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IMPROVING ASPEN/SP COMPUTER MODEL OF GREAT PLAINS COAL GASIFIERS

by

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Bachelor of Science, Bangladesh University of
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Submitted to the Graduate Faculty
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This thesis, submitted by Md. Moazzem Hossain in partial fulfillment of the requirements for the degree of Master of Science from the University of North Dakota, has been read by the Faculty Advisory Committee under whom the work has been done and is hereby approved.

John Erjavec
(Chairperson)

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Charles F. Moretti

This thesis meets the standards for appearance, conforms to the style and format requirements of the Graduate School of the University of North Dakota, and hereby approved.

Harvey Knull
Dean of the Graduate School

6-29-95

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Title	Improving ASPEN/SP Computer Model of Great Plains Coal Gasifiers.
Department	Chemical Engineering
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Date 06-21-95

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ABSTRACT

The Great Plains Gasification Plant located in Beulah, North Dakota, operated by the Dakota Gasification Company (DGC) is the only commercial production plant in the United States making synthetic natural gas (SNG) from coal. DGC operates 14 Lurgi gasifiers to produce 158 million ft^3/day of SNG from 17,000 tons of North Dakota lignite coal. As the first step in constructing a model of the entire plant to control its operation and optimize the economic performance, an ASPEN/SP computer model (called RGAS) of a Lurgi gasifier was developed with the combined effort of several researchers. RGAS will predict the impact of changes in inputs on production rates and efficiency.

The model parameters (i.e., kinetic constants, heat transfer coefficient to the reactor wall, heat capacity of the volatiles, etc.) were previously optimized in different stages to obtain the best possible model predictions. Unfortunately, the model did not predict the output variables within desirable accuracy, necessitating further improvements to the RGAS model. In this study some model improvements were made or tried.

The FORTRAN routine, which models the combustion and gasification zones in the gasifier, requires an iterative approach for solution. The efficiency of the FORTRAN code has been enhanced by changing the convergence scheme, which reduced the simulation time by 75%. In addition, a Hooke-Jeeves pattern search algorithm has been

included in the RGAS subroutine URE09, so that any optimization of parameters can be done automatically. This made optimization easy and efficient.

Contrary to the actual volatile evolution, RGAS assumes devolatilization to be a linear, temperature dependent evolution of volatile matter. However, limited data on North Dakota lignite and available literature information indicate that the temperature dependence of volatile evolution is non-linear. A non-linear devolatilization model was tried, but it did not result in any significant improvements in the RGAS predictions so, the simple linear model was retained.

An optimized value of 1.7 for the activity of carbon was included in the definition of the equilibrium constants of the reversible reactions (previously it was assumed to be unity), which improved the flow predictions significantly. This can be justified by the fact that amorphous carbon from lignite coal has higher free energies than graphite.

This research project has been very successful. After the improvements were incorporated into the RGAS model, it predicted nine of the ten responses studied (the exception being reactor steam utilization) within the accuracy of the data.

The RGAS model is now complete, in terms of giving good predictions for the coal (lignite) used during the study period. However, kinetic parameters vary with coal composition since several of the reactions are catalyzed by the metals present in the coal. The addition of metal composition catalytic effects would allow predictions to take into account changing coal composition. This is recommended as the next step in making the RGAS model even more valuable as an optimization and control tool for the DGC plant in Beulah, North Dakota.

Chapter 1

INTRODUCTION

Coal represents a substantial fraction of the estimated recoverable fossil fuel resources of the world and may become an increasingly important source of hydrocarbon fuels and feedstocks. In the United States, where coal is estimated to be about 70% of recoverable fossil fuel resources (1), petroleum and natural gas resources are so low that an alternative is imperative. National recognition of the immediate and long-range potential of coal has resulted in substantial efforts toward the development of economically and environmentally viable coal utilization technologies.

Interest in clean gaseous fuels from coal has been stimulated by the introduction of environmental constraints and the significant decline of proven and recoverable U.S. natural gas reserves. Natural gas is currently abundant in U.S. reservoirs and could last 35 years before the supplies run short. But coal supplies within U.S. borders are expected to last 300 years (2), and one way to extend the natural gas supply is to develop coal gasification technologies. Cleanliness and energy efficiency are bringing coal gasification from the pilot plant stage into commercial application.

The United States depends heavily on oil (Figure 2) (2), of which 42% is imported from potentially unreliable foreign suppliers. From past experience everybody recognizes the effect of a change in oil supply on economic stability. Concerns over continued U.S.

dependence on imported oil, and more importantly, increasing environmental restrictions on conventional coal fired power plants, are driving research and development of alternative energy sources. One alternative energy process being developed is coal gasification. The main concerns with conventional coal burning are the emissions of NO_x and SO_x which are regulated by the Environmental Protection Agency. Coal gasification involves converting coal to a synthetic gas by heating it under pressure in the presence of steam and oxygen. Coal is the most abundant fossil fuel in the United States, with

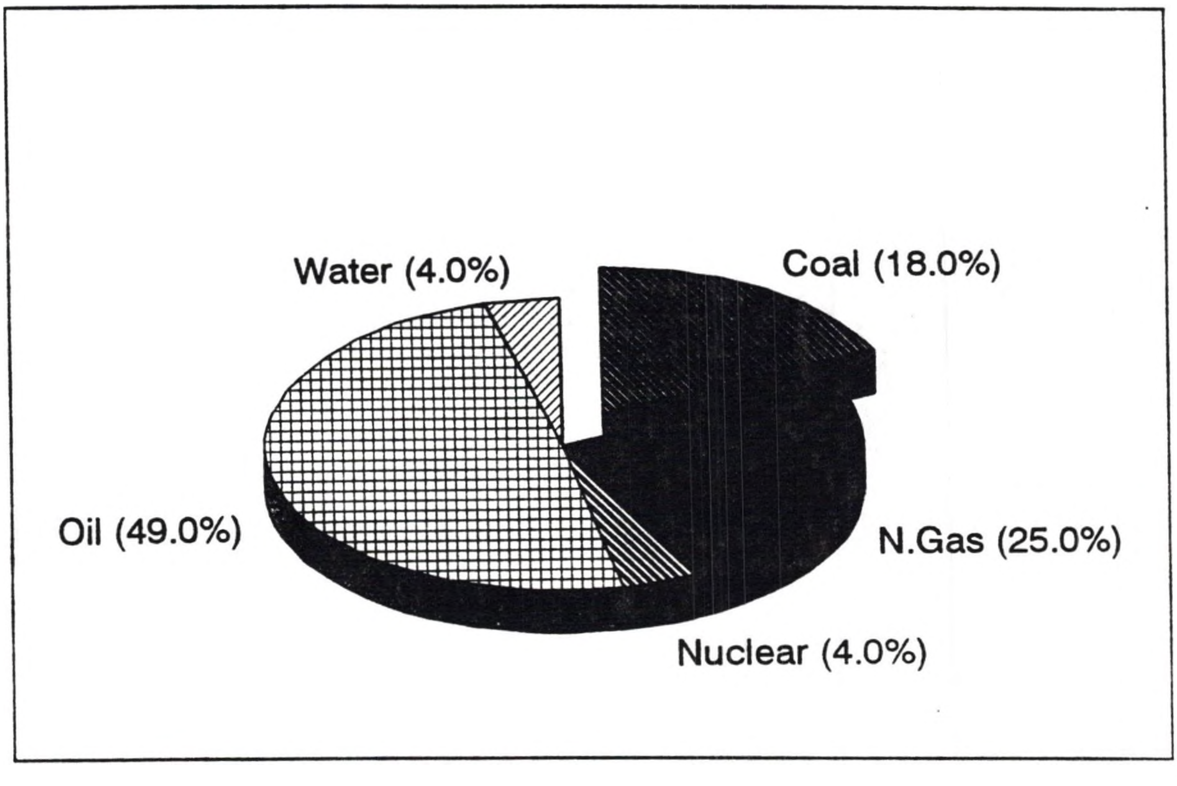

Figure 1 Source wise U.S. Energy Consumption

reserves far in excess of oil or gas (as stated earlier), and neither embargo nor war will endanger the flow of fuel for this technology.

It is expected that gasification will be the core technology for future power generation. The primary driving factors for coal gasification development are the environmental regulations which restrict the amount of SO_x, NO_x, and particulates that can be produced by coal burning plants. An inherent environmental advantage of coal gasification over conventional coal fired power plants, is the ease of sulfur removal in the former process. In gasification sulfur is removed in almost pure form and can be sold commercially at a profit. Using coal gasification, a fuel gas can be manufactured to any level of cleanliness. In addition to readily available domestic sources and a favorable environmental record, coal gas plants are 10 to 20 percent more energy-efficient than conventional coal-fired power plants (11).

The main problem that coal gasification still faces is the challenge of high construction costs -- up to 15 percent higher than conventional coal-fired power plants (11). It costs about $1400 per kilowatt of installed capacity, compared to $1300 for a traditional coal-fired power plant. Increasing the efficiency of coal gasification plants even further could make up for the higher capital costs of plant construction. Among the companies that have incorporated combined-cycle systems and gas turbines into their coal gas technologies are Shell Oil Co., Dow Chemical Co., and Texaco Inc. Because of their cleaner performance, coal gasification plants could pass through the permitting process more easily than conventional coal-burning plants. As environmental restrictions increase, the older coal-burning power plants are facing difficulties maintaining EPA performance standards. They need to be upgraded or replacement. Clearly, coal gasification should create an economic opportunity for companies pursuing this technology, to provide a clean and efficient supply of energy.

Coal by nature is a complex substance in its structure and composition. Because of this complex nature, many complex reactions occur during coal gasification and much research is needed to understand the gasification process and to locate optimum operating conditions.

The Great Plains Gasification Plant located in Beulah, North Dakota, operated by the Dakota Gasification Company (DGC) is the only commercial production plant in the United States making synthetic natural gas (SNG) from coal. DGC operates 14 Lurgi gasifiers to produce 158 million ft^3/day of SNG from 17,000 tons of North Dakota lignite coal.

The production process at DGC uses conventional moving bed Lurgi gasification technology (which produces mainly CO and H_2) followed by methanation. This plant can produce a nearly pure methane product, and continued research on it is of prime importance to present and future generations of energy consumers. DGC has a long range goal of developing a computer model of the entire plant which they can use for optimization and supervisory control. As the first step of this goal, an ASPEN/SP computer model (called RGAS) of a Lurgi gasifier was developed and soon after, the GPGP optimization phase was initiated. The goal of the optimization phase was to obtain the best possible model predictions by adjusting the model and reaction parameters. Operating data from DGC was available for comparison. The model and reaction parameters (i.e., heat transfer coefficient, kinetic constants, heat capacity of volatiles, etc.) were previously adjusted in different stages to improve the model predictions. But it did not predict the output variables within desired accuracy, necessitating a further improvement of the RGAS model.

Chapter 2

BACKGROUND

The concept for a gasification plant - feeding North Dakota lignite and using water from the nearby Lake Sakakawea reservoir - surfaced in the early 1970s with a national commitment to greater energy independence. A consortium of five energy companies invested about $550 million in the project and financed the remaining cost of the $2.1 billion project with federally guaranteed loans (16). Basin Electric Power Cooperative, headquartered in Bismarck, North Dakota, worked with the consortium in developing joint mine, rail and water delivery facilities during the construction of the gasification plant and the Antelope Valley Station (AVS).

Construction of the synfuels plant began in 1980 and, in April 1984, the plant produced its first synthetic natural gas. It began manufacturing gas for sale in July that year. However, when oil prices resumed a very low pre-recession level in the mid 80s, the revenue from the sale of natural gas in the market was too little to pay the financers. In 1985 when the U.S. Department of Energy (DOE) denied the consortium's request to get additional federal assistance, the five partners defaulted on their $1.5 billion loan and abandoned the project. In the same year the DOE foreclosed on the project, became its owner, and operated it for about three years.

In 1988, after going through a bidding process, the DOE sold the plant to Dakota Gasification Company (DGC), a Basin Electric subsidiary formed to own and operate the plant. The purchase of the synfuels plant by DGC included profit sharing. The government will share profits from sales of natural gas up to the full amount of the loan default by the original owners. The gas produced at Great Plains is purchased by four interstate pipeline companies. Under their agreements with DGC, the pipelines purchase 100 percent of the gas until the year 2009.

The Great Plains Gasification Plant made a commitment to understand and optimize plant operation. Since plant experimentation is both expensive and limited in terms of the number of variables that can be studied and their allowable ranges, the long range goal is to build a computer model of the whole plant for use in optimization and supervisory control. The process simulator software package, ASPEN/SP was selected by GPGP as the framework for this computer model. As the first step toward this goal, the FORTRAN model of a Lurgi Gasifier called RGAS (written in 1984 by B. Benjamin of Scientific Design Company, and modified in 1985 by J. Dweck of JSD Inc) was obtained from DOE. Further modifications were made between 1990 and 1993 by Simulation Sciences. A number of models had been developed and published for simulating the behavior of a moving bed gasifier. RGAS incorporates two of them and allows the user to select which one is to be used. The two models available are the DENN model, developed at the University of Delaware by Denn, Yoon, and Wei, and the WEN model, developed at the University of West Virginia. The performance of the two models was compared by J. Stefano of DOE. He found the DENN model to be superior in terms of convergence and it seemed to be as capable of predicting gasifier performance, so that model was selected for further attention.

The first phase of GPGP Gasifier Optimization, was done by Jonathan Kautz and supervised by John Erjavec (University of North Dakota), during the period of May 1990 to July 1991. In this study the volatiles had been thoroughly characterized. The mass fraction of each of 97 different organic species (in addition to O_2, H_2O, H_2, CO, CO_2,CH_4, N_2, and Ar) had been determined and split between the Rectisol naptha stream, the phenol stream, and the tar oils stream. The kinetic rate constants for gasification and combustion were also adjusted to fit plant data as close as possible. After these improvements, some of the ten responses examined were predicting reasonably well, but some of them were disappointing, and they recommended further study of other parameters such as equilibrium constants, heat transfer coefficient to the wall etc.

The second phase GPGP Gasifier Optimization was done by Bradley C. Carpenter (a graduate student supervised by John Erjavec,University of North Dakota) (2), during the period of May 1992 to May 1993. In this study the following model improvements had been made:

- The predicted flow of condensible volatile matter was corrected to allow for significant amount of noncondensible volatile matter produced during devolatilization.
- The heat transfer coefficient of the reactor vessel was reduced by matching steam production and enthalpy predictions to experimental data.
- The kinetic rate constants used in the RGAS model were adjusted to provide the best possible predictions.

- The predicted raw gas temperature was made to match the plant data by adjusting the specific heat of the volatiles.

After these improvements, the outlet gas compositions and temperature predictions were excellent, but the predictions of inlet coal flow, outlet gas flow, and fixed carbon conversion were very poor.

This thesis continues their work with the following objectives:

- Include a more realistic devolatilization mechanism in the RGAS model.
- Find a more appropriate value for the activity of carbon, which defines the equilibrium constants of the chemical reactions.
- Enhance the efficiency of the RGAS FORTRAN code in order to reduce simulation time.
- Optimize the rate constants further.

Chapter 3

RGAS DESCRIPTION

Overview of Process

The high-pressure Lurgi gasifier dominates oxygen blown, moving-bed gasification, since it is the essential part of the only viable process currently available for the production of Synthetic Natural Gas (SNG) from coal (4).

The Lurgi gasifier, the principal features of which are illustrated diagrammatically in Figure 3.1, has been progressively improved and refined by the developers of Lurgi Kohle und Mineraloltechnik GmbH of Frankfurt, Germany, since the first plant was built in 1936 (5). It employs a moving bed, it is steam and oxygen blown and it operates at pressures around 30 bar. Graded coal is supplied via a lock hopper to a distributor which spreads it uniformly across the top surface of the bed. An agitator is attached to the distributor to break up agglomerates as they form in the devolatilization zone. The coal bed is supported on a rotating grate through which the gasifying agents (steam and oxygen) are supplied and ash is withdrawn. Gases rise up the bed in counter-current heat exchange and mass transfer with the coal and leave the top of the reactor together with the unreacted steam at a temperature of about 500 F. The Lurgi gasifiers at the Beulah plant each have a reactor vessel 40 feet high with a diameter of 13 feet. The settling coal is first heated and dried by the countercurrent gas stream and then devolatilized. Those

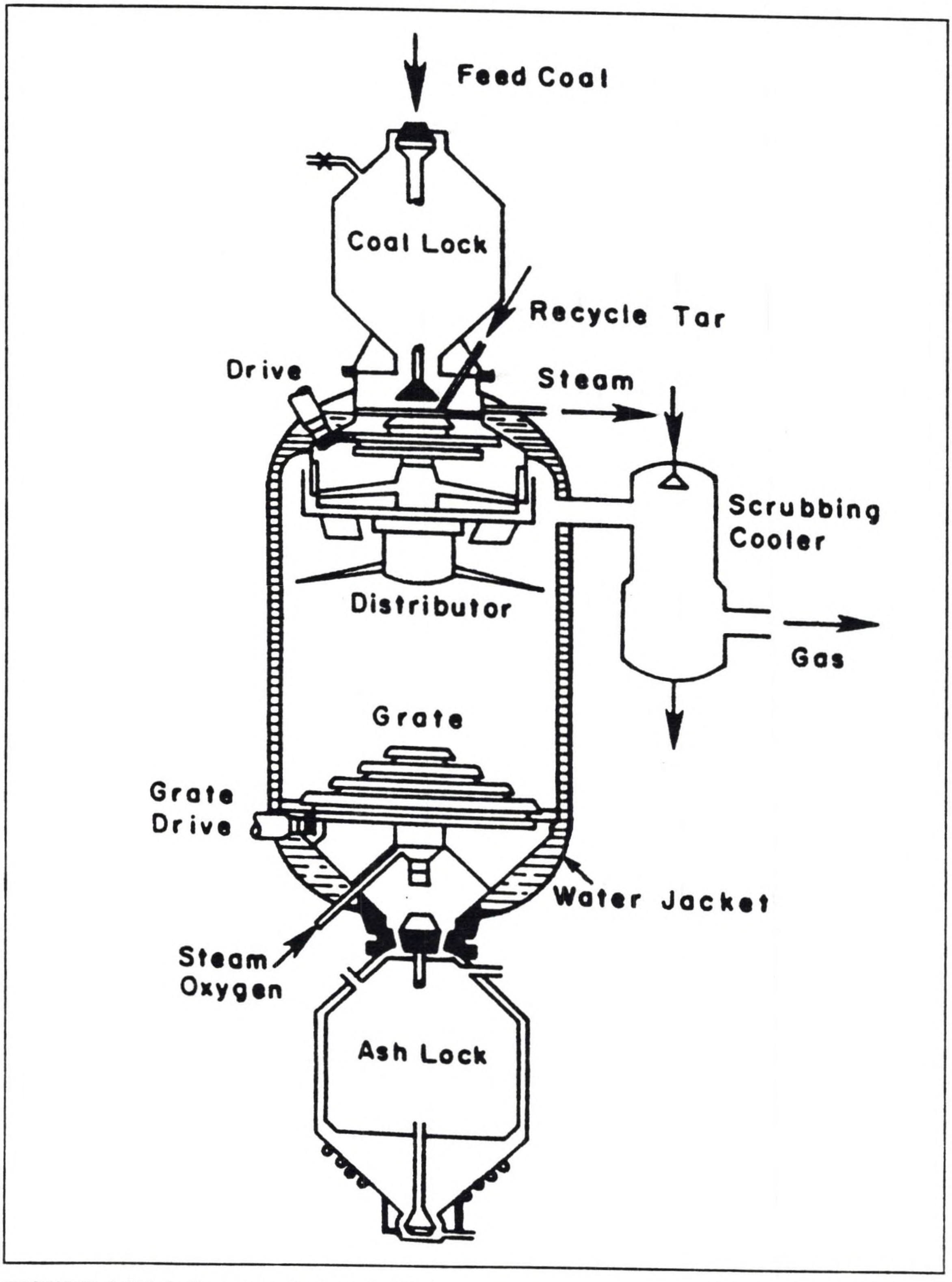

FIGURE 2 High Pressure Lurgi Gasifier

processes leave only fixed carbon to react with steam, hydrogen, and carbon monoxide. The exothermic combustion of a portion of the fixed carbon with oxygen occurs near the bottom of the reactor, which provides the heat needed for the endothermic gasification and drying.

A water jacket on the wall, where part of the process steam is produced, cools the coal and gas near the wall, and thus has a major effect on the energy balance there. The low thermal conductivity of the coal bed keeps the central portion of the gasifier unaffected by the heat loss. A steep radial temperature gradient results near the wall. The thermodynamic and kinetic properties are sensitive to the local temperature, which leads to a radial gradient of both gas composition and the extent of carbon conversion.

Zones in the gasifier

As the coal travels downward through the coal bed it is exposed to different temperatures and gas concentrations. Depending on these conditions, different processes may occur. Four zones have been identified in a gasifier (starting from the bottom): combustion, gasification, devolatilization, and drying. At the top of the bed, the coal is first heated and then water is vaporized in the drying zone. In the next zone, tars, oils, and light hydrocarbons present in the coal are evolved, and it is called the devolatilization zone. Fixed carbon formed in the devolatilization zone reacts with steam, hydrogen, and carbon dioxide under high temperature and pressure in the gasification zone. At the bottom of the coal bed, injected oxygen reacts with the remaining carbon to produce heat in the combustion zone.

ASPEN/SP

Advanced System for Process Engineering (ASPEN) is a software system for computer-aided process design was developed at M.I.T. during the period 1976 to 1981 under the sponsorship of the Department of Energy and 55 industrial participants. Simulation Sciences, a company headquartered in Denver, Colorado, has updated ASPEN and added an expert system front end (SPEXPERT) to make it more versatile and user-friendly. They market the updated version under the name, ASPEN/SP. ASPEN/SP is the package chosen by DGC to provide the framework for a model of their plant.

Several types of blocks can be defined in the input file for the purpose of process design and/or economic analysis. ASPEN/SP can incorporate user-defined design specification blocks that allow the operator to stipulate that a calculated (output) variable attain a specified value by varying an input variable. Partial or complete reports can be generated along with table and graph files. On many occasions it is necessary for the user to insert FORTRAN block statements into the flowsheet computations to perform auxiliary calculations. The advantage of using these techniques is that computer processing and user editing time is reduced since the input file needs only to be edited, compiled, and linked once.

An ASPEN/SP simulation is broken into four operations. First, the input translator processes the user input file, enters all data regarding the process into a file called a Problem Data File (PDF), and writes the main calling program. Any FORTRAN statements supplied by the user are converted into FORTRAN subroutines and a physical property initialization subroutine is written. Second, these subroutines are compiled and linked to create a simulation program. Third, the simulation program reads data from the PDF, makes the necessary calculations, and writes the results back to the same PDF. Finally, the Report Writer generates a report using the simulation results from the PDF.

The SPEXPERT system allows the user to construct a flow diagram by defining unit operation blocks, specifying component streams entering and leaving the blocks, and specifying the physical properties of the system. From this, the SPEXPERT system can generate an input file to be used by ASPEN/SP during the simulation.

Model Development

Based on the available literature review a one dimensional model was selected for ASPEN simulation work. The 1-D model assumes plug flow of gas and solids, and that there is no radial gradients in either temperature or composition. The latter is a good assumption if the reactor is adiabatic. However, for the Lurgi gasifier, which has a cooling jacket, there are significant radial profiles in parts of the bed. Differences between the raw gas compositions predicted by the one and two dimensional models are relatively small (3) and considered to be within the accuracy of the plant data available for validation.

The temperature profiles vary significantly in the vicinity of the wall. In a Lurgi gasifier, the variations in coal temperature are limited, through most of the bed height, to within a outer ring near the wall, and the area of this outer ring is about 30 percent of the cross sectional area of the gasifier. The maximum temperature predicted for the gasifier is the same regardless of which model is used. However, the location of the hotspot differs between the two models. It moves downward as the wall is approached. The two models also predict different raw gas temperatures. The one dimensional model predicts a raw gas temperature about 40 F higher than the 2-D model. The 2-D model also predicts about twice the steam generation rate as the two-zone 1-D model developed by Yoon et al. (15). It appears that the one-dimensional model predicts the raw composition and the maximum solids temperature about as well as a 2-D model. The discrepancy in steam generation rate can be reduced by adjusting the heat transfer coefficient to the wall. Based on these observation Benjamin and Ringard (7) concluded that the one dimensional model was adequate for ASPEN simulation work.

Mass and Energy Balances

Solid phase constituent mass balance: A mass balance on the jth solids constituent at a distance z from the bottom of the coal bed gives:

$$-\frac{d(Sx_j)}{dz} = Ac \sum_{k=1}^{N_k} a_{j,k} R_k \quad , \qquad j = 1, \ldots\ldots, N_s \tag{3.1}$$

where S is the solids flow rate,

x_j is the mole fraction of constituent j in the solids,

Ac is the cross sectional area of the gasifier,

R_k is the rate of the kth reaction in the solids,

$a_{j,k}$ is the stoichiometric coefficient for the jth constituent and the kth reaction in the solids,

N_k is the number of solid phase reactions included in the model,

N_s is the number of solid phase constituents included in the model.

For the solid phase there will be one mass balance for each element of the ultimate analysis (ash, carbon, hydrogen, nitrogen, chlorine, sulfur, and oxygen) and each component of the proximate analysis (water, fixed carbon, volatile matter, and ash).

Gas phase constituent mass balance: Each of the solid phase reactions produces one or more gas phase products. The generation rate of the i^{th} gas phase constituent denoted by g_i is given by:

$$g_i = Ac \sum_{k=1}^{N_k} b_{i,k} R_k \,, \qquad i = 1 \,, \ldots \ldots \ldots \ldots \,, N_g \qquad (3.2)$$

where

$b_{i,k}$ is the stoichiometric coefficient of the i^{th} gas phase constituent with respect to the k^{th} solid phase reaction

N_g is the number of gas phase constituents included in the model.

A component balance on the i^{th} constituent in the gas phase gives:

$$\frac{d(Gy_i)}{dz} = g_i + Ac \sum_{l=1}^{N_L} c_{i,l} R_l \,, \qquad i = 1 \,, \ldots \ldots \ldots \,, N_g \qquad (3.3)$$

where

G is the total gas flow rate,

y_i is the mole fraction of the i^{th} constituent in the gas phase,

R_l is the l^{th} gas phase reaction rate,

$c_{i,l}$ is the stoichiometric coefficient of the i^{th} gas phase constituent with respect to the l^{th} gas phase reaction,

N_L is the number of gas phase reactions included in the model.

For the gas phase, there will be one mass balance for each chemical species appearing in the raw gas, and one mass balance for oxygen.

Solid Phase Energy Balance: An energy balance on the solid phase gives:

$$-\frac{d(SHs)}{dz} = U_{GS}A_{GS}(T_G - T_S) - \sum_{i=1}^{N_i} g_i H_{Gi} + U_{cs}A_w(T_c - T_s) \tag{3.4}$$

where

H_S	is the enthalpy of the solids,
H_{Gi}	is the enthalpy of the ith component evaluated at the solids temperature T_S,
U_{GS}	is the heat transfer coefficient between the solids and the gas,
U_{CS}	is the heat transfer coefficient between the coolant in the jacket surrounding the reactor and the solids,
A_{GS}	is the heat transfer area per unit length of the gasifier,
A_W	is the heat transfer area of the coolant jacket wall per unit length,
T_S	is the temperature of the solids,
T_C	is the temperature of the coolant in the jacket,
T_G	is the temperature of the gas.

Gas Phase Energy Balance: An energy balance on the gas phase gives:

$$\frac{d(GH_G)}{dz} = U_{GS}A_{GS}(T_S - T_G) + \sum_{i=1}^{N_i} g_i H_{Gi} + U_{CG}A_W(T_C - T_G) \tag{3.5}$$

where

H_G	is the enthalpy of the gas,

U_{CG} is the heat transfer coefficient between the coolant in the jacket around the wall and the gas.

It is assumed that the enthalpies of the solids (H_S) and gas (H_G) can be evaluated using the ideal mixture rule:

$$H_S = \sum_{j=1}^{N_J} X_j H_{Sj} \, , \qquad H_G = \sum_{i=1}^{N_I} y_i H_{Gi} \tag{3.6}$$

where

H_{Sj} is the enthalpy of the jth solid phase constituent,

H_{Gi} is the enthalpy of the ith gas phase constituent.

The solid phase (and likewise, gas phase) enthalpy (H_S) can be written in terms of heat capacities and heats of reaction.

$$\frac{d(SH_S)}{dz} = H_S \frac{dS}{dz} + SC_{Pj} \frac{dT}{dz} + \sum_j \left(\frac{h_S}{y_j} \frac{dy_j}{dz} \right) \tag{3.7}$$

In order to complete the model we need to specify each of the reaction rates, i.e. the R_k and the R_l, as functions of pressure, temperature, and gas and solids compositions. These are evaluated using intrinsic kinetics for the gas phase reactions. Combined kinetics and mass transfer effects through porous media are used for the solid phase reactions. The University of Delaware model and the West Virginia University model, which specified those expressions were chosen from several available models for use in RGAS. These expressions are given in standard form, so the various derivatives with respect to z must be expanded and rearranged so that they become ordinary differential equations in the variables S, G, x_j, y_j, T_S, and T_G.

The solution to these equations is a multivariable boundary value problem. The flow rate, composition, and temperature of the gas entering the gasifier at the bottom are specified. So are the coal feed rate, temperature, and composition at the top. These are taken as simulation boundary conditions. An iterative procedure is required to determine the unknown initial conditions at the bottom for the solids phase variables so that integration of these equations from these initial conditions will match the corresponding boundary conditions at the top.

Kinetic Models

As stated earlier, two kinetic models (the University of Delaware (DENN) kinetic model, and the West Virginia University (WEN) kinetic model) were chosen from several available models for using in RGAS. Both models use the temperature dependent Arrhenius equation for the kinetic and equilibrium constants to determine reaction rates. The Arrhenius equation is written as:

$$K_j = A_j^{\circ}\exp\left(\frac{E_j^{\circ}}{RT}\right) \tag{3.8}$$

where,

A°	is a pre-exponential factor,
E°	is an activation energy,
K_j	is the kinetic or equilibrium constant for reaction j,
R	is the gas constant,
T	is the absolute temperature.

The kinetic parameters depend on the specific coal type, while the equilibrium parameters are fixed by thermodynamic properties. The DENN model (Table 3.1) includes five reactions. All reactions, except combustion, are reversible in this model. The first four reactions are heterogeneous, while the last reaction occurs in the gas phase. This reaction, the water gas shift, is catalyzed by coal particles.

TABLE 1 DENN Kinetic Model

Model Reactions	Rxn Heat (KJ/Kgmole)	Process	Equilibrium Parameters A°	E°(cal/mol)
1. $1^2/_3C + O_2 \rightarrow {}^2/_3CO + {}^2/_3CO_2$	393790	Combustion	-*	-*
2. $C + H_2O \rightarrow CO + H_2$	-175440	Steam-Carbon	$3.098(10^7)$	32457
3. $C + CO_2 \rightarrow 2CO$	-172580	Bouduard	$1.222(10^9)$	40300
4. $C + H_2 \rightarrow CH4$	74900	Hydrogasification	$1.472(10^{-6})$	-21854
5. $CO + H_2O \rightarrow CO_2 + H_2$	2853	Water-Gas Shift	0.0265	-7860

* Irreversible

There are various ways to physically model a coal pellet. The Ash Segration model assumes that the ash layer is removed from the coal pellet by melting or movement in the bed. The Shell Progressive model assumes that the ash remains in position around the coal during the course of any reactions, and the fixed carbon is contained in a shrinking core internal to the ash layer. The Homogeneous model assumes the ash and carbon are a homogeneous mixture. The Ash Segregation model was chosen for RGAS because it gives a higher peak temperature than the Shell Progressive model. The peak temperature is an indication of whether or not the ash from the coal will melt, thus causing gasifier operation to cease (because the type of Lurgi gasifier used by DGC can be operated only in dry ash condition). Therefore, the Ash Segregation model offers a more conservative estimation of the gasifier operating limits than does the Shell Progressive model.

The kinetic expressions for the net forward reaction rates using the Ash Segregation model are defined using intrinsic kinetics and an effectiveness factor. The rate expressions for the combustion and steam-carbon reactions (Reactions 1 & 2) are of the same form and are given by:

$$R_{i,j} = \frac{(1-\varepsilon_b)(P_i - P_i^*)V_c}{\dfrac{d_p{}^{\circ}(r_{part} - r_{core})}{6\ r_{core} K_{p,i}} + \dfrac{1}{\eta_i K_{r,j}[C]^{\circ}}} \qquad (3.9)$$

where $R_{i,j}$ is the j^{th} reaction rate of species i

$$K_{p,i} = \frac{2.06\ F_G{}^{0.425}}{P\varepsilon_b Sc^{0.092}}\left(\frac{PD_i}{d_p RT}\right) \quad \text{is the film mass transfer coefficient} \qquad (3.10)$$

$$\eta_j = \frac{3}{\phi_j^2}(\phi_j\ \coth\phi_j\ - 1) \quad \text{is the effectiveness factor for reaction j} \qquad (3.11)$$

$$\phi_j = \frac{d_p{}^{\circ} r_{core}}{6}\sqrt{\frac{K_{r,j}[C]^{\circ}RT}{\gamma_j\ D_{ei}\ r_{part}}} \quad \text{is the Thiele modulus} \qquad (3.12)$$

$$V_c = \frac{w\rho_c}{x\rho_a + (1-x)\rho_c\ f_{ash}} \qquad (3.13)$$

and w is the fraction of carbon remaining in a particle,

x	is the fractional conversion,
ρ_c	is the density of the original coal,
ρ_a	is the density of the ash,
f_{ash}	is the weight fraction of ash,
D_{ei}	is the effective diffusivity in particle core,
D_i	is the bulk gas diffusivity in particle core,
γ_j	is 1 for steam-carbon reaction, and 4/3 for combustion reaction,
P_i	is the partial pressure of component i,
P_i^*	is the equilibrium partial pressure (zero for combustion),
d_p^O	is the initial solid particle diameter,
r_{core}	is the radius of char core,
ε_b	is the bed void volume,
$[C]^O$	is the initial concentration of fixed carbon in the particle,
Sc	is the Schmidt number,
F_G	is the molar gas flow rate,
K_{rj}	is the reaction rate coefficient for reaction j.

The driving force of the reaction, $(P_i - P^*_i)$ in equation (3.1) can be represented as mole fractions and expanded to include each species in the reaction:

$$(P_i^{\nu_i} - P_i^{*\nu_i}) = P^{\nu_i}(y^{\nu_i} - y^{*\nu_i}) \tag{3.14}$$

where ν_i is the stoicheometric coefficient for species i. After substituting this in the driving force term, equation (3.1) becomes:

$$\left(y_{O_2} - \frac{y_{CO}^{\,q-1}\, y_{CO_2}^{\,2-q}}{K_{p1}^{eq}}\right) \qquad \text{for reaction 1 (combustion)} \tag{3.15}$$

$$P\left(y_{H_2O} - \frac{y_{CO}y_{H_2}}{K_{p2}^{eq}}\right) \qquad \text{for reaction 2 (steam - carbon)} \tag{3.16}$$

where y_i is mole fraction of species i and q is defined as the selectivity of the combustion reaction and represents the ratio of carbon monoxide and carbon dioxide produced during combustion (q = 2 for complete combustion, but presently it is 4/3 in RGAS). The equilibrium constant for combustion is infinite since the reaction is assumed to be irreversible.

The rate expression for the Bouduard reaction is:

$$R_3 = K_3\left(y_{CO_2} - \frac{Py_{CO}^{2}}{K_{p3}^{eq}}\right)\left(\frac{P}{RT}\right)(1-\varepsilon_b)[FC] \tag{3.17}$$

The rate expression for the hydrogasification is:

$$R_4 = K_4\left(y_{H_2}^{2} - \frac{y_{CH_4}}{PK_{p4}^{eq}}\right)\left(\frac{P}{RT}\right)^{2}(1-\varepsilon_b)[FC] \tag{3.18}$$

The rate expression for the water-gas shift reaction is:

$$R_5 = K_5\varepsilon_b\left(y_{H_2O}y_{CO} - \frac{y_{CO_2}y_{H_2}}{K_{p5}^{eq}}\right)\left(\frac{P}{RT}\right)^{2} \tag{3.19}$$

The West Virginia University (WEN) model contains six equations, five of which are the same as in the DENN model. The sixth equation allows the burning of hydrogen.

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \tag{3.20}$$

All of the six reactions are irreversible except the water-gas shift reaction. The combustion, steam-carbon, Bouduard, and hydrogasification are modeled as heterogeneous reactions while the water-gas shift and hydrogen burning reactions are modeled as gas phase reactions. The WEN model was selected for RGAS because of the extensive documentation available and its similarity to the DENN model (7). However, there was found to be no significant improvement in predictions using the WEN model, plus it was found to have occasional convergence problems. Therefore, it was designated as the backup to the DENN model in the RGAS.

Devolatilization

Devolatilization is a complex phenomenon. As coal is heated, various gaseous species or volatiles are evolved. Among these species are hydrogen, carbon monoxide, carbon dioxide, water, methane, ethane, ethylene, and wide variety of other compounds including aromatics, polyaromatics, pyridines, thiophenes, phenols, aliphatics, olefines, and ketones. The RGAS model simply incorporates a thermally neutral evolution of volatiles that is linearly scaled with temperature and is incrementally added to the gasification products to form the raw gas stream. The rate of volatile evolution with temperature is given by the expression:

$$\frac{dV}{dT} = K \qquad (3.21)$$

where V is the amount of the volatile matter produced up to temperature T, and K is the devolatilization constant. Devolatilization begins when the coal reaches the lower temperature for volatile matter release (T_L), and continues linearly until the upper temperature limit (T_U) is reached. Therefore the rate of volatile evolution for each species is constant. Since both gasification and devolatilization depend on temperature, these two zones may overlap. Therefore, the volatile species (specifically H_2, H_2O, CO, CO_2, and CH_4) will affect concentrations of the gasification reactants, and thus, the reaction rates.

Drying

RGAS does not model the drying of the coal in the same manner as it does the volatile matter. The effect of the initial heating and drying of the coal is calculated after the two point boundary problem has converged on the dry coal. Drying is assumed to take place instantaneously at the very top of the gasifier.

RGAS Structure and assumptions

The following assumptions are made with regard to the RGAS model:

- Each phase is assumed to move through the gasifier in plug flow, i.e., there are no radial temperature or concentration gradients within the bed.
- Heat transfer between the solids and the gas is sufficiently high so that the

temperatures of the two phases may be assumed to be identical at any axial distance in the gasification and devolatilization zones.

- The Grummel and Davis correlation for coal enthalpy was chosen because it was the only non-conventional enthalpy model in ASPEN which resulted in reasonable heats of formation for carbon dioxide, carbon monoxide, and methan at 298 K.
- The coal density and the heat capacity of the coal and ash used in the ASPEN routine are those provided by the West Virginia University researchers.
- The calculation of the heat capacity associated with volatile matter assumed the devolatilization process to be thermally neutral.
- The distinction between primary and secondary volatile matter was ignored.
- The ideal gas physical properties model, SYSOP0, was assumed to be adequate to describe a system where the fluid phase is always a vapor.

RGAS is designed to handle the counter-current flow system. A list of the RGAS routines and their functions are as follows:

URE08I: This is the interface routine for the RGAS. It defines storage areas, checks on report writing, and calls the model routine.

URE08R: This is the RGAS report writer. It is designed to print out input conditions and data, the gasifier temperature profile, and the value for coal conversion. In the event that the run can not converge, the report writer will print information on the cause of failure.

URE08: This is the model routine. This routine sets up the initial values of the state variable, supplies the integration weightings, initiates the integration, checks for convergence, and supplies new guesses for the two point boundary value problem when convergence is not achieved.

DRKGSA: This is a fourth order, variable step, double precision Runge-Kutta integration subroutine. The algorithm was originally obtained from the IBM Scientific Subroutine Package (originally named DRKGS). The only differences from the IBM version are the CALL statements and in the expansion of the step halving capability from tenth to twenty fifth order.

INTSTT: This routine outputs the result of each integration to the ASPEN history file. All state variables are provided, as well as the position along the gasifier and the degree to which the maximum allowable step size has been halved.

DELKIN: This is a routine which calculates the values of the derivatives for DRKGSA. The kinetic rate expression for combustion char gasification contained in this subroutine are based on the University of Delaware model. The differential equations for devolatilization are based on the ultimate yield-temperature relationship for coal.

The FORTRAN code for the routines cited above, and an example input file are included in Appendces A & B respectively.

Chapter 4

MODEL IMPROVEMENTS

RGAS Convergence Scheme

The FORTRAN routine (URE09), which models the combustion and gasification zones in the gasifier, solves a two point boundary value problem that requires an iterative approach for solution.

Original scheme: The composition, flow rate, and temperature of the reactants entering the bottom of the gasifier are known. Also known are the coal feed flow and the temperature of the coal at the top of the gasifier. To solve this problem, it is necessary to assume the amount of unreacted carbon in the ash. Now, all the variables at the bottom of the gasifier are known, and the differential mass and energy balance equations are integrated in the direction of gas flow from the bottom to the top of the gasifier. If the correct amount of unreacted carbon has been assumed, the calculated amount of coal feed entering the top will match the known value. If not, a new value of unreacted carbon is assumed and the integration is repeated (2).

Modified Scheme: The original scheme was giving a simulation error when the known coal flow was not high enough to allow the original algorithm to converge because the solution contained a physically impossible situation: a carbon conversion greater than one (or a negative unreacted carbon flow) (2). To prevent this, a carbon conversion "design specification" routine was added to the ASPEN/RGAS algorithm by Bradley C. Carpenter (2) which guessed the coal feed flow rate (using a secant convergence scheme) and calculated the carbon conversion. If the calculated carbon conversion did not match with the specified value a new guess was made and the calculations were repeated. The "design specification" in ASPEN is a user-defined routine used to specify that a flowsheet variable (i.e. carbon conversion) attain a specified value by freeing a previously specified variable (coal feed flow). After this change the modified algorithm contained a double-loop convergence scheme where it first guessed a coal feed flow then guessed a carbon conversion. The modified scheme first converged on carbon conversion, and then converged on coal feed flow rate. This was very inefficient algorithm because it made unnecessary calculations and iterations. Typically it took a total of 16 iterations for convergence. The solution could be found with just one loop by making programming adjustments to the original FORTRAN routine (URE09).

Current Scheme: The current scheme is based on the actual physical operating situation. In reality the coal feed flow rate is controled by reactor demand (as determined by the reactor top temperature) which depends mainly on the flow rates of the reactants (oxygen, and steam) entering at the bottom of the reactor and their pressure and temperature. For particular operating conditions, steam and oxygen flow rates are fixed which eventually fixes the inlet coal flow rate. So inlet coal flow rate cannot be a specified variable. If we specify the unreacted carbon flow (i.e. carbon conversion), everything is known at the bottom except the ash flow rate. The ash flow rate depends on the ash mass fraction (known) in the coal and coal feed flow rate. Once again, it becomes a two point boundary value problem. However, ash is not a reactant and contributes little to the mass and energy balances. The new routine guesses a coal feed flow rate, calculates ash flow rate from the specified carbon conversion and known ash mass fraction, and integrates the differential mass and energy balance equations from the bottom to the top which gives the calculated coal flow rate. If the calculated coal feed flow rate matches the value guessed (within tolerance), the run is converged. If not, a new guess is made and the whole process is repeated. Typically three iterations are required for convergence.

Devolatilization

Coal is the product of very slow decomposition of organic matter deposited in prehistoric times. The rate of decomposition can be increased by elevating the temperature. When coal is heated, the decomposition becomes apparent at 350 to 400 C, and the products consist of a carbon-rich residue and a hydrogen-rich volatile fraction. The decomposition continues until a temperature typically around 1000 C is reached, which if maintained for an extended time, results in a residue of nearly pure carbon. The accumulated volatiles are comprised of various gases and liquids; the relative amounts of each depend on the coal type and manner of heating. In the early 1960s investigators found that rapid heating techniques for coal permit substantially more volatiles than traditional slow heating methods. Much work has since focused on the kinetics, mechanism, and product distribution, to provide fundamental information of practical importance.

Most of the available data on coal devolatilization were obtained at temperatures below 1000 C, although some measurements at higher temperatures have been reported (4). The yields with temperature are less for shorter residence times, and they diminish further if only the heat up period of 0.4 seconds is considered. The additional weight loss observed between 0.4 to 30 seconds is roughly equivalent to the amount lost between 30 and seconds and 4 hours, which supports the existence of rapid initial decomposition followed by very slow degasification of char. Data obtained at higher temperatures suggest that additional devolatilization in short times may be observed by heating the coal to temperatures well beyond 1000 C. This seems reasonable because the absolute time required for a given degree of completion of devolatilization is much less for the higher temperatures.

Devolatilization Models: The complex decomposition and transport phenomena involved with coal devolatilization are not yet amenable to exact description. Many authors have approximated the overall process as a first order decomposition occurring uniformly throughout the particle. Thus, the rate of devolatilization is expressed as:

$$\frac{dV}{dt} = k\ (V^{*} - V\ ) \tag{4.1}$$

where V is the cumulative amount of volatiles produced up to time t, expressed as weight fraction of the initial coal, k is the rate constant, and $V \rightarrow V^{*}$ as $t \rightarrow \infty$. Thus V^{*} represents the effective volatile content of the coal. The unknown parameters k and V^{*} have usually been the focus of kinetic studies. The rate constant in equation (4.1) is typically correlated with temperature by an Arrhenius expression:

$$k = k_o \exp\left(-\frac{E}{RT}\right) \tag{4.2}$$

where

k_o is the pre-exponential factor,

E is the activation energy,

R is the gas constant, and

T is the absolute temperature.

There is little agreement among the currently available rate parameters (6). Many authors have contended that a simple first order model is inadequate. In one attempt to improve the utility of equation (4.1), devolatilization is described as a series of several first order processes occurring in different time intervals. Another approach has been to use an nth-order expression:

$$\frac{dV}{dt} = k\left(V^{*} - V\right)^{n} \tag{4.3}$$

Weiser et. al. (14) found that n = 2 gave the best fit to their data over the first 1 hour of weight loss, whereas n = 1 was perfect for longer times. Skyler et. al. (9) found that values of n from 2 to 8 were required to fit non isothermal devolatilization data for different coals. Pitt (6) successfully correlated his devolatilization data with the empirical relation:

$$\frac{V^{*} - V}{V^{*}} = A - B\ \log(t) \tag{4.4}$$

where, A and B are constants.

One of the most serious shortcomings of these equations is that the apparently asymptotic yield of volatiles observed after some time at the final temperature, that is, the value of V^*, is a function of final temperature. Since coal devolatilization is not a single reaction but rather a multiplicity of overlapping decompositions concentrated in different time and temperature intervals for the usual case of devolatilization, any one set of parameter values for these equations can not be expected to represent the complete situation accurately over a wide range of conditions.

As stated earlier, the RGAS model assumes that devolatilization is a linear temperature dependent evolution of volatile matter, which contradicts the above discussion. Furthermore, limited data on North Dakota lignite coal (2) indicates that volatile evolution versus temperature is not a linear relationship and can be approximated by the following equation:

$$\frac{V}{V^*} = \frac{1}{1 + \exp\ (-x)} \tag{4.5}$$

where x is scaled temperature and is defined as:

$$x = \frac{(T - T_{avg})}{25} \tag{4.6}$$

and T_{avg} is the average of the initial and final temperatures for devolatilization. Equation 4.5 is shown graphically in figure 4.1 along with the linear model.

The previous linear devolatilization model was replaced with the above nonlinear model to see if there were any improvements in the RGAS predictions. Both models gave similar results, so we decided to keep the linear model because of its is simplicity.

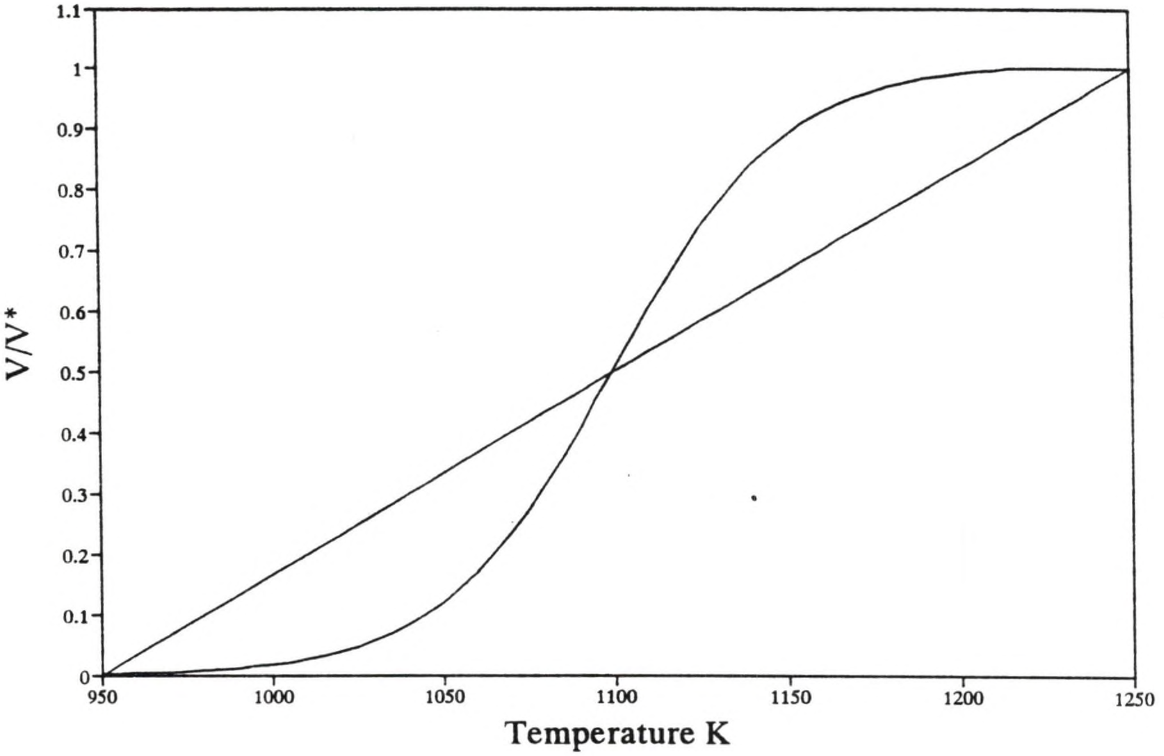

FIGURE 4.1 Devolatilization models

Thermodynamics

Thermodynamic considerations related to the gasification of coal and char are important to the theoretical evaluation of performance characteristics of individual process concepts and to the practical design of reactor systems. For these purposes the thermodynamic properties of coal gasification systems must be known or estimated, to permit a definition of heat effects and equilibrium or pseudo equilibrium behavior. Measurement of the thermodynamic properties of coals, however, is very difficult because of its complex and heterogeneous nature. Furthermore, there is uncertainty about the meaning of much of the available experimental information. The discussion in this section focuses on equilibrium activity coefficients, as they apply to coal gasification systems.

To determine the equilibrium characteristics of coal gasification systems, it is necessary to define the standard free energies of formation of the reactants and products. For major gaseous species involved in such systems, this information is available in a variety of tabulations and correlations. For coals, however, accurate experimental information is lacking, and relatively crude techniques have been used to estimate free energies of formation or equivalent parameters.

One technique for estimating coal thermodynamic properties has been to extrapolate or intrapolate from the properties of pure, solid aromatic compounds. It is not easy, however, to evaluate the uncertainties that result from using this technique, not even taking into consideration the complex, heterogeneous character of coal as well as its amorphous nature. The use of the estimated free energy of formation of coal itself in the thermodynamic analyses of coal gasification systems is perhaps most applicable for estimating overall potential performance characteristics of gasification concepts by accounting for second-law constraints.

Some investigators have interpreted experimental yields obtained during the gasification of coals in terms of pseudo-equilibrium constants, or equivalently, by assigning activity coefficients to the reacting carbon. Wen at al. (12) collected experimental data at apparent pseudo-equilibrium conditions during the gasification of low-temperature bituminous coal char at elevated pressure and temperature. Their data corresponds to a range of apparent carbon activity, a_C, from 1 to 7. Similarly, Squires (10) analyzed data obtained during steam-oxygen gasification of coals; these data show an apparent systematic trend in which values of a_C are generally greater than unity but decrease with increasing pressure, approaching unity at total pressures above 50 atm. Although apparent values of a_C are relatively independent of temperature from 700 to 900°C, values as high as $a_C = 20$ are indicated for data obtained at 1 atm total pressure. There are possible explanations for the experimental values of a_C greater than unity obtained in coal gasification systems. Squires suggested that amorphous carbon has a greater free energy than graphite. He also suggested that, in gases containing steam as well as hydrogen, the steam activates the carbon for gasification with hydrogen.

The rate at which reactions occur in the gasifier are described by the rate expressions given in Chapter 3. The net forward rate of reactions was determined by the deviation of actual reactant concentrations from equilibrium concentrations. So, the equilibrium constants play a direct role in the predictions made with the model. The definition of equilibrium constants in RGAS assumed that the activity of carbon is unity, which is not true if the carbon is not graphite. On the basis of the above discussion it is evident that the highly reactive lignite should have a higher activity than graphite. Since we do not know its value, we decided to include the activity as an adjustable variable in the RGAS model. After adjusting the activity of carbon, significant improvements were observed in the model predictions. An optimized value of $a_C = 1.7$ was found, which is in excellent agreement with the results reported in the literature.

CHAPTER 5

MODEL PREDICTIONS

Performance Index

The kinetic and equilibrium parameters were systematically adjusted using a Hooke-Jeeves pattern search method (13) to optimize the fit to plant data. Since ten responses were compared, an overall measure of fit was defined (called the performance index) to facilitate the optimization procedure. The performance index was calculated by first comparing simulation results with the plant data for the ten responses, normalizing the deviations (dividing by the actual value to put them all on a comparable basis), and summing the squares of the normalized errors. Mathematically, performance index (S) is defined as:

$$S = \sum \left(\frac{Y - Y^{*}}{Y} \right)^{2}$$

where, S is performance index, Y is plant data value, and Y^{*} is predicted value.

Previous Optimization Results

RGAS predictions have been improved in various stages. The predictions obtained prior to this work are given in Table 2 (2). The simulation predictions of raw gas composition and temperature are excellent. However, flow rates and reactor steam utilization predictions are poor. Predicted coal feed flow rate is reasonable (2.8% deviation from plant data), but predicted carbon conversion is only 97.25 percent compared to 99.48 percent for plant data. And note that for each percentage of carbon conversion increase, coal flow will decrease by about 1.5 percent (everything else remaining the same). So, if we are able to adjust the carbon conversion to a more appropriate (higher) value, the coal flow will deviate even more. The dry raw gas flow, raw gas water flow, and reactor steam utilization deviate from plant data by up to 20 percent.

TABLE 2 Previous Optimization Results

Response	Units	Plant Data	Prediction
Coal Feed Flow Rate	lb/hr.	104666	101743
Fixed Carbon Converted	%	99.480	97.250
Conc. of H_2 in Raw Gas	Mol%	0.3888	0.3891
Conc. of CO in Raw Gas	Mol%	0.1542	0.1507
Conc. of CO_2 in Raw Gas	Mol%	0.3165	0.3197
Conc. of CH_4 in Raw Gas	Mol%	0.1153	0.1151
Raw Gas Mass Flow	lb/hr.	130890	116970
Flow of Water Raw Gas	lb/hr.	88423	95562.0
Raw Gas Temperature	F	484.00	484.80
Reactor Steam Utilization	-	0.4852	0.4029
Performance Index, S	-	-	0.04851

Predictions with the Improved Convergence Scheme

After changing the RGAS convergence scheme, significant improvements were achieved in simulation time, and the prediction of carbon conversion. The simulation time is reduced by about 75%, and the predicted fixed carbon conversion is an exact match to plant data (Table 3). As expected, because of increased fixed carbon conversion the coal flow decreased. Consequently the raw gas flow rate decreased, and the raw gas temperature increased. The raw gas composition remained essentially same.

TABLE 3 Prediction with the Improved Convergence Scheme

Response	Units	Plant Data	Prediction
Coal Feed Flow Rate	lb/hr.	104666	98059
Fixed Carbon Converted	%	99.480	99.480
Conc. of H_2 in Raw Gas	Mol%	0.3888	0.3914
Conc. of CO in Raw Gas	Mol%	0.1542	0.1508
Conc. of CO_2 in Raw Gas	Mol%	0.3165	0.3202
Conc. of CH_4 in Raw Gas	Mol%	0.1153	0.1126
Raw Gas Mass Flow	lb/hr.	130890	115947
Flow of Water Raw Gas	lb/hr.	88423	94244.5
Raw Gas Temperature	F	484.00	509.53
Reactor Steam Utilization	-	0.4852	0.4028
Performance Index, S	-	-	0.0542

Further Optimization

In addition to changing the RGAS convergence scheme, a Hooke-Jeeves pattern search algorithm was also included in the RGAS subroutine URE09, so that any optimization of parameters could be done automatically. This automatic optimization is very important for ASPEN/RGAS accurate simulation, because every time the coal composition changes, the rate constants and several other parameters need to be adjusted. Now we can optimize rate constants and other parameters automatically in about 20 hours of computer time, whereas the process used to take about three months of human time.

At the end of the previous optimization study (2) it was found that the rate expression for Reaction 3 was coded incorrectly in the RGAS model, and it was thought that an optimization with the correct rate expression might improve the predictions. The re-optimization could not reasonably done by Carpenter et al. (2), but was a simple matter with the automatic search algorithm now incorporated into RGAS. The predictions with the optimized rate constants are given in Table 4. The predicted coal feed flow rate and raw gas flow rate improved slightly; compositions, and temperature predictions are as good as before, but the overall improvement is not significant.

TABLE 4 Results with corrected Reaction 3 expression and Re-Optimization

Response	Units	Plant Data	Prediction
Coal Feed Flow Rate	lb/hr.	104666	101730
Fixed Carbon Converted	%	99.480	99.480
Conc. of H_2 in Raw Gas	Mol%	0.3888	0.3866
Conc. of CO in Raw Gas	Mol%	0.1542	0.1507
Conc. of CO_2 in Raw Gas	Mol%	0.3165	0.3194
Conc. of CH_4 in Raw Gas	Mol%	0.1153	0.1183
Raw Gas Mass Flow (Dry)	lb/hr.	130890	119683
Flow of Water Raw Gas	lb/hr.	88423	94054.8
Raw Gas Temperature	F	484.00	485.45
Reactor Steam Utilization	-	0.4852	0.4190
Performance Index, S	-	-	0.03211

Predictions with Non-linear Devolatilization Model

RGAS assumes devolatilization to be a linear temperature dependent phenomenon, but on the basis of our limited data (2), and literature review (which was explained in more detailed in Chapter 4), the dependency should be nonlinear. The linear devolatilization model was replaced with a nonlinear one and an optimization was performed. The results are given in Table 5. No significant improvements were found in the predictions.

TABLE 5 Predictions with Non-linear Devolatilization Model

Response	Units	Plant Data	Prediction
Coal Feed Flow Rate	lb/hr.	104666	101979
Fixed Carbon Converted	%	99.480	99.480
Conc. of H_2 in Raw Gas	Mol%	0.3888	0.3857
Conc. of CO in Raw Gas	Mol%	0.1542	0.1506
Conc. of CO_2 in Raw Gas	Mol%	0.3165	0.3199
Conc. of CH_4 in Raw Gas	Mol%	0.1153	0.1188
Raw Gas Mass Flow (Dry)	lb/hr.	130890	119661
Flow of Water Raw Gas	lb/hr.	88423	94050.5
Raw Gas Temperature	F	484.00	483.36
Reactor Steam Utilization	-	0.4852	0.4200
Performance Index, S	-	-	0.0318

Predictions with the addition of a carbon activity

The definition of the equilibrium constants for the chemical reactions in RGAS assumes that the activity (a_C) of carbon is unity, which happens to be true for graphite. For more highly reactive carbon it could be anywhere between 1 to 20 at 1 atm pressure, and decreases with pressure (this was explained in Chapter 4). After including the activity of carbon in the definition of the equilibrium constants, an optimization was performed and a value of a_C= 1.7 was found for the best fit to plant data. The simulation predictions are given in Table 6. Significant improvements are made in flow rate predictions while maintaining the excellent composition predictions. The coal feed flow rate exactly matches plant data, but raw gas flow rate, and raw gas water flow rate still deviate from plant data by about 6 percent (average rate). But as described by Sears et al. (7) the gas flow measurement accuracy in plant data is ≥ 5.5 percent which justifies our flow rate prediction level.

TABLE 6 Predictions with the addition of carbon activity ($a_C = 1.7$)

Response	Units	Plant Data	Prediction
Coal Feed Flow Rate	lb/hr.	104666	104948
Fixed Carbon Converted	%	99.480	99.48
Conc. of H_2 in Raw Gas	Mol%	0.3888	0.3898
Conc. of CO in Raw Gas	Mol%	0.1542	0.1476
Conc. of CO_2 in Raw Gas	Mol%	0.3165	0.3190
Conc. of CH_4 in Raw Gas	Mol%	0.1153	0.1186
Raw Gas Mass Flow (Dry)	lb/hr.	130890	123442
Flow of Water Raw Gas	lb/hr.	88423	93225.0
Raw Gas Temperature	F	484.00	484.04
Reactor Steam Utilization	-	0.4852	0.4404
Performance Index, S	-	-	0.0174

Table 7 gives the kinetic constants obtained from the optimization studies for each stage in this project (i.e. the values used to obtain the predictions reported in each table in this chapter, Tables 2 - 6).

TABLE 7 Kinetic Rate Constants

	Table 5.1	Table 5.2	Table 5.3	Table 5.4	Table 5.5
PE1	2.70M	2.70M	3.51M	3.51M	3.51M
AE1	24.2K	24.2K	21.78K	21.78K	21.78K
PE2	610.0	610.0	805.0	820.0	810.0
AE2	39.0K	39.0K	35.1K	35.1K	35.1K
PE3	525.0	525.0	525.0	525.0	525.0
AE3	59.1K	59.1K	59.1K	59.1K	59.1K
PE4	4.78E-3	4.78E-3	5.87E-3	6.11E-3	6.11E-3
AE4	19.2K	19.2K	19.1K	19.1K	19.2K
PE5	26.3M	26.3M	32.3M	31.7M	32.3M
AE5	10.65K	10.65K	11.75K	11.75K	11.75K

PE = Pre-Exponential factor; AE = Activation Energy

Model Verification

The ASPEN model has been shown to be able to predict gasifier behavior at average operating conditions with reasonable accuracy. To gain confidence in the model, it was decided to check the model ability to predict the impacts of changing operating variables. Data on a single gasifier were collected in 1988 (ERNIE tests) to correlate operating variables with certain performance measures using a Box-Behnken design in three variables (oxygen flow, steam/oxygen ratio, and steam (agent) temperature) (7). The Box-Behnken test matrix (Table 8) consists of thirteen runs using scaled operating variables to represent low, average, and high values. To see how the ASPEN model predicts the impacts of these operating variable changes, the plant ERNIE test was repeated replacing the plant with the ASPEN model. The results of these ASPEN simulations were then fit by a quadratic equation in the three variables using regression analysis with coded variables (-1, 0, 1). The quadratic equations are given in Table 9

TABLE 8 Box-Behnken Test Matrix

Box-Behnken Design Values (coded value)			
O_2, % of Design (X_1)	H_2O/O_2 (X_2)	Temperature, F (X_3)	Run I.D. (Code Name)
0	-1	-1	F022
0	-1	+1	F021
0	+1	+1	F011
0	+1	-1	F012
-1	+1	0	F210
-1	-1	0	F220
+1	-1	0	F120
+1	+1	0	F110
-1	0	-1	F202
-1	0	+1	F201
+1	0	+1	F101
+1	0	-1	F102
0	0	0	F000

Definition of the variables:

X_1 = Coded Oxygen Flow = (O_2 Flow (scfs) - 66.64)/5.33

X_2 = Coded Steam/Oxygen Ratio = (Steam/Oxygen Ratio - 0.385)/0.02

X_3 = Coded Agent Temperature = (Agent Temperature (F) - 625)/15

TABLE 9 Constants and Significant Coefficients of Gasifier Regression Equations

Response	Constants	X_1	X_2	X_3	X_1^2	X_2^2	X_3^2
CO_2 in Raw Gas (Mol%)							
Plant	32.30 ± 0.36	--	0.31± 0.34	-0.40±0.34	--	--	0.37±0.44
ASPEN (old)	31.89	-0.09	0.62	-0.13	--	-0.04	--
ASPEN (new)	31.82	-0.12	0.52	-0.15	--	--	--
CH_4 in Raw Gas (Mol%)							
Plant	10.9 ± 0.1	-0.34 ± 0.13	-0.22±0.13	0.22±0.13	--	--	--
ASPEN (old)	11.47	-0.27	-0.30	0.03	--	--	--
ASPEN (new)	11.83	-0.20	-0.35	--	--	--	--
H_2 in Raw Gas (Mol%)							
Plant	40.88 ± 0.23	0.33 ± 0.21	0.64±0.21	-0.25±0.20	--	-0.28±0.32	--
ASPEN (old)	38.91	0.31	0.73	-0.04	--	--	--
ASPEN (new)	38.99	0.43	1.04	-0.10	--	--	--
CO in Raw Gas (Mol%)							
Plant	14.27 ± 0.30	-0.20 ± 0.23	-0.65±0.23	0.40±0.23	--	0.44±0.35	0.26±0.3
ASPEN (old)	15.19	0.08	-1.01	0.14	--	0.05	--
ASPEN (new)	14.88	0.06	-1.06	0.13	--	--	--
Raw Gas Temperature (F)							
Plant	482.0 ± 12	--	13.0±16.6	--	--	--	--
ASPEN (old)	484.0	9.91	19.7	-2.91	--	--	--
ASPEN (new)	486.4	--	28.31	--	--	--	--

No Cross Coefficients are significant
Error Limits are two standard deviations

along with the equations determined from the ERNIE tests. The coefficient of a particular variable X_i is the impact of changing that variable by one coded unit. Thus, the impacts predicted by ASPEN and those found from the ERNIE tests can be directly compared by examining the corresponding coefficients in the quadratic equations.

Many of the trends predicted by the ASPEN model for the ten responses are similar to those calculated from actual plant data. Methane, hydrogen, and carbon dioxide mole percents correlate with the operating variables with comparable coefficients, but others are not so similar. Raw gas temperature correlates with X_2 ,the steam/oxygen ratio in the same direction but with a different magnitude. The worst prediction is for mole percent of carbon monoxide; the ASPEN model predicts an effect that is in the opposite direction from that found in the ERNIE tests.

Chapter 6

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

Simulation time has been reduced significantly by changing the RGAS convergence scheme. Parameter optimization has been made much easier by including the Hooke-Jeeves pattern search algorithm in the RGAS routine URE09. Improvements in the prediction of raw gas and coal feed flow rate have been achieved by including the activity of carbon (a_C) with a value of 1.7, in the definition of equilibrium constants. The linear devolatilization model is simple and gives the same results as the nonlinear model, and so it was not replaced with a more realistic model.

Currently the model predicts almost all of the ten responses studied within their measurement accuracy. The coal feed flow rate, raw gas temperature and compositions are excellent, but the flow of raw gas, raw gas water flow rate, and reactor steam utilization are still not as good as we would like. Increasing water consumption within the reactor would improve model predictions by reducing raw gas water flow, which will increase raw gas flow rate and reactor steam utilization. However, because of the separation between the coal drying and gasification processes, the steam generated from drying of coal is not allowed to take part in gasification reactions. Allowing a portion of the drying water to be available in the gasification zone would probably eliminate the remaining minor discrepancies between the predictions and actual responses.

Recommendations

The RGAS model should be changed to allow the free water from coal drying to be available as a reactant. Since coal drying and volatile evolution are similar processes, they can be combined into a single process.

Kinetic parameters vary with coal compositions. We believe that the reactions are catalyzed by the metals present in coal. The addition of metal composition catalytic effects would allow predictions to take into account changing coal composition.

APPENDIX A

RGAS FORTRAN Routines

```
C$ #11 BY: SIMSCI DATE: 07/03/92 CORR. AVERAGES FOR PROX-,ULT-,SULFANAL
C$ #10 BY: MARINAN DATE: 09/01/81 DON'T MIX ATTRIBS. IF NONE THERE
C$ #9 BY: ZIEGLER DATE: 08/18/81 REMOVE UNLOCK NBTYPE
C$ #8 BY: CCCHEN DATE: 06/30/81 ADD COMMENTS AND CHANGE FLOW1 TO FLOW
C$ #7 BY: DWECK DATE: 04/10/81 CALC AVERAGE COMP ATTR FROM COMP FLOWS
C$ #6 BY: BRITT DATE: 03/27/81 UNLOCK BEADS
C$ #5 BY: CCCHEN DATE: 10/17/80 CODE REVIEW
C$ #4 BY: ZIEGLER DATE: 09/19/79 DON'T PRINT MSGG FOR 0 FLOW
C$ #3 BY: ZIEGLER DATE: 09/07/79 GET SIZE OF DESCRIPT RIGHT ( 4
C$ #2 BY: ZIEGLER DATE: 09/05/79 IMPROVED STUB ( DOES FLOW AVERAGE )
C$ #1 BY: CCCHEN DATE: 04/13/79 DUMMY FOR TEST
C-----------------------------------------------------------------------
C
C *---------------------------------------------------------------------
C *                   **** NOTICE ****
C *---------------------------------------------------------------------
C
C
C***********************************************************************************************************
C
C         COPYRIGHT (C) 1981-85
C         JAY S. DWECK, CONSULTANT, INC.
C
C***********************************************************************************************************
C
C
C       COPYRIGHT (C) 1980
C        MASSACHUSETTS INSTITUTE OF TECHNOLOGY
C        CAMBRIDGE, MA
C-----------------------------------------------------------------------
      SUBROUTINE CAMIX (IP    ,SS1    ,SS2    ,SSO    )
C
C    NAME OF MODULE:
C
C    MODULE TITLE:
C
C    PURPOSE:
C
C     TASK, SUBSYSTEM, SYSTEM:
C
C    WRITTEN BY:                  DATE WRITTEN:
C
C    READ BY:                     DATE READ:
C
C    APPROVED BY:                 DATE APPROVED:
C
C    CALLING SEQUENCE:
C
C         .
C
C    VARIABLES USED:
C
C    VARIABLES IN ARGUMENT LIST
C
C    VARIABLE  I/O  TYPE    DIMENSION    DESCRIPTION AND RANGE
C     IP        I    I        -          SUBSTREAM TYPE
C                                          1 OR 2: CONVENTIONAL
C                                          3: NONCONVENTIONAL
C      SS1      I    R                     1ST INPUT SUBSTREAM
C      SS2      I    R                     2ND INPUT SUBSTREAM
C      SSO      O    R                      OUTPUT SUBSTREAM
C
```

```
C    IMPORTANT INTERNAL VARIABLES
C
C     VARIABLE  I/O  TYPE    DIMENSION    DESCRIPTION AND RANGE
C
C    COMPONENTS OF VECTOR REAL
C
C    VARIABLE  I/O  TYPE    DIMENSION    DESCRIPTION AND RANGE
C
C
C   ERROR CONDITIONS:
C
C   NUMBER  LEVEL    TEXT
C
C   SUBROUTINES CALLED:
C
C      NAME -
C      DESCRIPTION -
C
C      NAME -
C      DESCRIPTION -
C
C       FILES:
C
C      FILE NAME -          - TITLE -
C      FORTRAN UNIT NUMBER -    - I/O -
C      CREATED BY / USED BY -
C      SEQUENCED ON -
C      ACCESS MODE -
C      DESCRIPTION -
C
C       SPECIFICATIONS, DECLARATIONS, DATA STATEMENTS, ETC.
C
      IMPLICIT REAL*8 (A-H,O-Z)
      LOGICAL IDRYFL
      DIMENSION IPROG(2), SS1(50), SS2(50), SSO(50), IDATT(2,3)
      COMMON /GLOBAL/ KPFLG1 ,KPFLG2 ,KPFLG3 ,LABORT ,NH     ,
     1           LDIAG  ,NCHAR  ,IMISS  ,MISSC1 ,MISSC2 ,
     2           LPDIAG ,IEBAL  ,IRFLAG ,MXBLKW ,ITYPRN ,
     3           LBNCP  ,LBCP   ,LSDIAG ,MAXNE  ,MAXNP1 ,
     4           MAXNP2 ,MAXNP3 ,IUPDAT ,IRSTRT ,LSFLAG ,
     5           LRFLAG ,KBLK1  ,KBLK2  ,KRFLAG ,IRNCLS
C     END COMMON /GLOBAL/ 06-22-79
       COMMON /RGLOB/ RMISS  ,RMIN   ,ABSMIN ,SCLMIN ,XMIN   ,
     1          HSCALE ,RELMIN ,SCLDEF ,TMAX   ,TNOW
C   END COMMON /RGLOB/ 10-13-78
      COMMON /PLEX/ IB(1)
      DIMENSION B(1)
      EQUIVALENCE (IB(1), B(1))
C   END COMMON /PLEX/ 10-13-78
      COMMON /PPCTBL/ NBCV   ,NBNC   ,NBAC   ,NBACC  ,NBCVAL ,
     1           NBNCAL ,NBACL
C   END COMMON /PPCTBL/ 8-29-79
      COMMON /NCOMP/ NCC    ,NNCC   ,NC     ,NAC    ,NACC   ,
     1               NVCP   ,NVNCP  ,NVACC  ,NVANCC
C   END COMMON /NCOMP/ 10-13-78
      COMMON /MW/ XMW(1)
      DATA IPROG/4HCAMI,4HX    /
      DATA IDATT /4HPROX,4HANAL,4HULTA,4HNAL ,4HSULF,4HANAL/
C    .
C    . ASSUME A CONVENTIONAL PHASE, CHANGE IF ITS NON-CONVENTIONAL
C    .
      N = NCC
```

```
      ISFLG = 1
      NBALOC = NBACL
      IF (IP .EQ. 3) N = NNCC
      IF (IP .EQ. 3) ISFLG = 2
      IF (IP .EQ. 3) NBALOC = NBNCAL
      IF (NBALOC .EQ. 0) GO TO 10000
      LBALOC = LOCATI(NBALOC)
C     .
C     . LOOP FOR EACH COMPONENT
C     .
      DO 500 K = 1,N
      FLOW1=SS1(K)*XMW(K)
      FLOW2=SS2(K)*XMW(K)
        IF(IP.EQ.3) FLOW1 = SS1(K)
        IF(IP.EQ.3) FLOW2 = SS2(K)
        FLOWO = FLOW1 + FLOW2
        IF (DABS(FLOWO) .LT. RMIN) GO TO 500
C
C     DETERMINE THE OFFSET TO THE FIRST ATTRIBUTE FOR THIS COMPONENT
C
        LATT1 = LCAOFF(ISFLG,K,1) + 1
C
C      SKIP TO NEXT COMPONENT IF NO ATTRIBUTES FOR THIS ONE
C
        IF (LATT1 .EQ. 1) GO TO 500
C
C     DETERMINE THE NUMBER OF ATTRIBUTES FOR THIS COMPONENT
C
        NATTR = NCTYPE(ISFLG,K)
C
C     DETECT IF PROXANAL IS AMONG ATTRIBUTES.  IF SO, CORRECT DRY-BASIS
C     MIXTURE VALUES WILL BE CALCULATED FOR PROXANAL, ULTANAL AND SULFANAL
C
        J = 1
        LATT = LATT1
        LOC1 = NCATID(ISFLG,K,J)
        LOCA = LOC1
        IDRYFL = .FALSE.
        DO 200 J = 1,NATTR
          IF (IB(LOCA).EQ.IDATT(1,1) .AND. IB(LOCA+1).EQ.IDATT(2,1))
     1      THEN
            DRY1 = FLOW1*(1D2 - SS1(LATT))*1D-2
            DRY2 = FLOW2*(1D2 - SS2(LATT))*1D-2
            DRYO = DRY1 + DRY2
            IDRYFL = .TRUE.
            GO TO 210
         END IF
         NUMELS = NCAVAR(ISFLG,K,J)
          LATT = LATT + NUMELS
          LOCA = LOCA + 4
  200   CONTINUE
  210    CONTINUE
C       .
C       . LOOP FOR EACH ATTRIBUTE
C       .
        LATT = LATT1
        LOCA = LOC1
        DO 400 J = 1,NATTR
        NUMELS = NCAVAR(ISFLG,K,J)
C         .
C         . INSERT COMPUTED GOTO HERE TO PROCESS DIFFERENT KINDS OF
C         . ATTRIBUTES.
```

```
C
      IF (IDRYFL) THEN
      IF (IB(LOCA).EQ.IDATT(1,1) .AND. IB(LOCA+1).EQ.IDATT(2,1))
     1 THEN
C
C             PROXANAL
C
        DO 230 I = 1,NUMELS
          II = LATT + I - 1
          IF (SS1(II).LT.RMISS .AND. SS2(II).LT.RMISS) THEN
          IF (I .EQ. 1) THEN
          SSO(II) = (SS1(II)*FLOW1 + SS2(II)*FLOW2)/FLOWO
          ELSE
          SSO(II) = (SS1(II)*DRY1 + SS2(II)*DRY2)/DRYO
          END IF
          ELSE
          SSO(II) = DMIN1 (SS1(II), SS2(II) )
          END IF
 230    CONTINUE
         GO TO 310
         END IF
       IF ((IB(LOCA).EQ.IDATT(1,2) .AND. IB(LOCA+1).EQ.IDATT(2,2))
     1 .OR. (IB(LOCA).EQ.IDATT(1,3) .AND. IB(LOCA+1).EQ.IDATT(2,3)))
     2 THEN
C
C             ULTANAL, SULFANAL
C
        DO 250 I = 1,NUMELS
          II = LATT + I - 1
          IF (SS1(II).LT.RMISS .AND. SS2(II).LT.RMISS) THEN
          SSO(II) = (SS1(II)*DRY1 + SS2(II)*DRY2)/DRYO
          ELSE
          SSO(II) = DMIN1 (SS1(II), SS2(II) )
          END IF
 250    CONTINUE
          GO TO 310
          END IF
          END IF
C
C       . THE FOLLOWING TAKES A TOTAL-FLOW-WEIGHTED AVERAGE
C       .
      DO 300 I = 1,NUMELS
       II = LATT + I - 1
       IF (SS1(II).LT.RMISS .AND. SS2(II).LT.RMISS) THEN
       SSO(II) = (SS1(II)*FLOW1 + SS2(II)*FLOW2) / FLOWO
       ELSE
       SSO(II) = DMIN1 (SS1(II), SS2(II) )
       END IF
 300  CONTINUE
 310   CONTINUE
      LATT = LATT + NUMELS
      LOCA = LOCA + 4
 400 CONTINUE
 500 CONTINUE
10000 IF(NBALOC.GT.0) CALL UNLOCK(NBALOC)
     RETURN
1111 CALL DMSTST
1112 CONTINUE
     END

C$ #1 BY: SIMSCI DATE: 07/03/92 NEW ROUTINE
```

```
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
      FUNCTION NCATID (ISSCNC, NCSEQ, J)
C
C     NAME OF MODULE: NCATID
C
C     PURPOSE: TO FIND PLEX LOCATION FOR BEGINNING OF ATTRIBUTE ID
C
C     TASK, SUBSYSTEM, SYSTEM: STREAM, STREAM HANDLING, ASPEN
C
C     WRITTEN BY: WILLIAM KEISTER       DATE WRITTEN: 07/03/92
C
C
C     CALLING SEQUENCE: LOC = NCATID (ISSCNC, NCSEQ)
C
C
C
C     VARIABLES USED:
C
C      VARIABLES IN ARGUMENT LIST
C
C       VARIABLE  I/O  TYPE     DIMENSION     DESCRIPTION AND RANGE
C
C       ISSCNC     I   INTEGER                  FLAG:
C                                  = 1 CONVENTIONAL SUBSTREAM
C                                  = 2 NON CONVENTIONAL
C                                     SUBSTREAM
C       NCSEQ      I   INTEGER                  ATTRIBUTED COMPONENT
C                                  SEQUENCE NUMBER
C       J          I   INTEGER                COMP ATTRIBUTE TYPE NO
C
C       NCATID     O   INTEGER                  PLEX LOCATION FOR FIRST INTEGER
C                                  WORD OF ATTRIBUTE ID
C
C      IMPORTANT INTERNAL VARIABLES
C
C       VARIABLE  I/O  TYPE     DIMENSION     DESCRIPTION AND RANGE
C
C       NBTBL      -   INTEGER                  BEAD NUMBER OF ATTRIBUTED
C                                  COMPONENT LOCATION
C       NBDEF      -   INTEGER                  BEAD NO OF ATTRIBUTE
C                                  DEFINITION
C
C     ERROR CONDITIONS:
C
C     NUMBER  LEVEL    TEXT
C
C     SUBROUTINES CALLED:
C
C       NAME - LOCATI
C       DESCRIPTION - TO LOCATE AN INTEGER BEAD
C
C        SPECIFICATIONS, DECLARATIONS, DATA STATEMENTS, ETC.
C
C** DOUBLE PRECISION
      IMPLICIT REAL*8 (A-H,O-Z)
C
      COMMON /PPCTBL/ NBCV  ,NBNC  ,NBAC  ,NBACC  ,NBCVAL  ,NBNCAL ,
     1                NBACL
C     COMMON /PPCTBL/ 3-27-79
      COMMON /NCOMP/ NCC   ,NNCC  ,NC    ,NAC   ,NACC   ,
     1                     NVCP  ,NVNCP  ,NVACC  ,NVANCC
```

```
C   END COMMON /NCOMP/ 10-13-78
      COMMON /PLEX/ IB(1)
      DIMENSION B(1)
      EQUIVALENCE (IB(1), B(1))
C   END COMMON /PLEX/ 10-13-78
C
C
C   CHECK STRUCTURE OF SUBSTREAM
C
      IF (ISSCNC .EQ. 2) GO TO 210
C
C   CONVENTIONAL SUBSTREAM
C
      NBTBL = NBCVAL
      GO TO 220
C
C   NON CONVENTIONAL SUBSTREAM
C
 210  CONTINUE
        NBTBL = NBNCAL
C
C       LOCATE BEAD NUMBER TO ATTRIBUTE DEFINITION BEAD
C
 220 CONTINUE

      LBTBL = LOCATI (NBTBL)
      NBDEF = IB(LBTBL + NCSEQ)
      LBDEF = LOCATI (NBDEF)
C
C   FIND ID LOCATION AND RETURN
C
      NCATID = LBDEF + 4 + 4*(J - 1)
      RETURN
      END


C$ #18 BY: BCC    DATE: 08/05/92 REMOVE LOOP EXIT AFTER 3150
C$ #17 BY: SIMSCI DATE: 07/14/92 INITIALIZE K AFTER 1200
C$ #16 BY: SIMSCI DATE: 03/08/91 ADD MIXED COMPS IN COAL FEED TO GAS
C$ #15 BY: SIMSCI DATE: 01/17/91 CLEAN-UP DIAGNOSTIC MESSAGES
C$ #14 BY: SIMSCI DATE: 01/17/91 CLEAN-UP ERROR HANDLING
C$ #13 BY: SIMSCI DATE: 01/15/91 ADD /RGAS1A/ AND USE REALK OFFSETS
C$ #12 BY: SIMSCI DATE: 09/25/90 FIX ILLEGAL GOTO FOR STATEMENT 2600
C$ #11 BY: KEW    DATE: 07/31/84 FIX FORMATS
C$ #10 BY: KEW    DATE: 07/31/84 RENAME TO URE09 FOR METC VAX SYSTEM
C$ #09 BY: BWB    DATE: 03/27/85 CONFORM TO ASPEN PROXANAL STANDARD
C$ #08 BY: BWB    DATE: 06/22/84 ADD EXPLANATORY TEXT FOR HISTORY
C$ #07 BY: BWB    DATE: 06/15/84 CORRECT REAL1 ORDER
C$ #06 BY: BWB    DATE: 05/04/84 CORRECT GAS OUT FOR HEATING COAL
C$ #05 BY: BWB    DATE: 05/04/84 MODIFY FOR VAX
C$ #04 BY: BWB    DATE: 05/02/84 ALLOW FOR VARIABLE ITERATIONS
C$ #03 BY: BWB    DATE: 04/23/84 ADD VMD,CONVERSION,MOISTURE
C$ #02 BY: BWB    DATE: 04/04/84 CORRECT MAXIMUM TEMPERATURE
C$ #01 BY: BWB    DATE: 04/04/84 NEW
C----------------------------------------------------------------------
C
C *--------------------------------------------------------------------
C *                  ****  NOTICE  ****
C *--------------------------------------------------------------------
C
C
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
C
C       COPYRIGHT (C) 1981-85
C       JAY S. DWECK, CONSULTANT, INC.
C
C
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
C
C-----------------------------------------------------------------
      SUBROUTINE URE09(LD    ,LVRIN ,LVROUT,LVRI3 ,LVRO3 ,LVRINC,
     1               LVROUC,NISCP ,ISCP  ,NPO   ,NBOPST,NIDS  ,
     2               IDS   ,NINT  ,INT   ,NREAL ,REAL  ,PEXP  ,
     3               ENGR  ,EXCN  ,COEF  ,NINT1 ,INT1  ,NINT2 ,
     4               INT2  ,NINT3 ,INT3  ,NREAL1,REAL1 ,NREAL2,
     5               REAL2 ,NREAL3,REAL3 ,NIWK1 ,IWK1  ,NIWK2 ,
     6               IWK2  ,NIWK3 ,IWK3  ,NWK1  ,WK1   ,NWK2  ,
     7               WK2   ,NWK3  ,WK3   ,NXLOC ,XLOC  ,TEMPPR,
     8               NSUBS ,NCQ   ,NCCQ  ,NR    ,NF    ,IWA   ,
     9               IDXSUB,JDXSUB,ITYPE ,JTYPE ,NWDIR ,IWDIR ,
     X               KINET ,PDROP ,QTRANS,Y     ,DERY  ,AUX   ,
     1               NSTATE,PRMT  )
C
C     NAME OF MODULE: GAS-ZONE
C
C     MODULE TITLE: COAL GASIFIER COMBUSTION/GASIFICATION ZONE
C
C     PURPOSE: THIS MODEL THE COMBUSTION/GASIFICATION ZONE OF A COAL
C           GASIFIER OF THE LURGI TYPE.  IT PROVIDES FOR COUNTER-
C           CURRENT FLOW OF GAS AND SOLID STREAMS.  THE FLOW OF
C           COOLANT IS ASSUMED TO BE CO-CURRENT TO THE GAS FLOW.
C           THE MODEL USES A MODIFIED FORM OF THE IBM SSP DRKGS
C           (VARIABLE STEP FOURTH ORDER RUNGE KUTTA) INTEGRATION
C           ROUTINE INSTEAD OF THE HARWELL GEAR PROVIDED WITH ASPEN.
C
C     TASK, SUBSYSTEM, SYSTEM: URE09, REACTOR, UOS
C
C    WRITTEN BY: BRUCE W.BENJAMIN     DATE WRITTEN: MARCH 20, 1984
C
C    CALLING SEQUENCE:
C
C    CALL URE09()
C
C     VARIABLES USED:
C
C      VARIABLES IN ARGUMENT LIST (SEE URE04)
C
C      SUBROUTINES CALLED:
C
C        NAME - TOTENT
C        DESCRIPTION - CALCULATE TOTAL STREAM ENTHALPY
C
C        NAME-SFLASH
C        DESCRIPTION-STREAM FLASH ROUTINE
C
C        SPECIFICATIONS, DECLARATIONS, DATA STATEMENTS, ETC.
C
      IMPLICIT REAL*8(A-H,O-Z)
      SAVE
      EXTERNAL KINET,INTSTT
      DIMENSION ITYPE(NSUBS),JTYPE(NSUBS),IDXSUB(NSUBS),JDXSUB(NSUBS)
      DIMENSION ISCP(NISCP),IDS(2,NIDS),NBOPST(2,NPO)
      DIMENSION INT(NINT),REAL(NREAL)
      DIMENSION INT1(NINT1),INT2(NINT2),INT3(NINT3)
```

```
      DIMENSION REAL1(NREAL1),REAL2(NREAL2),REAL3(NREAL3)
      DIMENSION IWK1(NIWK1),IWK2(NIWK2),IWK3(NIWK3)
      DIMENSION WK1(NWK1),WK2(NWK2),WK3(NWK3)
      DIMENSION ENGR(NR),PEXP(NCCQ),EXCN(NCCQ),COEF(NSUBS,NCQ,NR)
      DIMENSION XLOC(NXLOC),TEMPPR(NXLOC)
      DIMENSION IWDIR(NWDIR)
      DIMENSION Y(NSTATE),DERY(NSTATE),AUX(8,NSTATE),PRMT(10)
      COMMON /RGLOB/RMISS ,RMIN  ,ABSMIN,SCLMIN,XMIN  ,
     1          HSCALE,RELMIN,SCLDEF,TMAX  ,TNOW
C END COMMON /RGLOB/ 10-13-78
      COMMON /MW/XMW(1)
      COMMON /GLOBAL/KPFLG1,KPFLG2,KPFLG3,LABORT,NH    ,
     1            LDIAG ,NCHAR ,IMISS ,MISSC1,MISSC2,
     2            LPDIAG,IEBAL ,IRFLAG,MXBLKW,ITYPRN,
     3            LBNCP ,LBCP  ,LSDIAG,MAXNE ,MAXNP1,
     4            MAXNP2,MAXNP3,IUPDAT,IRSTRT,LSFLAG,
     5            LRFLAG,KBLK1 ,KBLK2 ,KRFLAG,IRNCLS,
     6            LSTHIS,IRETCD,JRFLAG,JSFLAG
C  END COMMON /GLOBAL/ 4-30-80
      COMMON /NCOMP/NCC   ,NNCC ,NC    ,NAC   ,NACC  ,
     1            NVCP  ,NVNCP ,NVACC ,NVANCC
C  END COMMON /NCOMP/ 10-13-78
      COMMON /STWORK/ NRETN  ,NIRETN ,NHXF   ,NHYF   ,NWYF   ,
     1             NSTW   ,KK1    ,KK2    ,KZ1    ,KZ2    ,
     2             KA1    ,KA2    ,KRET   ,KRSC   ,MF     ,
     3             MX     ,MX1    ,MX2    ,MY     ,MCS    ,
     4             MNC    ,MHXF   ,MHYF   ,MWY    ,MRETN  ,
     5             MIM    ,MIC    ,MIN    ,MPH    ,MIRETN ,
     6             NDUM   ,NBLM   ,NCOVAR ,NWR    ,NIWR   ,
     7             KEXT   ,KLNK   ,KFOUT  ,KPHV   ,KPHL   ,
     8             KLNGM  ,MSTOI  ,MLNKIN ,MZWK   ,MIZWK  ,
     9             IDUMX  ,HV     ,HL     ,HL1    ,HL2    ,
     1              SV    ,SL     ,SL1    ,SL2    ,VV     ,
     2             VL     ,VL1    ,VL2    ,XMWV   ,XMWL   ,
     3             XMWL1  ,XMWL2
C  END COMMON /STWORK/  2- 3-81
      COMMON /STWKWK/IDUM(6),DUM(26),WK(1)
      DIMENSION IWK(1)
      EQUIVALENCE(IWK(1),WK(1))
C  END COMMON /STWKWK/ 11-1-80
      COMMON /WORK/WORK(1)
      DIMENSION IWORK(1)
      EQUIVALENCE(WORK(1),IWORK(1))
C  END COMMON /WORK/ 12-6-78
      COMMON /PLEX/IB(1)
      DIMENSION B(1)
      EQUIVALENCE(IB(1), B(1))
C  END COMMON /PLEX/ 10-13-78
      COMMON /RGAS1A/ LRK1, LRK2, LRK3, LRK4, LRK5, LRK6, LRK7
      DIMENSION IPROG(2)
      DATA IPROG /4HURE0, 4H9    /
      DATA ICLASS /3/
C
C    Addition of Hooke-Jeeves Method
C    PP,PC,PO,D ARE VARIABLES USED FOR THE HOOKE-JEEVES METHOD
C
      DIMENSION PP(11)
      DIMENSION PC(11), PO(11)
      DIMENSION DSD(11)
      OPEN (UNIT=8, FILE='AVER.OUT', STATUS='UNKNOWN')
C
C REAL1(LRK1+1) IS THE RATE CONSTANT FOR THE FIRST REACTION REAL1(LRK1+2)
```

```
C IS THE ACTIVATION ENERGY FOR THE FIRST REACTION.

      PP(1)=REAL1(LRK1+1)
      PP(2)=REAL1(LRK1+2)
      PP(3)=REAL1(LRK1+3)
      PP(4)=REAL1(LRK1+4)
      PP(5)=REAL1(LRK1+5)
      PP(6)=REAL1(LRK1+6)
      PP(7)=REAL1(LRK1+7)
      PP(8)=REAL1(LRK1+8)
      PP(9)=REAL1(LRK1+9)
      PP(10)=REAL1(LRK1+10)
      PP(11)=REAL1(LRK1+11)
C
C  THE STARTING VALUE FOR THE EXPLOITORY MOVES IN THE HOOKE-JEEVES METHOD
C
      DSD(1)=35000.0
      DSD(2)=200.0
      DSD(3)=10.0
      DSD(4)=500.0
      DSD(5)=5.0
      DSD(6)=600.0
      DSD(7)=.00005
      DSD(8)=200.0
      DSD(9)=300000.0
      DSD(10)=120.0
      DSD(11)=0.050
C
C  IXIX IS A INDICATOR S,IS THE PERFORMACE INDEX MM, IS SET TO ONE BECAUSE
C  LOOKING FOR A MINIMUM L, IS A INTERNAL COUNTER
C
      IXIX=0
      S=0.0
      MM=1
      L=0
      JJ=2
      IRANK=6
C
C    START OF THE OPTIMIZATION SECTION
C

      DO 9001 ITIX=1,200
      WRITE(*,*)'iteration = ',ITIX
      WRITE(8,*)'iteration = ',ITIX

      B(LVRI3+IDXSUB(2)+NNCC-2)=13.20000000000000000
      GO TO (10,20,30,40,50,60),IRANK
 60   IF(IXIX .EQ. 0) THEN
        GO TO 8989
      ENDIF
C******************************************************************************************
C     HOOK-JEEVES PATTERN SEARCH METHOD
C******************************************************************************************
      NPRN=1
      LMAX=10000
      KKK=3
      DMIN=3.0
C
C    Put, Smin = 0.0005 for an optimization and
C    Smin = 10.0005 i.e. a big number for a single run
C
      SMIN= 10.0005
```

```
      R=2.
      NP=11
      DO 105 I=1,NP
        WRITE(8,*) I,PP(I)
        PC(I)=PP(I)
        PO(I)=PP(I)
 105 CONTINUE
        IF (NPRN) 80, 80, 81
 81   WRITE(*,*)
        WRITE(8,*) S, (PP(I),I=1,NP)
        IF(S.LE.SMIN) GO TO 1005
 80  GO TO (700,702), MM
700  S= -S
702  SO= S
100   SC=SO
        B(LVRI3+IDXSUB(2)+NNCC-2)=13.20000000000000000
        JJ=2

      DO 102 I=1,NP
102      PP(I)=PO(I)
1102      JJ=JJ+1
            IF(JJ.EQ.5.OR.JJ.EQ.6)GO TO 1102
 67     PP(JJ)=PP(JJ)+DSD(JJ)
          REAL1(LRK1+JJ)=PP(JJ)
          IRANK=1
          GO TO 8989
 10     IF (NPRN) 82,82,83
 83     WRITE(8,*) S,(PP(I), I=1,NP)
 82     GO TO (710,712), MM
710      S= -S
712      IF(SC -S) 403,404,404
404     PP(JJ)=PP(JJ)-2.0*DSD(JJ)
          REAL1(LRK1+JJ)=PP(JJ)
          IRANK=2
          GO TO 8989
 20     IF (NPRN) 84, 84, 85
 85     WRITE(8,*) S, (PP(I), I=1,NP)
 84     GOTO (720, 722), MM
720     S= -S
722     IF (SC-S) 403,407,407
407     PP(JJ)=PP(JJ)+DSD(JJ)
          REAL1(LRK1+JJ)=PP(JJ)
          GOTO 400
403     SC= S

400      IF(JJ .EQ. NP) THEN
          JJ=3
          GO TO 421
        ENDIF
4001     JJ=JJ+1
        IF(JJ.EQ.5.OR.JJ.EQ.6) GO TO 4001
        GO TO 67
421   CONTINUE

      IF(SC-SO) 300,300,200
200  DO 201 JJ=3,NP

      PO(JJ)=PC(JJ)
      PC(JJ)=PP(JJ)
      SO=SC
      IF(JJ.EQ.5.OR.JJ.EQ.6) GO TO 201
      PP(JJ)=PP(JJ)+PP(JJ)-PO(JJ)
```

```
      REAL1(LRK1+JJ)=PP(JJ)
 201  CONTINUE
      L=L+1
      IF (L-LMAX) 204,204,1000
 204  CONTINUE
      B(LVRI3+IDXSUB(2)+NNCC-2)=13.2000000000000000
      S11=S
      IRANK=3
      GOTO 8989
  30  SC=S
C     IF(SC-SO) 333,333,335
C 333  DO 334 I=1,NP
C     PP(I)=PC(I)
C     REAL1(LRK1+I)=PP(I)
C 334  CONTINUE
C 335  CONTINUE
      S=S11
      JJ=2
      IF (NPRN) 86,86, 87
  87  WRITE(8,*) SC, (PP(I), I=1,NP)
  86  GOTO (730,732), MM
 730  SC= -SC
7301  JJ=JJ+1
      IF(JJ.EQ.5.OR.JJ.EQ.6) GO TO 7301
 732  PP(JJ)=PP(JJ)+DSD(JJ)
      REAL1(LRK1+JJ)=PP(JJ)
      IRANK=4
      GO TO 8989
  40  IF (NPRN) 88,88, 89
  89  WRITE(8,*) S,(PP(I), I=1,NP)
  88  GOTO (740,742),MM
 740  S= -S
 742  IF (SC-S) 503,504,504
 504  PP(JJ)=PP(JJ) -2.0*DSD(JJ)
      REAL1(LRK1+JJ)=PP(JJ)
      IRANK=5
      GO TO 8989
  50  IF (NPRN) 90,90,91
  91  WRITE(8,*) S, (PP(I), I=1,NP)
  90  GO TO (750,752), MM
 750  S=-S
 752  IF (SC-S) 503,507,507
 507  PP(JJ)=PP(JJ)+DSD(JJ)
      REAL1(LRK1+JJ)=PP(JJ)
      GOTO 500
 503  SC=S
 500  IF(JJ .EQ. NP) THEN
       JJ=3
       GO TO 521
      ENDIF
      JJ=JJ+1
      GOTO 732
 521  CONTINUE
      IF (SO-SC) 200,100,100
 300  IF(DSD(KKK)-DMIN) 1001,600,600
 600  DO 601 I=1,NP
      DSD(I)=DSD(I)/R
 601  CONTINUE
      B(LVRI3+IDXSUB(2)+NNCC-2)=13.2000000000000000
      JJ=2
      GOTO 100
1000 WRITE(8,*)
```

```
      GOTO (760,761),MM
 760 SC=-SC
 761 WRITE(8,*) SC
      DO 800 I=1,NP
      WRITE(8,*) REAL1(LRK1+I)
 800 WRITE(8,*) LPC(I)
      WRITE(8,*) NPROB
      WRITE(8,*) S
      GO TO 1002
1001 GO TO (770,771),MM
 770 S= -SC
      GO TO 1003
 771 S=SC
1003 IF(NPRN) 850,850,851
 850 WRITE(8,*)
      GO TO 852
 851 WRITE(8,*)
 852 DO 801 I=1,NP
 801 WRITE(8,*) LPP(I)
      GO TO (1004,1005),MM
1004 WRITE(8,*) S
      GO TO 1006
1005 WRITE(8,*) S
1006 WRITE(8,*) NPROB
1002 CONTINUE
      WRITE(*,*) 'ENTERED STOP NUMBER 1 ****************'
      WRITE(8,*) 'ENTERED STOP NUMBER 1 ****************'
      STOP
1007 CONTINUE
8989 CONTINUE
      IXIX=IXIX+1
      KRSTRT=ISCP(6)
      LODIAG=ISCP(1)
      LODIAF=LODIAG-3
      LOPDIA=ISCP(2)
      LCFLAG=-9999
      LIRETN=INT(25)
      LIRSF3=INT(61)
      LIRETC=INT(28)
      LRETN=INT(31)
      LRRSF3=INT(64)
      LRETNC=INT(32)
      LRATE=IWDIR(6)
      LFLUXM=IWDIR(7)
      LFLUXS=IWDIR(8)
      LFSTEP=IWDIR(9)
      LDFDZ=IWDIR(10)
      LWA=IWDIR(11)
      LXOUT=IWDIR(13)
C
C     GET INFO ABOUT IDXSUB AND ITYPE
C
      CALL STRVEC(LD,NSUBS,IDXSUB,ITYPE)
      Z=0.D+00
C
C     ISTATE:    PHASE STATE OF THE MIXED SUBSTREAM
C                1: VAPOR    2:LIQUID
C     XLONG:     REACTOR LENGTH
C     DIA:       REACTOR DIAMETER
C
      ISTATE=1
      NPKC=INT(5)
```

```
      KPHC=INT(6)
      MAXIT=INT(7)
      XLONG=REAL(1)
      DIA=REAL(2)
      PRES=REAL(3)
      PRESDP=REAL(4)
      UCP=REAL(5)
      UCM=REAL(6)
      UCS=REAL(7)
      USM=REAL(8)
      CPRES=REAL(13)
      CPDP=REAL(14)
      TOL=REAL(16)
      CTEMP=REAL(17)
      AREA=3.14159D+00*(DIA/2.D+00)**2
      CIRM=3.14159D+00*DIA
C
C     COMPOSE THE BLENDED VOLATILE MATTER COMPONENT DISTRIBUTION
C
      DO 1107 I = 1, NCC
        REAL1(LRK7+I) = REAL1(LRK3+6)*REAL1(LRK4+I)/XMW(I) +
     *                  REAL1(LRK3+7)*REAL1(LRK5+I)/XMW(I) +
     *                  REAL1(LRK3+8)*REAL1(LRK6+I)/XMW(I)
 1107 CONTINUE
C
C     THIS SECTION SET UP PARAMETERS TO CALL SFLASH.
C
      NSTRML=NVCP+NVNCP+NVANCC
      KODE=1
      NPKODE=1
      KPHASE=ISTATE
      IF(ISTATE.EQ.3) NPKODE=2
      SPEC1=0.D+00
      SPEC2=0.D+00
      ENTHST=0.D+00
      GUESS=RMISS
      KREST=1
      KDENS=2

C
C     DENSITY IN THE REACTOR IS ALWAYS CALCULATED
C
C
C     COPY INLET VAPOR STREAM TO OUTLET
C
      CALL SCOPY(LD,LVRIN,LVROUT)
C
C     CHECK ZERO FLOW, EXIT IF YES.
C
      CALL TOTMAS(B(LVROUT),NSUBS,IDXSUB,ITYPE,TMASS)
      IF(TMASS.GE.RMIN) GO TO 1200
      IF(MERRPT(IPROG,IDS,1,8684101,LODIAG,KPFLG3).EQ.0) GO TO 1100
      WRITE(NH,9100)
 1100 CALL ERROR(1,ICLASS)
      ISCP(5)=-1
      RETURN
 1200 CONTINUE
      K = 0
      DO 1400 I=1,NSUBS
      IF(ITYPE(I).NE.1) GO TO 1300
      MDXSUB=IDXSUB(I)
      GO TO 1400
```

```
 1300 K=K+1
      JTYPE(K)=ITYPE(I)
      JDXSUB(K)=IDXSUB(I)
 1400 CONTINUE
C
C     CHECK ZERO PRESSURE, EXIT IF YES.
C
      IF(PRES.GE.RMIN) GO TO 1600
      IF(MERRPT(IPROG,IDS,1,8684105,LODIAG,KPFLG3).EQ.0) GO TO 1500
      WRITE(NH,9200)
 1500 CALL ERROR(1,ICLASS)
      ISCP(5)=-5
      RETURN
 1600 CONTINUE
C
C     CHECK SUBSTREAM TYPE
C
      DO 2000 I=1,NSUBS
      IF (ITYPE(I)-2) 1700,1800,1900
C
C     MIXED SUBSTREAM
C
 1700 IWK1(1)=1
      GO TO 1900
C
C     CONVEN SOLID SUBSTREAM
C
 1800 IWK1(2)=1
      GO TO 1900
C
C     NONCONVEN SOLID SUBSTREAM
C
 1900 IWK1(3)=1
 2000 CONTINUE
      IF(IWK1(1).NE.0) GO TO 2100
      GO TO 2200
 2100 IF (IWK1(3).NE.0) GO TO 2400
 2200 IF (KPFLG3.EQ.0) GO TO 2300
      IF(MERRPT(IPROG,IDS,1,8684106,LODIAG,KPFLG3).EQ.0) GO TO 2300
      WRITE(NH,9300)
 2300 CALL ERROR(1,ICLASS)
      ISCP(5)=-6
      RETURN
 2400 CONTINUE
C
C     SET UP PRMT VECTOR FOR DRKGSA
C
      NOUT=10
      PRMT(1)=0.D+00
      PRMT(2)=XLONG
      PRMT(3)=REAL(11)
      IF(PRMT(3).LE.0.D+00) PRMT(3)=1.D-03
      PRMT(4)=REAL(9)
      IF(PRMT(4).LE.0.D+00) PRMT(4)=1.D-10
      DELINC=DFLOAT(NXLOC)-2.D+00
      PRMT(10)=PRMT(2)/DELINC
C
C     SET UP TEMPERATURE PROFILE
C
      XLOC(1)=0.D+00
      TEMPPR(1)=B(LVRIN+IDXSUB(1)+NCC)
      CALL SDUMMY(LD,LVRD,NBDUM)
```

```
C
C     CORRECT PROXANAL ANALYSIS FOR VMD NUMBER
C     BUILD SOLIDS PORTION OF COMBINED BOTTOMS STREAM
C     RANGE GIVEN BY REAL1(LRK3+4) TO REAL1(LRK3+5)

      XXX=0
      NIT=INT1(1)
      IT=1
C
C     START OF ITERATION METHOD TO CONVERGE ON A SOLUTION
C
      DO 4900 ITIT=1,5

      PRXMOD=1D0-B(LVRI3+IDXSUB(2)+NNCC+8)/100D0
      REAL3(1)=B(LVRI3+IDXSUB(2)+NNCC+8)
      REAL3(3)=B(LVRI3+IDXSUB(2)+NNCC+10)*REAL1(LRK3+1)*PRXMOD
      REAL3(4)=B(LVRI3+IDXSUB(2)+NNCC+11)*PRXMOD
      REAL3(2)=100.-REAL3(1)-REAL3(3)-REAL3(4)
      REAL3(6)=B(LVRI3+IDXSUB(2)+NNCC+13)-REAL3(2)/(1.-REAL3(1)/100.)
      ULTSUM=REAL3(6)
      DO 2500 I=1,5
      REAL3(6+I)=B(LVRI3+IDXSUB(2)+NNCC+13+I)
      ULTSUM=ULTSUM+REAL3(6+I)
 2500 CONTINUE
C     IF (ULTSUM.LE.0.D+00) GO TO 2600
      IF (ULTSUM.LE.0.D+00) GO TO 2650
      DO 2600 I=1,6
      REAL3(5+I)=REAL3(5+I)/ULTSUM
 2600 CONTINUE
 2650 CONTINUE
      REAL3(12)=0.
      DO 2700 I=1,NCC
      REAL3(12)=REAL3(12)+REAL1(LRK7+I)
 2700 CONTINUE
      WTCHRF=B(LVRI3+IDXSUB(2)+NNCC-2)*REAL3(2)/1.D+02
      WTASH=B(LVRI3+IDXSUB(2)+NNCC-2)*B(LVRI3+IDXSUB(2)+NNCC+11)
     1      *PRXMOD/1.D+02
      IF(IT-2) 2800,2900,3000
 2800 WTCHAR=REAL1(LRK3+4)*WTCHRF
      WK2(1)=WTCHAR
      GO TO 3200
 2900 GO TO 3200
 3000 GO TO 3200
 3200 WTTTL=WTASH+WTCHAR
      WRITE(*,*)'ITERATION ',ITIT

      CALL SCOPY(LD,LVRIN,LVROUT)
      B(LVROUT+IDXSUB(2)+NNCC+8)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+9)=1.D+02*WTCHAR/WTTTL
      B(LVROUT+IDXSUB(2)+NNCC+10)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+11)=1.D+02*WTASH/WTTTL
      B(LVROUT+IDXSUB(2)+NNCC+12)=1.D+02*WTASH/WTTTL
      B(LVROUT+IDXSUB(2)+NNCC+13)=1.D+02*WTCHAR/WTTTL
      B(LVROUT+IDXSUB(2)+NNCC+14)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+15)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+16)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+17)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+18)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+19)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+20)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC+21)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC-2)=WTTTL
```

```
      B(LVROUT+IDXSUB(2)+NNCC-1)=WTTTL
C
C     OUTLET CHAR/ASH MIXTURE ASSUMED TO BE AT INLET GAS TEMPERATURE
C
      SPEC1=B(LVRIN+IDXSUB(1)+NCC)
      SPEC2=B(LVRIN+IDXSUB(1)+NCC+1)
      CALL FLASH(B(LVROUT)    ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2      ,
     1           NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
     2           LODIAF,LOPDIA,KREST ,KDENS ,REAL(LRETN)  ,
     3           INT(LIRETN)  ,LCFLAG)
      CALL SCOPY(LD,LVROUT,LVRO3)
C
C     SET UP MAXIMUM TEMPERATURE
C
      XLOC(NXLOC)=0.D+00
      TEMPPR(NXLOC)=B(LVRIN+IDXSUB(1)+NCC)
      PRMT(9)=2.D+00
C
C     PACK INITIAL VALUES OF DEPENDENT VARIABLES
C     THERE WILL BE NCC + 18 STATE VARIABLES:
C        NCC - GAS COMPONENT MOLE FRACTIONS:
C           O2      H2O     H2      CO      CO2     CH4
C           N2      H2S     NH3     C3H8    C6H6    C6H6O
C           C11H10-2 C21H42  COS     CS2     C4H4S   COOLANT
C          1 - GAS MASS BALANCE
C          4 - SOLID COMPONENT PROXANAL WEIGHT FRACTIONS:
C          7 - SOLID COMPONENT ULTANAL WEIGHT FRACTIONS:
C          3 - SOLID COMPONENT SULFANAL WEIGHT FRACTIONS:
C          1 - SOLID MASS BALANCE
C          1 - PROCESS TEMPERATURE EQUATION
C          1 - COOLANT ENTHALPY BALANCE
C
      DO 3300 I=1,NCC
      Y(I)=B(LVROUT+IDXSUB(1)+I-2)/B(LVROUT+IDXSUB(1)+NCC-1)
 3300 CONTINUE
      Y(NCC+1)=B(LVROUT+IDXSUB(1)+NCC-1)
      DO 3400 I=1,14
      Y(NCC+I+1)=B(LVROUT+IDXSUB(2)+NNCC+I+7)/1.D+02
 3400 CONTINUE
      Y(NCC+16)=B(LVROUT+IDXSUB(2)+NNCC-1)
      Y(NCC+17)=B(LVROUT+IDXSUB(1)+NCC)
      Y(NCC+18)=0.D+00
C
C     SET UP ERROR TEST WEIGHTING FACTORS FOR DRKGSA
C
      LX=NCC+18
      DO 3500 I=1,LX
      DERY(I)=REAL2(I)
 3500 CONTINUE
C
C     INTEGRATION STARTS HERE.
C
      CALL DRKGSA(PRMT  ,Y     ,DERY  ,LX    ,IHLF  ,KINET ,INTSTT,
     1           AUX   ,NOUT  ,NSUBS ,IDXSUB,ITYPE ,NINT  ,INT   ,
     2           NREAL1,REAL1 ,NIDS  ,IDS   ,NPO   ,NBOPST,NWK1  ,
     3           WK1   ,NCQ   ,WORK(LRATE)  ,WORK(LFLUXM) ,
     4           WORK(LFLUXS) ,XLONG ,AREA  ,CIRM  ,LVROUT,UCP   ,
     5           LD    ,REAL  ,NREAL ,LRETN ,LIRETN,LVRIN ,PRESDP,
     6           LVRINC,NPKODE,KPHASE,MAXIT ,TOL   ,GUESS ,LODIAF,
     7           LOPDIA,KREST ,KDENS ,LCFLAG,ISTATE,NX    ,LVRD  ,
     8           LVRI3 ,LVRO3 ,NXLOC ,XLOC  ,TEMPPR,NREAL3,REAL3 )
C
```

```
C     INTEGRATION COMPLETE - CHECK CONVERGENCE
C

      IF(IHLF.LT.26) GO TO 3600
      IF(MERRPT(IPROG,IDS,2,8684104,LODIAG,KPFLG3).EQ.0) GO TO 3550
      WRITE(NH,9400)
 3550 CALL ERROR(2,ICLASS)
      ISCP(5)=-4
      RETURN
C
C     REBUILD OUTLET PROCESS STREAM VECTOR
C
 3600 CONTINUE
      DO 3700 I=1,NCC
      B(LVROUT+IDXSUB(1)+I-2)=Y(I)*Y(NCC+1)
 3700 CONTINUE
C     B(LVROUT+IDXSUB(1)+NCC-1)=Y(NCC+1)
      DO 3800 I=1,14
      B(LVROUT+IDXSUB(2)+NNCC+I+7)=1.D+02*Y(NCC+I+1)
 3800 CONTINUE
      B(LVROUT+IDXSUB(2)+NNCC-2)=Y(NCC+16)

C     B(LVROUT+IDXSUB(2)+NNCC-1)=Y(NCC+16)
      B(LVROUT+IDXSUB(1)+NCC)=Y(NCC+17)
      TEMPP=Y(NCC+17)
      REAL(12)=-Y(NCC+18)
      PRESO=PRES-PRESDP
      DO 4100 J=1,NSUBS
      NM=ITYPE(J)
      IF(NM.EQ.3) GO TO 3900
C
C     CALCULATE TOTAL FLOWRATES AND MOLECULAR  WEIGHT
C
      DUM1=SAVEMW(LVROUT+IDXSUB(J)-1)
      GO TO 4100
 3900 CONTINUE
      DUM1=0.D+00
      DO 4000 I=1,NNCC
      DUM1=DUM1+B(LVROUT+IDXSUB(J)+I-2)
 4000 CONTINUE
      B(LVROUT+IDXSUB(J)+NNCC-1)=DUM1
 4100 CONTINUE
      SPEC2=PRESO
      SPEC1=TEMPP
      CALL SETP(B(LVROUT),NSUBS,IDXSUB,ITYPE,PRES)
      CALL SETH(B(LVROUT),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVROUT)    ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2     ,
     1           NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
     2           LODIAF,LOPDIA,KREST ,KDENS ,REAL(LRETN)   ,
     3           INT(LIRETN)   ,LCFLAG)
C
C     CHECK FOR PROCESS STREAM PHASE STATE SPECIFIED.
C
      VAP=B(LVROUT+MDXSUB+NCC+3)
      IF(LODIAG.GE.6) WRITE(*,*) VAP
      DVAP=DABS(VAP-1D+00)
      IF(ISTATE.EQ.1.AND.DVAP.GT.RMIN) GO TO 4200
      IF(ISTATE.EQ.2.AND.DABS(VAP).GT.RMIN) GO TO 4200
      GO TO 4400
 4200 CONTINUE
      IF(MERRPT(IPROG,IDS,1,8684102,LODIAG,KPFLG3).EQ.0) GO TO 4300
      WRITE(*,*)
```

```
 4300 CALL ERROR(1,ICLASS)
      ISCP(5)=-2
 4400 CONTINUE
C
C     PREPARE NEXT ITERATION
C     DETERMINE INLET CARBON FLOW AND COMPARE
C
      TPCHRF=B(LVROUT+IDXSUB(2)+NNCC+9)
     1         *B(LVROUT+IDXSUB(2)+NNCC-2)/1.D+02
      DLTCHR=WTCHRF-TPCHRF

      ADC=DABS(DLTCHR)
      IF(ADC.LE. .005) THEN
       XXX=1
      ENDIF
      WK2(1)=WTCHAR
      WK2(2)=TPCHRF
      WK2(3)=WTCHAR
      WK2(4)=TPCHRF

      WRITE(*,*)'WTCHRF',WTCHRF
      WRITE(*,*)'TPCHRF',TPCHRF
      WRITE(*,*)' Tin=',REAL1(LRK3+2)
C
C     RESET DEVOLATILIZATION LOW TEMPERATURE TO GAS OUTLET TEMPERATURE
C
      REAL1(LRK3+2)=B(LVROUT+IDXSUB(1)+NCC)
        WRITE(*,*)' Tin=',B(LVROUT+IDXSUB(1)+NCC)

C     IF(MERRPT(IPROG,IDS,2,8684108,LODIAG,KPFLG3).EQ.0) GO TO 4950
C     WRITE(NH,9700) NIT
C 4950 CALL ERROR(2,ICLASS)
C     ISCP(5)=-8


 5000 CONTINUE

C
C     DETERMINE TOTAL ENTHALPY OF HEATED DRIED COAL STREAM
C
      SLOENT=B(LVROUT+IDXSUB(2)+NNCC-1)*B(LVROUT+IDXSUB(2)+NNCC+2)
C
C     REMOVE SOLIDS FROM GAS OUTLET STREAM (LVROUT)
C
      DO 5100 I=1,NNCC
      B(LVROUT+IDXSUB(2)+I-2)=0.D+00
 5100 CONTINUE
      B(LVROUT+IDXSUB(2)+NNCC-1)=0.D+00
      B(LVROUT+IDXSUB(2)+NNCC)=RMISS
      B(LVROUT+IDXSUB(2)+NNCC+2)=RMISS
      B(LVROUT+IDXSUB(2)+NNCC+3)=RMISS
      B(LVROUT+IDXSUB(2)+NNCC+4)=RMISS
      DO 5200 I=1,NVANCC
      B(LVROUT+IDXSUB(2)+NNCC+7+I)=RMISS
 5200 CONTINUE
C
C     REMOVE GAS FROM SOLID OUTLET STREAM (LVRO3)
C
      PHOLD=B(LVRO3+IDXSUB(1)+NCC+1)
      DO 5300 I=1,NCC
      B(LVRO3+IDXSUB(1)+I-2)=0.D+00
 5300 CONTINUE
```

```
      B(LVRO3+IDXSUB(1)+NCC-1)=0.D+00
      DO 5400 I=2,9
      B(LVRO3+IDXSUB(1)+NCC+I-2)=RMISS
 5400 CONTINUE
      B(LVRO3+IDXSUB(1)+NCC+1)=PHOLD
C
C     ADD MIXED SUBSTREAM COMPONENTS FROM INLET COAL FEED (LVRI3)
C     TO PRODUCT GAS (LVROUT)
C
      FMOLI = B(LVRI3+IDXSUB(1)+NCC-1)
      IF ( FMOLI .GT. RMIN .AND. FMOLI .LT. RMISS ) THEN
        DO 5410 I = 1, NCC
          IOFF = IDXSUB(1) + I - 2
          B(LVROUT+IOFF) = B(LVROUT+IOFF) + B(LVRI3+IOFF)
 5410   CONTINUE
        FMOLO = B(LVROUT+IDXSUB(1)+NCC-1)
        FMASI = B(LVRI3+IDXSUB(1)+NCC+7) * FMOLI
        FMASO = B(LVROUT+IDXSUB(1)+NCC+7) * FMOLO
        HGASI = B(LVRI3+IDXSUB(1)+NCC+2)
        HGASO = B(LVROUT+IDXSUB(1)+NCC+2)
        FMOLM = FMOLI + FMOLO
        FMASM = FMASI + FMASO
        IF ( FMOLM .LE. RMIN .OR. FMOLM .GE. RMISS ) THEN
          FMOLM = 0D0
          FMASM = 0D0
        END IF
        HGASM = 0D0
        IF ( FMASM .GT. RMIN ) HGASM = (HGASI*FMASI+HGASO*FMASO)/FMASM
        B(LVROUT+IDXSUB(1)+NCC-1) = FMOLM
        B(LVROUT+IDXSUB(1)+NCC+2) = HGASM
        B(LVROUT+IDXSUB(1)+NCC+7) = 0D0
        IF ( FMOLM .GT. RMIN ) B(LVROUT+IDXSUB(1)+NCC+7) = FMASM/FMOLM
      END IF
C
C     ADD WATER VAPORIZED FROM COAL FEED
C
      CDRY=B(LVRI3+IDXSUB(2)+NNCC+8)*B(LVRI3+IDXSUB(2)+NNCC-1)/1801.5
      SLIENT=B(LVRI3+IDXSUB(2)+NNCC-1)*B(LVRI3+IDXSUB(2)+NNCC+2)
      GSIENT=B(LVROUT+IDXSUB(1)+NCC-1)*B(LVROUT+IDXSUB(1)+NCC+2)
     1     *B(LVROUT+IDXSUB(1)+NCC+7)
      SPEC1=B(LVROUT+IDXSUB(1)+NCC+1)
      SPEC2=GSIENT+SLIENT-SLOENT
      B(LVROUT+IDXSUB(1))=B(LVROUT+IDXSUB(1))+CDRY
      B(LVROUT+IDXSUB(1)+NCC-1)=B(LVROUT+IDXSUB(1)+NCC-1)+CDRY
      DUM1=SAVEMW(LVROUT+IDXSUB(1)-1)
      CALL SETH(B(LVROUT),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVROUT)    ,NSUBS ,IDXSUB,ITYPE ,NBOPST,1     ,
     1          NPKC  ,KPHC  ,MAXIT ,TOL   ,SPEC1 ,SPEC2 ,GUESS ,
     2          LODIAF,LOPDIA,KREST ,KDENS ,REAL(LRETN)  ,
     3          INT(LIRETN)  ,LCFLAG)
C
C     CONVERSION CALCULATION
C
      IT=IT+1
      REAL3(5)=100.-100.
     1          *B(LVRO3+IDXSUB(2)+NNCC+13)*B(LVRO3+IDXSUB(2)+NNCC-1)
     2          /B(LVRI3+IDXSUB(2)+NNCC+13)/B(LVRI3+IDXSUB(2)+NNCC-1)
     3          /(1.-B(LVRI3+IDXSUB(2)+NNCC+8)/100.)


      IF(XXX .EQ. 1) THEN
        GO TO 8999
```

```
      ENDIF


      WTCHAR=((1-.9948)*B(LVRI3+IDXSUB(2)+NNCC+13)
     1           *B(LVRI3+IDXSUB(2)+NNCC-1)
     2           *(1.-B(LVRI3+IDXSUB(2)+NNCC+8)/100.))/100.0
C
C     SETS B(LVRI3+IDXSUB(2)+NNCC-2) THE NEXT GUESS OF COAL FLOW TO MATCH
C     OUTLET CONDITIONS AT THE BOTTOM OF THE REACTOR
C
      IF(ITTIT.GT.3)THEN
      B(LVRI3+IDXSUB(2)+NNCC-2)=(B(LVRI3+IDXSUB(2)+NNCC-2)
     + *(TPCHRF+WTCHRF)/(2*WTCHRF))
      ELSE
      B(LVRI3+IDXSUB(2)+NNCC-2)=(B(LVRI3+IDXSUB(2)+NNCC-2)*TPCHRF/WTCHRF)
      ENDIF
      B(LVRI3+IDXSUB(2)+NNCC-1)=B(LVRI3+IDXSUB(2)+NNCC-2)

      WRITE(*,*)'REAL3(5)',REAL3(5)
      WRITE(*,*)'B(LVRI3+IDXSUB(2)+NNCC-1)= ',B(LVRI3+IDXSUB(2)+NNCC-1)

 4900 CONTINUE
 8999 CONTINUE
C
C     CHECK IF MAXIMUM TEMPERATURE HIGH ENOUGH FOR DEVOLATILIZATION
C
      IF(TEMPPR(NXLOC).GE.REAL1(LRK3+3)) GO TO 5500
      IF(MERRPT(IPROG,IDS,1,8684109,LODIAG,KPFLG3).EQ.0) GO TO 5450
      WRITE(NH,9800)
 5450 CALL ERROR(1,ICLASS)
      ISCP(5)=-9
 5500 CONTINUE
C
C     COOLANT CALCULATION
C
      CALL SCOPY(LD,LVRINC,LVROUC)
C     CALL TOTENT(B(LVRINC),NSUBS,IDXSUB,ITYPE,HCOOLI)
C     CALL SETP(B(LVROUC),NSUBS,IDXSUB,ITYPE,CPRES)
      CALL SETH(B(LVROUC),NSUBS,IDXSUB,ITYPE,ENTHST)
      SPEC1=B(LVRINC+IDXSUB(1)+NCC+1)-CPDP
      SPEC2=B(LVRINC+IDXSUB(1)+NCC-1)*B(LVRINC+IDXSUB(1)+NCC+2)
     1    *B(LVRINC+IDXSUB(1)+NCC+7)-REAL(12)
      CALL FLASH(B(LVROUC)    ,NSUBS  ,IDXSUB,ITYPE  ,NBOPST,1      ,
     1          NPKC   ,KPHC   ,MAXIT  ,TOL    ,SPEC1  ,SPEC2  ,GUESS  ,
     2          LODIAF,LOPDIA,KREST  ,KDENS  ,REAL(LRETN)   ,
     3          INT(LIRETN)   ,LCFLAG)



      CALL URE09R (NSIN   ,NBSIN  ,NSOUT  ,NBSOUT,NINT   ,INT    ,
     1            NREAL  ,REAL   ,NPO    ,NBOPST,NIDS   ,IDS    ,
     2            NISCP  ,ISCP   ,NISIZE,ISIZE  ,NB, S)


 9001 CONTINUE
      WRITE(8,*) 'ENTERED STOP NUMBER 2 ***************'
      WRITE(*,*) 'ENTERED STOP NUMBER 2 ***************'
      STOP
C
C     FORMAT STATEMENTS
C
 9000 FORMAT(/6X,'BEGINNING OF ITERATIONS:',
```

```
     1      //6X,'IHLF IS INTERVAL HALVING, X IS REACTOR POSITION',
     2       /6X,'FIRST NCC VARIABLES IN Y ARE GAS MOLE FRACTIONS',
     3       /6X,'VARIABLE NCC+1 IS THE GAS MOLE FLOW',
     4       /6X,'VARIABLES NCC+2 TO NCC+5 IS THE PROXANAL ANALYSIS',
     5       /6X,'VARIABLES NCC+6 TO NCC+12 IS THE ULTANAL ANALYSIS',
     6       /6X,'VARIABLES NCC+13 TO NCC+15 IS THE SULFANAL ANALYSIS',
     7       /6X,'VARIABLE NCC+16 IS THE SOLID WEIGHT FLOW',
     8       /6X,'VARIABLE NCC+17 IS THE PROCESS TEMPERATURE',
     9       /6X,'VARIABLE NCC+18 IS HEAT LOSS TO THE COOLANT')
 9100 FORMAT( 6X,'TOTAL FLOW IS ZERO.')
 9200 FORMAT( 6X,'TOTAL PRESSURE IS ZERO.')
 9300 FORMAT( 6X,'MIXED SUBSTREAM AND A NONCONVENTIONAL SUBSTREAM',
     1         1X,'EXPECTED BUT ONE OR BOTH NOT PRESENT.')
 9350 FORMAT( 6X,'SPECIFIED INLET COAL FLOW IS TOO LOW.')
 9400 FORMAT( 6X,'RUNGE-KUTTA INTEGRATION HAS HALVED OUT.')
 9500 FORMAT(/6X,'VAPOR FRACTION = ',G12.5)
 9600 FORMAT( 6X,'OUTLET PROCESS STREAM PHASE SPEC. IS INCORRECT.')
 9700 FORMAT( 6X,'NO CONVERGENCE IN ',I3,' ITERATIONS.')
 9800 FORMAT( 6X,'TEMPERATURE IS TOO LOW FOR DEVOLATILIZATION.')
 9900 FORMAT(/6X,'SECANT CALCULATION FOR CONVERGENCE:',
     1      //6X,'ESTIMATED WEIGHT FRACTION OUTLET FIXED CARBON ',G12.5,
     2       /6X,'ESTIMATED WEIGHT OF FIXED CARBON IN OUTLET    ',G12.5,
     3       /6X,'ESTIMATED TOTAL WEIGHT CHAR-ASH OUTLET        ',G12.5,
     4       /6X,'CALCULATED WEIGHT FRACTION INLET FIXED CARBON ',G12.5,
     5       /6X,'CALCULATED INLET WEIGHT DRY COAL              ',G12.5,
     6       /6X,'CALCULATED INLET WEIGHT FIXED CARBON          ',G12.5,
     7       /6X,'DIFFER. BETWEEN CALCULATED AND DESIRED RESULT ',G12.5)
      RETURN
      END


C$ #07 BY: SIMSCI DATE: 07/17/92 REPORT COAL FEED FLOW RATE
C$ #06 BY: SIMSCI DATE: 07/15/92 SET UNIT NUMBER FOR SPECIAL REPORT FILE
C$ #05 BY: SIMSCI DATE: 11/18/91 ADD ATOMBAL POSSIBILITY
C$ #04 BY: SIMSCI DATE: 06/14/91 CONTROL LOGIC FOR PRINTING SPECIAL FILE
C$ #03 BY: SIMSCI DATE: 04/03/91 PRINT SUMMARY IN SPECIAL FILE
C$ #02 BY: SIMSCI DATE: 03/08/91 ADD STEAM UTILIZATION CALCULATION
C$ #01 BY: SIMSCI DATE: 01/18/91 NEW
C

      SUBROUTINE  URE09R (NSIN  ,NBSIN ,NSOUT ,NBSOUT,NINT  ,INT  ,
     1            NREAL ,REAL  ,NPO   ,NBOPST,NIDS  ,IDS   ,
     2            NISCP ,ISCP  ,NISIZE,ISIZE ,NB, S)

C
C---------------------------------------------------------------------
C
C *-------------------------------------------------------------------
C *                       **** NOTICE ****
C *-------------------------------------------------------------------
C
C
C%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%
C
C                      COPYRIGHT (C) 1991
C                    SIMULATION SCIENCES INC.
C
C
C%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%
```

```
C
C-----------------------------------------------------------------------
C
C   NAME: URE09R
C
C   DESC: REPORT WRITER FOR URE09 (RGAS).
C
C   SYST: SP
C
C   AUTH: STEVEN C. LYTHGOE
C
C   DATE: 01/18/91
C
C-----------------------------------------------------------------------
C
C   VARIABLES IN ARGUMENT LIST:
C
C     VARIABLE  I/O  TYPE  DIMENSION  DESCRIPTION
C
C     NSIN      I    I                NUMBER OF INLET STREAMS
C
C     NBSIN     I    I     NSIN       BEAD NUMBERS OF INLET STREAMS
C
C     NSOUT     I    I                NUMBER OF OUTLET STREAMS
C
C     NBSOUT    I    I     NSOUT      BEAD NUMBERS OF OUTLET STREAMS
C
C     NINT      I    I                NUMBER OF INTEGER VARIABLES
C
C     INT       I    I     NINT       INTEGER VARIABLES
C
C     NREAL     I    I                NUMBER OF REAL VARIABLES
C
C     REAL      I    R     NREAL      REAL VARIABLES
C
C     NPO       I    I                NUMBER OF PROP. OPTION SETS
C
C     NBOPST    I    I     NPO        PROPERTY OPTION SETS
C
C     NIDS      I    I                NUMBER OF BLOCK IDS
C
C     IDS       I    I     NIDS       BLOCK IDS
C
C     NISCP     I    I                NUMBER OF SIM. CONTROL PARAM
C
C     ISCP      I    I     NISCP      SIMULATION CONTROL PARAM
C
C     NIREP     I    I                NUMBER OF REPORT CONTROL FLAGS
C
C     IREP      I    I     NIREP      REPORT CONTROL FLAGS
C
C     NB        I    I                BLOCK BEAD NUMBER
C
C-----------------------------------------------------------------------
C
C   IMPORTANT INTERNAL VARIABLES:
C
C     VARIABLE  I/O  TYPE  DIMENSION   DESCRIPTION
C
C-----------------------------------------------------------------------
C
C   SUBROUTINES CALLED:
```

```
C
C      NAME - LABCTR
C      DESC - LABEL CENTERING UTILITY
C
C      NAME - LOCATI
C      DESC - LOCATE AN INTEGER BEAD
C
C      NAME - LOCATM
C      DESC - LOCATE A MIXED INTEGER/REAL BEAD
C
C      NAME - LOCATS
C      DESC - LOCATE A STREAM BEAD
C
C      NAME - LOCATR
C      DESC - LOCATE A REAL BEAD
C
C      NAME - NPHASE
C      DESC - RETRIEVE THE NUMBER OF SUBSTREAMS FOR A STREAM CLASS
C
C      NAME - RCONV1
C      DESC - UNIT CONVERSION UTILITY
C
C      NAME - RPTBAL
C      DESC - HMB BALANCE REPORT
C
C      NAME - RPTHDR
C      DESC - REPORT PAGINATION UTILITY
C
C      NAME - STRVEC
C      DESC - UTILITY TO RETRIEVE STREAM STRUCTURE FOR A STREAM CLASS
C
C      NAME - UOBOX
C      DESC - BLOCK DIAGRAM PRINTING UTILITY
C
C      NAME - UOSHDR
C      DESC - REPORT SECTION HEADER UTILITY
C
C-----------------------------------------------------------------------
C
C    *** DOUBLE PRECISION ***
C
      IMPLICIT REAL*8 (A-H,O-Z)
C
C      COMMON STATEMENTS
C
      COMMON /PLEX  / IB(1)
      DIMENSION B(1)
      EQUIVALENCE (IB(1), B(1))
C     END COMMON /PLEX  / 10-13-78
C
      COMMON /WORK  / WORK(1)
      DIMENSION IWORK(1)
      EQUIVALENCE (IWORK(1),WORK(1))
C
      COMMON /GLOBAL/ KPFLG1 ,KPFLG2 ,KPFLG3 ,LABORT ,NH     ,
     1               LDIAG  ,NCHAR  ,IMISS  ,MISSC1 ,MISSC2 ,
     2               LPDIAG ,IEBAL  ,IRFLAG ,MXBLKW ,ITYPRN ,
     3               LBNCP  ,LBCP   ,LSDIAG ,MAXNE  ,MAXNP1 ,
     4               MAXNP2 ,MAXNP3 ,IUPDAT ,IRSTRT ,LSFLAG ,
     5               LRFLAG ,KBLK1  ,KBLK2  ,KRFLAG ,IRNCLS ,
     6               LSTHIS ,IRETCD ,JRFLAG ,JSFLAG ,ICOMTP
C     END COMMON /GLOBAL/ 07-21-81
```

```
C
      COMMON /RGLOB / RMISS  ,RMIN   ,ABSMIN ,SCLMIN ,XMIN   ,
     1               HSCALE ,RELMIN ,SCLDEF ,TMAX   ,TNOW
C     END COMMON /RGLOB / 10-13-78
C
      COMMON /PPGLOB/ PREF, TREF, RGAS
C
      COMMON /RPTGLB/ IREPFL ,ISUB(10)
C     END COMMON /RPTGLB/ 09-06-79
C
      COMMON /FLES  / IFLS(30)
      EQUIVALENCE (IFLS(1),NID   ), (IFLS(2),NDSPFR), (IFLS(3),NINFOR),
     1           (IFLS(4),NDSFTE), (IFLS(5),IJNK01), (IFLS(6),IJNK02),
     2           (IFLS(7),NWWWW ), (IFLS(8),NDSFIN), (IFLS(9),NTOC  ),
     3           (IFLS(10),NSD  ), (IFLS(11),NPF  ), (IFLS(12),NPD  ),
     4           (IFLS(13),NPH  ), (IFLS(14),NR   ), (IFLS(15),NMP  )
      EQUIVALENCE (IFLS(16),NIS  ), (IFLS(17),NLCF ), (IFLS(18),MPD  ),
     1           (IFLS(19),NAD  ), (IFLS(20),NCI  ), (IFLS(21),NP1  ),
     2           (IFLS(22),NP2  ), (IFLS(23),NP3  ), (IFLS(24),NP4  ),
     3           (IFLS(25),NP5  ), (IFLS(26),NA1  ), (IFLS(27),NA2  ),
     4           (IFLS(28),NA3  ), (IFLS(29),NA4  ), (IFLS(30),NA5  )
C     END COMMON /FLES  / 04-05-79
C
      COMMON /STWORK/ NRETN  ,NIRETN ,NHXF   ,NHYF   ,NWYF   ,
     1               NSTW   ,KK1    ,KK2    ,KZ1    ,KZ2    ,
     2               KA1    ,KA2    ,KRET   ,KRSC   ,MF     ,
     3               MX     ,MX1    ,MX2    ,MY     ,MCS    ,
     4               MNC    ,MHXF   ,MHYF   ,MWY    ,MRETN  ,
     5               MIM    ,MIC    ,MIN    ,MPH    ,MIRETN
C     END COMMON /STWORK/ 7-28-81
C
      COMMON /STWKWK/ IDUM(6),DUM(26),WK(1)
      DIMENSION IWK(1)
      EQUIVALENCE (IWK(1),WK(1))
C     END COMMON /STWKWK/ 11-1-80
C
      COMMON /NCOMP / NCC    ,NNCC   ,NC     ,NAC    ,NACC   ,
     1               NVCP   ,NVNCP  ,NVACC  ,NVANCC
C     END COMMON /NCOMP / 10-13-78
C
      COMMON /IDSCC / IDSCC(2,1)
C
      COMMON /FRMULA/ FRMULA(3,1)
      INTEGER FRMULA
C
      COMMON /MW    / XMW(1)
C
      COMMON /RGAS1A/ LRK1, LRK2, LRK3, LRK4, LRK5, LRK6, LRK7
C
C        DIMENSION STATEMENTS
C
      DIMENSION NBSIN(1), NBSOUT(1), INT(1), REAL(1),
     1         NBOPST(1), IDS(2,1), ISCP(1), IREP(1)
      DIMENSION LABEL1(4), STRNG1(8), LABEL2(4), STRNG2(8)
      DIMENSION IFORM(3,6), ICOMP(6), IDSS(2)
C
C        DATA STATEMENTS
C
      DATA IFORM  / 4HO2   , 4H    , 4H    ,
     1             4HH2   , 4H    , 4H    ,
     2             4HCO   , 4H    , 4H    ,
     3             4HCO2  , 4H    , 4H    ,
```

```
     4         4HCH4  , 4H    , 4H    ,
     5         4HH2O  , 4H    , 4H    /
      DATA IDSS / 4HNC  , 4H    /
C
C     EXECUTABLE CODE
C
      IFLAG = IREP(2) + IREP(3) + IREP(4) + IREP(5) + IREP(6)
C      IF ( IFLAG .EQ. 0 ) GO TO 9999
C
C     INITIALIZE CONTROL VARIABLES
C
      IHD = 0
      IFF = 1
      ISC = 3
      IFM = 0
      IPR = 0
      IERR = 0
      KEEP = 5
      IOPT = 1

C******************************************************************************************
C
C CALCULATION OF PERFORMANCE INDEX
C
C******************************************************************************************

C    WEIGHT FACTOR (ITSTEV) NEEDS TO BE CHANGED FOR EACH CALCULATION
C    INVOLVING THE PERFORMANCE INDEX CALCULATION
C
C    PERFOR= CARRIES THE PERFORMANCE INDEX CALCULAION NUBER

      ITSTEV=0
      PERFOR=0
      NPTS = INT(10)
      INT9 = INT(9)
      RVAL0 = 0D0
      IF ( NPTS .GT. 0 ) RVAL0 = REAL(INT9+NPTS-1)
      CALL RCONV1 ( 22, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
C
C     PEAK TEMPERATURE
C

      WRITE(8,1470) (LABEL1(I),I=1,4), RVAL1

      IOFF = INT(59)
C
C     CARBON CONVERSION
C
      ITSTEV=1

      WRITE(8,1460) REAL(IOFF+4)
C
C     CALCULATE PERFOMANCE INDEX FOR CARBON CONFERSION
C
      CCCCC=(ITSTEV*(((REAL(IOFF+4)-99.48)**2.0)/(99.48**2)))
C      WRITE(8,*) CCCCC
      PERFOR=PERFOR+CCCCC

      NBSIN(2)=100000057
      LVII2=91893
      LVRI2=45953
      LDI2=20169
```

```
      NBSI2=100000532

      CALL FIPHN(IDSS,LDI2,ISEQ)

      ISS0 = LPHASE(LDI2,ISEQ)
      RVAL0 = B(LVRI2+ISS0)
      CALL RCONV1 ( 10, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
C
C      COAL FLOW RATE
C
      ITSTEV=1
      WRITE (8,1455) (LABEL1(I),I=1,4), RVAL1
      CCCFC=(ITSTEV*(((RVAL1-104666.)**2.0)/(104666.**2)))

C       WRITE(8,*) CCCFC
      PERFOR=PERFOR+CCCFC

      NSUM = 70
      LINES = 19
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(8,1450)
      DO 250 K = 1, 6
        ICOMP(K) = 0
        DO 240 J = 1, NCC
            IF ( FRMULA(1,J) .EQ. IFORM(1,K) .AND.
     1           FRMULA(2,J) .EQ. IFORM(2,K) .AND.
     2           FRMULA(3,J) .EQ. IFORM(3,K) ) ICOMP(K) = J
  240   CONTINUE
  250 CONTINUE
      NBSOUT(1)=100000058
      LVIO=92401
      LVRO=46207
      LDO=20169
      NBSO=100000532


      NSUBS = NPHASE ( LDO )
      CALL STRVEC ( LDO, NSUBS, IWK(MPH+NSUBS), IWK(MPH) )
      IMIXED = 0
      DO 260 I = 1, NSUBS
        IF ( IWK(MPH+I-1) .EQ. 1 ) IMIXED = I
  260 CONTINUE
      IF ( IMIXED .GT. 0 ) THEN
        IOFF = LVRO + IWK(MPH+NSUBS+IMIXED-1) - 1
        DRYFLO = B(IOFF+NCC) - B(IOFF+ICOMP(6)-1)
        IF ( DRYFLO .GT. 0D0 ) THEN
          DO 270 I = 1, 5
            J = ICOMP(I)
            RVAL1 = B(IOFF+J-1) / DRYFLO
C
C     CONC. OF H2 CO CO2 CH4
C
            WRITE(8,1480) IDSCC(1,J), IDSCC(2,J), RVAL1
            IF(I .EQ. 2)THEN
              ITSTEV=1
              H2=(ITSTEV*(((RVAL1-.3888)**2)/(.3888**2)))
CC                WRITE(8,*) 'H2 ',H2
              PERFOR=PERFOR+H2
            ENDIF
            IF(I .EQ. 3)THEN
              ITSTEV=1
              CO=(ITSTEV*(((RVAL1-.1542)**2)/(.1542**2)))
```

```
CC             WRITE(8,*) 'CO ',CO
            PERFOR=PERFOR+CO

          ENDIF
          IF(I .EQ. 4)THEN
            ITSTEV=1
            CO2=(ITSTEV*(((RVAL1-.3165)**2)/(.3165**2)))
CC             WRITE(8,*) 'CO2 ',CO2
            PERFOR=PERFOR+CO2
          ENDIF
          IF(I .EQ. 5)THEN
            ITSTEV=1
            CH4=(ITSTEV*(((RVAL1-.1153)**2)/(.1153**2)))
            PERFOR=PERFOR+CH4
          ENDIF


 270       CONTINUE
        RVAL0 = B(IOFF+NCC) * B(IOFF+NCC+8) -
   1            B(IOFF+ICOMP(6)-1) * XMW(ICOMP(6))
        CALL RCONV1 ( 10, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
C
C        RAW GAS MASS FLOW RATE (DRY)
C
        ITSTEV=1
        WRITE(8,1490) (LABEL1(I),I=1,4), RVAL1
        RAWFL=(ITSTEV*(((RVAL1-130890.)**2)/(130890.**2)))
CC         WRITE(8,*) 'RAW GAS FLOW RATE',RAWFL

        PERFOR=PERFOR+RAWFL
        RVAL0 = DRYFLO * RGAS * 273.15D0 / PREF
        CALL RCONV1 ( 50, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(8,1500) (LABEL1(I),I=1,4), RVAL1

      END IF

    NBSIN(3)=100000072
    LVII=94797
    LVRI=47405
    LDI=20169
    NBSI=100000532

    NBSOUT(3)=100000061
    LVIO=93153
    LVRO=46583
    LDO=20169
    NBSO=100000532

    NSUBS = NPHASE ( LDO )
    CALL STRVEC ( LDO, NSUBS, IWK(MPH+NSUBS), IWK(MPH) )
    IMIXED = 0
    DO 280 I = 1, NSUBS
      IF ( IWK(MPH+I-1) .EQ. 1 ) IMIXED = I
 280 CONTINUE
    IF ( IMIXED .GT. 0 ) THEN
      IOFFI = LVRI + IWK(MPH+NSUBS+IMIXED-1) - 1
      IOFFO = LVRO + IWK(MPH+NSUBS+IMIXED-1) - 1
      RVAL0 = B(IOFFO+NCC) * B(IOFFO+NCC+8) * B(IOFFO+NCC+3) -
   1          B(IOFFI+NCC) * B(IOFFI+NCC+8) * B(IOFFI+NCC+3)
      CALL RCONV1 ( 13, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
      WRITE(8,1530) (LABEL1(I),I=1,4), RVAL1
```

```
        RVAL0 = B(IOFFO+NCC) * B(IOFFO+NCC+4) * B(IOFFO+NCC+8)
        CALL RCONV1 ( 10, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(8,1540) (LABEL1(I),I=1,4), RVAL1

        RVAL0 = B(IOFFO+NCC+1)
        CALL RCONV1 ( 22, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(8,1550) (LABEL1(I),I=1,4), RVAL1

        END IF
        RVAL0 = B(IOFF+ICOMP(6)-1) * XMW(ICOMP(6))
        CALL RCONV1 ( 10, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
C
C        FLOW OF WATER IN RAW GAS
C
        ITSTEV=1

        WRITE(8,1510) (LABEL1(I),I=1,4), RVAL1
        FH2O=(ITSTEV*(((RVAL1-88423.)**2)/(88423.**2)))
        PERFOR=PERFOR+FH2O

        RVAL0 = B(IOFF+NCC+1)
        CALL RCONV1 ( 22, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
C
C        RAW GAS TEMPERATURE
C
        ITSTEV=1

        WRITE(8,1520) (LABEL1(I),I=1,4), RVAL1
        RTEMP=(ITSTEV*(((RVAL1-484.)**2)/(484.**2)))
        PERFOR=PERFOR+RTEMP
      END IF


      NBSIN(1)=100000056
      LVII1=91351
      LVRI1=45682
      LDI1=20169
      NBSI1=100000532
      NBSIN(2)=100000057
      LVII2=91893
      LVRI2=45953
      LDI2=20169
      NBSI2=100000532
      NBSOUT(1)=100000058
      LVIO1=92401
      LVRO1=46207
      LDO1=20169
      NBSO1=100000532

      NSUBS = NPHASE ( LDO1 )
      CALL STRVEC ( LDO1, NSUBS, IWK(MPH+NSUBS), IWK(MPH) )
      IMIXED = 0
      INCSOL = 0
      DO 290 I = 1, NSUBS
        IF ( IWK(MPH+I-1) .EQ. 1 ) IMIXED = I
        IF ( IWK(MPH+I-1) .EQ. 3 ) INCSOL = I
  290 CONTINUE
      IF ( IMIXED .GT. 0 .AND. INCSOL .GT. 0 ) THEN
        IOFFI1 = LVRI1 + IWK(MPH+NSUBS+IMIXED-1) - 1
        IOFFI2 = LVRI2 + IWK(MPH+NSUBS+IMIXED-1) - 1
        IOFFI3 = LVRI2 + IWK(MPH+NSUBS+INCSOL-1) - 1
        IOFFO1 = LVRO1 + IWK(MPH+NSUBS+IMIXED-1) - 1
```

```
        STMIN1 = B(IOFFI1+ICOMP(6)-1)
        STMIN2 = B(IOFFI2+ICOMP(6)-1)
        STMIN3 = B(IOFFI3+NNCC)*B(IOFFI3+NNCC+9)/1D2/XMW(ICOMP(6))
        STMOU1 = B(IOFFO1+ICOMP(6)-1)
        STUTIL = 0D0
        IF ( STMIN1 .GT. 0D0 ) THEN
          STUTIL = (STMIN1-(STMOU1-(STMIN2+STMIN3))) / STMIN1
        END IF
        ITSTEV=1
C
C        REACTOR STEAM UTILIZATION
C
        WRITE(8,1560) STUTIL
        UTIL=(ITSTEV*(((STUTIL-.4852)**2)/(.4852**2)))
CC          WRITE(8,*)'UTIL',UTIL
        PERFOR=PERFOR+UTIL
      END IF
        S=PERFOR

C         WRITE(8,*) 'S= ',S
        WRITE(*,*) 'S= ',S
      RETURN
C************************************************************

      CALL UOSHDR ( NIDS, IDS )
C
C        PRINT THE HEADER AND THE BLOCK DESCRIPTION
C
      LINES = 1
      CALL LOCATM ( NB, LBI, LBR, IOFF )
      NBDESC = IB(LBI+2)
      IF ( NBDESC .NE. 0 ) THEN
        LBDESC = LOCATI(NBDESC)
        LNDESC = LENTHI(NBDESC)
        LINES = LINES + 1
        CALL RPTHDR ( LINES, IFF, ISC, ISUB )
        WRITE(NR,1000) (IB(LBDESC+I-1),I=1,LNDESC)
      ELSE
        CALL RPTHDR ( LINES, IFF, ISC, ISUB )
      END IF
C
C        PRINT THE BLOCK DIAGRAM SHOWING THE INLET AND OUTLET STREAMS
C
      CALL UOBOX ( NB, NBSIN, NSIN, NBSOUT, NSOUT, IDS, NIDS,
     1             NBOPST, NPO )
C
C        CHECK ISCP(5) FOR ERROR CONDITIONS DURING THE SIMULATION
C
      IF ( ISCP(5) .EQ. -9999 ) THEN
        LINES = 7
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2000)
        IERR = 1
      END IF
      IF ( ISCP(5) .EQ. -IMISS ) THEN
        LINES = 7
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2000)
        IERR = 1
      END IF
      IF ( ISCP(5) .EQ. -1 ) THEN
        LINES = 8
```

```
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2010)
        IERR = 1
      END IF
      IF ( ISCP(5) .EQ. -2 ) THEN
        LINES = 8
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2020)
      END IF
      IF ( ISCP(5) .EQ. -4 ) THEN
        LINES = 8
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2040)
      END IF
      IF ( ISCP(5) .EQ. -5 ) THEN
        LINES = 8
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2050)
        IERR = 1
      END IF
      IF ( ISCP(5) .EQ. -6 ) THEN
        LINES = 8
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2060)
        IERR = 1
      END IF
      IF ( ISCP(5) .EQ. -7 ) THEN
        LINES = 8
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2070)
      END IF
      IF ( ISCP(5) .EQ. -8 ) THEN
        LINES = 7
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2080)
      END IF
      IF ( ISCP(5) .EQ. -9 ) THEN
        LINES = 7
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,2090)
      END IF
      IF ( IERR .NE. 0 ) GO TO 9999
C
C       REPORT THE MATERIAL BALANCE
C
      IFLAG = IREP(2) + 2*IREP(3) + 4*IREP(6)
      CALL RPTBAL ( NSIN, NBSIN, NSOUT, NBSOUT, WORK(1), WORK(NCC+1),
     1              WORK(2*NCC+1), WORK(2*NCC+NNCC+1), IFLAG, 3 )
C
C       RETRIEVE THE REPORT OPTION AND CHECK FOR SUMMARY OPTION
C
      IOFF = INT(49) + 1
      IOPT = INT(IOFF)
      IF ( IOPT .EQ. 2 ) GO TO 200
C
C       REPORT THE INPUT DATA
C
      IF ( IREP(4) .EQ. 0 ) GO TO 200
      LINES = 2
      CALL RPTHDR ( LINES, IFF, ISC, ISUB )
      WRITE(NR,1010)
C
```

```
C       GENERAL PARAMETERS
C
        LINES = 14
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1020)
        IVALI = INT(1)
        WRITE(NR,1030) IVALI
        IVALI = INT(4)
        WRITE(NR,1040) IVALI
        IVALI = INT(2)
        WRITE(NR,1050) IVALI
        IVALI = INT(15)
        WRITE(NR,1060) IVALI
        RVAL0 = REAL(1)
        CALL RCONV1 ( 17, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1070) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(2)
        CALL RCONV1 ( 17, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1080) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(3)
        CALL RCONV1 ( 20, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1090) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(4)
        CALL RCONV1 ( 20, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1100) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(5)
        CALL RCONV1 ( 16, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1110) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(11)
        CALL RCONV1 (  0, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1120) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(9)
        CALL RCONV1 (  0, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1130) (LABEL1(I),I=1,4), RVAL1
C
C       COOLANT PARAMETERS
C
        LINES = 9
        IF ( IABS(INT(5)) .EQ. 1 ) LINES = LINES + 1
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1140)
        RVAL0 = REAL(13)
        CALL RCONV1 ( 20, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1150) (LABEL1(I),I=1,4), RVAL1
        RVAL0 = REAL(14)
        CALL RCONV1 ( 20, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1160) (LABEL1(I),I=1,4), RVAL1
        IVALI = INT(5)
        WRITE(NR,1170) IVALI
        IF ( IABS(INT(5)) .EQ. 1 ) THEN
          IVALI = INT(6)
          WRITE(NR,1180) IVALI
        END IF
        RVAL0 = REAL(15)
        CALL RCONV1 ( 22, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1190) (LABEL1(I),I=1,4), RVAL1
        IVALI = INT(7)
        WRITE(NR,1200) IVALI
        RVAL0 = REAL(16)
        CALL RCONV1 (  0, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        WRITE(NR,1210) (LABEL1(I),I=1,4), RVAL1
C
```

```
C       REACTION STOICHIOMETRY
C
      MR = INT(15)
      IF ( MR .GT. 0 ) THEN
        NSUBS = INT(12)
        LINES = 3 + MR*(2+NSUBS*2)
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1220)
        CALL LOCATS ( NBSOUT(1), LVIO, LVRO, LDO, NBSO )
        CALL STRVEC ( LDO, NSUBS, IWK(MPH+NSUBS), IWK(MPH) )
        INT11 = INT(11)
        INT14 = INT(14)
        CALL RPSTOI ( MR, INT(INT11), NSUBS, IWK(MPH), NC,
     1                REAL(INT14) )
      END IF
C
C       DIMENSIONS FOR USER VECTORS
C
      LINES = 6
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1230)
      IOFF = 36
      WRITE(NR,1240) (INT(IOFF+I-1),I=1,12)
C
C       INTK ARRAY
C
      IOFF = INT(49)
      LINES = 5
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1250)
      WRITE(NR,1260) INT(IOFF), INT(IOFF+1)
C
C       REALK ARRAY
C
      IOFF = INT(51)
      LINES = 23
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1270)
      WRITE(NR,1280) (REAL(IOFF+LRK1+I-1),I=1,20)
      LINES = 21
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1290) (REAL(IOFF+LRK2+I-1),I=1,20)
      LINES = 21
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1300) (REAL(IOFF+LRK3+I-1),I=1,20)
      LINES = 1
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1310)
      DO 100 I = 1, NCC
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1320) IDSCC(1,I), IDSCC(2,I), REAL(IOFF+LRK4+I-1)
  100 CONTINUE
      LINES = 1
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1310)
      DO 110 I = 1, NCC
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1330) IDSCC(1,I), IDSCC(2,I), REAL(IOFF+LRK5+I-1)
  110 CONTINUE
      LINES = 1
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1310)
```

```
      DO 120 I = 1, NCC
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1340) IDSCC(1,I), IDSCC(2,I), REAL(IOFF+LRK6+I-1)
  120 CONTINUE
C
C       REALP ARRAY
C
      IOFF = INT(55)
      LINES = 3 + KEEP
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1350)
      LINES = 1
      DO 130 I = 1, NCC
        IF ( I .GT. KEEP ) CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1360) IDSCC(1,I), IDSCC(2,I), REAL(IOFF+I-1)
  130 CONTINUE
      LINES = 18
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1370) (REAL(IOFF+NCC+I-1),I=1,18)
C
C       REPORT THE RESULTS
C
  200 CONTINUE
      IF ( IREP(5) .EQ. 0 ) GO TO 9999
      LINES = 2
      CALL RPTHDR ( LINES, IFF, ISC, ISUB )
      WRITE(NR,1380)
      IF ( IOPT .EQ. 2 ) GO TO 230
C
C       WET BASIS PROXIMATE ANALYSIS FOR COAL
C
      IOFF = INT(59)
      LINES = 7
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1390)
      WRITE(NR,1400) (REAL(IOFF+I-1),I=1,4)
C
C       DEVOLATILIZATION CONSTANTS
C
      IOFF = INT(51)
      LINES = 3 + KEEP
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1410)
      LINES = 1
      DO 210 I = 1, NCC
        IF ( I .GT. KEEP ) CALL RPTHDR ( LINES, IHD, ISC, ISUB )
        WRITE(NR,1420) IDSCC(1,I), IDSCC(2,I), REAL(IOFF+LRK7+I-1)
  210 CONTINUE
C
C       TEMPERATURE PROFILE
C
      NPTS = INT(10)
      IF ( NPTS .GT. 0 ) THEN
        INT8 = INT(8)
        INT9 = INT(9)
        RVAL0 = 0D0
        CALL RCONV1 ( 17, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
        CALL RCONV1 ( 22, RVAL0, RVAL2, LABEL2, IFM, IPR, STRNG2 )
        CALL LABCTR ( LABEL1, 4, 12 )
        CALL LABCTR ( LABEL2, 4, 12 )
        LINES = 6 + KEEP
        CALL RPTHDR ( LINES, IHD, ISC, ISUB )
```

```
        WRITE(NR,1430) (LABEL1(I),I=1,3), (LABEL2(I),I=1,3)
        LINES = 1
        IEND = NPTS - 1
        DO 220 I = 1, IEND
          RVAL0 = REAL(INT8+I-1)
          CALL RCONV1 ( 17, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
          RVAL0 = REAL(INT9+I-1)
          CALL RCONV1 ( 22, RVAL0, RVAL2, LABEL1, IFM, IPR, STRNG1 )
          IF ( I .GT. KEEP ) CALL RPTHDR ( LINES, IHD, ISC, ISUB )
          WRITE(NR,1440) RVAL1, RVAL2
 220    CONTINUE
      END IF
C
C       PERFORMANCE SUMMARY
C
 230 CONTINUE
      NSUM = 70
      LINES = 19
      CALL RPTHDR ( LINES, IHD, ISC, ISUB )
      WRITE(NR,1450)
      IF (NSUM.NE.0) WRITE(NSUM,1450)
C
C       COAL FEED FLOW RATE
C
      CALL LOCATS ( NBSIN(2) , LVII2, LVRI2, LDI2, NBSI2 )
      CALL FIPHN(IDSS,LDI2,ISEQ)
      ISS0 = LPHASE(LDI2,ISEQ)
      RVAL0 = B(LVRI2+ISS0)
      CALL RCONV1 ( 10, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
      WRITE (NR,1455) (LABEL1(I),I=1,4), RVAL1
      IF (NSUM.NE.0) WRITE (NSUM,1455) (LABEL1(I),I=1,4), RVAL1
      RETURN

 9999 CONTINUE
      RETURN
C
C       FORMAT STATEMENTS - INPUT DATA AND RESULTS
C
 1000 FORMAT( 1X,16A4)
 1010 FORMAT(/3X,27X,'***  INPUT DATA  ***')
 1020 FORMAT(/3X,'GENERAL PARAMETERS:')
 1030 FORMAT(/5X,'CALCULATION OPTION CODE                  ',16X,I4)
 1040 FORMAT( 5X,'NUMBER OF INTEGRATION INCREMENTS         ',16X,I4)
 1050 FORMAT( 5X,'PHASE CODE FOR THE PROCESS STREAM        ',16X,I4)
 1060 FORMAT( 5X,'NUMBER OF REACTIONS                      ',16X,I4)
 1070 FORMAT( 5X,'REACTOR LENGTH                 ',4A4,6X,G13.6)
 1080 FORMAT( 5X,'REACTOR DIAMETER               ',4A4,6X,G13.6)
 1090 FORMAT( 5X,'REACTOR INLET PRESSURE         ',4A4,6X,G13.6)
 1100 FORMAT( 5X,'REACTOR PRESSURE DROP          ',4A4,6X,G13.6)
 1110 FORMAT( 5X,'HEAT TRANSFER COEFFICIENT, UCP ',4A4,6X,G13.6)
 1120 FORMAT( 5X,'MAXIMUM INTEGRATION STEP SIZE  ',4A4,6X,G13.6)
 1130 FORMAT( 5X,'CONVERGENCE TOLERANCE          ',4A4,6X,G13.6)
 1140 FORMAT(/3X,'COOLANT PARAMETERS:')
 1150 FORMAT(/5X,'COOLANT INLET PRESSURE         ',4A4,6X,G13.6)
 1160 FORMAT( 5X,'COOLANT PRESSURE DROP          ',4A4,6X,G13.6)
 1170 FORMAT( 5X,'NUMBER OF PHASES                         ',16X,I4)
 1180 FORMAT( 5X,'SINGLE PHASE CODE                        ',16X,I4)
 1190 FORMAT( 5X,'INITIAL TEMPERATURE ESTIMATE   ',4A4,6X,G13.6)
 1200 FORMAT( 5X,'MAXIMUM NUMBER OF FLASH ITERATIONS       ',16X,I4)
 1210 FORMAT( 5X,'FLASH CONVERGENCE TOLERANCE    ',4A4,6X,G13.6)
 1220 FORMAT(/3X,'REACTION STOICHIOMETRY:'/)
 1230 FORMAT(/3X,'DIMENSIONS FOR USER VECTORS:')
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1240 FORMAT(/5X,'NINTK  = ',I4,5X,'NREALK = ',I4,
   1      5X,'NIWK   = ',I4,5X,'NWK    = ',I4,
   2     /5X,'NINTP  = ',I4,5X,'NREALP = ',I4,
   3      5X,'NIWP   = ',I4,5X,'NWP    = ',I4,
   4     /5X,'NINTQ  = ',I4,5X,'NREALQ = ',I4,
   5      5X,'NIWQ   = ',I4,5X,'NWQ    = ',I4)
1250 FORMAT(/3X,'INTK ARRAY:')
1260 FORMAT(/5X,'MAXIMUM NUMBER OF ITERATIONS              ',15X,I4,
   1     /5X,'REPORT OPTION: 1 = STANDARD, 2 = SUMMARY  ',15X,I4)
1270 FORMAT(/3X,'REALK ARRAY:')
1280 FORMAT(/5X,'RATE CONSTANT FOR REACTION #1          ',15X,G13.6,
   1     /5X,'ACTIVATION ENERGY FOR REACTION #1      ',15X,G13.6,
   2     /5X,'RATE CONSTANT FOR REACTION #2          ',15X,G13.6,
   3     /5X,'ACTIVATION ENERGY FOR REACTION #2      ',15X,G13.6,
   4     /5X,'RATE CONSTANT FOR REACTION #3          ',15X,G13.6,
   5     /5X,'ACTIVATION ENERGY FOR REACTION #3      ',15X,G13.6,
   6     /5X,'RATE CONSTANT FOR REACTION #4          ',15X,G13.6,
   7     /5X,'ACTIVATION ENERGY FOR REACTION #4      ',15X,G13.6,
   8     /5X,'RATE CONSTANT FOR REACTION #5          ',15X,G13.6,
   9     /5X,'ACTIVATION ENERGY FOR REACTION #5      ',15X,G13.6,
   +     /5X,'UNUSED                        ',15X,G13.6,
   1     /5X,'UNUSED                        ',15X,G13.6,
   2     /5X,'UNUSED                        ',15X,G13.6,
   3     /5X,'UNUSED                        ',15X,G13.6,
   4     /5X,'UNUSED                        ',15X,G13.6,
   5     /5X,'UNUSED                        ',15X,G13.6,
   6     /5X,'UNUSED                        ',15X,G13.6,
   7     /5X,'UNUSED                        ',15X,G13.6,
   8     /5X,'UNUSED                        ',15X,G13.6,
   9     /5X,'UNUSED                        ',15X,G13.6)
1290 FORMAT(/5X,'BED VOID FRACTION                      ',15X,G13.6,
   1     /5X,'COAL VOID FRACTION                   ',15X,G13.6,
   2     /5X,'INITIAL COAL PARTICLE DIAMETER    CM  ',15X,G13.6,
   3     /5X,'RESERVED FOR UWV MODEL                ',15X,G13.6,
   4     /5X,'INITIAL DENSITY OF CHAR        G/CM3 ',15X,G13.6,
   5     /5X,'INITIAL DENSITY OF ASH         G/CM3 ',15X,G13.6,
   6     /5X,'RATIO OF C TO O2 IN REACTION #4       ',15X,G13.6,
   7     /5X,'SCHMIDT NUMBER                       ',15X,G13.6,
   8     /5X,'DIFFUSION CONSTANT FOR OXYGEN    CM2/S ',15X,G13.6,
   9     /5X,'DIFFUSION CONSTANT FOR WATER     CM2/S ',15X,G13.6,
   +     /5X,'KINETIC MODEL: 1=AS, 2=SP, 3=HOMO     ',15X,G13.6,
   1     /5X,'UNUSED                        ',15X,G13.6,
   2     /5X,'UNUSED                        ',15X,G13.6,
   3     /5X,'UNUSED                        ',15X,G13.6,
   4     /5X,'UNUSED                        ',15X,G13.6,
   5     /5X,'UNUSED                        ',15X,G13.6,
   6     /5X,'UNUSED                        ',15X,G13.6,
   7     /5X,'UNUSED                        ',15X,G13.6,
   8     /5X,'UNUSED                        ',15X,G13.6,
   9     /5X,'UNUSED                        ',15X,G13.6)
1300 FORMAT(/5X,'FRACTION VM RELEASED BY PYROLYSIS      ',15X,G13.6,
   1     /5X,'FINAL TEMPERATURE FOR VM RELEASE  K    ',15X,G13.6,
   2     /5X,'INITIAL TEMPERATURE FOR VM RELEASE K   ',15X,G13.6,
   3     /5X,'CONVERSION OF FIXED CARBON, 1ST ITERATION ',15X,G13.6,
   4     /5X,'CONVERSION OF FIXED CARBON, 2ND ITERATION ',15X,G13.6,
   5     /5X,'MASS FRACTION OF RECTISOL NAPHTHA IN VM  ',15X,G13.6,
   6     /5X,'MASS FRACTION OF CRUDE PHENOL IN VM     ',15X,G13.6,
   7     /5X,'MASS FRACTION OF TAR OILS IN VM        ',15X,G13.6,
   8     /5X,'UNUSED                        ',15X,G13.6,
   9     /5X,'UNUSED                        ',15X,G13.6,
   +     /5X,'UNUSED                        ',15X,G13.6,
   1     /5X,'UNUSED                        ',15X,G13.6,
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   2     /5X,'UNUSED                          ',15X,G13.6,
   3     /5X,'UNUSED                          ',15X,G13.6,
   4     /5X,'UNUSED                          ',15X,G13.6,
   5     /5X,'UNUSED                          ',15X,G13.6,
   6     /5X,'UNUSED                          ',15X,G13.6,
   7     /5X,'UNUSED                          ',15X,G13.6,
   8     /5X,'UNUSED                          ',15X,G13.6,
   9     /5X,'UNUSED                          ',15X,G13.6)
1310 FORMAT( 1X)
1320 FORMAT( 5X,'MASS FRACTION OF ',2A4,' IN RECTISOL NAPHTHA',
   1     12X,G13.6)
1330 FORMAT( 5X,'MASS FRACTION OF ',2A4,' IN CRUDE PHENOL    ',
   1     12X,G13.6)
1340 FORMAT( 5X,'MASS FRACTION OF ',2A4,' IN TAR OILS        ',
   1     12X,G13.6)
1350 FORMAT(/3X,'REALP ARRAY:'/)
1360 FORMAT( 5X,'INTEGRATION WEIGHTING FOR ',2A4,23X,G13.6)
1370 FORMAT( 5X,'INTEGRATION WEIGHTING FOR TOTAL GAS FLOW  ',15X,G13.6,
   1     /5X,'INTEGRATION WEIGHTING FOR PROXANAL(1)     ',15X,G13.6,
   2     /5X,'INTEGRATION WEIGHTING FOR PROXANAL(2)     ',15X,G13.6,
   3     /5X,'INTEGRATION WEIGHTING FOR PROXANAL(3)     ',15X,G13.6,
   4     /5X,'INTEGRATION WEIGHTING FOR PROXANAL(4)     ',15X,G13.6,
   5     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(1)      ',15X,G13.6,
   6     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(2)      ',15X,G13.6,
   7     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(3)      ',15X,G13.6,
   8     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(4)      ',15X,G13.6,
   9     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(5)      ',15X,G13.6,
   +     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(6)      ',15X,G13.6,
   1     /5X,'INTEGRATION WEIGHTING FOR ULTANAL(7)      ',15X,G13.6,
   2     /5X,'INTEGRATION WEIGHTING FOR SULFANAL(1)     ',15X,G13.6,
   3     /5X,'INTEGRATION WEIGHTING FOR SULFANAL(2)     ',15X,G13.6,
   4     /5X,'INTEGRATION WEIGHTING FOR SULFANAL(3)     ',15X,G13.6,
   5     /5X,'INTEGRATION WEIGHTING FOR TOTAL SOLID FLOW',15X,G13.6,
   6     /5X,'INTEGRATION WEIGHTING FOR PROCESS TEMP    ',15X,G13.6,
   7     /5X,'INTEGRATION WEIGHTING FOR HEAT TRANSFER   ',15X,G13.6)
1380 FORMAT(/3X,28X,'***  RESULTS  ***')
1390 FORMAT(/3X,'WET BASIS PROXIMATE ANALYSIS FOR COAL:')
1400 FORMAT(/5X,'MOISTURE (WET)                 WT%   ',15X,G13.6,
   1     /5X,'FIXED CARBON (WET)             WT%   ',15X,G13.6,
   2     /5X,'VOLATILE MATTER (WET)          WT%   ',15X,G13.6,
   3     /5X,'ASH (WET)                      WT%   ',15X,G13.6)
1410 FORMAT(/3X,'DEVOLATILIZATION CONSTANTS:'/)
1420 FORMAT( 5X,'KGMOL OF ',2A4,' PER KG OF VOLATILE MATTER',14X,G13.6)
1430 FORMAT(/3X,'TEMPERATURE PROFILE:',
   1     //5X,18X,'  LOCATION  ',5X,' TEMPERATURE ',
   2     /5X,18X,3A4,6X,3A4,
   3     /5X,18X,'------------',5X,'------------')
1440 FORMAT( 5X,18X,G13.6,5X,G13.6)
1450 FORMAT(/3X,'PERFORMANCE SUMMARY:')
1455 FORMAT(/5X,'COAL FEED FLOW RATE                ',4A4,6X,G13.6)
1460 FORMAT( 5X,'FIXED CARBON CONVERTED             ','%',21X,G13.6)
1470 FORMAT( 5X,'PEAK TEMPERATURE                   ',4A4,6X,G13.6)
1480 FORMAT( 5X,'CONC. OF ',2A4,' IN RAW GAS (DRY) MOL%   ',14X,G13.6)
1490 FORMAT( 5X,'RAW GAS MASS FLOW RATE (DRY)       ',4A4,6X,G13.6)
1500 FORMAT( 5X,'RAW GAS VOLUME FLOW RATE (DRY)     ',4A4,6X,G13.6)
1510 FORMAT( 5X,'FLOW OF WATER IN RAW GAS           ',4A4,6X,G13.6)
1520 FORMAT( 5X,'RAW GAS TEMPERATURE                ',4A4,6X,G13.6)
1530 FORMAT( 5X,'HEAT TRANSFERRED TO STEAM JACKET   ',4A4,6X,G13.6)
1540 FORMAT( 5X,'MASS FLOW OF STEAM PRODUCED        ',4A4,6X,G13.6)
1550 FORMAT( 5X,'OUTLET STEAM TEMPERATURE           ',4A4,6X,G13.6)
1560 FORMAT( 5X,'REACTOR STEAM UTILIZATION          ',16X,6X,G13.6)
C
```

```
C     FORMAT STATEMENTS - ERROR MESSAGES
C
 2000 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',23X,'BLOCK WAS NOT EXECUTED',23X,'*',
     2       /5X,'*',68X,'*',/5X,70('*'))
 2010 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',23X,'ZERO FEED TO THE BLOCK',23X,'*',
     2       /5X,'*',23X,'BLOCK WAS NOT EXECUTED',23X,'*',
     3       /5X,'*',68X,'*',/5X,70('*'))
 2020 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',12X,'OUTLET PROCESS STREAM PHASE SPEC IS',
     2        1X,'INCORRECT',11X,'*',
     3       /5X,'*',12X,'BLOCK EXITED IN THE MIDDLE OF THE',
     4        1X,'SIMULATION',12X,'*',
     5       /5X,'*',68X,'*',/5X,70('*'))
 2040 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',17X,'RUNGE-KUTTA INTEGRATION HALVED OUT',17X,'*',
     2       /5X,'*',12X,'BLOCK EXITED IN THE MIDDLE OF THE',
     3        1X,'SIMULATION',12X,'*',
     4       /5X,'*',68X,'*',/5X,70('*'))
 2050 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',23X,'TOTAL PRESSURE IS ZERO',23X,'*',
     2       /5X,'*',23X,'BLOCK WAS NOT EXECUTED',23X,'*',
     3       /5X,'*',68X,'*',/5X,70('*'))
 2060 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',18X,'INCORRECT STREAM CLASS STRUCTURE',18X,'*',
     2       /5X,'*',23X,'BLOCK WAS NOT EXECUTED',23X,'*',
     3       /5X,'*',68X,'*',/5X,70('*'))
 2070 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',16X,'SPECIFIED INLET COAL FLOW IS TOO',
     2        1X,'LOW',16X,'*',
     3       /5X,'*',12X,'BLOCK EXITED IN THE MIDDLE OF THE',
     4        1X,'SIMULATION',12X,'*',
     5       /5X,'*',68X,'*',/5X,70('*'))
 2080 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',20X,'CONVERGENCE WAS NOT ACHIEVED',20X,'*',
     2       /5X,'*',68X,'*',/5X,70('*'))
 2090 FORMAT(//5X,70('*'),/5X,'*',68X,'*',
     1       /5X,'*',12X,'TEMPERATURE IS TOO LOW FOR',
     2        1X,'DEVOLATILIZATION',13X,'*',
     3       /5X,'*',68X,'*',/5X,70('*'))
      END


C$ #09 BY; SSIWPK DATE: 03/04/93 C$ 7 CUT OUT FOR DELIVERY TO U.N.D.
C$ #08 BY: SSIWPK DATE: 03/03/93 SAVE INPUT VOL.MATTER RELEASE TEMP.
C$ #07 BY: SSIKRC DATE: 02/05/93 ADD CALL FOR TRANSPORT PROPERTY CALCS.
C$ #06 BY: SIMSCI DATE: 01/15/91 ADD /RGAS1A/ AND CALC. REALK OFFSETS
C$ --------------------- V8 CHANGES START ABOVE ----------------------
C$ #05 BY: JSDINC DATE: 11/16/88 UPDATE /GLOBAL/ AND ARG LIST
C$ #04 BY: BWB    DATE: 03/20/84 TRANSMIT ALL PROCESS STREAMS
C$ #03 BY: BWB    DATE: 03/20/84 REMOVE TRANSMISSION OF WORK STREAMS
C$ #02 BY: JSDINC DATE: 03/20/84 RETRIEVE WORK AREA OFFSETS
C$ #01 BY: JSDINC DATE: 03/15/84 NEW
C-------------------------------------------------------------------
C
C *-----------------------------------------------------------------
C *                      ****  NOTICE  ****
C *-----------------------------------------------------------------
C
C
C*****************************************************************************************************
```

```
C
C        COPYRIGHT (C) 1981-85
C        JAY S. DWECK, CONSULTANT, INC.
C
C*********************************************************************************************************
C
C------------------------------------------------------------------
      SUBROUTINE URE09I(NB    ,NISCP ,ISCP  ,NIDS  ,IDS   ,
     1                  NPO   ,NBOPST,NWDIR ,IWDIR ,NINT  ,
     2                  INT   ,NREAL ,REAL  ,NSIN  ,NBSIN ,
     3                  NSOUT ,NBSOUT,NINFI ,NINFO ,NISIZE,
     4                  ISIZE ,NSIZE ,SIZE  ,MODEL ,KINET ,
     5                  PDROP ,QTRANS,MODELE)
C
C   NAME OF MODULE:
C
C   TASK, SUBSYSTEM, SYSTEM:      URE09I, URE09, UOS
C
C   WRITTEN BY: MICHAEL MENDELSON       DATE WRITTEN: 03/15/84
C
C
C
C      NAME - URE09 (.....)
C      DESCRIPTION -  MODEL
C
C      NAME -  SUNLCK
C      DESCRIPTION -  TO UNLOCK STREAMS
C
C
C
C      SPECIFICATIONS, DECLARATIONS, DATA STATEMENTS, ETC.
C
C** DOUBLE PRECISION
      IMPLICIT REAL*8 (A-H,O-Z)
      SAVE
      EXTERNAL MODEL, KINET, PDROP, QTRANS, MODELE
      DIMENSION ISCP(NISCP) ,IDS(2,NIDS) ,NBOPST(2,NPO) ,IWDIR(NWDIR),
     1          INT(NINT)   ,REAL(NREAL) ,NBSIN(NSIN)  ,NBSOUT(NSOUT),
     2          ISIZE(NISIZE),SIZE(NSIZE)
      COMMON /USER/ RUMISS, IUMISS, NGBAL , IPASS , IRESTR , ICONVG ,
     $              LMSG , LPMSG , KFLAG , NHSTRY , NRPT   , NTRMNL
C     END COMMON /USER/ 05-26-80
      COMMON /WORK/ WORK(1)
      DIMENSION IWORK(1)
      EQUIVALENCE (WORK(1),IWORK(1))
      COMMON /NCOMP/ NCC    ,NNCC  ,NC    ,NAC   ,NACC  ,
     1                 NVCP   ,NVNCP ,NVACC ,NVANCC
C     END COMMON /NCOMP/ 10-13-78
      COMMON /RGLOB/ RMISS  ,RMIN   ,ABSMIN ,SCLMIN ,XMIN   ,
     1               HSCALE ,RELMIN ,SCLDEF ,TMAX   ,TNOW
C     END COMMON /RGLOB/ 10-13-78
      COMMON /GLOBAL/ KPFLG1 ,KPFLG2 ,KPFLG3 ,LABORT ,NH     ,
     1                LDIAG  ,NCHAR  ,IMISS  ,MISSC1 ,MISSC2 ,
     2                LPDIAG ,IEBAL  ,IRFLAG ,MXBLKW ,ITYPRN ,
     3                LBNCF  ,LBCP   ,LSDIAG ,MAXNE  ,MAXNP1 ,
     4                MAXNP2 ,MAXNP3 ,IUPDAT ,IRSTRT ,LSFLAG ,
     5                LRFLAG ,KBLK1  ,KBLK2  ,KRFLAG ,IRNCLS ,
     6                LSTHIS ,IRETCD ,JRFLAG ,JSFLAG ,ICOMTP
C     END COMMON /GLOBAL/ 7-21-81
      COMMON /RPTGLB/ IREPFL,ISUB(10)
C     END COMMON /RPTGLB/ 09-06-79
      COMMON /PLEX/ IB(1)
```

```
      DIMENSION B(1)
      EQUIVALENCE (IB(1), B(1))
C     END COMMON /PLEX/ 10-13-78
      COMMON /RGAS1A/ LRK1, LRK2, LRK3, LRK4, LRK5, LRK6, LRK7
      DATA VMRT,VMRTF /0D0,0D0/
C     .
C     . FORMAT STATEMENTS
C     .
 10   FORMAT (6X,'INCONSISTENT HMB FLAG. SIZING CALCULATIONS WILL NOT',
     1' BE DONE.')
C
C        CHECK FOR REPORT PASS
C
      IF(IREPFL .EQ. 0)GO TO 202
      CALL URE09R (NSIN  ,NBSIN ,NSOUT ,NBSOUT,NINT  ,INT   ,
     1            NREAL ,REAL  ,NPO   ,NBOPST,NIDS  ,IDS   ,
     2            NISCP ,ISCP  ,NISIZE,ISIZE ,NB, S)


      GO TO 10000
C     .
C     . SET THE HMB RESULT FLAG
C     .
  202 IF(JRFLAG.EQ.0) GO TO 9999
      IF(JRFLAG.NE.2) ISCP(5)=-9999
C-----------------------------------------------------------------------
C       GET THE STREAM INFORMATION
C-----------------------------------------------------------------------
      CALL LOCATS(NBSOUT(1),LVIOUT,LVROUT,LD,NBD)
      CALL LOCATS(NBSOUT(2),LVIO3,LVRO3,LD,NBD)
      CALL LOCATS(NBSOUT(3),LVIOUC,LVROUC,LD,NBD)
C-----------------------------------------------------------------------
C      SET UP FEED STREAM TO CALL MODEL (URE09)
C-----------------------------------------------------------------------
      CALL LOCATS(NBSIN(1),LVIIN,LVRIN,LD,NBD)
      CALL LOCATS(NBSIN(2),LVI3,LVRI3,LD,NBD)
      CALL LOCATS(NBSIN(3),LVIINC,LVRINC,LD,NBD)
      NXLOC = INT(10)
      LXLOC = INT(8)
      LTEMP = INT(9)
      NREACT = INT(15)
      LCOEF = INT(14)
      LPEXP = INT(17)
      LENGR = INT(18)
      LEXCN = INT(22)
C      LIRSF1 = INT(25)
C      LIRSF2 = INT(28)
C      LRRSF1 = INT(31)
C      LRRSF2 = INT(34)
C      LIRSF3 = INT(61)
C      LRRSF3 = INT(64)
      NINK   = INT(36)
      NRK    = INT(37)
      NIWK   = INT(38)
      NWK    = INT(39)
      NINP   = INT(40)
      NRP    = INT(41)
      NIWP   = INT(42)
      NWP    = INT(43)
      NINQ   = INT(44)
      NRQ    = INT(45)
      NIWQ   = INT(46)
```

```
      NWQ    = INT(47)
      LINK   = INT(49)
      LRK    = INT(51)
      LINP   = INT(53)
      LRP    = INT(55)
      LINQ   = INT(57)
      LRQ    = INT(59)
C-------------------------------------------------------------------
C   INITIALIZE THE REALK OFFSET VARIABLES
C-------------------------------------------------------------------
      LRK1 = 0
      LRK2 = LRK1 + 20
      LRK3 = LRK2 + 20
      LRK4 = LRK3 + 20
      LRK5 = LRK4 + NCC
      LRK6 = LRK5 + NCC
      LRK7 = LRK6 + NCC
C
C   INITIALIZE OR RESTORE VOLATILE MATTER RELEASE TEMPERATURE
C
      IF (VMRT .EQ. 0D0) THEN
        VMRT = REAL(LRK+LRK3+1)
      ELSE
        IF (REAL(LRK+LRK3+1) .EQ. VMRTF) THEN
          REAL(LRK+LRK3+1) = VMRT
        ELSE
          VMRT = REAL(LRK+LRK3+1)
        END IF
      END IF
C-------------------------------------------------------------------
C   FIND THE TOTAL NUMBER OF COMPONENT
C-------------------------------------------------------------------
      NSUBS=NPHASE(LD)
      NX= 0
      DO  580 I = 1 , NSUBS
      KTYPE = IPTYPE(LD,I)
      GO TO(550,560,570),KTYPE
  550 CONTINUE
      NX = NX + NCC
      GO TO 580
  560 CONTINUE
      NX = NX + NCC
      GO TO 580
  570 CONTINUE
      NX = NX + NNCC
  580 CONTINUE
      LX = NX + 2
      NF = 17*LX
      IWA = 2*LX*LX
      NSTATE=NCC+40
C-------------------------------------------------------------------
C    GET VECTOR ADDRESS LOCATION
C-------------------------------------------------------------------
      LITYPE = IWDIR(2)
      LJTYPE = IWDIR(3)
      LIDXSU = IWDIR(4)
      LJDXSU = IWDIR(5)
      LIWK = IWDIR(14)
      LWK = IWDIR(15)
      LIWP = IWDIR(16)
      LWP = IWDIR(17)
      LIWQ = IWDIR(18)
```

```
      LWQ = IWDIR(19)
      LWSTAT = IWDIR(20)
      LWDERV = IWDIR(22)
      LWAUX = IWDIR(24)
      LPRMT = IWDIR(26)
C-----------------------------------------------------------------------
C      CALL MODEL
C-----------------------------------------------------------------------
C
C       LOAD COMMON USER FROM GLOABL AND ISCP
C
      IUMISS = IMISS
      RUMISS = RMISS
      NGBAL = ISCP(3)
      IPASS = JRFLAG
      IF(IREPFL.EQ.1) IPASS = 4
      IRESTR = ISCP(6)
      LMSG = ISCP(1)
      LPMSG = ISCP(2)
      KFLAG = KPFLG3
      NHSTRY = NH
      NRPT = NR
      NTRMNL = NTERM
C
C
      CALL MODEL(LD     ,LVRIN ,LVROUT,LVRI3 ,LVRO3 ,LVRINC,LVROUC,
     1          NISCP ,ISCP  ,NPO   ,NBOPST,NIDS  ,IDS   ,NINT  ,
     2          INT   ,NREAL ,REAL  ,REAL(LPEXP) ,REAL(LENGR) ,
     3          REAL(LEXCN) ,REAL(LCOEF) ,NINK  ,INT(LINK)    ,
     4          NINP  ,INT(LINP)     ,NINQ  ,INT(LINQ)     ,NRK   ,
     5          REAL(LRK)     ,NRP   ,REAL(LRP)     ,NRQ   ,
     6          REAL(LRQ)     ,NIWK  ,IWORK(LIWK) ,NIWP  ,
     7          IWORK(LIWP)  ,NIWQ  ,IWORK(LIWQ) ,NWK   ,
     8          WORK(LWK)     ,NWP   ,WORK(LWP)     ,NWQ   ,
     9          WORK(LWQ)     ,NXLOC ,REAL(LXLOC)  ,REAL(LTEMP)  ,
     X           NSUBS ,NC    ,NCC   ,NREACT,NF    ,IWA   ,
     1          IWORK(LIDXSU),IWORK(LJDXSU),IWORK(LITYPE),
     2          IWORK(LJTYPE),NWDIR ,IWDIR ,KINET ,PDROP ,QTRANS ,
     3          WORK(LWSTAT) , WORK(LWDERV),WORK(LWAUX)  ,NSTATE ,
     4          WORK(LPRMT)  )
      VMRTF = REAL(LRK+LRK3+1)
      IF(ISCP(5).EQ.-9999) ISCP(5)=0
C-----------------------------------------------------------------------
C
 9999 IF(JSFLAG .EQ. 0) GO TO 10000
C
C-----------------------------------------------------------------------
C
C           UNLOCK THE STREAMS
C
10000 CALL SUNLCK(NSIN,NBSIN,NSOUT,NBSOUT)
      RETURN
      END


C$ #13 BY: SIMSCI DATE: 01/26/93 PROTECT AGAINST DIV./0 AROUND LINE 353
C$ #12 BY: SIMSCI DATE: 08/28/92 PROTECT AGAINST DIV./0 AROUND LINE 350
C$ #11 BY: SIMSCI DATE: 12/10/91 NPKODE=3 TEST FIRST FOR MIXED RESULTS
C$ --------------------- V8 CHANGES START ABOVE ----------------------
C$ #10 BY: JSDINC DATE: 04/25/89 CHANGE FREE TO FREESP
C$ #9 BY: JSDINC DATE: 12/04/88 CORRECT SOLID MW NAME IN DENSITY CALC
C$ #8 BY: JSDINC DATE: 05/13/87 DIMENSN. DD TO 15
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C$ #7 BY: JSDINC DATE: 09/29/85 DIMENSN. DD TO 16
C$ #6 BY: JSDINC DATE: 10/10/86 UPDATE FOR SOLIDS
C$ #5 BY: JSDINC DATE: 07/07/86 CORRECT MW CALCULATION
C$ #4 BY: JSDINC DATE: 06/27/86 STREAM LINE CODE
C$ #3 BY: JSDINC DATE: 04/21/86 CORRECT MASS VOLUME CALC
C$ #2 BY: CHEN DATE: 11/13/81 ADD ARGS.
C$ #1 BY: CCCHEN DATE: 10/26/81 SPLIT APART
C-----------------------------------------------------------------
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C       JAY S. DWECK, CONSULTANT, INC.
C       DENVER, COLORADO  80222
C-----------------------------------------------------------------
C       COPYRIGHT (C) 1980
C        MASSACHUSETTS INSTITUTE OF TECHNOLOGY
C        CAMBRIDGE, MA
C-----------------------------------------------------------------
      SUBROUTINE FLASHA(B     ,NPH    ,LPB    ,IPHASE ,NBOPST ,
     1               NCPM   ,NCPCS  ,SCS    ,NCPNCS ,SNCS   ,
     2               HM     ,NPKODE ,KPHASE ,LOPDIA ,KDENS  ,MJ,
     3               X      ,IDX    ,NX     ,X1     ,IDX1,  NX1,
     4               X2     ,IDX2   ,NX2    ,Y      ,IDY    ,NY ,
     5               F      ,IDF    ,NF)
C
C   NAME OF MODULE: FLASHA
C
C   MODULE TITLE: STREAM FLASH ROUTINE  (APPENDIX)
C
C
C   PURPOSE: THIS ROUTINE IS USED TO CALCULATE AND STORE STREAM
C          PROPERITIES AFTER A FLASH.
C          NO DEFUALT IS PROVIDED, ALL VALUES HAVE TO BE SPECIFIED.
C
C   TASK, SUBSYSTEM, SYSTEM: STREAM FLASH, UTILITY ROUTINE, UOS
C
C   WRITTEN BY: CHAU-CHYUN CHEN       DATE WRITTEN: JUNE 9, 1980
C
C   READ BY:                       DATE READ:
C
C   APPROVED BY:                     DATE APPROVED:
C
C   CALLING SEQUENCE:
C
C          CALL FLASH
C
C   VARIABLES USED:
C
C    VARIABLES IN ARGUMENT LIST:
C
C  VARIABLE  I/O  TYPE   DIM   DESCRIPTION AND RANGE
C   I/O:  INPUT/OUTPUT
C   DIM:  DIMENSION
C
C  SVEC      I/O  R    (1)    STREAM VECTOR
C  NSUBS      I   I    --    NUMBER OF SUBSTREAMS IN THE STREAM
C  IDSUBS     I   I    NSUBS  LOCATION VECTOR OF SUBSTREAM SEGMENTS
C                         IN THE STREAM VECTOR
C  ITYPE     I   I    NSUBS  SUBSTREAM TYPE VECTOR
C                         1: MIXED SUBSTREAM
C                         2: CSOLID SUBSTREAM
C                         3: NCSOLID SUBSTREAM
C  NBOPST     I   I   (3,NPO) PHYSICAL PROPERTY OPTION SET
C  KODE       I   I   --    FLASH OPTION KODE
```

```
C                       1:PQ 2:TP 3:PV 4:TQ 5:TV
C                       IF NPKODE=1, 1:Q 2:T
C  NPKODE   I   I   --   NUMBER OF PHASES IN THE MIXED SUBSTREAM
C                       IF NPKODE=1  WFLASH IS CALLED
C                       IF NPKODE=2  XFLASH IS CALLED
C                       IF NPKODE=3  YFLASH IS CALLED
C  KPHASE   I   I   --   KEY PHASE FOR NPKODE=1 (WFLASH)
C                       1:VAPOR 2:LIQUID 3:SOLID
C  MXIT     I   I   --  MAXIMUM NUMBER OF ITERATIONS
C  TOL      I   R   --  ITERATION TOLERANCE
C  SPEC1    I   R   --   FIRST SPECIFIED VARIBLE
C                       IF KODE=1  SPEC1=P
C                       IF KODE=2  SPEC1=T
C                       IF KODE=3  SPEC1=P
C                       IF KODE=4  SPEC1=T
C                       IF KODE=5  SPEC1=T
C  SPEC2    I   R   --   SECOND SPECIFIED VARIABLE
C                       IF KODE=1  SPEC2=Q
C                       IF KODE=2  SPEC2=P
C                       IF KODE=3  SPEC2=V
C                       IF KODE=4  SPEC2=Q
C                       IF KODE=5  SPEC2=V
C      FOR SPEC1 AND SPEC2: P CAN BE < OR = 0D0
C  GUESS    I   R   --   INITIAL GUESS
C                       IF KODE=1  GUESS=T
C                       IF KODE=2  NO GUESS REQUIRED
C                       IF KODE=3  GUESS=T
C                       IF KODE=4  GUESS=P
C                       IF KODE=5  GUESS=P
C          NOTE: INITIAL VALUES ARE NOT REQUIRED; DEFAULT PROVIDED
C  LODIAG   I   I   --   LOCAL DIAGNOSTIC MESSAGE FLAG
C  LOPDIA   I   I   --   LOCAL PHYSICAL PROPERTY DIAGNOSTIC FLAG
C  KSIM     I   I   --  SIMULATION RESTART FLAG
C  KDENS    I   I   --   RESULT CALCULATION FLAG
C                        KDENS=0  NOT RESULT PASS
C                        KDENS=1  RESULT PASS
C  RETN     R   R  NRETN   REAL RETENTION VECTOR
C                        NRETN=6*NCC+31
C  IRETN    R   I  NIRETN  INTEGER RETENTION VECTOR
C                        NIRETN=6
C  LCFLAG   O   I   --   LOCAL CONVERGENCE FLAG
C                       IF LCFLAG=0  CONVERGED
C                       IF LCFLAG=-1  NOT CONVERGED
C
C
C    COMPONENTS OF VECTOR RETN:
C    (SEE XFLASH AND YFLASH TECHNICAL DOCUMENTATIONS)
C      K1(NCC)
C      K2(NCC)
C      Z1(NCC)
C      Z2(NCC)
C      ALPHA1(NCC)
C      ALPHA2(NCC)
C      RET(20)
C      RSCLAR(11)
C
C     COMPONENTS OF VECTOR WK AND IWK
C    F(NCC)
C    X(NCC)
C    X1(NCC)
C    X2(NCC)
C    Y(NCC)
```

```
C    XCS(NCC)
C    XNCS(NNCC)
C    HXF(NHXF) NHXF=(NCC+8)**2
C    HYF(NHYF) NHYF=(2*NCC+10)**2
C    WYF(NWYF) NWYF=20*NCC+45
C    IDXM(NCC)
C    IDXCS(NCC)
C    IDXNCS(NNCC)
C    IPHASE(NPH)
C    LPB(NPH)
C
C
C    ERROR CONDITIONS:
C
C      NUMBER  LEVEL    TEXT
C
C    SUBROUTINES CALLED:
C
C      NAME - CPACK (SUBROUTINE)
C      DESCRIPTION - CONVENTIONAL PHASES PACKING
C
C      NAME - TEMPC (SUBROUTINE)
C      DESCRIPTION - CONVENTIONAL PHASE TEMPERATURE CALCULATION
C
C      NAME - NCPACK (SUBROUTINE)
C      DESCRIPTION - NON-CONVENTIONAL PHASES PACKING
C
C      NAME - TEMPNC (SUBROUTINE)
C      DESCRIPTION - NON-CONVENTIONAL SOLID PHASE TEMPERATURE
C               CALCULATION
C
C      NAME - SPACK (SUBROUTINE)
C      DESCRIPTION - ADDING AND PACKING SOLID PHASES OF A STREAM
C
C      NAME - WFLASH (SUBROUTINE)
C      DESCRIPTION - GENERAL PURPOSE SINGLE PHASE FLASH
C
C      NAME - XFLASH (SUBROUTINE)
C      DESCRIPTION - GENERAL PURPOSE TWO PHASE FLASH
C
C      NAME - YFLASH (SUBROUTINE)
C      DESCRIPTION - GENERAL PURPOSE THREE PHASE FLASH
C
C      NAME - AVEMW (FUNCTION)
C      DESCRIPTION - AVERAGE MOLECULAR WEIGHT
C
C      NAME - TEMPS (SUBROUTINE)
C      DESCRIPTION - TEMPERATURE CALCULATION OF SOLID PHASES
C
C      NAME - VMTHRM (SUBROUTINE)
C      DESCRIPTION - VAPOR MIXTURE THERMAL MONITOR
C
C      NAME - VOLS (SUBROUTINE)
C      DESCRIPTION - SOLID VOLUME MONITOR
C
C      NAME - LMTHRM (SUBROUTINE)
C      DESCRIPTION - LIQUID MIXTURE THERMAL MONITOR
C
C      NAME - DENSTY
C      DESCRIPTION - NON-CONVENTIONAL DENSITY MONITOR
C
C      NAME - ENTHAL
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C       DESCRIPTION - NON-CONVENTIONAL ETHALPY MONITOR
C
C       NAME - ENTROP
C       DESCRIPTION - NON-CONVENTIONAL ENTROPY MONITOR
C
C       NAME - SIMISS
C       DESCRIPTION - STREAM VECTOR INITIALIZATION ROUTINE
C
C       NAME - SMTHRM
C       DESCRIPTION - SOLID MIXTURE THERMAL MONITOR
C       NAME - LERRPT (FUNCTION)
C       DESCRIPTION - ERROR MESSAGE CHECKING
C
C       NAME - ERRSP (SUBROUTINE)
C       DESCRIPTION - ERROR HANDLING ROUTINE
C
C    FILES:
C
C       FILE NAME - HISTORY   - TITLE -
C       FORTRAN UNIT NUMBER -     - I/O -
C       CREATED BY / USED BY -
C       SEQUENCED ON -
C       ACCESS MODE -
C       DESCRIPTION -
C
C       SPECIFICATIONS, DECLARATIONS, DATA STATEMENTS, ETC.
C
C*    DABS(X)=ABS(X)
C** DOUBLE PRECISION
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /PLEX/ IPB(1)
      LOGICAL SOLIDS
      DIMENSION PB(1)
      EQUIVALENCE (IPB(1),PB(1))
C     END COMMON /PLEX/ 10-13-78
      COMMON /ICHWRK/ JWORK(1)
C     END COMMON /ICHWRK/ 6-20-85
      COMMON /CHWRK/ WORK(1)
C     END COMMON /CHWRK/ 6-20-85
      COMMON /IDXNCC/ IDXNCC(1)
      COMMON /GLOBAL/ KPFLG1 ,KPFLG2 ,KPFLG3 ,LABORT ,NH      ,
     1              LDIAG  ,NCHAR  ,IMISS  ,MISSC1 ,MISSC2 ,
     2              LPDIAG ,IEBAL  ,IRFLAG ,MXBLKW ,ITYPRN ,
     3              LBNCP  ,LBCP   ,LSDIAG ,MAXNE  ,MAXNP1 ,
     4              MAXNP2 ,MAXNP3 ,IUPDAT ,IRSTRT ,LSFLAG ,
     5              LRFLAG ,KBLK1  ,KBLK2  ,KRFLAG
C     END COMMON /GLOBAL/ 05-02-79
      COMMON /RGLOB/ RMISS  ,RMIN   ,ABSMIN ,SCLMIN ,XMIN   ,
     1              HSCALE ,RELMIN ,SCLDEF ,TMAX   ,TNOW
C     END COMMON /RGLOB/ 10-13-78
      COMMON /NCOMP/ NCC    ,NNCC   ,NC     ,NAC    ,NACC   ,
     1                     NVCP   ,NVNCP  ,NVACC  ,NVANCC
C     END COMMON /NCOMP/ 10-13-78
      DIMENSION B(1)
      DIMENSION NBOPST(3,1),IPHASE(NPH),LPB(NPH)
      COMMON /STWORK/ NRETN  ,NIRETN ,NHXF   ,NHYF   ,NWYF   ,
     1              NSTW   ,KK1    ,KK2    ,KZ1    ,KZ2    ,
     2              KA1    ,KA2    ,KRET   ,KRSC   ,MF     ,
     3              MX     ,MX1    ,MX2    ,MY     ,MCS    ,
     4              MNC    ,MHXF   ,MHYF   ,MWY    ,MRETN  ,
     5              MIM    ,MIC    ,MIN    ,MPH    ,MIRETN ,
     6              NDUM   ,NBLM   ,NCOVAR ,NWR    ,NIWR   ,
```

```
     7          KEXT   ,KLNK   ,KFOUT ,KPHV   ,KPHL   ,
     8          KLNGM  ,MSTOI  ,MLNKIN ,MZWK   ,MIZWK  ,
     9          IDUMX  ,HV     ,HL     ,HL1    ,HL2    ,
     1          SV     ,SL     ,SL1    ,SL2    ,VV     ,
     2          VL     ,VL1    ,VL2    ,XMWV   ,XMWL   ,
     3          XMWL1  ,XMWL2  ,NPO    ,CALCL  , HS    ,
     4          SS     ,VS     ,XMWS
C    END COMMON /STWORK/ 10-10-86
      COMMON /STWKWK/  NCPMOO,NCPCSO,NCPNCO,NTRIAL,KRSTRT,IDUMY,
     1 TCALC,PCALC,VCALC,QCALC,BETA,T,P,VFRAC,Q,TINIT,PINIT,
     2 DD(15),WK(1)
      DIMENSION IWK(1), X1(1), IDX1(1), X2(1), IDX2(1), Y(1), IDY(1),
     1        F(1),  IDF(1), X(1), IDX(1)
      EQUIVALENCE (IWK(1),WK(1))
C    END COMMON /STWKWK/ 11-1-80
C
C    CALCULATE RETENTION VECTOR LOCATION
C
C    KK1=1
C    KK2=KK1+NCC
C    KZ1=KK2+NCC
C    KZ2=KZ1+NCC
C    KA1=KZ2+NCC
C    KA2=KA1+NCC
C     KRET=KA2+NCC
C    KRSC=KRET+26
C
C     CALCULATE WORK AND IWORK VECTOR LOCATION
C
C    MF=1
C    MX=MF+NCC
C    MX1=MX+NCC
C    MX2=MX1+NCC
C    MY=MX2+NCC
C    MCS=MY+NCC
C    MNC=MCS+NCC
C    MHXF=MNC+NNCC
C    MHYF=MHXF+NHXF
C    MWY=MHYF+NHYF
C    MIM=1
C    MIC=MIM+NCC
C    MIN=MIC+NCC
  100 CONTINUE
C
C     FILL OUTPUT STREAM SOLID PHASES
C
      IONE = 1
      IZER = 0
      DO 200 I =1, NPH
      IF(IPHASE(I).EQ.1) GO TO 200
      NCD=NCC
      IF(IPHASE(I).EQ.3) NCD=NNCC
      INDEX=LPB(I)
      INDEX0=INDEX+NCD
      INDEX1=INDEX+NCD+1
      INDEX2=INDEX+NCD+2
      INDEX3=INDEX+NCD+3
      INDEX4=INDEX+NCD+4
      INDEX5=INDEX+NCD+5
      INDEX6=INDEX+NCD+6
      INDEX7=INDEX+NCD+7
      INDEX8=INDEX+NCD+8
```

```
      B(INDEX2)=PCALC
      IF(B(INDEX0).LE.RMIN) GO TO 200
      B(INDEX1)=TCALC
      B(INDEX4)=0D0
      B(INDEX5)=0D0
      IF(IPHASE(I).EQ.3) GO TO 150
      CALL CPACK(B(INDEX),NCPCS,IWK(MIC),WK(MCS),SCS)
      CALL SMTHRM (TCALC ,PCALC ,WK(MCS),NCPCS ,IWK(MIC),
     1            NBOPST ,LOPDIA ,IONE   ,IZER   ,IONE   ,
     2            KDENS  ,IZER   ,KDENS  ,DUMMY  ,HCS    ,
     3            SS     ,DUMMY  ,VOL    ,DUMMY  ,DUMMY  ,
     4            DUMMY  ,DUMMY  ,DUMMY  ,KER    )
      B(INDEX3)=HCS/B(INDEX8)
      IF(KDENS.EQ.1) B(INDEX7)=B(INDEX8)/VOL
      IF(KDENS.EQ.1) B(INDEX6)=SS/B(INDEX8)
      GO TO 200
  150 CALL NCPACK(B(INDEX),NCPNCS,IWK(MIN),WK(MNC),SNCS)
      HNCS=0D0
      IF(KDENS.EQ.1) VOL=0D0
      IF(KDENS.EQ.1) SS=0D0
      JDEX=INDEX+NVNCP
      DO 175 K=1, NCPNCS
      J=IWK(MIN+K-1)
      CALL ENTHAL(IDXNCC(J),B(JDEX),TCALC,PCALC,LOPDIA,
     1           1      ,HTEMP ,DUMMY  ,KER  )
      HNCS=HNCS+WK(MNC+K-1)*HTEMP
      IF(KDENS.EQ.0) GO TO 175
      CALL ENTROP(IDXNCC(J),B(JDEX),TCALC  ,PCALC  ,LOPDIA ,
     1           1      ,SS1    ,DUMMY  ,KER    )
      SS=SS+SS1*WK(MNC+K-1)
      IF(SS1.EQ.RMISS) SS=RMISS
      CALL DENSTY (IDXNCC(J),B(JDEX),TCALC  ,PCALC  ,LOPDIA ,
     1           1      ,RHO    ,DUMMY  ,KER    )
      IF (RHO .GT. RMIN) VOL=VOL+WK(MNC+K-1)/RHO
  175 CONTINUE
      B(INDEX3)=HNCS
      IF (KDENS.EQ.1) THEN
        B(INDEX7) = RMISS
        IF (VOL .GT. RMIN) B(INDEX7)=1D0/VOL
        B(INDEX6)=SS
      END IF
  200 CONTINUE
      IF (NPO .LT. 1 .OR. NPO .GT. 2) NPO=1
C
C      OUTPUT STREAM MIXED PHASE
C
      INDEX=LPB(MJ)+NCC
      INDEX1=INDEX+1
      INDEX2=INDEX+2
      INDEX3=INDEX+3
      INDEX4=INDEX+4
      INDEX5=INDEX+5
      INDEX8=INDEX+8
      B(INDEX2)=PCALC
      B(INDEX1)=TCALC
      SS = 0D0
      VS = 0D0
      XMWV = 0D0
      XMWL = 0D0
      XMWS = 0D0
C
C     CHECK FOR SOLIDS
```

```
C
     SOLIDS = .FALSE.
     CHECK = VCALC + CALCL + RMIN
     IF (CHECK .LT. 1.0D0) SOLIDS = .TRUE.
     NPO2 = 1
     IF (BETA .EQ. 0D0) NPO2 = NPO
C
C     CHECK FOR AQUEOUS CHEMISTRY
C
     IF (NPO .EQ. 1) GOTO 250
C
C     CALCULATE MOLECULAR WEIGHT OF MIXED PHASE
C
     IF (.NOT. SOLIDS) GOTO 250
     LOFF = IWORK(1)
     CALL ALLOCI (NF, NBI, LBI)
     CALL ALLOCR (NF, NBR, LBR)
     CALL CPACK(WORK(LOFF), NS, IPB(LBI), PB(LBR), TFLOW)
C
C     CALCULATE THE AVERAGE MOLECULAR WEIGHT OF THE SOLIDS
C
     XMWS = AVEMW(NCPM, IPB(LBI), PB(LOFF))
C
C     CALCULATE THE PROPERTIES OF THE SOLIDS
C
     IF (KDENS .NE. 0)
    1CALL SMTHRM(TCALC  ,PCALC   ,PB(LBR),NCPM,IWK(MIM),
    2    NBOPST(1,NPO) ,LOPDIA  ,IONE   ,IZER   ,IZER   ,IONE ,
    3    IZER   ,IONE   ,DUMMY  ,DUMMY  ,SS     ,DUMMY  ,VS    ,
    4    DUMMY  ,DUMMY  ,DUMMY  ,DUMMY  ,DUMMY  ,KER     )
C
     CALL FREEBD(NBI)
     CALL FREEBD(NBR)
C
 250 CONTINUE
     IF (IABS(NPKODE) .GT. 1) GOTO 380
       IF (KPHASE .NE. 1) GOTO 300
         XMWV = AVEMW(NY,IDY,Y)
         VCALC = 1D0
         B(INDEX4) = 1D0
         B(INDEX5) = 0D0
         GOTO 500
 300   CONTINUE
       IF (KPHASE .NE. 2) GOTO 500
         XMWL = AVEMW(NX,IDX,X)
         B(INDEX4) = 0D0
         B(INDEX5) = 1D0
         GOTO 500
 380 XMWV = AVEMW(NY,IDY,Y)
     IF(NPKODE.EQ.3) GO TO 400
       XMWL = AVEMW(NX,IDX,X)
       GO TO 500
 400 XMWL1 = 0D0
     XMWL2 =0D0
     IF (NX1 .GT. 0) XMWL1 = AVEMW(NX1,IDX1,X1)
     IF (NX2 .GT. 0) XMWL2 = AVEMW(NX2,IDX2,X2)
     XMWL = BETA * XMWL1 + (1D0 - BETA) * XMWL2
C
 500 B(INDEX8) = XMWV*VCALC + XMWL*CALCL + XMWS*(1D0-VCALC-CALCL)
     IF(NPKODE.EQ.1) B(INDEX3)=HM/B(INDEX8)
     IF(NPKODE.EQ.2) B(INDEX3)=(HL*CALCL+HV*VCALC+HS*(1D0-VCALC-CALCL))
     1 /B(INDEX8)
```

```
      IF(NPKODE.EQ.3) B(INDEX3)=(HV*VCALC+HL1*CALCL*BETA+
     1 HL2*CALCL*(1D0-BETA)+HS*(1D0-VCALC-CALCL))/B(INDEX8)
      IF(NPKODE.EQ.1 .AND. KPHASE.EQ.1) B(INDEX4)=1D0
      IF(NPKODE.EQ.1 .AND. KPHASE.NE.1) B(INDEX4)=0D0
      IF(NPKODE.NE.1) B(INDEX4)=VCALC
      B(INDEX5)=1D0-B(INDEX4)
      IF(NPKODE.EQ.1 .AND. KPHASE.EQ.3) B(INDEX5)=0D0
C
C      CHECK LOCAL RESULT SWITCH
C
      IF(KDENS .EQ.0) GO TO 999
C
C      MIXED PHASE RESULT PASS CALCULATION
C
      INDEX7=INDEX+7
      INDEX6=INDEX+6
      IF(NPKODE.EQ.3) GO TO 900
      IF(B(INDEX4).EQ.1D0) GO TO 600
      IF(B(INDEX5).EQ.1D0) GO TO 700
      IF(B(INDEX4).EQ.0D0 .AND. B(INDEX5).EQ.0D0) GO TO 800
      CALL VMTHRM(TCALC ,PCALC ,Y     ,NY    ,IDY   ,
     1          NBOPST ,LOPDIA ,IONE   ,IZER   ,IZER   ,IONE   ,
     2          IZER   ,IONE   ,DUMMY  ,DUMMY  ,SV     ,DUMMY  ,
     3          VV     ,DUMMY  ,DUMMY  ,DUMMY  ,DUMMY  ,DUMMY  ,
     4          KER    )
      CALL LMTHRM(TCALC ,PCALC ,X     ,NX    ,IDX   ,
     1          NBOPST(1,NPO2) ,LOPDIA ,IONE   ,IZER   ,IZER   ,IONE,
     2          IZER   ,IONE   ,DUMMY  ,DUMMY  ,SL     ,DUMMY  ,
     3          VL     ,DUMMY  ,DUMMY  ,DUMMY  ,DUMMY  ,DUMMY  ,
     4          KER    )
      AVMWX=AVEMW(NX  ,IDX   ,X)
      AVMWY=AVEMW(NY  ,IDY   ,Y)
      B(INDEX6)=(VCALC*SV+(CALCL)*SL
     1        +(1D0-VCALC-CALCL)*SS)/B(INDEX8)
      B(INDEX7)=(VCALC*AVMWY + CALCL*AVMWX + (1D0 -VCALC -CALCL)*XMWS)
     1       / (VV*VCALC+VL*CALCL+VS*(1D0-VCALC-CALCL))
      GO TO 999
  600 CALL VMTHRM(TCALC ,PCALC ,F     ,NF    ,IDF   ,NBOPST ,
     1   LOPDIA ,IONE   ,IZER   ,IZER   ,IONE   ,IZER   ,IONE   ,
     2   DUMMY  ,DUMMY  ,SV     ,DUMMY  ,VV     ,DUMMY  ,DUMMY  ,
     3   DUMMY  ,DUMMY  ,DUMMY  ,KER    )
      B(INDEX7)=B(INDEX8)/VV
      B(INDEX6)=SV/B(INDEX8)
      GO TO 999
  700 CALL LMTHRM(TCALC ,PCALC ,F     ,NF    ,IDF,NBOPST(1,NPO2),
     1    LOPDIA ,IONE   ,IZER   ,IZER   ,IONE   ,IZER   ,IONE   ,
     2    DUMMY  ,DUMMY  ,SL     ,DUMMY  ,VL     ,DUMMY  ,DUMMY  ,
     3    DUMMY  ,DUMMY  ,DUMMY  ,KER    )
      B(INDEX7)=B(INDEX8)/VL
      B(INDEX6)=SL/B(INDEX8)
      GO TO 999
  800 CALL SMTHRM(TCALC ,PCALC ,F     ,NF    ,IDF   ,NBOPST(1,NPO),
     1    LOPDIA ,IONE   ,IZER  ,IZER   ,IONE   ,IZER   ,IONE   ,
     2    DUMMY  ,DUMMY  ,SS     ,DUMMY  ,VS     ,DUMMY  ,DUMMY  ,
     3    DUMMY  ,DUMMY  ,DUMMY ,KER    )
      B(INDEX7)=B(INDEX8)/VS
      B(INDEX6)=SS/B(INDEX8)
      GO TO 999
  900 CALL VMTHRM(TCALC ,PCALC ,Y     ,NY    ,IDY   ,NBOPST ,
     1    LOPDIA ,IONE   ,IZER   ,IZER   ,IONE   ,IZER   ,IONE   ,
     2    DUMMY  ,DUMMY  ,SV     ,DUMMY  ,VV     ,DUMMY  ,DUMMY  ,
     3    DUMMY  ,DUMMY  ,DUMMY  ,KER    )
```

```
      SL1 = 0D0
      VL1 = 0D0
      IF (NX1 .GT. 0)
     1CALL LMTHRM(TCALC ,PCALC ,X1   ,NX1   ,IDX1  ,NBOPST,
     2    LOPDIA ,IONE   ,IZER  ,IZER ,IONE   ,IZER   ,IONE   ,
     3    DUMMY  ,DUMMY  ,SL1   ,DUMMY ,VL1    ,DUMMY  ,DUMMY  ,
     4    DUMMY  ,DUMMY  ,DUMMY ,KER   )
      SL2 = 0D0
      VL2 = 0D0
      IF (NX2 .GT. 0)
     1CALL LMTHRM(TCALC ,PCALC  ,X2   ,NX2   ,IDX2,NBOPST(1,NPO),
     2    LOPDIA ,IONE   ,IZER  ,IZER  ,IONE  ,IZER   ,IONE   ,
     3    DUMMY  ,DUMMY  ,SL2   ,DUMMY ,VL2   ,DUMMY  ,DUMMY  ,
     4    DUMMY  ,DUMMY  ,DUMMY  ,KER   )
      AVMWY=AVEMW(NY,IDY,Y)
      AVMWX1=XMWL1
      AVMWX2 = XMWL2
      B(INDEX7)=(VCALC*AVMWY + CALCL*BETA*AVMWX1 + CALCL
     1         *(1D0-BETA)*AVMWX2 + (1D0-VCALC-CALCL)*XMWS)/
     2          (VV*VCALC+VL1*CALCL*BETA+VL2*CALCL*(1D0-BETA)+
     3           VS*(1D0-CALCL-VCALC))
      B(INDEX6)=(VCALC*SV+SL1*CALCL*BETA+SL2*CALCL*(1D0-BETA)+
     1         SS*(1D0-VCALC-CALCL))/B(INDEX8)
      SL = BETA * SL1 + (1.D0 - BETA) * SL2
      VL = BETA * VL1 + (1.D0 - BETA) * VL2
  999 CONTINUE
      RETURN
      END


C$ #07 BY: BRAD C DATE: 03/12/93 CORRECT RXN 3 CO2 EQUILIBRIUM
C$ #06 BY: SIMSCI DATE: 01/15/91 ADD /RGAS1A/ AND USE REALK OFFSETS
C$ #05 BY: JSDINC DATE: 04/30/85 REMOVE SYSTEM DEPEND. REALS
C$ #04 BY: JSDINC DATE: 01/31/85 DOUBLE PREC. CONSTANTS
C$ #03 BY: BWB    DATE: 03/27/85 CONFORM TO ASPEN PROXANAL STANDARD
C$ #02 BY: BWB    DATE: 06/15/84 CORRECT REAL1 ORDER
C$ #01 BY: BWB    DATE: 06/11/84 NEW
C-----------------------------------------------------------------
C
C *---------------------------------------------------------------
C *                     ****  NOTICE  ****
C *---------------------------------------------------------------
C
C
C*************************************************************************************************
C
C       COPYRIGHT (C) 1981-85
C       JAY S. DWECK, CONSULTANT, INC.
C
C
C*************************************************************************************************
C
C-----------------------------------------------------------------
C
C   KINETIC MODEL FOR PLUG FLOW COAL GASIFIER ( DENN MODEL )
C
      SUBROUTINE DELKIN(Z     ,SOUT  ,DERIV ,NSUBS ,IDXSUB,ITYPE ,
     1                 NINT  ,INT   ,NREAL1,REAL1 ,NIDS  ,IDS   ,
     2                 NPO   ,NBOPST,NW    ,W     ,NCQ   ,RATES ,
     3                 FLUXG ,FLUXS ,XLONG ,LX    ,AREA  ,CIRM  ,
     4                 LVROUT,UCP   ,LD    ,REAL  ,NREAL ,LRETN ,
```

```
     5          LIRETN,LVRIN ,PRESDP,LVRINC,NPKODE,KPHASE,
     6          MAXIT ,TOL   ,GUESS ,LODIAF,LOPDIA,KREST ,
     7          KDENS ,LCFLAG,ISTATE,NX    ,H     ,LVRD  ,
     8          LVRI3 ,LVRO3 ,NXLOC ,XLOC  ,TEMPPR,NREAL3,
     9          REAL3 )
      IMPLICIT REAL*8 (A-H,O-Z)
      SAVE
      DIMENSION SOUT(LX),DERIV(LX),IDXSUB(NSUBS),ITYPE(NSUBS),
     1     INT(NINT),REAL1(NREAL1),IDS(2,NIDS),NBOPST(2,NPO),
     2     W(NW),RATES(NCQ),FLUXG(NCQ),FLUXS(NCQ),REAL(NREAL),
     3     XLOC(NXLOC),TEMPPR(NXLOC),REAL3(NREAL3)
      DIMENSION IPROG(2)
      DIMENSION AKI(5),EKI(5),AKEQ(5),HKEQ(5),BKEQ(5),BKI(5)
      DIMENSION D(2),DT(2),DE(2),DM(2),AKG(2),ATH(2),EFF(2),BKG(2)
      COMMON/USER/RMISS,IMISS,NGBAL,IPASS,IRESTR,ICONVG,LMSG,LPMSG,
     1      KFLAG,NHSTRY,NRPT,NTRMNL
      COMMON/NCOMP/NCC,NNCC,NC,NAC,NACC,NVCP,NVNCP,NVACC,NVANCC
      COMMON/IDSCC/IDSCC(2,1)
      COMMON/IDSNCC/IDSNCC(2,1)
      COMMON/MW/XMW(1)
      COMMON /PLEX/ IB(1)
      DIMENSION B(1)
      EQUIVALENCE (IB(1), B(1))
C     END COMMON /PLEX/ 10-13-78
      COMMON /GLOBAL/ KPFLG1 ,KPFLG2 ,KPFLG3 ,LABORT ,NH     ,
     1          LDIAG  ,NCHAR  ,IMISSX ,MISSC1 ,MISSC2 ,
     2          LPDIAG ,IEBAL  ,IRFLAG ,MXBLKW ,ITYPRN ,
     3          LBNCP  ,LBCP   ,LSDIAG ,MAXNE  ,MAXNP1 ,
     4          MAXNP2 ,MAXNP3 ,IUPDAT ,IRSTRT ,LSFLAG ,
     5          LRFLAG ,KBLK1  ,KBLK2  ,KRFLAG ,IRNCLS ,
     6          LSTHIS ,IRETCD ,JRFLAG ,JSFLAG
C     END COMMON /GLOBAL/ 4-30-80
      COMMON /STWORK/ NRETN  ,NIRETN ,NHXF   ,NHYF   ,NWYF   ,
     1          NSTW   ,KK1    ,KK2    ,KZ1    ,KZ2    ,
     2          KA1    ,KA2    ,KRET   ,KRSC   ,MF     ,
     3          MX     ,MX1    ,MX2    ,MY     ,MCS    ,
     4          MNC    ,MHXF   ,MHYF   ,MWY    ,MRETN  ,
     5          MIM    ,MIC    ,MIN    ,MPH    ,MIRETN ,
     6          NDUM   ,NBLM   ,NCOVAR ,NWR    ,NIWR   ,
     7          KEXT   ,KLNK   ,KFOUT  ,KPHV   ,KPHL   ,
     8          KLNGM  ,MSTOI  ,MLNKIN ,MZWK   ,MIZWK  ,
     9          IDUMX  ,HV     ,HL     ,HL1    ,HL2    ,
     1          SV     ,SL     ,SL1    ,SL2    ,VV     ,
     2          VL     ,VL1    ,VL2    ,XMWV   ,XMWL   ,
     3          XMWL1  ,XMWL2
C     END COMMON /STWORK/ 2-3-81
      COMMON /STWKWK/NCPMOO,NCPCSO,NCPNCO,NTRIAL,KRSTRT,IDUMY,
     1 TCALC,PCALC,VCALC,QCALC,BETA,T,P,VFRAC,Q,TINIT,PINIT,
     2 DD(15),WK(1)
      DIMENSION IWK(1)
      EQUIVALENCE (IWK(1),WK(1))
C     END COMMON /STWKWK/ 11-1-80
      COMMON /IDXNCC/IDXNCC(1)
      COMMON /RGAS1A/ LRK1, LRK2, LRK3, LRK4, LRK5, LRK6, LRK7
      DATA IPROG/4HDELK,4HIN  /
      DATA AKEQ/0.D0,3098.0D+04,1222.D+06,1472.D-09,0.0265D0/
      DATA HKEQ/0.,32457D0,40300D0,-21854D0,-7860.0D0/
C
C     THERE WILL BE NCC + 18 STATE VARIABLES:
C       NCC - GAS COMPONENT MOLE FRACTIONS:
C         O2     H2O    H2     CO     CO2    CH4
C         N2     AR     HCL    H2S    H3N    COS
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C        CS2     CHN      C2H4     C2H4O2-1 C2H6     C3H6-2
C        C3H6O-1  C3H8     C4H4S    C4H8-1   C4H8-2   C4H8-3
C        C4H8O-3  C4H10-1  C5H5N    C6H6     C6H6O    C6H14-1
C        C7H8     C7H8O-3  C10H8    C10H22-1 COOL
C        1 - GAS MASS BALANCE
C        4 - SOLID COMPONENT PROXANAL WEIGHT FRACTIONS:
C        7 - SOLID COMPONENT ULTANAL WEIGHT FRACTIONS:
C        3 - SOLID COMPONENT SULFANAL WEIGHT FRACTIONS:
C        1 - SOLID MASS BALANCE
C        1 - PROCESS TEMPERATURE EQUATION
C        1 - COOLANT ENTHALPY BALANCE
C
C     CALCULATE PROCESS STREAM CONDITIONS
C
      PRES=B(LVRIN+IDXSUB(1)+NCC+1)-PRESDP*Z/XLONG
      PRESA=PRES/101300.D0
      ENTHST=0.D0
C
C     CALCULATE REACTION RATES USING DELAWARE MODEL
C
C     REACTION 1:      Q  * C   + 1.0 * O2 --- 2 * ( Q - 1.0 ) * CO
C                                          + ( 2.0 - Q ) * CO2
C     REACTION 2:     1.0 * H2O + 1.0 * C  === 1.0 * CO  + 1.0 * H2
C     REACTION 3:     1.0 * CO2 + 1.0 * C  === 2.0 * CO
C     REACTION 4:     2.0 * H2  + 1.0 * C  === 1.0 * CH4
C     REACTION 5:     1.0 * H2O + 1.0 * CO === 1.0 * CO2 + 1.0 * H2
C
C     ONLY REACTION 1 IS NOT REVERSIBLE
C     REACTION 5 WILL NOT BE AT EQUILIBRIUM
C
      RMINV = 1D0/RMISS
      DO 1100 I=1,NCQ
      RATES(I)=0.D0
      FLUXG(I)=0.D0
      FLUXS(I)=0.D0
 1100 CONTINUE
      DO 1200 I=1,NW
      W(I)=0.D0
 1200 CONTINUE
      DO 1300 I=1,LX
      DERIV(I)=0.D0
 1300 CONTINUE
      GSHRNK=0.D0
      SSHRNK=0.D0
C
C     EXPONENTIAL FAILSAFES FOR OVERLY LARGE STEP SIZE
C
      TIDLGS=DMAX1(1D0,SOUT(NCC+17))
      COALLO=DMAX1(RMINV,SOUT(NCC+3))
      COALIM=DMIN1(1D0-1D-10,COALLO)
C
C     TEST FOR MINIMUM REACTION TEMPERATURE
C
      IF(TIDLGS.LT.300D0) GO TO 2400
C
C     CALCULATE REACTION RATES
C
C     REAL1     1 = KGMOLES OF VOLATILE O2  MADE/KG VOLATILE MATTER
C     REAL1     2 = KGMOLES OF VOLATILE H2O MADE/KG VOLATILE MATTER
C     REAL1     3 = KGMOLES OF VOLATILE H2  MADE/KG VOLATILE MATTER
C     REAL1     4 = KGMOLES OF VOLATILE CO  MADE/KG VOLATILE MATTER
C     REAL1     5 = KGMOLES OF VOLATILE CO2 MADE/KG VOLATILE MATTER
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C     REAL1       6 = KGMOLES OF VOLATILE CH4 MADE/KG VOLATILE MATTER
C     REAL1       7 = KGMOLES OF VOLATILE N2  MADE/KG VOLATILE MATTER
C     REAL1       8 = KGMOLES OF VOLATILE ??? MADE/KG VOLATILE MATTER
C     ...
C     REAL1   NCC-1 = KGMOLES OF VOLATILE ??? MADE/KG VOLATILE MATTER
C     REAL1     NCC = 0. (DUMMY SPACE FOR COOLANT)
C     REAL1 NCC+ 1 = RATE CONSTANT OF REACTION 1
C     REAL1 NCC+ 2 = ACTIVATION ENERGY OF REACTION 1
C     REAL1 NCC+ 3 = RATE CONSTANT OF REACTION 2
C     REAL1 NCC+ 4 = ACTIVATION ENERGY OF REACTION 2
C     REAL1 NCC+ 5 = RATE CONSTANT OF REACTION 3
C     REAL1 NCC+ 6 = ACTIVATION ENERGY OF REACTION 3
C     REAL1 NCC+ 7 = RATE CONSTANT OF REACTION 4
C     REAL1 NCC+ 8 = ACTIVATION ENERGY OF REACTION 4
C     REAL1 NCC+ 9 = RATE CONSTANT OF REACTION 5
C     REAL1 NCC+10 = ACTIVATION ENERGY OF REACTION 5
C     REAL1 NCC+21 = BED VOID FRACTION
C     REAL1 NCC+22 = COAL VOID FRACTION
C     REAL1 NCC+23 = INITIAL PARTICLE DIAMETER (CM)
C     REAL1 NCC+25 = INITIAL DENSITY OF CHAR FEED (GM/CU.CM.)
C     REAL1 NCC+26 = INITIAL DENSITY OF ASH FEED (GM/CU.CM.)
C     REAL1 NCC+27 = RATIO OF C  TO O2  IN REACTION 4
C     REAL1 NCC+28 = SCHMIDT NUMBER
C     REAL1 NCC+29 = DIFFUSION CONSTANT FOR OXYGEN (SQ.CM./SEC)
C     REAL1 NCC+30 = DIFFUSION CONSTANT FOR WATER (SQ.CM./SEC)
C     REAL1 NCC+31 = MODEL TYPE: 1 = ASH SEGREGATION
C                                2 = SHELL PROGRESSIVE
C                                3 = HOMOGENEOUS
C     REAL1 NREAL1-4 = FRACTION VOLATILE MATTER RELEASED BY PYROLYSIS
C     REAL1 NREAL1-3 = FINAL TEMPERATURE FOR VOLATILE MATTER RELEASE
C     REAL1 NREAL1-2 = INITIAL TEMPERATURE FOR VOLATILE MATTER RELEASE
C     REAL1 NREAL1-1 = FRACTION UNCONVERTED FIXED CARBON 1ST ITERATION
C     REAL1 NREAL1 = FRACTION UNCONVERTED FIXED CARBON 2ND ITERATION
C
      D(1)=REAL1(LRK2+9)
      D(2)=REAL1(LRK2+10)
      MODEL=REAL1(LRK2+11)
      ITIP=ITIP+1

      AKI(1)=REAL1(LRK1+1)
      EKI(1)=REAL1(LRK1+2)

      AKI(2)=REAL1(LRK1+3)
      EKI(2)=REAL1(LRK1+4)
      AKI(3)=REAL1(LRK1+5)
      EKI(3)=REAL1(LRK1+6)
      AKI(4)=REAL1(LRK1+7)
      EKI(4)=REAL1(LRK1+8)
      AKI(5)=REAL1(LRK1+9)
      EKI(5)=REAL1(LRK1+10)
      AC=REAL1(LRK1+11)
      IF(ITIP .GT. 2000) THEN
        ITIP=0

        WRITE(*,*) AKI(1)
        WRITE(*,*) EKI(1)
        WRITE(*,*) AKI(2)
        WRITE(*,*) EKI(2)
        WRITE(*,*) AKI(3)
        WRITE(*,*) EKI(3)
        WRITE(*,*) AKI(4)
        WRITE(*,*) EKI(4)
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        WRITE(*,*) AKI(5)
        WRITE(*,*) EKI(5)
        WRITE(*,*) AC
        ITIP=0

      ENDIF

      PRXMOD=1D0-B(LVRI3+IDXSUB(2)+NNCC+8)/100D0
      CC0=REAL1(LRK2+5)*B(LVRI3+IDXSUB(2)+NNCC+9)*PRXMOD/12.01115D0
     1    /100D0
      VFC2=REAL1(LRK2+2)*REAL1(LRK2+2)
      VFS=REAL1(LRK2+2)+(1D0-REAL1(LRK2+2))*B(LVRI3+IDXSUB(2)+NNCC+9)
     1     /(B(LVRI3+IDXSUB(2)+NNCC+9)+B(LVRI3+IDXSUB(2)+NNCC+11))
      VFS2=VFS*VFS
      RTW2=82.05D0*B(LVRINC+IDXSUB(1)+NCC)
      AKG0=(2.06D0/REAL1(LRK2+1)/PRESA)*(REAL1(LRK2+8)**(-0.092D0))
     1     *((PRESA/REAL1(LRK2+3)/82.05D0)**0.575D0)
      DO 1500 I=1,2
      DT(I)=D(I)*(B(LVRINC+IDXSUB(1)+NCC)**0.8D0)/(352.3D0**1.8D0)
      DE(I)=DT(I)*VFC2
      DM(I)=DT(I)*VFS2
      AKG(I)=AKG0*(DT(I)**.575D0)
 1500 CONTINUE
      ATH(1)=REAL1(LRK2+3)*DSQRT(CC0*82.05D0/REAL1(LRK2+7)/DE(1))/2D0
      ATH(2)=REAL1(LRK2+3)*DSQRT(CC0*82.05D0/DE(2))/2D0
      APH=(1.-REAL1(LRK2+1))*PRESA*1D2*XLONG
      APHC=APH*CC0
      AWGS=REAL1(LRK2+1)*1D2*XLONG*PRESA*PRESA/RTW2/RTW2
      YFC=COALIM
      APHCVC=APHC*YFC/(YFC+(1D0-YFC)*REAL1(LRK2+5)*0.01D0
     1       *B(LVRI3+IDXSUB(2)+NNCC+11)*PRXMOD/REAL1(LRK2+6))
      FDP=YFC**(1D0/3D0)
      DP=REAL1(LRK2+3)*FDP
      TTW=TIDLGS/B(LVRINC+IDXSUB(1)+NCC)
      RT1=1.987D0*TIDLGS
C     RT2=82.05D0*TIDLGS
      DO 1600 I=1,5
      BKEQ(I)=AKEQ(I)*DEXP(-HKEQ(I)/RT1)
 1600 CONTINUE
C************************************************************************************
C     Addition of activity coefficient for Carbon
C************************************************************************************
      DO 16001 I=1,4
      BKEQ(I)=BKEQ(I)*AC
16001 CONTINUE
C************************************************************************************
      XEQO2=0.
      XEQH2O=DMAX1(PRESA*SOUT(3)*SOUT(4)/BKEQ(2),0.D+00)
      XEQCO2=DMAX1(PRESA*SOUT(4)*SOUT(4)/BKEQ(3),0.D+00)
      XEQH22=DMAX1(SOUT(6)/PRESA/BKEQ(4),0.D+00)
      XEQWGS=DMAX1(SOUT(3)*SOUT(5)/BKEQ(5),0.D+00)
      DO 1700 I=1,5
      BKI(I)=AKI(I)*DEXP(-EKI(I)/RT1)
 1700 CONTINUE
      DO 1900 I=1,2
      THIELE=ATH(I)*FDP*DSQRT(BKI(I)/(TTW**(0.8D0)))
      IF(THIELE.LE.0.02D0) GO TO 1800
      EFF(I)=(3D0/THIELE)*(1D0/DTANH(THIELE)-1D0/THIELE)
      GO TO 1900
 1800 EFF(I)=1D0
 1900 CONTINUE
      FGAS=1D3*SOUT(NCC+1)/AREA/1D2/1D2
```

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      IF(FGAS.LE.0D0) FGAS = RMINV
      BKGO=(FGAS**(0.425D0))*(TTW**(0.46D0))
      IF(MODEL.EQ.1)BKGO=BKGO/(FDP**(0.575D0))
      DO 2000 I=1,2
      BKG(I)=BKGO*AKG(I)
 2000 CONTINUE
      S1=DMAX1(0.D0,SOUT(1))
      S2=DMAX1(0.D0,SOUT(2))
      S3=DMAX1(0.D0,SOUT(3))
      S4=DMAX1(0.D0,SOUT(4))
      S5=DMAX1(0.D0,SOUT(5))
      GO TO (2100,2200,2300),MODEL
C     ASH SEGREGATION MODEL
 2100 CONTINUE

      W(NC+1)=10.*APHCVC*(S1-XEQO2)
     1        /(CC0*DP/6./BKG(1)+REAL1(LRK2+7)/EFF(1)/BKI(1))
      W(NC+2)=10.*APHCVC*(S2-XEQH2O)
     1        /(CC0*DP/6./BKG(2)+1./EFF(2)/BKI(2))
      W(NC+3)=10.*APHCVC*(S5-XEQCO2)*BKI(3)
      W(NC+4)=10.*APHCVC*PRESA*(S3*S3-XEQH22)*BKI(4)
      W(NC+5)=10.*AWGS*(S2*S4-XEQWGS)*BKI(5)/TTW/TTW
      GO TO 2400
C     SHELL PROGRESSIVE MODEL
 2200 CONTINUE
C     COMMENT BELOW REPRESENTS ORIGINAL FORM (RT2 COMMENTED ABOVE)
      W(NC+1)=10.*APH*(S1-XEQO2)
     1        /(REAL1(LRK2+3)/6./BKG(1)
     2        +REAL1(LRK2+3)*REAL1(LRK2+3)*(1.-FDP)*82.05
     3        /12./FDP/DM(1)/(TTW**(0.8))
     4        +REAL1(LRK2+7)/EFF(1)/YFC/BKI(1)/CC0)
      W(NC+2)=10.*APH*(S2-XEQH2O)
     1        /(REAL1(LRK2+3)/6./BKG(2)
     2        +REAL1(LRK2+3)*REAL1(LRK2+3)*(1.-FDP)*82.05
C    2         +REAL1(LRK2+3)*REAL1(LRK2+3)*(1.-FDP)*RT2
     3        /12./FDP/DM(2)/(TTW**(0.8))
     4        +1./EFF(2)/YFC/BKI(2)/CC0)
      W(NC+3)=10.*APHC*YFC*(S5-XEQCO2)*BKI(3)
      W(NC+4)=10.*APHC*YFC*PRESA*(S3*S3-XEQH22)*BKI(4)
      W(NC+5)=10.*AWGS*(S2*S4-XEQWGS)*BKI(5)/TTW/TTW
      GO TO 2400
C     HOMOGENEOUS MODEL

 2300 CONTINUE
      W(NC+1)=10.*APHC*(S1-XEQO2)
     1        /(CC0*REAL1(LRK2+3)/6./BKG(1)
     2        +REAL1(LRK2+7)/EFF(1)/BKI(1)/YFC)
      W(NC+2)=10.*APHC*(S2-XEQH2O)
     1        /(CC0*REAL1(LRK2+3)/6./BKG(2)
     2        +1./EFF(2)/BKI(2)/YFC)
      W(NC+3)=10.*APHC*(S5-XEQCO2)*BKI(3)*YFC
      W(NC+4)=10.*APHC*PRESA*(S3*S3-XEQH22)*BKI(4)*YFC
      W(NC+5)=10.*AWGS*(S2*S4-XEQWGS)*BKI(5)/TTW/TTW
 2400 CONTINUE

      O2LIM=SOUT(1)*SOUT(NCC+1)/H/AREA
      IF(O2LIM.LE.0.D+00) O2LIM=0.D+00
      IF(W(NC+1).GT.O2LIM) W(NC+1)=O2LIM
C
C     REBUILD OUTLET PROCESS STREAM VECTOR
C
      DO 2500 I=1,NCC
```

```
      B(LVROUT+IDXSUB(1)+I-2)=SOUT(I)*SOUT(NCC+1)
 2500 CONTINUE
C     B(LVROUT+IDXSUB(1)+NCC-1)=SOUT(NCC+1)
      DO 2600 I=1,14
      B(LVROUT+IDXSUB(2)+NNCC+I+7)=1.D+02*SOUT(NCC+I+1)
 2600 CONTINUE
      B(LVROUT+IDXSUB(2)+NNCC-2)=SOUT(NCC+16)
C     B(LVROUT+IDXSUB(2)+NNCC-1)=SOUT(NCC+16)
      B(LVROUT+IDXSUB(1)+NCC)=SOUT(NCC+17)
      DO 2900 J=1,NSUBS
      NM=ITYPE(J)
      IF(NM.EQ.3) GO TO 2700
C
C     CALCULATE TOTAL FLOWRATES AND MOLECULAR  WEIGHT
C
      DUM1=SAVEMW(LVROUT+IDXSUB(J)-1)
      GO TO 2900
 2700 CONTINUE
      DUM1=0.D+00
      DO 2800 I=1,NNCC
      DUM1=DUM1+B(LVROUT+IDXSUB(J)+I-2)
 2800 CONTINUE
      B(LVROUT+IDXSUB(J)+NNCC-1)=DUM1
 2900 CONTINUE
      SPEC2=PRES
      SPEC1=TIDLGS
      CALL SETP(B(LVROUT),NSUBS,IDXSUB,ITYPE,PRES)
      CALL SETH(B(LVROUT),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVROUT)    ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2      ,
     1          NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
     2          LODIAF,LOPDIA,KREST ,KDENS ,REAL(LRETN)  ,
     3          INT(LIRETN)  ,LCFLAG)
C
C     CALCULATE FORMATION RATE FOR FIXED CARBON
C
      SSHRNK=12.01115*(REAL1(LRK2+7)*W(NC+1)+W(NC+2)+W(NC+3)+W(NC+4))
C
C     OBTAIN DHGDT

C
      CALL SCOPY(LD,LVROUT,LVRD)
      CALL CPACK(B(LVROUT),NCPGG,IWK(MIC),WK(MCS),TGFLOW)
      CALL IDLGAS(TIDLGS,WK(MCS)      ,NCPGG ,IWK(MIC)     ,
     1           KDIAG ,1     ,0     ,0     ,0     ,2     ,0     ,
     2           0      ,HI    ,SI    ,GI    ,DHI   ,DSI   ,DGI   ,
     3           H      ,S     ,G     ,DHGDTT,DS    ,DG    ,KER   )
C
C     OBTAIN DHFDT
C

      CALL NCPACK(B(LVROUT+IDXSUB(2)-1),NCPSS,IWK(MIN),WK(MNC),TSFLOW)
      DHSDTT=0.D0
      JDEX=LVROUT+IDXSUB(2)+NNCC+8
      DO 3000 I=1,NCPSS
      J=IWK(MIN+I-1)
      CALL ENTHAL (IDXNCC(J)   ,B(JDEX)      ,TIDLGS,PRES   ,
     1            LOPDIA,2    ,HSOLID,DHSDT ,KER   )
      CALL DENSTY (IDXNCC(J)   ,B(JDEX)      ,TIDLGS,PRES   ,
     1            LOPDIA,1    ,RHO   ,DRHO  ,KER   )
      DHSDTT=DHSDTT+WK(MNC+I-1)*DHSDT
 3000 CONTINUE
C
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```
C     OBTAIN DEVOLATILIZATION TERM OF RHS
      TT=TIDLGS
      TAV=(REAL1(LRK3+2)+REAL1(LRK3+3))/2.0
      XX=(TT-TAV)/25.0
      HFMVG=0.D+00
      HFMVS=0.D+00
      ZMV=0.D+00
      IF(TEMPPR(NXLOC).LT.REAL1(LRK3+3).OR.
     1  SOUT(NCC+17).GT.REAL1(LRK3+3)) GO TO 3600

      ZMV=-B(LVRI3+IDXSUB(2)+NNCC+10)/100.
     1   /(REAL1(LRK3+3)-REAL1(LRK3+2))

C    2   /(1.-B(LVRI3+IDXSUB(2)+NNCC+8)/100.)

C
C       Non-linear devolatilization Model
C
C       ZMV=(-B(LVRI3+IDXSUB(2)+NNCC+10)/100.)*(1.01/25.)*DEXP(-XX)
C     1  /((1.+DEXP(-XX))**2)
C

      DO 3100 I=1,NCC
      FLUXS(I)=SOUT(NCC+16)*ZMV*REAL1(LRK7+I)/(1.-SOUT(NCC+4))
 3100 CONTINUE
      B(LVRD+IDXSUB(1)+NCC-1)=0.D+00
      DO 3200 I=1,NCC
      B(LVRD+IDXSUB(1)+I-2)=FLUXS(I)
      B(LVRD+IDXSUB(1)+NCC-1)=B(LVRD+IDXSUB(1)+NCC-1)
     1                     +B(LVRD+IDXSUB(1)+I-2)
 3200 CONTINUE
      B(LVRD+IDXSUB(2)+NNCC-2)=0.D0
      B(LVRD+IDXSUB(2)+NNCC-1)=0.D0
      DO 3300 I=1,14
      B(LVRD+IDXSUB(2)+NNCC+7+I)=0.D0
 3300 CONTINUE
      DUM1=SAVEMW(LVRD+IDXSUB(1)-1)
      CALL SETP(B(LVRD),NSUBS,IDXSUB,ITYPE,PRES)
      CALL SETH(B(LVRD),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVRD)      ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2     ,
     1          NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
     2          LODIAF,LOPDIA,KREST ,0      ,WK(MRETN)     ,
     3          IWK(MIRETN)  ,LCFLAG)
      CALL TOTENT(B(LVRD),NSUBS,IDXSUB,ITYPE,HFMVG)
C
C     OBTAIN VOLATILE MATTER TERM OF RHS
C
      B(LVRD+IDXSUB(1)+NCC-1)=0.D+00
      DO 3400 I=1,NCC
      B(LVRD+IDXSUB(1)+I-2)=0.D0
 3400 CONTINUE
      B(LVRD+IDXSUB(2)+NNCC-2)=SOUT(NCC+16)*ZMV/(1.-SOUT(NCC+4))
      B(LVRD+IDXSUB(2)+NNCC-1)=SOUT(NCC+16)*ZMV/(1.-SOUT(NCC+4))
      B(LVRD+IDXSUB(2)+NNCC+10)=1.D+02
      DO 3500 I=1,6
      B(LVRD+IDXSUB(2)+NNCC+12+I)=1.D+02*REAL3(5+I)
 3500 CONTINUE
      DUM1=SAVEMW(LVRD+IDXSUB(1)-1)
      CALL SETP(B(LVRD),NSUBS,IDXSUB,ITYPE,PRES)
      CALL SETH(B(LVRD),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVRD)      ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2     ,
     1          NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
```

```
     2         LODIAF,LOPDIA,KREST ,0     ,WK(MRETN)    ,
     3         IWK(MIRETN)  ,LCFLAG)
      CALL TOTENT(B(LVRD),NSUBS,IDXSUB,ITYPE,HFMVS)
C
C     CALC THE NET ENTHALPY FLUX RESULTING FROM REACTIONS
C
 3600 CONTINUE
      DO 3700 I=1,NCC
      FLUXS(I)=SOUT(NCC+4)*SSHRNK*REAL1(LRK7+I)/(1.-SOUT(NCC+4))
 3700 CONTINUE
      FLUXG(1)=+1.0*W(NC+1)
      FLUXG(2)=+1.0*W(NC+2)+1.0*W(NC+5)
      FLUXG(3)=+2.0*W(NC+4)
      FLUXG(4)=+1.0*W(NC+5)
      FLUXG(5)=+1.0*W(NC+3)
      FLUXS(2)=FLUXS(2)
      FLUXS(3)=FLUXS(3)+1.0*W(NC+2)+1.0*W(NC+5)
      FLUXS(4)=FLUXS(4)+1.0*W(NC+2)+2.0*W(NC+3)
     1         +2.0*(REAL1(LRK2+7)-1.0)*W(NC+1)
      FLUXS(5)=FLUXS(5)+(2.0-REAL1(LRK2+7))*W(NC+1)+1.0*W(NC+5)
      FLUXS(6)=FLUXS(6)+1.0*W(NC+4)
      B(LVRD+IDXSUB(1)+NCC-1)=0.D+00
      DO 3800 I=1,NCC
      B(LVRD+IDXSUB(1)+I-2)=FLUXG(I)
      B(LVRD+IDXSUB(1)+NCC-1)=B(LVRD+IDXSUB(1)+NCC-1)
     1                  +B(LVRD+IDXSUB(1)+I-2)
 3800 CONTINUE

      B(LVRD+IDXSUB(2)+NNCC-2)=SSHRNK/(1.-SOUT(NCC+4))
      B(LVRD+IDXSUB(2)+NNCC-1)=SSHRNK/(1.-SOUT(NCC+4))
      DO 3900 I=1,14
      B(LVRD+IDXSUB(2)+NNCC+7+I)=0.D0
 3900 CONTINUE

      B(LVRD+IDXSUB(2)+NNCC+9)=1.D+02*(1.-SOUT(NCC+4))
      B(LVRD+IDXSUB(2)+NNCC+10)=1.D+02*SOUT(NCC+4)
      DO 4000 I=1,6
      B(LVRD+IDXSUB(2)+NNCC+12+I)=1.D+02*SOUT(NCC+4)*REAL3(5+I)
 4000 CONTINUE
      B(LVRD+IDXSUB(2)+NNCC+13)=B(LVRD+IDXSUB(2)+NNCC+13)
     1                  +1.D+02*(1.-SOUT(NCC+4))
      DUM1=SAVEMW(LVRD+IDXSUB(1)-1)
      CALL SETP(B(LVRD),NSUBS,IDXSUB,ITYPE,PRES)
      CALL SETH(B(LVRD),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVRD)      ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2     ,
     1         NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
     2         LODIAF,LOPDIA,KREST ,0     ,WK(MRETN)    ,
     3         IWK(MIRETN)  ,LCFLAG)
      CALL TOTENT(B(LVRD),NSUBS,IDXSUB,ITYPE,HCALR)
      B(LVRD+IDXSUB(1)+NCC-1)=0.D+00
      DO 4100 I=1,NCC
      B(LVRD+IDXSUB(1)+I-2)=FLUXS(I)
      B(LVRD+IDXSUB(1)+NCC-1)=B(LVRD+IDXSUB(1)+NCC-1)
     1                  +B(LVRD+IDXSUB(1)+I-2)

 4100 CONTINUE

      B(LVRD+IDXSUB(2)+NNCC-2)=0.D+00
      B(LVRD+IDXSUB(2)+NNCC-1)=0.D+00
      DO 4200 I=1,14
      B(LVRD+IDXSUB(2)+NNCC+7+I)=0.D0
 4200 CONTINUE
```

```
      CALL SETP(B(LVRD),NSUBS,IDXSUB,ITYPE,PRES)
      CALL SETH(B(LVRD),NSUBS,IDXSUB,ITYPE,ENTHST)
      CALL FLASH(B(LVRD)      ,NSUBS ,IDXSUB,ITYPE ,NBOPST,2      ,
     1       NPKODE,KPHASE,MAXIT ,TOL    ,SPEC1 ,SPEC2 ,GUESS ,
     2       LODIAF,LOPDIA,KREST ,0      ,WK(MRETN)     ,
     3       IWK(MIRETN)  ,LCFLAG)
      CALL TOTENT(B(LVRD),NSUBS,IDXSUB,ITYPE,HCALP)

C
C     CALCULATE HEAT TRANSFER FROM REACTION MIXTURE TO COOLANT STREAM
C
      QTCP=CIRM*UCP*(B(LVRINC+IDXSUB(1)+NCC)-SOUT(NCC+17))
      DHTDT=SOUT(NCC+1)*DHGDTT-SOUT(NCC+16)*DHSDTT+HFMVG-HFMVS

      DERIV(NCC+17)=((HCALR-HCALP)*AREA+QTCP)/DHTDT

      DERIV(NCC+18)=-QTCP
C
C     COMPUTE FUNCTIONS AND PACK FOR INTEGRATION ROUTINE
C
      DERIV(NCC+4)=ZMV*DERIV(NCC+17)
      RV=(SOUT(NCC+16)*DERIV(NCC+4)/AREA+SOUT(NCC+4)*SSHRNK)
     1  /(1.-SOUT(NCC+4))
      DERIV(NCC+16)=(AREA*SSHRNK+SOUT(NCC+16)*DERIV(NCC+4))
     1         /(1.-SOUT(NCC+4))
      DERIV(NCC+2)=0.
      DERIV(NCC+3)=(AREA*SSHRNK-SOUT(NCC+3)*DERIV(NCC+16))/SOUT(NCC+16)
      DERIV(NCC+5)=-SOUT(NCC+5)*DERIV(NCC+16)/SOUT(NCC+16)
      DERIV(NCC+6)=-SOUT(NCC+6)*DERIV(NCC+16)/SOUT(NCC+16)
      DERIV(NCC+7)=(AREA*(SSHRNK+RV*REAL3(6))
     1         -SOUT(NCC+7)*DERIV(NCC+16))/SOUT(NCC+16)
      DO 4300 I=1,5
      DERIV(NCC+7+I)=(AREA*RV*REAL3(6+I)
     1         -SOUT(NCC+7+I)*DERIV(NCC+16))/SOUT(NCC+16)
 4300 CONTINUE
      GSHRNK=(REAL1(LRK2+7)-1.0)*W(NC+1)+W(NC+2)+W(NC+3)
     1     -W(NC+4)+RV*REAL3(12)
      DO 4400 I=1,NCC
      RATES(I)=REAL1(LRK7+I)*RV-SOUT(I)*GSHRNK
 4400 CONTINUE
      RATES(1)=-W(NC+1)+RATES(1)
      RATES(2)=-1.0*W(NC+2)-1.0*W(NC+5)+RATES(2)
      RATES(3)=-2.0*W(NC+4)+1.0*W(NC+2)+1.0*W(NC+5)+RATES(3)
      RATES(4)=-1.0*W(NC+5)+1.0*W(NC+2)+2.0*W(NC+3)+RATES(4)
     1     +2.0*(REAL1(LRK2+7)-1.0)*W(NC+1)
      RATES(5)=-1.0*W(NC+3)+1.0*W(NC+5)+RATES(5)
     1     +(2.0-REAL1(LRK2+7))*W(NC+1)
      RATES(6)=+1.0*W(NC+4)+RATES(6)
      DO 4500 I=1,NCC
      DERIV(I)=RATES(I)*AREA/SOUT(NCC+1)
 4500 CONTINUE
      DERIV(NCC+1)=AREA*GSHRNK
      B(LVROUT+IDXSUB(2)+NNCC+6)=RHO
      B(LVRO3+IDXSUB(2)+NNCC+6)=RHO
      RETURN
      END
```

APPENDIX B

RGAS Input File

```
;
TITLE 'GASIFIER SIMULATION USING DENN KINETICS - UND CASE AVER'
;
DESCRIPTION "BEULAH LIGNITE IN LURGI MARK IV USING DENN KINETICS WITH
        MODIFIED KINETIC PARAMETERS.  RECYCLE TAR-OIL IS MIXED
        WITH THE FRESH COAL FEED BEFORE INTRODUCING THE COAL TO
        THE GASIFIER.  THE RECYCLE TAR OIL IS MODELED USING A
        SLATE OF PURE COMPONENTS AND INCLUDES COAL FINES AND ASH.
        THIS IS FOR AN AVERAGE PRODUCTION MONTH 7/90."
;
;---------------------------------------------------------------------------
;                          Global Parameters
;---------------------------------------------------------------------------
;
IN-UNITS SI
OUT-UNITS ENG
;
HISTORY MSG-LEVEL PROPERTIES=2 SIMULATION=4
HISTORY-UNITS SI
;
SIM-OPTIONS RESULTS-PASS=1 HMB-RESULTS=2
;
RUN-CONTROL MAX-ERRORS=5000 MAX-TIME=900000
;
;---------------------------------------------------------------------------
;                          Report Options
;---------------------------------------------------------------------------
;
REPORT FLOWSHEET PROPERTIES BLOCKS STREAMS
;
STREAM-REPORT
  STREAMS ALL
  FLOW-FRAC MIXED BASES=MOLE MOLE-FRAC MASS MASS-FRAC /
        NC   BASES=MASS MASS-FRAC
  PHASE-SPLITS MOLE
  INTENSIVE-PROPS MIXED PROPS=TEMP PRES ENTH DENS MW BASES=MOLE MASS /
            NC   PROPS=TEMP PRES ENTH DENS BASES=MASS
  ATTRIBUTES NC COMPONENT
;
;---------------------------------------------------------------------------
;                          Components
;---------------------------------------------------------------------------
;
;  Oxygen, water, hydrogen, carbon-monoxide, carbon-dioxide, and methane
;  must be the first six components listed in the COMPONENTS paragraph,
;  and they must be listed in this order.  In order to include more or
;  different components, modify the COMPONENTS paragraph and the REALK
;  and REALP arrays in the RGAS model.
;
COMPONENTS O2  OXYGEN                   /
        H2O    WATER                    /
        H2     HYDROGEN                 /
        CO     CARBON-MONOXIDE          /
        CO2    CARBON-DIOXIDE           /
        CH4    METHANE                  /
        N2     NITROGEN                 /
        AR     ARGON                    /
        H2S    HYDROGEN-SULFIDE         /
        C2H6   ETHANE                   /
        C3H6   PROPYLENE                /
        C3C8   PROPANE                  /
        CH4S   METHYL-MERCAPTAN         /
```

```
CH4O       METHANOL                      /
C2H3N      ACETONITRILE                  /
C2H4       ETHYLENE                      /
C2H4O-1    ACETALDEHYDE                  /
C2H6S-1    ETHYL-MERCAPTAN               /
C2H6S-2    DIMETHYL-SULFIDE              /
C3H5N      PROPIONITRILE                 /
C3H6O-1    ACETONE                       /
C4H4S      THIOPHENE                     /
C4H5N-2    PYRROLE                       /
C4H8O-3    METHYL-ETHYL-KETONE           /
C5H5N      PYRIDINE                      /
C5H6       CYCLOPENTADIENE               /
C5H8-1     CYCLOPENTENE                  /
C5H8-4     1,4-PENTADIENE                /
C5H8O      CYCLOPENTANONE                /
C5H10O-2   METHYL-N-PROPYL-KETONE        /
C5H10O-3   METHYL-ISOPROPYL-KETONE       /
C5H12S     1-PENTANETHIOL                /
C6H6       BENZENE                       /
C6H6S      PHENYL-MERCAPTAN              /
C6H6O      PHENOL                        /
C6H6O2     P-HYDROQUINONE                /
C6H7N-1    ANILINE                       /
C6H7N-2    4-METHYLPYRIDINE              /
C6H10-2    CYCLOHEXENE                   /
C6H10O     CYCLOHEXANONE                 /
C6H12-3    1-HEXENE                      /
C6H14-1    N-HEXANE                      /
C7H8       TOLUENE                       /
C7H8O-1    METHYL-PHENYL-ETHER           /
C7H8O-5    P-CRESOL                      /
C7H8O2     P-METHOXYPHENOL               /
C7H9N-5    METHYLPHENYLAMINE             /
C7H9N-10   2,6-DIMETHYLPYRIDINE          /
C7H14-6    METHYLCYCLOHEXANE             /
C7H14-7    1-HEPTENE                     /
C7H14O-10  5-METHYL-2-HEXANONE           /
C7H16-1    N-HEPTANE                     /
C8H8O2     METHYL-BENZOATE               /
C8H8O2-3   P-TOLUIC-ACID                 /
C8H10-2    M-XYLENE                      /
C8H10-4    ETHYLBENZENE                  /
C8H10O-3   P-ETHYLPHENOL                 /
C8H10O-5   2,3-XYLENOL                   /
C8H11N     N,N-DIMETHYLANILINE           /
C8H16-3    TRANS-1,2-DIMETHYLCYCLOHEXANE/
C8H18-1    N-OCTANE                      /
C8H18-3    3-METHYLHEPTANE               /
C8H18-5    2,2-DIMETHYLHEXANE            /
C8H18-8    2,5-DIMETHYLHEXANE            /
C9H7N-1    ISOQUINOLINE                  /
C9H7N-2    QUINOLINE                     /
C9H10      ALPHA-METHYL-STYRENE          /
C9H10O2    ETHYL-BENZOATE                /
C9H12-1    N-PROPYLBENZENE               /
C9H12-3    1-METHYL-2-ETHYLBENZENE       /
C9H12-7    1,2,4-TRIMETHYLBENZENE        /
C9H14O     ISOPHORONE                    /
C10H8      NAPHTHALENE                   /
C10H10-1   M-DIVINYLBENZENE              /
C10H12     1,2,3,4-TETRAHYDRONAPHTHALENE /
```

```
        C10H14-3   SEC-BUTYLBENZENE             /
        C10H14O    P-TERT-BUTYLPHENOL           /
        C10H14O2   P-TERT-BUTYLCATECHOL         /
        C10H22-1   N-DECANE                     /
        C10H23N    N-DECYLAMINE                 /
        C11H10-1   1-METHYLNAPHTHALENE          /
        C11H10-2   2-METHYLNAPHTHALENE          /
        C11H16O    P-TERT-AMYLPHENO             /
        C11H24     N-UNDECANE                   /
        C12H9N     DIBENZOPYRROLE               /
        C12H10     DIPHENYL                     /
        C12H10-2   ACENAPHTHENE                 /
        C12H10O    DIPHENYL-ETHER               /
        C12H11N    DIPHENYLAMINE                /
        C13H10     FLUORENE                     /
        C13H10O    BENZOPHENONE                 /
        C13H12     DIPHENYLMETHANE              /
        C14H10-1   ANTHRACENE                   /
        C14H10-2   PHENANTHRENE                 /
        C14H12-2   TRANS-STILBENE               /
        C14H30     N-TETRADECANE                /
        C15H16O    P-CUMYLPHENOL                /
        C15H32     N-PENTADECANE                /
        C16H10-1   FLUORANTHENE                 /
        C16H10-2   PYRENE                       /
        C16H26     N-DECYLBENZENE               /
        C16H34     N-HEXADECANE                 /
        C18H12     CHRYSENE                     /
        C18H14-1   O-TERPHENYL                  /
        C18H14-2   M-TERPHENYL                  /
        C18H38     N-OCTADECANE                 /
        C19H40     N-NONADECANE                 /
        C20H42     N-EICOSANE                   /
        C26H20     TETRAPHENYLETHYLENE          /
        COAL
;
FORMULA O2 O2 / H2O H2O / H2 H2 / CO CO / CO2 CO2 / CH4 CH4
;
COMP-NAMES COAL 'BEULAH LIGNITE'
;
ATTR-COMPS COAL PROXANAL ULTANAL SULFANAL
;
;------------------------------------------------------------------------------
;                              Properties
;------------------------------------------------------------------------------
;
PROPERTIES SYSOP0
;
NC-PROPS COAL ENTHALPY HCOALGEN 3 1 1 1 / DENSITY DCHARIGT
;
PROP-DATA
  PROP-LIST CP1C
  PVAL COAL 1.0 0.0 0.0 0.0            & ; MOISTURE
          0.223 0.000218 0.0 0.0     & ; FIXED CARBON (WEN)
          0.025 0.0 0.0 0.0 & ; PRIMARY VOLATILES (NEUTRAL)
          0.025 0.0 0.0 0.0 & ; SECONDARY VOLATILES (NEUTRAL)
          0.180 0.00014 0.0 0.0          ; ASH
;
;------------------------------------------------------------------------------
;                    Process Flowsheet Connectivity
;------------------------------------------------------------------------------
;
```

```
FLOWSHEET
  BLOCK  GASMIX    IN= STM-FD O2-FD          OUT= STM-O2
  BLOCK  COALMIX   IN= COAL-FD TAR-REC        OUT= COAL-TAR
  BLOCK  GASIFIER  IN= STM-O2 COAL-TAR COOL-IN  OUT= PROD-GS CHAR COOL-OUT
;
DEF-STREAMS MIXNC ALL
;
;-----------------------------------------------------------------------------
;                    Feed Stream Specifications
;-----------------------------------------------------------------------------
;
STREAM STM-FD
  SUBSTREAM MIXED TEMP=600.900 PRES=3.175055D+06
    MASS-FLOW H2O 11.73000
;
STREAM O2-FD
  SUBSTREAM MIXED TEMP=600.900 PRES=3.175055D+06
    MASS-FLOW O2 2.558567 / AR 0.040221 / N2 0.003074
;
STREAM COAL-FD
  SUBSTREAM NC TEMP=288.70 PRES=3.266756D+06
    MASS-FLOW COAL 13.20
    COMP-ATTR COAL PROXANAL (35.96 46.34 44.16 9.50) / ; Dry Basis
              ULTANAL  (9.52 65.70 4.52 0.88 0.00 0.96 18.41) /
              SULFANAL (0.0 0.0 0.0)
;
;   The coal fines and ash are lumped together as coal.  The
;   proximate and ultimate analyses for fresh coal were assumed
;   for the coal fines and then adjusted to reflect the extra ash.
;   This method is preferable over the case where Na2SO4 is used
;   to model the ash because the enthalpy calculation for ash will
;   be more accurate.  The available Na2SO4 property constants are
;   not sufficient for our purposes.
;
STREAM TAR-REC
  SUBSTREAM MIXED TEMP=298.15              PRES=3.266756D+06
  MASS-FLOW H2O  0.4307          /         C2H3N      0.00001215     /
          C2H6S-1   0.0006075    /         C3H6O-1    0.0000729      /
          C4H5N-2   0.0001215    /         C4H8O-3    0.0001215      /
          C5H5N     0.0000243    /         C5H8O      0.0001215      /
          C5H10O-2  0.0001215    /         C5H10O-3   0.0001215      /
          C5H12S    0.0006075    /         C6H6       0.0006075      /
          C6H6S     0.00013365   /         C6H6O      0.001944       /
          C6H6O2    0.00941215   /         C6H7N-1    0.0001215      /
          C6H7N-2   0.00020655   /         C7H8       0.001701       /
          C7H8O-1   0.00001215   /         C7H8O-5    0.004617       /
          C7H8O2    0.00159165   /         C7H9N-5    0.00042525     /
          C7H9N-10  0.0001215    /         C7H14O-10  0.0001215      /
          C8H8O2    0.001215     /         C8H10-2    0.0018255      /
          C8H10-4   0.0008505    /         C8H10O-3   0.000972       /
          C8H10O-5  0.0038637    /         C8H11N     0.0005346      /
          C9H7N-1   0.00088695   /         C9H7N-2    0.0017253      /
          C9H10     0.0003645    /         C9H10O2    0.0001215      /
          C9H12-3   0.00052245   /         C9H12-7    0.000243       /
          C9H14O    0.0025515    /         C10H8      0.00307395     /
          C10H10-1  0.0001215    /         C10H12     0.001458       /
          C10H14-3  0.001215     /         C10H14O    0.001215       /
          C10H14O2  0.0006075    /         C10H23N    0.00144585     /
          C11H10-2  0.006075     /         C11H16O    0.00438615     /
          C11H24    0.000243     /         C12H9N     0.000729       /
          C12H10    0.001215     /         C12H10-2   0.00686475     /
          C12H10O   0.00243      /         C12H11N    0.0010449      /
```

```
             C13H10     0.0061965      /        C13H10O    0.006318      /
             C13H12     0.0033291      /        C14H10-1   0.0006075     /
             C14H10-2   0.0025515      /        C14H12-2   0.004374      /
             C14H30     0.0001701      /        C15H16O    0.0004131     /
             C15H32     0.0047385      /        C16H10-1   0.00198045    /
             C16H10-2   0.0001215      /        C16H26     0.001701      /
             C16H34     0.0006075      /        C18H12     0.0008505     /
             C18H14-1   0.000486       /        C18H14-2   0.0183465     /
             C18H38     0.0007776      /        C19H40     0.00057105    /
             C20H42     0.0148589      /        C26H20     0.0021627     /

SUBSTREAM NC TEMP=298.15 PRES=3.266756D+06
   MASS-FLOW COAL 0.0188
   COMP-ATTR COAL PROXANAL (13.58 12.96 12.35 74.69) / ; Dry Basis
              ULTANAL  (74.69 18.37 1.27 0.25 0.00 0.27 5.15) /
              SULFANAL (0.0 0.0 0.0)
;
STREAM COOL-IN
  SUBSTREAM MIXED PRES=3.185398D+06 V=0.0
   MASS-FLOW H2O 1.1552746
;
;-----------------------------------------------------------------------------
;                   Unit Operation Specifications
;-----------------------------------------------------------------------------
;
BLOCK COALMIX MIXER
;
BLOCK GASMIX MIXER
;
BLOCK GASIFIER RGAS
  BLOCK-OPTIONS SIM-LEVEL=4
  SUBROUTINE KINET=DELKIN
  PARAM CODE=6 NOUT=10 STATE=1 &
      LENGTH=3.0 DIAM=4.0 &
      PRES=3.1026D+06 PRESDP=0.0 UCP=105.0 &
      ESP=0.03 TEST1=0.001
  COOLANT CPRES=3.892468D+06 NPK=2 TINIT=672.049
  STOICH  1 NC     COAL -4  /   MIXED O2  -3     / MIXED CO  2      / MIXED CO2 2    /
          2 NC     COAL -1  /   MIXED H2O -1     / MIXED CO  1      / MIXED H2  1    /
          3 NC     COAL -1  /   MIXED CO2 -1     / MIXED CO  2      /
          4 NC     COAL -1  /   MIXED H2  -2     / MIXED CH4 1      /
          5 MIXED  CO   -1  /   MIXED H2O -1     / MIXED CO2 1      / MIXED H2  1    /

T-PROF   0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0 /    0.0 0.0 /    0.0 0.0 /   0.0 0.0 /
         0.0 0.0 /  0.0 0.0
;
;  Dimensions for User Vectors:
;  ---------------------------
;
;     NCC          = 109     = Number of Conventional Components
;     NNCC         = 1       = Number of Nonconventional Components
;     NR           = 5       = Number of Reactions
;
;     NINTK        = 2
;     NREALK       = 60 + 4*NCC
```

```
;   NIWK        = 3
;   NWK         = NCC + NNCC + NR
;   NREALP      = NCC + 18
;   NWP         = 4
;   NREALQ      = 12
;
 UVEC NINTK=2 NREALK=496 NIWK=3 NWK=115 NREALP=127 NWP=4 NREALQ=12
;
 INTK   10            & ; Maximum Number of Iterations
        1             & ; Report Option: 1 = Standard, 2 = Summary
;
 REALK  3.5100E+06    & ; Rate Constant for Reaction #1
        21780.0       & ; Activation Energy for Reaction #1
        810.00        & ; Rate Constant for Reaction #2
        35100.0       & ; Activation Energy for Reaction #2
        525.00        & ; Rate Constant for Reaction #3
        59100.0       & ; Activation Energy for Reaction #3
        6.11000E-03   & ; Rate Constant for Reaction #4
        19200.0       & ; Activation Energy for Reaction #4
        3.2300E+07    & ; Rate Constant for Reaction #5
        11750.0       & ; Activation Energy for Reaction #5
        1.7000000     & ; Activity of carbon, Ac
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.4           & ; Bed Void Fraction
        0.6           & ; Coal Void Fraction
        2.367         & ; Initial Coal Particle Diameter (cm)
        0.0           & ; Reserved for UWV Model
        1.3           & ; Initial Density of Char Feed (g/cm3)
        0.5           & ; Initial Density of Ash Feed (g/cm3)
        1.333333      & ; Ratio of C to O2 in Reaction 4
        0.6           & ; Schmidt Number
        0.01408       & ; Diffusion Constant for Oxygen (sqcm/sec)
        0.01408       & ; Diffusion Constant for Water (sqcm/sec)
        1.0           & ; Model: 1=Ash Seg, 2=Shell Prog, 3=Homogeneous
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
        1.0           & ; Fraction Volatile Matter Released by Pyrolysis
        975.0         & ; Final Temperature for Volatile Matter Release
        1255.3822     & ; Initial Temperature for Volatile Matter Release
        0.001         & ; Fraction Unconverted Fixed Carbon, 1st iteration
        0.500         & ; Fraction Unconverted Fixed Carbon, 2nd iteration
        0.1055        & ; Mass Fraction of Rectisol Naphtha in Volatile Matter
        0.2155        & ; Mass Fraction of Crude Phenol in Volatile Matter
        0.6790        & ; Mass Fraction of Tar Oils in Volatile Matter
        0.0           & ; Unused
        0.0           & ; Unused
        0.0           & ; Unused
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0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.0            & ; Unused
0.00000E+00    & ;  Mass Fraction of O2              in Rectisol Naphth
2.48412E-01    & ;  Mass Fraction of H2O     *       in Rectisol Naphth
1.19491E-03    & ;  Mass Fraction of H2      *       in Rectisol Naphth
1.91569E-01    & ;  Mass Fraction of CO      *       in Rectisol Naphth
1.00331E-01    & ;  Mass Fraction of CO2     *       in Rectisol Naphth
1.94512E-01    & ;  Mass Fraction of CH4     *       in Rectisol Naphth
1.89609E-02    & ;  Mass Fraction of N2      *       in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of AR      *       in Rectisol Naphth
2.22983E-02    & ;  Mass Fraction of H2S     *       in Rectisol Naphth
2.89799E-02    & ;  Mass Fraction of C2H6    *       in Rectisol Naphth
5.79367E-03    & ;  Mass Fraction of C3H6    *       in Rectisol Naphth
5.20389E-03    & ;  Mass Fraction of C3H8    *       in Rectisol Naphth
3.04931E-04    & ;  Mass Fraction of CH4S            in Rectisol Naphth
2.69056E-04    & ;  Mass Fraction of CH4O            in Rectisol Naphth
1.97308E-04    & ;  Mass Fraction of C2H3N           in Rectisol Naphth
4.68328E-03    & ;  Mass Fraction of C2H4            in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C2H4O-1         in Rectisol Naphth
5.91924E-04    & ;  Mass Fraction of C2H6S-1         in Rectisol Naphth
1.97308E-04    & ;  Mass Fraction of C2H6S-2         in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C3H5N           in Rectisol Naphth
7.10309E-03    & ;  Mass Fraction of C3H6O-1         in Rectisol Naphth
1.14797E-03    & ;  Mass Fraction of C4H4S           in Rectisol Naphth
1.43497E-04    & ;  Mass Fraction of C4H5N-2         in Rectisol Naphth
8.12550E-03    & ;  Mass Fraction of C4H8O-3         in Rectisol Naphth
5.38113E-05    & ;  Mass Fraction of C5H5N           in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C5H6            in Rectisol Naphth
1.79371E-04    & ;  Mass Fraction of C5H8-1          in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C5H8-4          in Rectisol Naphth
2.69056E-03    & ;  Mass Fraction of C5H8O           in Rectisol Naphth
1.07623E-03    & ;  Mass Fraction of C5H10O-2        in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C5H10O-3        in Rectisol Naphth
9.86540E-04    & ;  Mass Fraction of C5H12S          in Rectisol Naphth
7.89232E-02    & ;  Mass Fraction of C6H6            in Rectisol Naphth
2.33182E-04    & ;  Mass Fraction of C6H6S           in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C6H6O           in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C6H6O2          in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C6H7N-1         in Rectisol Naphth
8.96855E-04    & ;  Mass Fraction of C6H7N-2         in Rectisol Naphth
8.96855E-04    & ;  Mass Fraction of C6H10-2         in Rectisol Naphth
8.96855E-04    & ;  Mass Fraction of C6H10O          in Rectisol Naphth
4.12553E-03    & ;  Mass Fraction of C6H12-3         in Rectisol Naphth
3.40805E-03    & ;  Mass Fraction of C6H14-1         in Rectisol Naphth
3.35424E-02    & ;  Mass Fraction of C7H8            in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C7H8O-1         in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C7H8O-5         in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C7H8O2          in Rectisol Naphth
3.58742E-04    & ;  Mass Fraction of C7H9N-5         in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C7H9N-10        in Rectisol Naphth
1.97308E-03    & ;  Mass Fraction of C7H14-6         in Rectisol Naphth
2.88787E-03    & ;  Mass Fraction of C7H14-7         in Rectisol Naphth
1.61434E-03    & ; Mass Fraction of C7H14O-10        in Rectisol Naphth
4.12553E-03    & ;  Mass Fraction of C7H16-1         in Rectisol Naphth
0.00000E+00    & ;  Mass Fraction of C8H8O2          in Rectisol Naphth
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0.00000E+00   & ;  Mass Fraction of C8H8O2-3      in Rectisol Naphth
3.40805E-03   & ;  Mass Fraction of C8H10-2       in Rectisol Naphth
7.78470E-03   & ;  Mass Fraction of C8H10-4       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C8H10O-3      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C8H10O-5      in Rectisol Naphth
3.58742E-04   & ;  Mass Fraction of C8H11N        in Rectisol Naphth
5.38113E-04   & ;  Mass Fraction of C8H16-3       in Rectisol Naphth
1.79371E-03   & ;  Mass Fraction of C8H18-1       in Rectisol Naphth
3.58742E-04   & ;  Mass Fraction of C8H18-3       in Rectisol Naphth
8.96855E-04   & ;  Mass Fraction of C8H18-5       in Rectisol Naphth
5.38113E-04   & ;  Mass Fraction of C8H18-8       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C9H7N-1       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C9H7N-2       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C9H10         in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C9H10O2       in Rectisol Naphth
8.96855E-04   & ;  Mass Fraction of C9H12-1       in Rectisol Naphth
8.96855E-04   & ;  Mass Fraction of C9H12-3       in Rectisol Naphth
7.17484E-04   & ;  Mass Fraction of C9H12-7       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C9H14O        in Rectisol Naphth
5.38113E-05   & ;  Mass Fraction of C10H8         in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C10H10-1      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C10H12        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C10H14-3      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C10H14O       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C10H14O2      in Rectisol Naphth
7.17484E-04   & ;  Mass Fraction of C10H22-1      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C10H23N       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C11H10-1      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C11H10-2      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C11H16O       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C11H24        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C12H9N        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C12H10        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C12H10-2      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C12H10O       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C12H11N       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C13H10        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C13H10O       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C13H12        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C14H10-1      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C14H10-2      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C14H12-2      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C14H30        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C15H16O       in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C15H32        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C16H10-1      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C16H10-2      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C16H26        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C16H34        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C18H12        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C18H14-1      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C18H14-2      in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C18H38        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C19H40        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C20H42        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C26H20        in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of O2            in Crude Phenol
2.54008E-01   & ;  Mass Fraction of H2O           in Crude Phenol
1.19491E-03   & ;  Mass Fraction of H2            in Crude Phenol
1.91569E-01   & ;  Mass Fraction of CO            in Crude Phenol
1.00331E-01   & ;  Mass Fraction of CO2           in Crude Phenol
1.94512E-01   & ;  Mass Fraction of CH4           in Crude Phenol
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1.89609E-02   & ;  Mass Fraction of N2           in Crude Phenol
0.00000E+00   & ;  Mass Fraction of AR           in Crude Phenol
2.22983E-02   & ;  Mass Fraction of H2S          in Crude Phenol
2.89799E-02   & ;  Mass Fraction of C2H6         in Crude Phenol
5.79367E-03   & ;  Mass Fraction of C3H6         in Crude Phenol
5.20389E-03   & ;  Mass Fraction of C3H8         in Crude Phenol
0.00000E+00   & ;  Mass Fraction of CH4S         in Crude Phenol
0.00000E+00   & ;  Mass Fraction of CH4O         in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C2H3N        in Crude Phenol
4.41422E-03   & ;  Mass Fraction of C2H4         in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C2H4O-1      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C2H6S-1      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C2H6S-2      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C3H5N        in Crude Phenol
1.25560E-04   & ;  Mass Fraction of C3H6O-1      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C4H4S        in Crude Phenol
1.79371E-04   & ;  Mass Fraction of C4H5N-2      in Crude Phenol
3.58742E-05   & ;  Mass Fraction of C4H8O-3      in Crude Phenol
5.38113E-04   & ;  Mass Fraction of C5H5N        in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C5H6         in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C5H8-1       in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C5H8-4       in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C5H8O        in Crude Phenol
1.61434E-04   & ;  Mass Fraction of C5H10O-2 i   n Crude Phenol
0.00000E+00   & ;  Mass Fraction of C5H10O-3     in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C5H12S       in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C6H6         in Crude Phenol
4.30490E-04   & ;  Mass Fraction of C6H6S        in Crude Phenol
6.18292E-02   & ;  Mass Fraction of C6H6O        in Crude Phenol
3.58742E-03   & ;  Mass Fraction of C6H6O2       in Crude Phenol
8.96855E-05   & ;  Mass Fraction of C6H7N-1      in Crude Phenol
7.17484E-04   & ;  Mass Fraction of C6H7N-2      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C6H10-2      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C6H10O       in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C6H12-3      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C6H14-1      in Crude Phenol
1.25560E-04   & ;  Mass Fraction of C7H8         in Crude Phenol
1.25560E-04   & ;  Mass Fraction of C7H8O-1      in Crude Phenol
3.82060E-02   & ;  Mass Fraction of C7H8O-5      in Crude Phenol
1.94617E-02   & ;  Mass Fraction of C7H8O2       in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C7H9N-5      in Crude Phenol
1.79371E-03   & ;  Mass Fraction of C7H9N-10     in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C7H14-6      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C7H14-7      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C7H14O-10    in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C7H16-1      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H8O2       in Crude Phenol
1.75783E-02   & ;  Mass Fraction of C8H8O2-3     in Crude Phenol
2.51119E-04   & ;  Mass Fraction of C8H10-2      in Crude Phenol
1.25560E-04   & ;  Mass Fraction of C8H10-4      in Crude Phenol
4.66364E-03   & ;  Mass Fraction of C8H10O-3     in Crude Phenol
1.32734E-02   & ;  Mass Fraction of C8H10O-5     in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H11N       in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H16-3      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H18-1      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H18-3      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H18-5      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C8H18-8      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C9H7N-1      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C9H7N-2      in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C9H10        in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C9H10O2      in Crude Phenol
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0.00000E+00  & ; Mass Fraction of C9H12-1     in Crude Phenol
0.00000E+00  & ; Mass Fraction of C9H12-3     in Crude Phenol
1.79371E-04  & ; Mass Fraction of C9H12-7     in Crude Phenol
2.69056E-03  & ; Mass Fraction of C9H14O      in Crude Phenol
1.79371E-05  & ; Mass Fraction of C10H8       in Crude Phenol
0.00000E+00  & ; Mass Fraction of C10H10-1    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C10H12      in Crude Phenol
1.79371E-04  & ; Mass Fraction of C10H14-3    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C10H14O     in Crude Phenol
3.94616E-03  & ; Mass Fraction of C10H14O2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C10H22-1    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C10H23N     in Crude Phenol
1.79371E-04  & ; Mass Fraction of C11H10-1    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C11H10-2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C11H16O     in Crude Phenol
0.00000E+00  & ; Mass Fraction of C11H24      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C12H9N      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C12H10      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C12H10-2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C12H10O     in Crude Phenol
0.00000E+00  & ; Mass Fraction of C12H11N     in Crude Phenol
1.79371E-03  & ; Mass Fraction of C13H10      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C13H10O     in Crude Phenol
0.00000E+00  & ; Mass Fraction of C13H12      in Crude Phenol
1.79371E-04  & ; Mass Fraction of C14H10-1    in Crude Phenol
1.79371E-04  & ; Mass Fraction of C14H10-2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C14H12-2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C14H30      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C15H16O     in Crude Phenol
8.96855E-05  & ; Mass Fraction of C15H32      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C16H10-1    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C16H10-2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C16H26      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C16H34      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C18H12      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C18H14-1    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C18H14-2    in Crude Phenol
0.00000E+00  & ; Mass Fraction of C18H38      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C19H40      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C20H42      in Crude Phenol
0.00000E+00  & ; Mass Fraction of C26H20      in Crude Phenol
0.00000E+00  & ; Mass Fraction of O2          in Tar Oils
2.52232E-01  & ; Mass Fraction of H2O         in Tar Oils
1.19491E-03  & ; Mass Fraction of H2          in Tar Oils
1.91569E-01  & ; Mass Fraction of CO          in Tar Oils
1.00331E-01  & ; Mass Fraction of CO2         in Tar Oils
1.94512E-01  & ; Mass Fraction of CH4         in Tar Oils
1.89609E-02  & ; Mass Fraction of N2          in Tar Oils
0.00000E+00  & ; Mass Fraction of AR          in Tar Oils
2.22983E-02  & ; Mass Fraction of H2S         in Tar Oils
2.89799E-02  & ; Mass Fraction of C2H6        in Tar Oils
5.79367E-03  & ; Mass Fraction of C3H6        in Tar Oils
5.20389E-03  & ; Mass Fraction of C3H8        in Tar Oils
0.00000E+00  & ; Mass Fraction of CH4S        in Tar Oils
0.00000E+00  & ; Mass Fraction of CH4O        in Tar Oils
1.79371E-05  & ; Mass Fraction of C2H3N       in Tar Oils
4.41422E-03  & ; Mass Fraction of C2H4        in Tar Oils
0.00000E+00  & ; Mass Fraction of C2H4O-1     in Tar Oils
8.96855E-04  & ; Mass Fraction of C2H6S-1     in Tar Oils
0.00000E+00  & ; Mass Fraction of C2H6S-2     in Tar Oils
0.00000E+00  & ; Mass Fraction of C3H5N       in Tar Oils
1.07623E-04  & ; Mass Fraction of C3H6O-1     in Tar Oils
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0.00000E+00   & ;  Mass Fraction of C4H4S          in Tar Oils
1.79371E-04   & ;  Mass Fraction of C4H5N-2        in Tar Oils
1.79371E-04   & ;  Mass Fraction of C4H8O-3        in Tar Oils
3.58742E-05   & ;  Mass Fraction of C5H5N          in Tar Oils
0.00000E+00   & ;  Mass Fraction of C5H6           in Tar Oils
0.00000E+00   & ;  Mass Fraction of C5H8-1         in Tar Oils
0.00000E+00   & ;  Mass Fraction of C5H8-4         in Tar Oils
1.79371E-04   & ;  Mass Fraction of C5H8O          in Tar Oils
1.79371E-04   & ;  Mass Fraction of C5H10O-2       in Tar Oils
1.79371E-04   & ;  Mass Fraction of C5H10O-3       in Tar Oils
8.96855E-04   & ;  Mass Fraction of C5H12S         in Tar Oils
8.96855E-04   & ;  Mass Fraction of C6H6           in Tar Oils
1.97308E-04   & ;  Mass Fraction of C6H6S          in Tar Oils
2.86993E-03   & ;  Mass Fraction of C6H6O          in Tar Oils
1.79371E-05   & ;  Mass Fraction of C6H6O2         in Tar Oils
1.79371E-04   & ;  Mass Fraction of C6H7N-1        in Tar Oils
3.04931E-04   & ;  Mass Fraction of C6H7N-2        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C6H10-2        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C6H10O         in Tar Oils
0.00000E+00   & ;  Mass Fraction of C6H12-3        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C6H14-1        in Tar Oils
2.51119E-04   & ;  Mass Fraction of C7H8           in Tar Oils
1.79371E-05   & ;  Mass Fraction of C7H8O-1        in Tar Oils
6.81609E-03   & ;  Mass Fraction of C7H8O-5        in Tar Oils
2.34976E-03   & ;  Mass Fraction of C7H8O2         in Tar Oils
6.27798E-04   & ;  Mass Fraction of C7H9N-5        in Tar Oils
1.79371E-04   & ;  Mass Fraction of C7H9N-10       in Tar Oils
0.00000E+00   & ;  Mass Fraction of C7H14-6        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C7H14-7        in Tar Oils
1.79371E-04   & ;  Mass Fraction of C7H14O-10      in Tar Oils
0.00000E+00   & ;  Mass Fraction of C7H16-1        in Tar Oils
1.79371E-03   & ;  Mass Fraction of C8H8O2         in Tar Oils
0.00000E+00   & ;  Mass Fraction of C8H8O2-3       in Tar Oils
2.69056E-03   & ;  Mass Fraction of C8H10-2        in Tar Oils
1.25560E-03   & ;  Mass Fraction of C8H10-4        in Tar Oils
1.43497E-03   & ;  Mass Fraction of C8H10O-3       in Tar Oils
5.70399E-03   & ;  Mass Fraction of C8H10O-5       in Tar Oils
7.89232E-04   & ;  Mass Fraction of C8H11N         in Tar Oils
0.00000E+00   & ;  Mass Fraction of C8H16-3        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C8H18-1        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C8H18-3        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C8H18-5        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C8H18-8        in Tar Oils
1.30941E-03   & ;  Mass Fraction of C9H7N-1        in Tar Oils
2.54707E-03   & ;  Mass Fraction of C9H7N-2        in Tar Oils
5.38113E-04   & ;  Mass Fraction of C9H10          in Tar Oils
1.79371E-04   & ;  Mass Fraction of C9H10O2        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C9H12-1        in Tar Oils
7.71295E-04   & ;  Mass Fraction of C9H12-3        in Tar Oils
3.58742E-04   & ;  Mass Fraction of C9H12-7        in Tar Oils
3.76679E-03   & ;  Mass Fraction of C9H14O         in Tar Oils
4.53808E-03   & ;  Mass Fraction of C10H8          in Tar Oils
1.79371E-04   & ;  Mass Fraction of C10H10-1       in Tar Oils
2.15245E-03   & ;  Mass Fraction of C10H12         in Tar Oils
1.79371E-03   & ;  Mass Fraction of C10H14-3       in Tar Oils
1.79371E-03   & ;  Mass Fraction of C10H14O        in Tar Oils
8.96855E-04   & ;  Mass Fraction of C10H14O2       in Tar Oils
0.00000E+00   & ;  Mass Fraction of C10H22-1       in Tar Oils
2.13451E-03   & ;  Mass Fraction of C10H23N        in Tar Oils
0.00000E+00   & ;  Mass Fraction of C11H10-1       in Tar Oils
8.96855E-03   & ;  Mass Fraction of C11H10-2       in Tar Oils
6.47529E-03   & ;  Mass Fraction of C11H16O        in Tar Oils
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         3.58742E-04   & ;  Mass Fraction of C11H24        in Tar Oils
         1.07623E-03   & ;  Mass Fraction of C12H9N        in Tar Oils
         1.79371E-03   & ;  Mass Fraction of C12H10        in Tar Oils
         1.01345E-02   & ;  Mass Fraction of C12H10-2      in Tar Oils
         3.58742E-03   & ;  Mass Fraction of C12H10O       in Tar Oils
         1.54259E-03   & ;  Mass Fraction of C12H11N       in Tar Oils
         9.14792E-03   & ;  Mass Fraction of C13H10        in Tar Oils
         9.32729E-03   & ;  Mass Fraction of C13H10O       in Tar Oils
         4.91476E-03   & ;  Mass Fraction of C13H12        in Tar Oils
         8.96855E-04   & ;  Mass Fraction of C14H10-1      in Tar Oils
         3.76679E-03   & ;  Mass Fraction of C14H10-2      in Tar Oils
         6.45735E-03   & ;  Mass Fraction of C14H12-2      in Tar Oils
         2.51119E-04   & ;  Mass Fraction of C14H30        in Tar Oils
         6.09861E-04   & ;  Mass Fraction of C15H16O       in Tar Oils
         6.99547E-03   & ;  Mass Fraction of C15H32        in Tar Oils
         2.92375E-03   & ;  Mass Fraction of C16H10-1      in Tar Oils
         1.79371E-04   & ;  Mass Fraction of C16H10-2      in Tar Oils
         2.51119E-03   & ;  Mass Fraction of C16H26        in Tar Oils
         8.96855E-04   & ;  Mass Fraction of C16H34        in Tar Oils
         1.25560E-03   & ;  Mass Fraction of C18H12        in Tar Oils
         7.17484E-04   & ;  Mass Fraction of C18H14-1      in Tar Oils
         2.70850E-02   & ;  Mass Fraction of C18H14-2      in Tar Oils
         1.14797E-03   & ;  Mass Fraction of C18H38        in Tar Oils
         8.43043E-04   & ;  Mass Fraction of C19H40        in Tar Oils
         8.25106E-04   & ;  Mass Fraction of C20H42        in Tar Oils
         3.19280E-03   & ;  Mass Fraction of C26H20        in Tar Oils
;
  REALP  0.025         & ; Integration Weighting for O2
         0.025         & ; Integration Weighting for H2O
         0.025         & ; Integration Weighting for H2
         0.025         & ; Integration Weighting for CO
         0.025         & ; Integration Weighting for CO2
         0.025         & ; Integration Weighting for CH4
         0.0           & ; Integration Weighting for N2
         0.0           & ; Integration Weighting for AR
         0.0           & ; Integration Weighting for H2S
         0.0           & ; Integration Weighting for C2H6
         0.0           & ; Integration Weighting for C3H6
         0.0           & ; Integration Weighting for C3H8
         0.0           & ; Integration Weighting for CH4S
         0.0           & ; Integration Weighting for CH4O
         0.0           & ; Integration Weighting for C2H3N
         0.0           & ; Integration Weighting for C2H4
         0.0           & ; Integration Weighting for C2H4O-1
         0.0           & ; Integration Weighting for C2H6S-1
         0.0           & ; Integration Weighting for C2H6S-2
         0.0           & ; Integration Weighting for C3H5N
         0.0           & ; Integration Weighting for C3H6O-1
         0.0           & ; Integration Weighting for C4H4S
         0.0           & ; Integration Weighting for C4H5N-2
         0.0           & ; Integration Weighting for C4H8O-3
         0.0           & ; Integration Weighting for C5H5N
         0.0           & ; Integration Weighting for C5H6
         0.0           & ; Integration Weighting for C5H8-1
         0.0           & ; Integration Weighting for C5H8-4
         0.0           & ; Integration Weighting for C5H8O
         0.0           & ; Integration Weighting for C5H10O-2
         0.0           & ; Integration Weighting for C5H10O-3
         0.0           & ; Integration Weighting for C5H12S
         0.0           & ; Integration Weighting for C6H6
         0.0           & ; Integration Weighting for C6H6S
         0.0           & ; Integration Weighting for C6H6O
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0.0          & ; Integration Weighting for C6H6O2
0.0          & ; Integration Weighting for C6H7N-1
0.0          & ; Integration Weighting for C6H7N-2
0.0          & ; Integration Weighting for C6H10-2
0.0          & ; Integration Weighting for C6H10O
0.0          & ; Integration Weighting for C6H12-3
0.0          & ; Integration Weighting for C6H14-1
0.0          & ; Integration Weighting for C7H8
0.0          & ; Integration Weighting for C7H8O-1
0.0          & ; Integration Weighting for C7H8O-5
0.0          & ; Integration Weighting for C7H8O2
0.0          & ; Integration Weighting for C7H9N-5
0.0          & ; Integration Weighting for C7H9N-10
0.0          & ; Integration Weighting for C7H14-6
0.0          & ; Integration Weighting for C7H14-7
0.0          & ; Integration Weighting for C7H14O-10
0.0          & ; Integration Weighting for C7H16-1
0.0          & ; Integration Weighting for C8H8O2
0.0          & ; Integration Weighting for C8H8O2-3
0.0          & ; Integration Weighting for C8H10-2
0.0          & ; Integration Weighting for C8H10-4
0.0          & ; Integration Weighting for C8H10O-3
0.0          & ; Integration Weighting for C8H10O-5
0.0          & ; Integration Weighting for C8H11N
0.0          & ; Integration Weighting for C8H16-3
0.0          & ; Integration Weighting for C8H18-1
0.0          & ; Integration Weighting for C8H18-3
0.0          & ; Integration Weighting for C8H18-5
0.0          & ; Integration Weighting for C8H18-8
0.0          & ; Integration Weighting for C9H7N-1
0.0          & ; Integration Weighting for C9H7N-2
0.0          & ; Integration Weighting for C9H10
0.0          & ; Integration Weighting for C9H10O2
0.0          & ; Integration Weighting for C9H12-1
0.0          & ; Integration Weighting for C9H12-3
0.0          & ; Integration Weighting for C9H12-7
0.0          & ; Integration Weighting for C9H14O
0.0          & ; Integration Weighting for C10H8
0.0          & ; Integration Weighting for C10H10-1
0.0          & ; Integration Weighting for C10H12
0.0          & ; Integration Weighting for C10H14-3
0.0          & ; Integration Weighting for C10H14O
0.0          & ; Integration Weighting for C10H14O2
0.0          & ; Integration Weighting for C10H22-1
0.0          & ; Integration Weighting for C10H23N
0.0          & ; Integration Weighting for C11H10-1
0.0          & ; Integration Weighting for C11H10-2
0.0          & ; Integration Weighting for C11H16O
0.0          & ; Integration Weighting for C11H24
0.0          & ; Integration Weighting for C12H9N
0.0          & ; Integration Weighting for C12H10
0.0          & ; Integration Weighting for C12H10-2
0.0          & ; Integration Weighting for C12H10O
0.0          & ; Integration Weighting for C12H11N
0.0          & ; Integration Weighting for C13H10
0.0          & ; Integration Weighting for C13H10O
0.0          & ; Integration Weighting for C13H12
0.0          & ; Integration Weighting for C14H10-1
0.0          & ; Integration Weighting for C14H10-2
0.0          & ; Integration Weighting for C14H12-2
0.0          & ; Integration Weighting for C14H30
0.0          & ; Integration Weighting for C15H16O
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        0.0             & ; Integration Weighting for C15H32
        0.0             & ; Integration Weighting for C16H10-1
        0.0             & ; Integration Weighting for C16H10-2
        0.0             & ; Integration Weighting for C16H26
        0.0             & ; Integration Weighting for C16H34
        0.0             & ; Integration Weighting for C18H12
        0.0             & ; Integration Weighting for C18H14-1
        0.0             & ; Integration Weighting for C18H14-2
        0.0             & ; Integration Weighting for C18H38
        0.0             & ; Integration Weighting for C19H40
        0.0             & ; Integration Weighting for C20H42
        0.0             & ; Integration Weighting for C26H20
        0.010           & ; Integration Weighting for Gas Mass Balance
        0.0             & ; Integration Weighting for Coal Proxanal(1)
        0.010           & ; Integration Weighting for Coal Proxanal(2)
        0.005           & ; Integration Weighting for Coal Proxanal(3)
        0.005           & ; Integration Weighting for Coal Proxanal(4)
        0.005           & ; Integration Weighting for Coal Ultanal(1)
        0.005           & ; Integration Weighting for Coal Ultanal(2)
        0.0             & ; Integration Weighting for Coal Ultanal(3)
        0.0             & ; Integration Weighting for Coal Ultanal(4)
        0.0             & ; Integration Weighting for Coal Ultanal(5)
        0.0             & ; Integration Weighting for Coal Ultanal(6)
        0.0             & ; Integration Weighting for Coal Ultanal(7)
        0.0             & ; Integration Weighting for Coal Sulfanal(1)
        0.0             & ; Integration Weighting for Coal Sulfanal(2)
        0.0             & ; Integration Weighting for Coal Sulfanal(3)
        0.010           & ; Integration Weighting for Solid Mass Balance
        0.800           & ; Integration Weighting for Process Temperature Equation
        0.0             &; Integration Weighting for Coolant Enthalpy Balance
;
 REALQ 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
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REFERENCES

1. Averitt, P.: "Coal Resources of United States," U.S. Geological survey bulletin, No. 1412, 1975.

2. Carpenter, B.C.: "Optimization of Great Plains Coal Gasification Plant using ASPEN/SP," Master's Thesis, May 1993.

3. Denn, M.M., J. Wei, W.C. Yu, and R. Cwiklinski: "Detailed simulation of a Moving-Bed Gasifier," EPRI, Palo Alto, California, September, 1982, AP - 2576

4. Elliott, M.A.: "*Chemistry of Coal Utilization*," second supplementary volume, John Wiley and Sons, New York, 1981.

5. Howard-Smith, I. and G.J. Werner: "Coal Conversion Technology," Noyes Data Corporation, Park Ridge, N.J., 1976.

6. Pitt, G.J. "The Kinetics of Evolution of Volatile products from coal," Fuel, **41**, 1962.

7. Ringard, I.H., and B.W. Benjamin: "Great Plains ASPEN Model development: Gasifier Model, Literature Review, and Model Specification," Final Topical Report, January, 1985, DOE/MC/19163 - 1782 (DE85003388).

8. Sears, R., W. Wilson, R. Shockey, S. Cisney, J. Erjavec, G. Gruber, D. Johnson, and B. Birk: "Great Plains Gasification Plant, Gasifier Optimization," DOE Contract DE-FC21-86MC10637, January 31, 1989.

9. Skyler, M.G., V.I. Shustikov, and I.V. Virozub: "Investigation of the kinetics of thermal decomposition of coals," International Chemical Engineering, **9**, 1969.

10. Squires, A.M.: Trans Institute of Chemical Engineering, London, **39**, 1961.

11. Valenti, M.: "Coal Gasification: an alternative energy source is coming of age," Mechanical Engineering, **114**, January, 1992.

12. Wen, C.Y., O.C. Abraham, and A.T. Talwalker: American Chemical Society, Advanced Chemical Series, No. 69, 1967.

13. Wilde, D.J.: "*Optimum Seeking Methods*," Prentice-Hall, Inc., Englewood Cliffs, N.J., 1964.

13. Wiser, W.H., G.R. Hill, and N.J. Kertamus: "Kinetic study of the pyrolysis of a high-volatile Bituminous Coal," Industrial Engineering Chemistry, Process Design and Development, **6**, 1967.

14. Yoon, H., J. Wei, and M.M. Denn: "A model for Moving-Bed Coal Gasification Reactors," AIChE Journal, **24**(5), 1978.

15. Great Plains Synfuels Plant brochure, 1994.