATE = ',1PE12.3,' <KG/HR> STONE = ',
*1PE12.3)
PAIR=(AIR(6)-1.0)*100.0
WRITE(IOUT,510)PAIR,GG(2)
510 FORMAT(' % EXCESS AIR = ',1PE12.3,' CA/S RATIO = ',
*1PE12.3)
WRITE(IOUT,511)GG(36),GG(4)
511 FORMAT(' BED CHAR FRACTION = ',1PE12.3,' RECYCLE RATIO= ',
*1PE12.3)
A=GG(36)*GG(37)*3600.0
WRITE(IOUT,512)A
512 FORMAT(' CARBON LOSS STREAMS ',12X,' KG/HR OVERFLOW=',
*1PE12.3)
B=GG(43)*3600.0
C=GG(44)*3600.0
WRITE(IOUT,513)C,B
513 FORMAT(' RECYCLE PRODUCT = ',1PE12.3,' BAGHOUSE = ',
*1PE12.3)
WRITE(IOUT,565)ENO(2,3),ENO(2,12)
565 FORMAT(' COAL ENERGY IN' = ',1PE12.3,' J/S COOLING LOAD=',
*1PE12.3)
WRITE(IOUT,525)GG(47),GG(49)
525 FORMAT(' HEAT TRANS. COEFF= ',1PE12.3,' W/M2.K RADIATION=',
*1PE12.3,/)
WRITE(IOUT,514)
514 FORMAT(' GAS STREAMS TOP OF BED ... COMPOSITION MOLE FRACTION',
*/,21X,' EMULSION PHASE ',11X,' BUBBLE PHASE')
WRITE(IOUT,515)GASX(10,1),GASB(10,1)
515 FORMAT(' CO ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,516)GASX(10,2),GASB(10,2)
516 FORMAT(' CO2 ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,517)GASX(10,3),GASB(10,3)
517 FORMAT(' H2 ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,518)GASX(10,4),GASB(10,4)
518 FORMAT(' H2O ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,519)GASX(10,5),GASB(10,5)
519 FORMAT(' NO ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,520)GASX(10,6),GASB(10,6)
520 FORMAT(' NO2 ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,521)GASX(10,7),GASB(10,7)
521 FORMAT(' N2 ',1PE12.3,18X,1PE12.3)

```

```

WRITE(IOUT,522)GASX(10,8),GASB(10,8)
522 FORMAT('      O2              ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,523)GASX(10,9),GASB(10,9)
523 FORMAT('      SO2              ',1PE12.3,18X,1PE12.3)
WRITE(IOUT,524)GASX(10,10),GASB(10,10)
524 FORMAT('      CH4              ',1PE12.3,18X,1PE12.3,/)
WRITE(IOUT,530)
530 FORMAT('      GAS STREAM LEAVING BED ...
*/ ,21X, '      TOP OF BED          ',12X, 'TOP OF UNIT')
DO 590 I=1,20
BUO(1,1,I)=GASX(10,I)*GASX(10,21)+GASB(10,I)*GASB(10,21)
590 BUO(1,1,I)=BUO(1,1,I)/(GASX(10,21)+GASB(10,21))
WRITE(IOUT,515)BUO(1,1,1),EMO(1,1,1)
WRITE(IOUT,516)BUO(1,1,2),EMO(1,1,2)
WRITE(IOUT,517)BUO(1,1,3),EMO(1,1,3)
WRITE(IOUT,518)BUO(1,1,4),EMO(1,1,4)
WRITE(IOUT,519)BUO(1,1,5),EMO(1,1,5)
WRITE(IOUT,520)BUO(1,1,6),EMO(1,1,6)
WRITE(IOUT,521)BUO(1,1,7),EMO(1,1,7)
WRITE(IOUT,522)BUO(1,1,8),EMO(1,1,8)
WRITE(IOUT,523)BUO(1,1,9),EMO(1,1,9)
WRITE(IOUT,524)BUO(1,1,10),EMO(1,1,10)
C
C      CALCULATE CARBON EFFICIENCY, SULPHUR CAPTURE, AND NOX EMISSIONS
C
      FED=PTX(7,1)*3600.0
C      DRY BASIS
      FED=FED*(1.0-COAL(1))
      FEDC=FED*COAL(6)
      EFC=(FEDC-(A+B+C))/FEDC
      EFC=EFC*100.0
C      SULPHUR AND NOX
      FEDS=FED*COAL(10)
      FEDN=FED*COAL(9)
C      SULPHUR OUT
      SOUT=EMO(1,1,9)*GASX(11,22)*BED(1)*0.032064*3600.0
      EFS=(FEDS-SOUT)/FEDS
      EFS=EFS*100.0
C      NOX OUT
      XX=(EMO(1,1,5)+EMO(1,1,6))*GASX(11,22)*BED(1)*0.0140067*3600.0
      EFN=XX/FEDN
      EFN=EFN*100.0
      WRITE(IOUT,541)
541 FORMAT('      ',/, '      EFFICIENCIES %: ')
      WRITE(IOUT,542)EFC,EFS,EFN
542 FORMAT('      CARBON:',1PE12.3, ' S CAPTURE:',1PE12.3,
*/ ' NO/COAL N:',1PE12.3)
C
C      CARBON BALANCE ON SYSTEM
C      OPTIONAL : TO EXECUTE REMOVE C'S
C      CIN=FEDC+PTX(7,2)*GG(3)*432.0*GG(38)

```



```
C      COUT=(A+B+C)*CM(1)
C      EALL=EMO(1,1,1)+EMO(1,1,2)+EMO(1,1,10)
C      COUT=COUT+EALL*GASX(11,22)*0.012*BED(1)*3600.0
C      COUT=100.0*COUT/CIN
C      WRITE(IOUT,543)COUT
C543  FORMAT('      C % BALANCE OUT/IN = ',1PE12.3)
      RETURN
      END
```

```

SUBROUTINE XFACTR
C
C
C
CALCULATE INTERPHASE TRANSFER FACTOR
COMMON/OERALL/NS,XH,XL,TBU(2),EMO(2,2,20),BUO(2,2,20),ENO(2,20)
COMMON/BEDPAR/TB,BED(10),AIR(10),COAL(10),HOT(10),PTX(10,3)
COMMON/CONST/PP(5,20),GG(50)
C
C
C
ORIFICE JET HEIGHT
A=BED(1)*(AIR(1)-AIR(2))/GG(15)
A=A**0.35
B=125.0*PTX(4,3)/(0.0007+55.6*PTX(4,3))
BED(10)=B*A
C
LIMIT JET TO HALF OF BED HEIGHT
C=BED(8)*0.5
IF(BED(10).GT.C) BED(10)=C
C
C
C
BUBBLING THEORY TRANSFER FACTOR
C
C
C
BUBBLE DIAMETER
HF=0.8*BED(8)
IF(HF.GT.1.0) HF=1.0
HF=(1.0+6.8*HF)**1.2
HF=0.0085*HF*((1.0+27.0*(AIR(1)-AIR(2)))**0.3333)
C
BED DIAMETER AND FACTOR
ZETA=0.64
BD=2.0*((BED(1)/3.141593)**0.5)
IF(BD.GT.0.1) ZETA=1.60*(BD**0.4)
IF(BD.GT.1.0) ZETA=1.60
IF(HF.GT.BD) HF=BD
GG(45)=HF
C
C
C
TRANSFER FACTOR - X -
C
C
CHI=GG(17)
X=4.5*CHI*AIR(2)*BED(7)/(ZETA*HF)
X=X/((9.80665*HF)**0.5)
C
X/LMF
GG(46)=X/BED(7)
C
FACTOR MUST FALL WITHIN ACCEPTABLE BOUNDS
C
LIMITS 3< X/LMF <10
IF(GG(46).LT.3.0)GG(46)=3.0
IF(GG(46).GT.10.0)GG(46)=10.0
RETURN
END

```

FILE1 CONTAINS INPUT DATA 830309 -3/8+3/16C -6+20L

SPECIES

CO CO2 H2 H2O NO NO2 N2 O2 SO2 CH4 ????????????

BED

951.0 0.381 0.406 3.34 0.45
1100.0 7.0 8.0 9.0 0.10

AIR

1.90 2.0 101000.0 4.0 305.0
6.0 0.208 0.782 0.01 10.0

COAL

0.03 0.200 0.336 0.464 28172000.
0.647 0.041 0.047 0.011 0.054

HOT

16.0 0.380 0.0213 278.0 328.0
600.0 300.0 4184.0 298.0 0.2

PTX

0.71 0.71 0.71
1400.0 2200.0 1800.0
840.0 840.0 840.0

GG

10.0 3.00 0.98 0.857 0.90
1.0 10.0 5.0 9.0 0.0070
0.35 0.004 9000.0 -18000.0 400.0
0.8 0.45 0.0002 720.0 0.5

SIV ----->

COAL	LIME	BED
25.0	0.0	0.0
19.0	0.0	0.0
12.5	0.0	0.0
9.5	0.0223	0.0000
6.3	0.5879	0.0000
4.0	0.3232	0.0020
2.8	0.0232	0.0440
2.0	0.0160	0.2690
1.4	0.0038	0.4050
1.0	0.0023	0.2300
0.71	0.0000	0.0340
0.5	0.0017	0.0050
0.355	0.0013	0.0035
0.25	0.0014	0.0075
0.18	0.0015	0.0000
0.125	0.0024	0.0000
0.090	0.0016	0.0000
0.063	0.0029	0.0000
0.045	0.0000	0.0000
0.0	0.0085	0.0000

EQUIL

0603

1.00.01.00.00.0
1.00.02.00.00.0
0.02.00.00.00.0
0.02.01.00.00.0

0.00.01.01.00.0

0.00.02.01.00.0

0.00.00.02.00.0

0.00.02.00.00.0

0.00.02.00.01.0

1.04.00.00.00.0

DATA OK

ENDOS

FLUIDIZED BED COMBUSTION OF COAL MODEL
STEADY STATE

TEMPERATURE= 1.224E+03 K
 BED AREA= 1.547E-01 M2 BED HEIGHT= 6.133E-01 M
 OP. PRESSURE= 1.010E+05 PA PRESSURE DROP= 4.854E+03 PA
 MIN. AIR VEL.= 9.322E-01 M/S ACTUAL AIR VEL.= 1.900E+00 M/S
 DP (MM) COAL:STONE:BED = 1.611E+00 1.572E+00 1.572E+00

PARAMETERS:

 INTERPHASE FACTOR X/LMF 9.113E+00 RESIDENCE MULT.= 1.000E+01
 SO2 CAPTURE CONSTANT 3.500E-01 NOX REDUCTION = 7.000E-03
 CHAR KINETICS CONSTS. 9.000E+03 <--A E--> -1.800E+04
 CHAR COMB DIJ 298 2.000E-04 FRAGMENT. FACTOR 5.000E-01

RESULTS:

 COAL FEEDRATE = 2.918E+01<KG/HR> STONE = 1.461E+01
 % EXCESS AIR = 3.388E+00 CA/S RATIO = 3.000E+00
 BED CHAR FRACTION = 4.979E-03 RECYCLE RATIO= 8.570E-01
 CARBON LOSS STREAMS KG/HR OVERFLOW= 5.090E-02
 RECYCLE PRODUCT = 4.949E-02 BAGHOUSE = 3.845E-02
 COAL ENERGY IN = 2.284E+05 J/S COOLING LOAD= 9.479E+04
 HEAT TRANS. COEFF= 2.530E+02 W/M2.K RADIATION= 9.906E+01

GAS STREAMS TOP OF BED ... COMPOSITION MOLE FRACTION

	EMULSION PHASE	BUBBLE PHASE
CO	1.401E-03	1.459E-05
CO2	1.605E-01	1.387E-01
H2	3.819E-04	3.965E-06
H2O	7.230E-02	5.936E-02
NO	1.421E-03	1.348E-03
NO2	9.502E-07	9.619E-07
N2	7.434E-01	7.525E-01
O2	1.821E-02	4.671E-02
SO2	1.780E-03	1.382E-03
CH4	5.728E-04	5.937E-06

GAS STREAM LEAVING BED ...

	TOP OF BED	TOP OF UNIT
CO	6.660E-04	5.092E-04
CO2	1.489E-01	1.503E-01
H2	1.815E-04	8.832E-05
H2O	6.544E-02	6.635E-02
NO	1.382E-03	1.386E-03
NO2	9.564E-07	9.561E-07
N2	7.482E-01	7.480E-01
O2	3.332E-02	3.168E-02
SO2	1.569E-03	1.584E-03
CH4	2.722E-04	1.325E-04

EFFICIENCIES %:

CARBON: 9.924E+01 S CAPTURE: 6.351E+01 NO/COAL N: 6.853E+01