5-1-1993

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Recommended Citation

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OPTIMIZATION OF GREAT PLAINS
COAL GASIFICATION USING ASPEN/SP

by

Bradley C. Carpenter
Bachelor of Science
University of Minnesota, 1989

A Thesis

Submitted to the Graduate Faculty

of the

University of North Dakota

in partial fulfillment of the requirements

for the degree of

Master of Science

Grand Forks, North Dakota

May 1993

This thesis, submitted by Bradley C. Carpenter 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)

Thomas C. Owens

N. S. Grewal

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 is hereby approved.

Harvey Knull
Dean of the Graduate School
4-23-93

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Title	Optimization of Great Plains Coal Gasification Using ASPEN/SP
Department	Chemical Engineering
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Signature Bradley Carpenter

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ACKNOWLEDGEMENTS

The author wishes to express his appreciation to the Dakota Gasification Company and the Department of Energy for providing resources and financial assistance for this project.

A special thanks is extended to Professor John Erjavec for his aid and guidance throughout this project. The author also wishes to express his gratitude to Professor Tom Owens, Chairman of the Chemical Engineering Department, and Professor Nanak Grewal for reviewing this thesis.

Appreciaction is expressed to Bill Keister from Simulation Sciences who spent much time debugging and discussing model algorithms. Additional thanks goes to Steve Poliet and Terry Towers from the Dakota Gasification Company for providing plant model information.

The author would also like to acknowledge Ron Timpe and laboratory personnel at the Energy and Environmental Research Center for performing Differential Scanning Calorimetry experiments, and Sriram Srinavasen, a fellow graduate student, who performed numerous computer simulations.

ABSTRACT

The Dakota Gasification Company in Beulah, North Dakota operates the only commercial coal-to-synthetic natural gas (SNG) plant in the United States, and continued research on the plant's operations is of prime importance. An ASPEN/SP model of a Lurgi coal gasifier that will predict the impact of variable input parameters, such as coal composition and reactant feed flows, on production rates and efficiency is the first step in constructing a model of the entire plant to control its operation and optimize the economic performance of producing SNG.

A model, called RGAS, was developed with the combined effort of several researchers (Benjamin, Denn, Dweck, etc.) during the Great Plains ASPEN Model Development project phase. This model contains parameters (i.e., equilibrium and kinetic constants, heat transfer coefficient to the jacket, and volatile heat capacity) that were verified to be the best established values or were optimized using a pattern search to obtain model predictions used for statistical analysis and comparison to plant data. The volatile heat capacity assumes that the energy associated with devolatilization is thermally neutral. However, pressure differential scanning calorimeter tests of five North Dakota lignite coal samples indicate this energy is exothermic.

In this study, some significant model improvements have been made.

- The predicted flow of condensible volatile matter (naphtha, phenol, tar oil) was corrected to allow for the significant amount of non-condensible volatile matter produced during devolatilization. (Previously, all volatile matter was assumed to be condensible.)

- The heat transfer coefficient of the reactor vessel was reduced from 170 to 105 W/m^{2}K by matching steam production and enthalpy predictions to experimental data.
- The kinetic rate constants used in the RGAS model were adjusted to provide predictions that would match plant data as closely as possible. Results provided predictions within 2% (relative) of plant data for raw gas mole fractions on a dry basis (i.e., H_2, CO, CO_2, CH_4). However, the raw gas and water mass flow rates and steam utilization predictions are still in error by as much as 8%, 10%, and 20%, respectively.
- The predicted raw gas temperature was made to match the plant data by adjusting the specific heat of the volatile matter from $0.43862 + 1.5414(10^{-4})T$ to 0.17. We can justify this change by rejecting the previous assumption that the heat of devolatilization is neutral, since it is an exothermic process for many lignite coals (13). This was experimentally verified using a differential scanning calorimeter at operating conditions similar to those in a Lurgi gasifier for five representative samples of plant lignite.

We have proceeded as far as possible in our model improvement efforts without changing the model itself. The next logical step is to include a kinetic model of, and incorporate the drying of coal into, the devolatilization process. Since there is considerable overlap between the gasification and devolatilization zones the evolution of volatile products will affect the concentration of gasification reactants, and thus the reaction rates. The current devolatilization model is a simple, linear, temperature dependant evolution of volatile matter and does not reflect actual volatile evolution. A kinetic model of Beulah lignite devolatilization with drying, the next phase of the Great Plains Gasifier Plant Optimization project, would be much more realistic and hopefully give better mass flow predictions.

Chapter I

INTRODUCTION

Coal as an Energy Alternative

The U.S. depends heavily on oil (Figure 1, (22)), of which 42% is imported from potentially unreliable foreign suppliers. Recall from past experience the effect of a small change in the oil supply on economic stability. Concerns over continued U.S. dependence on imported oil and increasing environmental restrictions on conventional

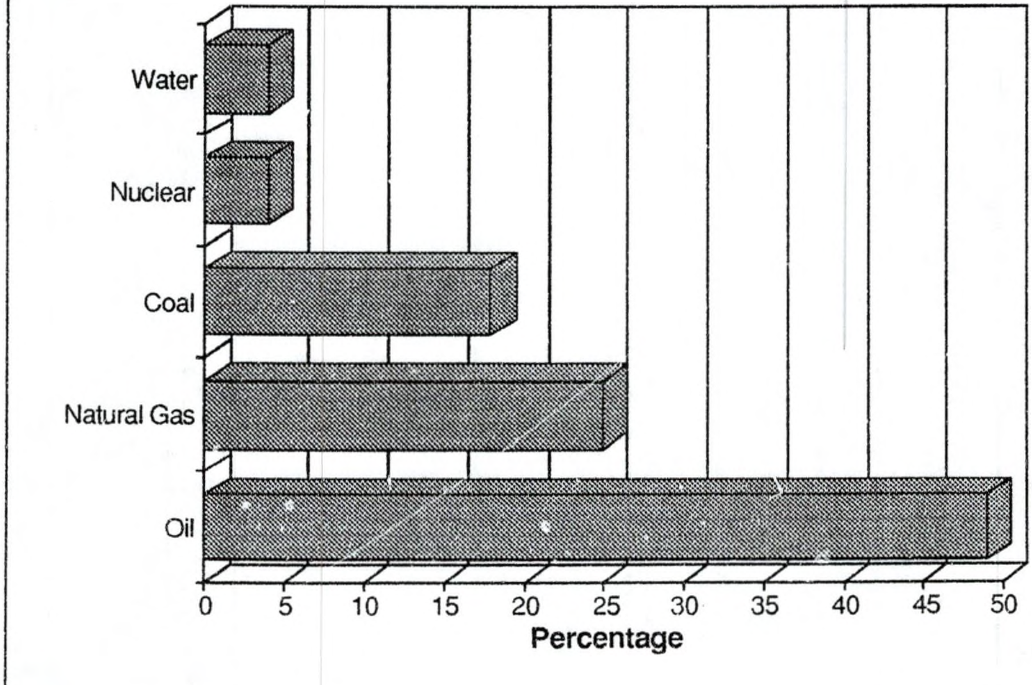

Figure 1. U.S. Energy Consumption By Source

coal fired power plants are driving the research and development of alternative energy sources.

Coal supplies within U.S. borders are projected to last 300 years. However, coal is generally thought to be an environmentally harmful energy source. Natural gas is currently abundant in U.S. reservoirs and could last 35 years before supplies run short. A way to extend the natural gas supply is to develop coal gasification technologies.

The main concerns with burning coal are oxidized emissions of nitrogen and sulfur, which contribute to acid rain and are regulated by the Environmental Protection Agency. Technologies have emerged in which coal is gasified at very high temperatures and pressures to provide an efficient, clean, and inexpensive source of fuel. Gasification is the anaerobic reaction of the carbon within coal with steam and carbon oxide reactants. It produces the reduced form of nitrogen and sulfur which are more easily removed with adsorbent materials.

Because of the complex reactions that occur and the variability of the coal composition much research is being done to understand the gasification process and predict optimum operating conditions. The Energy and Environmental Research Center in Grand Forks, North Dakota is administering the University of North Dakota's research activities on the Great Plains Gasifier Plant (GPGP) Optimization project. GPGP Optimization is jointly sponsored by the Department of Energy and the Dakota Gasification Company, and it has an ultimate goal of optimizing the production of synthetic natural gas. The reason for the Department of Energy's interest is the development of this alternative energy source to reduce the United States' dependence on foreign energy supplies. Lignite coal, vast deposits of which are present in the northern great plains province (North and South Dakota and Montana), is ideal for the

Lurgi gasification process. Lignite is also scattered in gulf province fields (Texas, Arkansas, Louisiana, Mississippi, Alabama). Bituminous and subbituminous coals are also abundant in fields throughout much of the United States. These are valuable deposits and are expected to play an important role in the future energy supply.

Methane Production in North Dakota

The Dakota Gasification Company (DGC), located in Beulah, North Dakota, operates 14 Lurgi gasifiers to produce 158 million cubic ft/day of synthetic natural gas (equivalent to 25,000 barrels of oil) from 17,000 tons of North Dakota lignite coal. Beulah is located in western North Dakota adjacent to the Freedom Mine and expansive reserves of lignite coal. Mining equipment and mining rights are owned by the Dakota Coal Company, a subsidiary of Basin Electric. The adjacent Antelope Valley Station electric generation plant is part of a regional power supply system operated by Basin Electric and works in conjunction with the gasification plant by sharing water supply, water treatment, coal handling, rail and electrical transmission facilities.

The production process at DGC was designed in the 1970's and uses conventional moving bed Lurgi gasification technology with methanation. A unique characteristic of this plant is its ability to produce a nearly pure methane product. In fact, it is the only commercial coal-to-SNG plant in the USA, and continued research on it is of prime importance to the present and future generations of energy consumers.

The Dakota Gasification Company has made a commitment to understand plant operation, and they have a long range goal to build a computer model of the entire plant to be used for optimization and supervisory control. The first step toward this goal is to develop a model of the Lurgi gasifiers; thus the GPGP ASPEN Model Development project was initiated and soon followed by the GPGP Optimization phase. Ultimately, the model should allow building a control system that will measure important variables and make adjustments that optimize plant operation. The goal of the Optimization phase was to improve model predictions by validating equilibrium constants and optimizing kinetic rate constants, the heat transfer coefficient to the jacket, and other parameters. As a verification of the simulation, data were available from a statistically designed (i.e., Box-Behnken) plant test in three operating variables: production rate, steam-oxygen ratio, and steam temperature.

Producing Electricity From Coal Gasification

Alternative technologies such as fluidized and entrained bed gasification have been developed by Exxon Corporation, Babcock & Wilcox, Westinghouse Electric Corporation, and others (14). In addition Shell Oil Company, Dow Chemical Company, and Texaco Incorporated have included high efficiency integrated gasification combined cycle gas turbines and produce electricity rather than methane. The gasification process produces a hydrogen, carbon monoxide mixture called syngas that is burned to produce steam. A power plant built by Texaco in southern California produces 120 megawatts of electricity from 1000 tons/day of coal. This particular plant is very environmentally sound. It has gasified high-sulfur coals, including Pittsburgh No. 8, with 3% sulfur content, while removing 97% of the sulfur. Airborne emissions were a fraction of the EPA's performances standards (23).

Although these plants use promising technologies, they are small in comparison to the Great Plains plant. In addition, production of synthetic natural gas is more efficient than electricity because of high power losses in transmission lines. The development of a reliable supply and distribution system would promote the use of natural gas for transportation, heating and cooling requirements, and cogeneration units.

As the environmental restrictions increase, the number of older coal-burning power plants operating outside EPA performance standards increase. They are in need of upgrading or replacement. Clearly, gasification and a worldwide abundance of coal should create an economic opportunity for companies pursuing this technology, in addition to creating jobs and providing a clean, efficient supply of energy.

Chapter II

BACKGROUND

The Gasification Plant

Early stages of the planning process for a coal gasification synfuels plant began in the mid 1970's because of concerns over foreign energy dependence. Construction of the gasification plant was completed in 1984 by a consortium of five energy companies. Financing was provided by a federally secured loan of $2.1 billion along with a $550 million company investment. However, when oil prices resumed a pre-recession level in the mid 80's, the revenue from the sale of natural gas in a depressed market was too little to pay financers. Foreclosure proceedings resulted in the plant being administered by the Department of Energy for two years prior to selling it in 1988 to the Dakota Gasification Company, a subsidiary of Basin Electric Power Cooperative. The federal government shares revenues from natural gas sales because of a partnership agreement, and the operation has had positive cash flows in recent years.

Great Plains ASPEN Model Development

A FORTRAN unit operation model of a Lurgi gasifier (RGAS) was developed for incorporation into the ASPEN software package in 1984 by Bruce Benjamin of Scientific Design Company (2). This mechanistic model was later modified in 1985 by Jay Dweck of JSD Incorporated and further modifications were made between 1990 and 1993 by

Simulation Sciences. By specifying the gasifier configuration, inlet stream flows, kinetic and equilibrium constants, and other physical parameters RGAS (ASPEN/SP) will perform mass and energy balances to predict outlet stream flows, compositions, and thermal conditions.

Several kinetic reaction models for simulating the behavior of a moving-bed gasifier have been developed and published (i.e., General Electric, IBM, Washington University, University of Minnesota models). From these, two were selected to be used to model the reaction kinetics within the gasification zone of a Great Plains gasifier (17). These are the DENN and WEN models developed by Denn, Yoon, and Wei of the University of Delaware (5) and C.Y. Wen of the University of West Virginia (24), respectively. J. Stefano of the Department of Energy compared the performance of the two models and found the DENN model to be superior to the WEN model, since it was simpler yet it gave comparable results (21).

GPGP Optimization and ERNIE Tests

In order to assess the adequacy of the RGAS model, plant data were collected at three operating rates to be used for validation and kinetic optimization studies. The data collected for the low (93.11%, August '90), average (98.35%, July '90), and high (103.79%, November '89) gasification rates are used as both simulation input parameters and output target levels.

The Great Plains Gasifier Plant (GPGP) Optimization study was initiated to improve the RGAS model in phases:

- Revise the devolatilization product schedule and adjust the gasification and combustion kinetics.

- Develop a kinetic model of Beulah lignite devolatilization.
- Add lignite metal composition catalytic effects.
- Add ash phase chemistry.

J. Kautz, J. Erjavec,and R. Sears of the University of North Dakota began the optimization phase of the project by upgrading the raw gas component list to 105 to include the characterized phenol, naphtha, and tar oil streams, and performing an optimization study of the kinetic rate constants in the DENN model (4).

Data on a single gasifier was collected in 1988 (ERNIE tests) to determine the effects of three operating variables (oxygen flow, steam/oxygen ratio, and agent temperature) on gasifier performance (using a Box-Behnken statistical experimental design) (20). Once the RGAS kinetics were optimized as well as possible, the model was then used to rerun the ERNIE test "on paper". Quadratic equations were obtained from regression analysis of the Box-Behnken design predictions, and compared with those from the ERNIE tests. The work of Kautz and Erjavec showed promise but did not adequately predict outlet temperatures as well as other responses and effects from variable input parameters. This thesis continues their work (GPGP Optimization phase one) with one objective being to optimize the kinetic reaction constants as well as other parameters.

Chapter III

MODEL DESCRIPTION

Lurgi Gasifier Configuration

A Lurgi moving-bed dry-ash coal gasifier (Figure 2) produces synthetic natural gas (SNG) from the gasification of coal and steam. Coal is crushed into 1/4 to 2 inch diameter chunks and screened to remove smaller particles. Coal and recycled tar, fed at the top of the Lurgi reactor from the lock hopper after depressurization, move downward by gravity through an upward flowing gas stream. Steam and oxygen enter the bottom of the reactor and flow upward to provide reactants for combustion and gasification. The product gases exit at the top while ash and unreacted char collect in the bottom lock hopper. A Lurgi gasifier at the Beulah plant has a reactor vessel (minus the lock hoppers) that is 40 feet high with a 13 foot diameter.

The settling coal chunks are first heated and dried by the countercurrent gas stream and then devolatilized which leaves fixed carbon to react with steam, hydrogen gas, and carbon monoxide. Combustion of a portion of the fixed carbon with the injected oxygen occurs near the bottom of the reactor and is needed to provide energy for endothermic gasification reactions. A moving grate at the bottom acts as a gas distributer and removes dry powdered ash. At the top, a coal distributor is used to provide the feed for a nearly uniform plug flow reaction within the vessel. A water jacket surrounds the vessel to control temperatures.

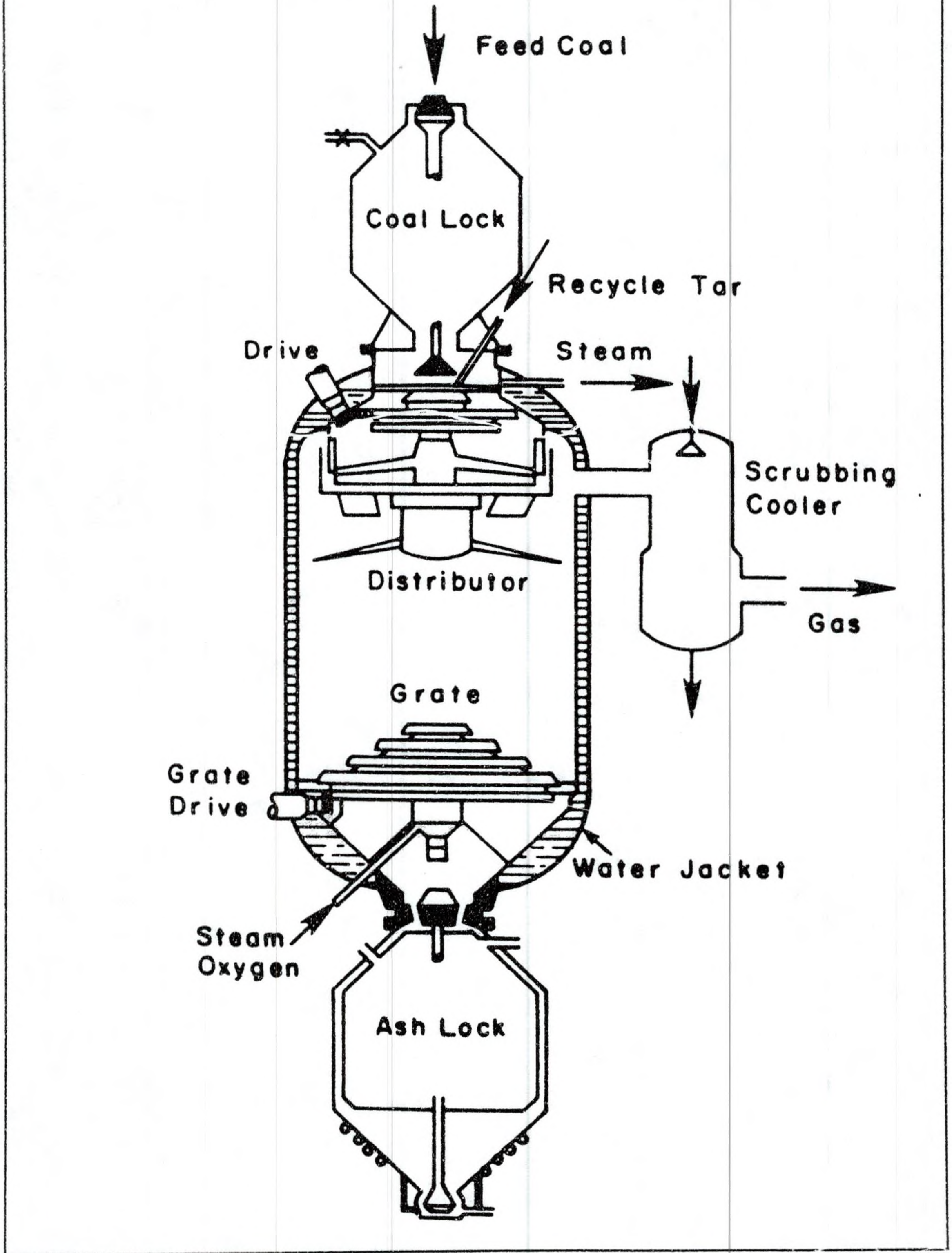

FIGURE 2. Lurgi Pressurized Gasifier.

Downstream Operations

A wet scrubber separates crude product gas from gas liquor by condensing tars, oils, phenols, ammonia, and steam and is the main source of waste water. The crude gas undergoes shift conversion to increase the ratio of hydrogen to carbon monoxide from 2.2:1 to 3:1. Cobalt-molybdenum catalytic reactors convert some of the carbon monoxide and water to hydrogen and carbon dioxide. Acid gas and organic impurities are removed in Rectisol by passing the raw gas through a cold (-95°F) methanol wash. The methanol is recycled by distillation; a naphtha distillate is incinerated while sulfur is recovered in the Sulfolin process. Finally, the clean raw gas undergoes methanation where the carbon monoxide reacts witn free hydrogen in the presence of a nickel catalyst. The product gas is dried, compressed, and piped to distribution centers.

Most of the oil and tar in the gas liquor stream is removed in a closed settling tank clarifier where tar settles and is drained while oil is skimmed from the top. The lighter oils are sold while the tars are reinjected into the gasifiers. Diisopropyl ether is used to extract the remaining phenol and residual oil and tar. Phenol is recovered and sold as a byproduct after evaporating the organic solvent.

Ammonia is recovered using an ammonium phosphate solvent and sold as a fertilizer. The stripped gas liquor stream is now ready for BOD (biological oxygen demand) removal using a biological treatment process.

RGAS Model

RGAS models a moving-bed dry-ash Lurgi gasifier as a one-dimensional countercurrent plug flow reactor with no axial dispersion. In other words, no radial temperature and concentration gradients are present. This is a good assumption if the reactor is adiabatic. However, a cooling water jacket creates a significant temperature gradient near the reactor wall, particularly at the bottom of the coal bed where combustion creates the peak temperature. This gradient is extreme but is generally limited to the one foot thick outer ring. Denn compared his two-dimensional model to a one-dimensional model (Yoon) and found a relatively small difference between the raw gas compositions (18). However, the one-dimensional model predicts a raw gas temperature about 40°F higher and a steam generation rate of one-half that of the two-dimensional model. These incongruities can be reduced by adjusting the heat transfer coefficient. Ringard and Benjamin concluded that a one-dimensional model was adequate for ASPEN simulation work and the relatively small differences between the models are generally within the accuracy of the plant data available for validation.

Mass and Energy Balance

A mass balance on the j^{th} solids constituent at a distance z from the bottom of the bed gives:

$$-\frac{d(S\,x_j)}{dz} = Ac \sum_{k=1}^{N_K} a_{j,k} R_k \,, \qquad j = 1\,, \ldots, N_J \tag{3.1}$$

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 k^{th} reaction in the solids,

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

N_K is the number of solid phase reactions included in the model, and

N_J 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). For example, a mass balance on the volatile proximate component results in:

$$\frac{d(Sx_v)}{dz} = S\frac{dx_v}{dz} + x_v\frac{dS}{dz} = A_c R_v \tag{3.2}$$

where R_v is the rate of devolatilization. An overall mass balance on all proximate components produces:

$$\frac{dS}{dz} = A_c(R_1 + R_2 + R_3 + R_4 + R_v) \tag{3.3}$$

where reaction rates one through four are due to fixed carbon reactions (the reaction rate of ash and water in the solid phase is zero).

Each of the solid phase reactions produce one or more gas phase products. The generation of the i^{th} gas phase constituent is given by:

$$g_i = Ac\sum_{k=1}^{N_K} b_{i,k}R_k\,, \qquad i = 1\,, \ldots, N_I \tag{3.4}$$

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

N_I is the number of gas phase constituents included in the model (i.e., from the proximate and ultimate analysis).

A component balance on the ith constituent in the gas phase gives:

$$\frac{d(G\,y_i)}{dz} = g_i + S\sum_{l=1}^{N_L} c_{i,l}R_l\,, \qquad i = 1\,,\ldots,\,N_l \tag{3.5}$$

where	G	is the total gas flow rate,
	y_i	is the mole fraction of the ith constituent in the gas phase,
	R_l	is the lth gas phase reaction rate,
	$c_{i,l}$	is the stoichiometric coefficient of the ith gas phase constituent with respect to the lth gas phase reaction, and
	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 in the raw gas and one for oxygen.

An energy balance on the solid phase gives:

$$-\frac{d(S\,H_S)}{dz} = U_{GS}\,A_{GS}\,(T_G - T_S) - \sum_{i=1}^{N_i} g_i\,H_{G_i}\{T_S\} + U_{CS}\,A_W\,(T_C - T_S) \tag{3.6}$$

where	H_S	is the enthalpy of the solids,
	H_{G_i}	is the enthalpy of the ith component evaluated at the solids temperature Ts,
	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}	in the heat transfer area per unit length of 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, and

T_G is the temperature of the gas.

An energy balance on the gas phase gives:

$$\frac{d(G\,H_G)}{dz} = U_{GS}\,A_{GS}\,(T_S - T_G) + \sum_{i=1}^{N_i} g_i H_{G_i}\{T_S\} + U_{CG}\,A_W\,(T_C - T_G) \qquad \textbf{(3.7)}$$

where H_G is the enthalpy of the gas, and

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 the gas (H_G) can be evaluated using the ideal mixture rule:

$$H_S = \sum_{j=1}^{N_J} x_j H_{S_j}\{T_S\}\,, \qquad H_G = \sum_{i=1}^{N_i} y_i H_{G_i}\{T_G\} \qquad \textbf{(3.8), (9)}$$

where H_{S_j} is the enthalpy of the jth solid phase constituent.

The solid phase (and likewise, gas phase) enthalpy can be written using heat capacities.

$$\frac{d(SH_S)}{dz} = H_S\frac{dS}{dz} + SC_{p_j}\frac{dT_S}{dz} + \sum_j\left(\frac{h_S}{y_j}\frac{dy_j}{dz}\right) \qquad \textbf{(3.10)}$$

The heat capacity (C_{pj}) of the j^{th} solid phase constituent is written in polynomial form as a function of temperature.

These equations can be integrated and rearranged to produce ordinary differential equations in the variables S, G, x_j, y_i, T_S, and T_G. The conditions for these variables (i.e., feed flow rates, composition, and temperatures of the coal and blast gas) are specified at both the top and bottom of the gasifier. This is a two point boundary value problem that requires an iterative procedure to determine exit flows, compositions and thermal conditions. The enthalpies, heat transfer coefficients, and transfer areas are known or can be measured and represented by numerical values or correlations as a function of temperature. This model was simplified by assuming the temperatures of the gas and solids to be equal at any one axial position in the gasifier. This is a good approximation for the devolatilization and gasification zones (the drying zone is modeled differently).

The remaining unknown parameters in the mass balance equations are the reaction rates R_k and R_l. These are evaluated using chemical reaction kinetic theory in the gas phase and incorporating diffusion in a porous catalyst pellet for the solid phase reactions. Two reaction kinetic models were chosen (the DENN and WEN models) from several available models for use in RGAS (17).

Process Zones and Kinetic Model

As a coal particle travels downward through the coal bed it is exposed to different temperatures and gas concentrations. Depending on these conditions, different processes may occur. Four process zones can be defined in the gasifier: combustion, gasification, devolatilization, and drying (see Figure 3). At the top of the bed, the coal is first heated and then water is vaporized in the drying zone. Next, tars and oils present in the feed coal are evolved during devolatilization. Gasification reactions of carbon with steam, hydrogen, and carbon dioxide occur under high temperatures and anaerobic conditions. At the bottom of the coal bed, injected oxygen reacts with the remaining fixed carbon to produce heat and the consequent peak temperatures in the combustion zone.

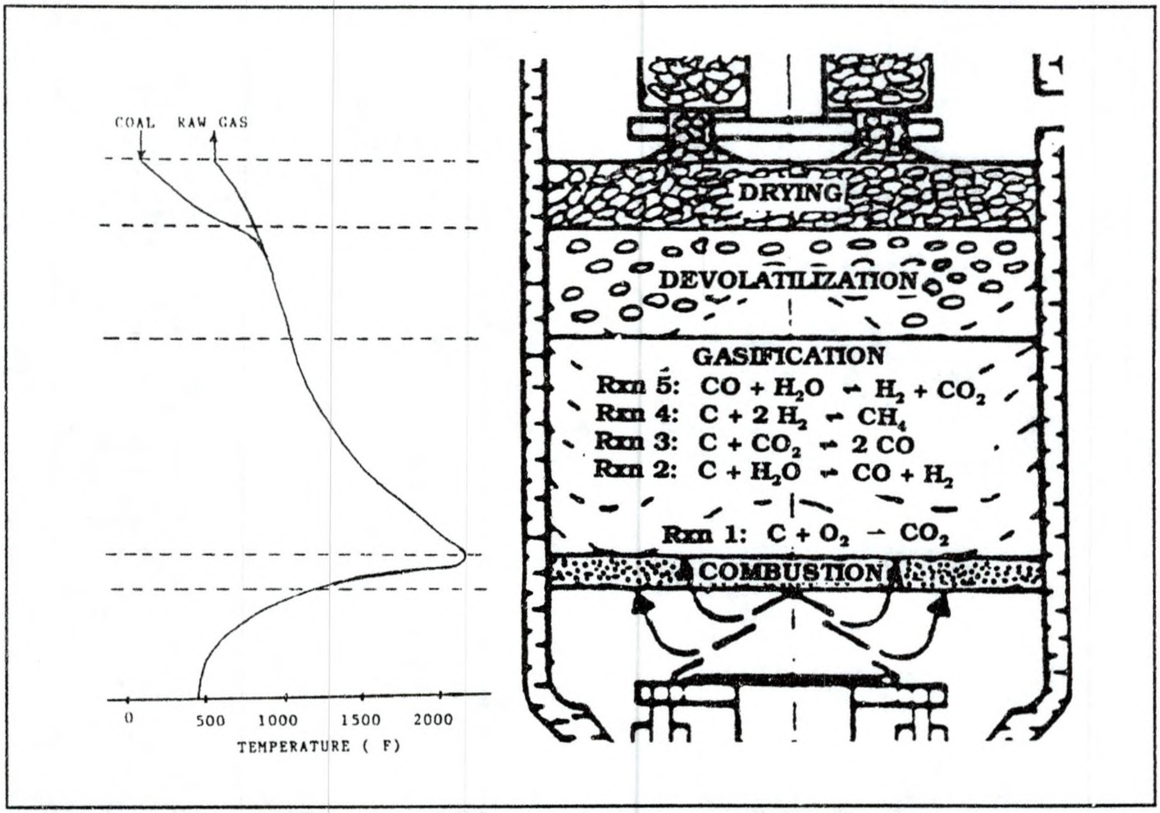

FIGURE 3. Process Zones and Temperatures in Lurgi Gasification.

Combustion and Gasification

DENN Model - In the combustion and gasification zones, the University of Delaware (DENN) kinetic model (Table 1) uses the temperature dependent Arrhenius equation for both the kinetic and equilibrium constants used to determine reaction rates in a porous catalyst pellet. The kinetic parameters (pre-exponential factor and activation energy) depend on the specific coal type used while the equilibrium parameters are fixed by measured thermodynamic values. The reactions produce carbon monoxide, carbon dioxide, hydrogen gas, and methane from fixed carbon, steam, and oxygen reactants. The combustion reaction (Reaction 1) is fast and assumed irreversible while the gasification reactions may go in either direction.

TABLE 1. DENN Kinetic Model

	DENN Kinetic Model Reactions			Rxn Heat (KJ/Kgmol)	Process	Equilibrium Parameters	
						A°	E°(cal/mol)
1.	$1\frac{1}{3}C + O_2$	$\rightarrow$	$\frac{2}{3}CO_2 + \frac{2}{3}CO$	+393,790*	Combustion	infinite	(irreversible)
2.	$H_2O + C$	$\rightleftharpoons$	$CO + H_2$	-175,440	Steam-Carbon	$3.098(10^7)$	32,457
3.	$CO_2 + C$	$\rightleftharpoons$	$2CO$	-172,580	Bouduard	$1.222(10^9)$	40,300
4.	$2H_2 + C$	$\rightleftharpoons$	CH_4	+74,900	Hydrogasification	$1.472(10^{-6})$	-21,854
5.	$H_2O + CO$	$\rightleftharpoons$	$CO_2 + H_2$	+2,853	Water-Gas Shift	0.0265	-7,860

* For complete combustion

The Arrhenius equation is written as:

$$K_{pj} = A_j{}^o \exp\left(-\frac{E_j{}^o}{RT}\right) \tag{3.11}$$

where A° = pre-exponential factor,

E° = activation energy,

K_{pj} = the dimensionless kinetic or equilibrium constant for reaction j,

R and T are the gas constant and temperature.

Reactions 1 through 4 are heterogeneous, while the last occurs in the gas phase. This reaction, the water-gas shift, is catalyzed by coal particles and is not assumed to be at equilibrium. Once the oxygen is consumed the gasification reactions dominate and continue throughout the length of the coal bed.

The kinetic expressions for the forward reaction rates using the Ash Segregation model are defined using diffusion theory in a catalyst pellet (17). The rate expressions for the combustion and steam-carbon reactions (Reactions 1 and 2) are of the same form

The rate expressions for the Ash Segregation Model are:

$$R_{i,j} = \frac{(1-\epsilon_b)(P_i - P_i^*)\,V_c}{\dfrac{d_p^0\,(r_{part} - r_{core})}{6\,r_{core}\,k_{p,i}} + \dfrac{1}{\eta_i\,K_{pj}\,[C]^0}} = j^{\text{th}} \text{ rxn rate of species } i \tag{3.12}$$

$$\text{where } k_i = \frac{2.06\,F_G^{0.425}}{P\,\epsilon_b\,Sc^{0.092}}\left(\frac{P\,D_i}{d_p\,R\,T}\right)^{0.575} = \text{mass transfer coefficient} \tag{3.13}$$

$$\eta_j = \frac{3}{\phi_j^2}\,(\phi_j \coth\phi_j - 1) = \text{effectiveness factor for reaction } j \tag{3.14}$$

$$\phi_j = \frac{d_p^0\,r_{core}}{6}\sqrt{\frac{K_{pj}[C]^0\,R\,T}{\gamma_j\,D_{e_i}\,r_{part}}} = \text{Thiele modulus} \tag{3.15}$$

$$V_c = \frac{w\,\rho_c}{x\,\rho_a + (1-x)\,\rho_c\,f_{ash}} \tag{3.16}$$

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,

De_i is the effective diffusivity in particle core,

D_i is the bulk gas diffusivity in particle core,

γ_i = 1 for steam-carbon reaction,

= q for combustion reaction (presently designated as 4/3),

P_i is the partial pressure of component i,

P_i^*	is the equilibrium partial pressure (zero for combustion),
d_p^0	is the initial solid particle diameter,
r_{core}	is the radius of char core,
ε_b	is the bed void volume,
$[C]^0$	is the initial concentration of fixed carbon in the particle,
Sc	is the Schmidt number,
F_G	is the molar gas flow, and
K_j	is the kinetic reaction rate coefficient from the Arrhenius equation.

The driving force of the reaction rate, $P_i - P_i^*$, in Equation 3.12 can be represented as mole fractions and expanded to include each species in the reaction:

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

$$= \left(y_{O_2} - \frac{y_{CO}^{q-1}\, y_{CO_2}^{2-q}}{K_{p1}^{eq}} \right) \qquad \text{for Reaction 1 (combustion)} \qquad \textbf{(3.17)}$$

$$= P\left(y_{H_2O} - \frac{y_{CO}\, y_{H_2}}{K_{p2}^{eq}} \right) \qquad \text{for Reaction 2 (steam - carbon)} \qquad \textbf{(3.18)}$$

where y is mole fraction and q is defined as the selectivity of the combustion reaction and represents a ratio of carbon monoxide and carbon dioxide produced during combustion (q = 2 for complete combustion but is presently designated as 1⅓ in RGAS). For the combustion reaction the equilibrium constant, K_{p1}^{eq}, is infinite since the reaction is assumed irreversible.

The Bouduard rate expression is:

$$R_3 = K_3\left(y_{CO_2} - \frac{P y_{CO}^2}{K_{p3}^{eq}}\right)\left(\frac{P}{RT}\right)(1 - \epsilon_b)[FC] \tag{3.19}$$

where [FC] is the concentration of fixed carbon.

For the hydrogasification reaction we have:

$$R_4 = K_4\left(y_{H_2}^2 - \frac{y_{CH_4}}{P K_{p4}^{eq}}\right)\left(\frac{P}{RT}\right)^2 (1 - \epsilon_b)[FC]\,. \tag{3.20}$$

The water-gas shift reaction is a gas phase reaction with the rate expression defined as:

$$R_5 = K_5\,\epsilon_b\left(y_{H_2O}y_{CO} - \frac{y_{CO_2}y_{H_2}}{K_{p5}^{eq}}\right)\left(\frac{P}{RT}\right)^2. \tag{3.21}$$

The Ash Segregation model assumes that the ash layer is removed from the coal pellet by melting or movement in the bed. The Ash Segregation model was chosen by Benjamin (2) because it yields a higher peak temperature and is a more conservative prediction since the ash melting temperature will be reached at lower gasification rates. RGAS also incorporates two other physical models that can be selected to model a coal pellet as it is transformed to raw gas products and ash. The Shell Progressive model assumes that the ash remains in position around the coal during the course of the reaction. In other words, the fixed carbon is contained in a shrinking core internal to the ash layer. In the Homogenous model the ash and fixed carbon are assumed to be a homogeneous mixture.

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

$$H_2 + \frac{1}{2} O_2 \rightleftharpoons H_2O$$

All six reactions are irreversible except the water-gas shift reaction. The combustion reaction is modeled as a heterogeneous reaction on a catalyst surface with mass transfer coefficients for both diffusion into the ash layer and across a thin film. The steam-carbon, Bouduard, and hydrogasification reactions are modeled as heterogeneous reactions while the water-gas shift and hydrogen burning reactions occur in the gas phase.

The WEN model was selected for RGAS because of the extensive documentation available and simplicity and similarity to the DENN model (17). It was designated as the backup to the DENN model because of convergence difficulties and very high peak temperatures. Ringard and Benjamin suggest that the convergence problem is a result of an infinite derivative of the combustion reaction rate with respect to carbon concentration, and the high peak temperatures are caused by integration errors due to high hydrogen burning reaction rates.

Devolatilization

As coal is heated, devolatilization of hydrocarbons, water and carbon oxides, and compounds containing nitrogen and sulfur such as aromatics, pyridines, thiophenes, phenols, aliphatics, olefins, and ketones occur at various rates. In addition, this volatile evolution involves cracking reactions that have not yet been well-defined. 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 for species i is:

$$\frac{dV_i}{dT} = K_i \tag{3.22}$$

where V is the amount of the volatile produced up to temperature T and K is a devolatilization constant. Devolatilization begins when the coal temperature reaches the lower temperature for volatile matter release, T_L, and continues linearly until the upper temperature limit, T_U, is reached. Actually, this is reversed in the simulation since discretization begins at the bottom of the coal bed. Therefore, the rate of volatile evolution for each species is constant and equivalent relative to their ultimate concentration in the raw gas stream.

If the devolatilization constant is assumed independent of temperature, an integration of Equation 3.22 results in:

$$V_i^0 = K_i(T_U - T_L) \tag{3.23}$$

where V_i^0 is the ultimate mass of volatile species i in the raw gas. V_i^0, T_U, and T_L are defined input values to the model and therefore K_i is determined and used in Equation 3.22 to determine evolution rates.

Note that since both gasification and devolatilization depend on temperature these two zones may overlap. Therefore, the non-condensible volatile matter (specifically H_2, H_2O, CO, CO_2, and CH_4) will affect gasification reactant concentrations, and thus, the reaction rates.

Drying

Water released during drying consists of inherent and surface moisture contained in cracks and capillaries and also includes physically and chemically absorbed moisture. Water produced from decomposition and mineral dehydration is not modeled in the drying zone because it requires energy to break chemical bonds, but is evolved within the devolatilization zone. The drying zone is modeled as an instantaneous transfer of mass and energy after convergence of reaction zone calculations and so does not affect the reactant concentrations. These are simple one-step calculations that involve the proximate water mass fraction and physical properties in the ASPEN/SP physical property data bank.

Chapter IV

COMPUTER SIMULATION

ASPEN/SP

ASPEN/SP (Advanced System for Process ENgineering) is a software system for computer-aided process design being marketed by Simulation Sciences in Denver, Colorado. ASPEN, a predecessor to ASPEN/SP, was developed at M.I.T. during the period 1976-81 under the sponsorship of the Department of Energy and 55 industrial participants. Simulation Sciences has updated ASPEN with an expert system (SPEXPERT) to make it more versatile and user-friendly.

Several types of blocks can be defined in the input file for the purpose of process design and statistical 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 (parameter). Other useful techniques used to study the operating parameters of the gasifier are case-study and optimization blocks. A case-study is used to perform a series of runs during one simulation by specifying that a variable have a sequence of values. Partial or complete reports can be generated along with table and graph files. An optimization block will maximize (or minimize) the value of a design specification variable. 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.

The ASPEN/SP simulation can be broken into four operations. First, the input translator processes the user input file, enters all data regarding the process into a Problem Data File (PDF), and writes the main calling program. Any FORTRAN statements supplied by the user are converted into FORTRAN subprograms and a physical property initialization subprogram is written. Second, these programs are compiled and linked to create a tailor-made 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 operator to construct a flow diagram by defining unit operation blocks, specifying component streams entering and leaving the block, and specifying the physical properties in the system (i.e., the ideal gas law). From this the SPEXPERT system can generate an input file to be used by ASPEN/SP during a simulation.

Verification of Equilibrium Constants

The rate at which reactions occur in the gasifier are described by the DENN model rate expressions given in Chapter III (Equations 3.12 through 3.21). The values of the rate expressions are 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 temperature dependence of each equilibrium constant in the DENN model follows the Arrhenius form:

$$K_i^{eq} = K_i^o \exp\left(\frac{E_i^o}{RT}\right) \qquad \textbf{(4.1)}$$

where K_i^{eq} = equilibrium constant for reaction i,

K^o = pre-exponential factor,

E^o = activation energy,

and R & T are the gas constant and temperature, respectively.

The values for the equilibrium parameters K^o and E^o are given in Table 1 and originated from sources by Hottel and Howard (7) and Parent and Katz (15).

Lavrov, et. al. (12) used experimental thermochemical data and statistical thermodynamics to calculate equilibrium constants from:

$$R\,LOG(K_i^{eq}) = \frac{-\Delta H_i^o}{T} + \Delta\Phi_i \qquad \textbf{(4.2)}$$

where $\mathbf{\Delta H_i^o}$ and $\mathbf{\Delta\Phi_i}$ are the sums of the heats of formation and chemical potentials of all species in reaction i.

A comparison of the equilibrium constants used in the ASPEN/SP simulation with theoretical values from Lavrov for Reactions 2 through 5 of the DENN model are plotted versus temperature in Figures 4 through 7. Note that Reaction 1, the combustion of fixed carbon, is considered irreversible so no equilibrium constants are needed in the model. Since there is nearly perfect agreement with the thermodynamic values, it can be concluded that the equilibrium parameters given in the DENN model are theoretically correct.

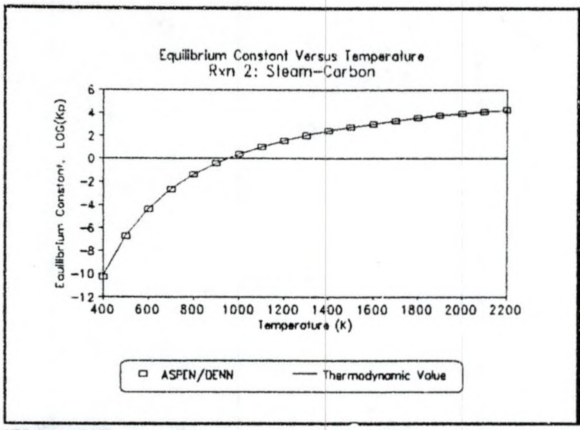

FIGURE 4. Steam-Carbon Reaction.

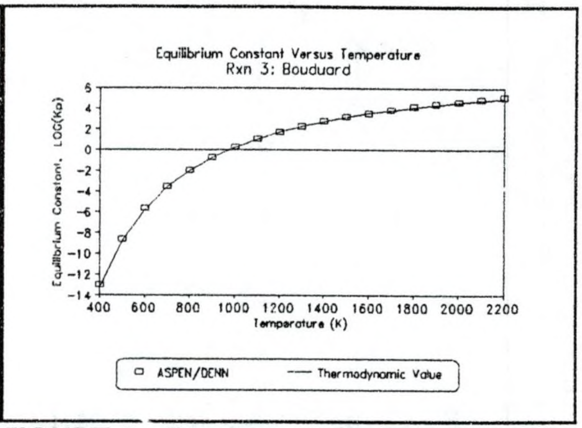

FIGURE 5. Bouduard Reaction.

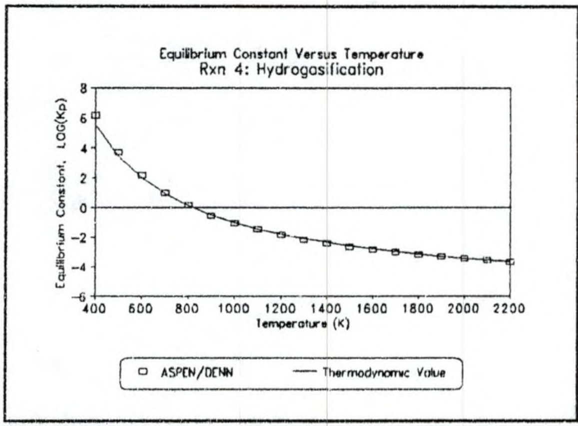

FIGURE 6. Hydrogasification Reaction.

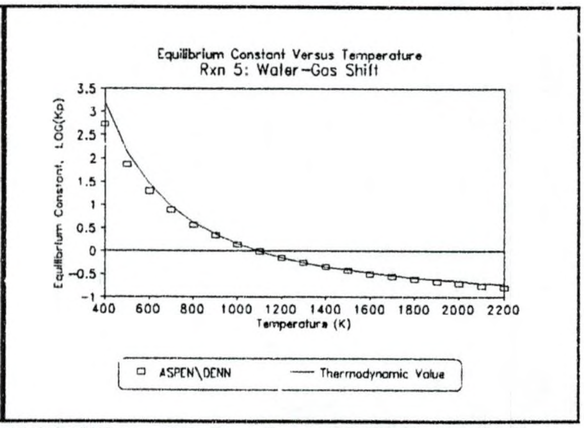

FIGURE 7. Water-Gas Shift Reaction.

Input Adjustment

Several problems and inconsistencies were found with the input to the RGAS model. For example, preliminary simulations produced a high volatile stream flow of 6 mol% of the dry raw gas flow while plant data used for validation and kinetic optimization of the ASPEN/RGAS model showed 2½ mol%. In addition, a simulation error was reported on many occasions which indicated that the simulation was pre-empted before convergence because of a low coal feed flow. Some of the major improvements made to the input are listed below.

- The mass fractions of the volatile components were adjusted to reduce condensible volatile flows, and four non-condensible raw gas components were added to the volatile matter (H_2S, C_2H_6, C_3H_6, and C_3H_8).
- A design specification ASPEN/SP routine was added which obtains a proper carbon conversion by iteratively adjusting the coal feed rate.
- The heat transfer coefficient was reduced from 170 to 105 W/m^{2}K in order to correctly predict the rate of steam generation in the gasifier jacket.
- The heat capacity of the volatile matter was reduced to obtain a raw gas temperature corresponding to plant data.
- The initial and final temperature for volatile release was reduced when a simulation produced the error message "Severe Error. Temperature too low for devolatilization".
- The kinetic rate constants were adjusted to improve response predictions using a weighted and normalized performance criterion.

These improvements are discussed in more detail in the following paragraphs. In addition to the input file changes, the RGAS FORTRAN files were revised by Simulation Sciences to update the report files and to correct initialization errors that were found as a result of the design specification's iterative nature.

Coal Gas in Volatile Stream

Coal is composed of aromatic clusters of fused rings. Heating causes the structure to decompose, producing an assortment of organic fragments. Many of the fragments are highly reactive free radicals which react with steam, hydrogen, and other fragments. Much of the volatile mass produced from these cracking reactions is non-condensible gas (coal gas). The volatile portion of the coal, as determined from the proximate analysis, was previously assumed to be condensible organic matter which ultimately can be separated into the tar oil, naphtha, and phenol streams

Adjustments were made to take into account the very significant fraction (~57%) of coal gas in the volatile matter. The amount of each coal gas component generated during devolatilization was estimated using an elemental mole balance on the components in the system. This was possible by using the proximate and ultimate analyses, the previously determined volatile slate of the tar oil, naphtha, and phenol streams, and by assuming the distribution of coal gas components. Once the elemental molar flow of non-condensible matter was determined by subtracting condensible volatile flows from total volatile flows, the elements were reassembled to form coal gas molecules. For example, all remaining nitrogen and sulfur were assumed to form nitrogen gas and hydrogen sulfide, respectively.[1] Since the current RGAS input file breaks the volatile matter into only three streams (tar oil, phenol, and naphtha), the fourth coal gas stream was nested in the other three streams. The assumptions provided results similar to devolatilization data obtained by Loison and Chauvin (1964) (5). The results of the elemental balance are given in Table 2.

---

[1] The procedure to determine coal gas component flows was done separately from the ASPEN simulation (on a spreadsheet) and the results were entered into the RGAS input. A FORTRAN routine is available to perform these calculations using a smaller volatile component list (i.e., 28) and slightly different coal gas distribution criteria (3).

TABLE 2. Mole Balance of Volatile Matter

	Molar Flows (lbmol/hr)				
	C	H	O	S	N
Condensible Volatile Molar Flows	362.0	445.4	28.5	0.73	2.10
Total Volatile Molar Flows	1079.4	3008.1	771.8	20.09	42.14
Non-condensible Volatile Flows	717.4	2562.7	743.3	19.36	40.04

Simultaneous Solution

Coal Gas Flows From Devolatilization

Component	Formula	lbmol/hr	lb/hr	Wt%
Hydrogen Gas	H_2	17.5	35.3	0.2%
Carbon Monoxide	CO	202.3	5666.5	33.4%
Carbon Dioxide	CO_2	67.4	2967.7	17.5%
Methane	CH_4	358.6	5753.6	33.9%
Ethane	C_2H_6	28.5	857.2	5.1%
Propane	C_3H_8	3.5	153.9	0.9%
Hydrogen Sulfide	H_2S	19.4	659.6	3.9%
Nitrogen Gas	N_2	20.0	560.9	3.3%
Ethylene	C_2H_4	4.7	130.6	0.8%
Propylene	C_3H_6	4.07	171.4	1.0%
TOTAL		726.0	16956.7	100%

Total Proximate Volatile Flows

Component	lbmol/hr	lb/hr	Wt%
Water	406.2	7317.1	24.7%
Coal Gas	726.0	16956.7	57.3%
Phenol	12.5	1143.5	3.9%
Naphtha	6.9	559.5	1.9%
Tar Oil	27.5	3602.7	12.2%
TOTAL	1179.1	29579.5	100%

Average Volatile Molecular Weight = 25.09

Simultaneous Equations

A	$717.39 = CH_4 + CO + 2C_2H_6 + 3C_3H_8 + 2C_2H_4 + 3C_3H_6$	
A	$2562.7 = 4CH_4 + 2H_2O + 6C_2H_6 + 8C_3H_8 + 2H_2S + 4C_2H_4 + 6C_3H_6$	
A	$743.33 = CO + 2CO_2 + H_2O$	
A	$19.356 = H_2S$	
A	$40.041 = 2N_2$	
B	$C_2H_6 = MOL*0.49/100$	
B	$C_3H_8 = MOL*0.06/100$	
B	$C_2H_4 = MOL*0.08/100$	
B	$C_3H_6 = MOL*0.07/100$	
B	MF = 125841 lb/hr	Mass flow rate of raw gas
B	MW = 21.63 lb/lbmol	Average molecular weight of raw gas
C	$CO + CO_2 + C_2H_6 + H_2 + N_2 + H_2S + C_3H_8 = CH_4$	50% methane in dry coal gas
C	$CO/CO_2 = 3$	3:1 carbon monoxide/carbon dioxide ratio
	MOL = MF/MW = 5817.9 lbmol/hr;	Mole flow rate of raw gas

Key
A => From Non-Condensible Molar Flows
B => From Plant Data (Appendix B)
C => Assumptions (based on Loison and Chauvin devolatilization data) (5)

Carbon Conversion Specification

The simulation error "Specified inlet coal flow is too low. Block exited in the middle of the simulation." was frequently reported. This indicates that the simulation was pre-empted before convergence because of a low coal feed flow. A design specification block (Table 3) was defined in the RGAS input file to specify the carbon conversion while varying the coal feed flow rate. Also, this is more realistic since the carbon conversion is known and the coal flow is determined by gasifier operating conditions.

TABLE 3. Carbon Conversion Design Specification

```
Design-Spec Spec1
   Define FCCLFD Comp-Attr-Var Stream=COAL-TAR Subs=NC Comp=COAL &
                 Attr=Proxanal Elem=2
   Define FCCHAR Comp-Attr-Var Stream=CHAR Subs=NC Comp=COAL
Attr=Proxanal &
                 Elem=2
   Define FLCHAR Mass-Flow Stream=CHAR Subs=NC Comp=COAL
   Define FLCLFD Mass-Flow Stream=COAL-TAR Subs=NC Comp=COAL
F     CC=1-FCCHAR*FLCHAR/FCCLFD/FLCLFD
   Spec 'CC' To '.975'
    Tol-Spec .0005
   Vary Substream-Var Stream=COAL-FD Subs=NC Var=Mass-Flow
   Limits Lower=11.5 Upper=14.5
```

For example, this routine will choose a coal feed flow rate using a secant convergence method, calculate predictions from the gasifier model, and compare the specified carbon conversion with the predicted value. If the predicted value is within the specified tolerance, the simulation is completed and ASPEN writes the report files; otherwise, a new coal feed flow rate is chosen for the next iteration.

A word of caution when using this routine: the first iteration must not result in the above mentioned error since this will produce a zero slope using the secant convergence method to predict a new coal flow, and no further iterations will be performed. The value given for the coal mass flow rate in the feed stream specification section of the input file is used for the initial iteration and should be chosen so the error does not occur.

The carbon conversion was specified at 0.975 rather than the 0.995 obtained from the plant. Carbon conversion values above this specification resulted in the simulation error. Not surprisingly, the change in the coal feed prediction was the largest effect (1.5% increase) per unit change in carbon conversion. While this adjustment had a small effect on the ultimate predictions it should not have hurt the ASPEN/RGAS model when being used to predict the impacts of changing operating variables.

Determination of Heat Transfer Coefficient

An energy balance was used to determine the heat transfer coefficient at the reactor wall. The following assumptions were made to simplify calculations:

- No heat loss to surroundings (adiabatic).
- No sensible heat change in water jacket (constant T and P).

With these assumptions the rate of energy passing through the gasifier wall can be determined from temperature, pressure, and mass flow measurements of the cooling water, which are available in the plant data sets.

A design specification block (listed in Appendix A) was used to determine the value of 105 W/m^{2}K for the heat transfer coefficient. It specifies the temperature of the exiting cooling water at a value slightly above that of the water entering the gasifier jacket. This assures that the entire cooling water flow is vaporized with a negligible degree of superheat. The predicted value of the heat transfer coefficient using this design specification block will change slightly with changing input parameters (such as kinetic reation rate constants).

Rather than determining a new heat transfer coefficient after each simulation the validity of the current value can be evaluated from the predicted outlet steam mass flow and temperature. These are the last two simulation responses listed in Tables 4 through 7. An outlet steam temperature of 460°F or below indicates a condition where a fraction of the cooling water is vaporized. This fraction can be determined by comparing predicted mass flows with plant data. An outlet steam temperature greater than 460°F indicates that the entire cooling water stream is vaporized and superheated. For example, the outlet steam temperatures in Table 4 (last prediction) are well above 460°F and indicates that the heat transfer coefficient is too high since the steam has a high degree of superheat.

Specific Heat of Volatile Matter

No provision was made in the RGAS model to directly allow for the enthalpy changes due to cracking reactions of the volatile matter. Rather, this was done indirectly. The total energy of devolatilization is the sum of the sensible heat, latent heat, and heat of reactions of all volatile components. The model currently assumes that devolatilization is thermally neutral (i.e., latent heat + heat of reactions = 0). The remaining sensible heat term is represented by the Kirov correlation specific heat value of 0.43862 + 1.5414(10^{-4})T, where T is temperature in Celsius. The size of this term was "fudged" to compensate for devolatilization not being thermally neutral by substituting the original Kirov correlation coefficients with an average value for the energy of devolatilization over the temperature range that this process occurs. In particular, the specific heat of the volatile matter was reduced from 0.43862 + 1.5414(10^{-4})T to 0.17 after the results of the kinetic parameter optimization provided little improvement in the predicted raw gas temperature. This will represent the significant exothermic nature of devolatilization that have been determined to occur with several North Dakota lignite samples (see Chapter VI). However, it should be noted that the specific value for this "fudged" heat capacity is expected to vary widely with different coal samples.

Temperature For Volatile Release

In the RGAS model, volatile matter is evolved at a rate that is linear with temperature. During the simulation, the gasifier is discretized from the bottom of the coal bed (high temperature) to the top (low temperature). If the temperature for volatile matter release is not reached, no volatile matter will evolve and a simulation error will be reported: "Severe Error. Temperature too low for devolatilization". The initial and final temperatures for volatile matter release were adjusted from 1255°K and 950°K to 1205°K and 750°K to prevent the simulation error when predicted temperatures did not reach this upper value (1255°K). There is evidence that devolatilization begins at temperatures below 750°K. However, during the simulation, the final (lower) temperature for volatile matter release is reset to the gas outlet temperature. Therefore, the input file value is only an initial guess and will not significantly affect predictions. The adjustment to the initial (upper) temperature for volatile matter release had only a minor effect on predictions. The concentration of methane had the largest percentage change (1.3%) while the other predictions changed by only a fraction of a percentage.

Optimization of Kinetic Reaction Rate Constants

The kinetic parameters were systematically adjusted using a Hooke-Jeeves pattern search (25) to optimize the fit to plant data. Since nine 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 plant data for the nine responses, normalizing the squared deviations (dividing by the average value of the three responses squared to put them all on a comparable basis), and summing the normalized deviations, each weighted by a multiplier between 1 and 10 to reflect its importance. Kinetic constants (pre-exponential factor and activation energy) for each of the five model reactions were sequentially varied, using the Hooke-Jeeves algorithm, to determine the direction to proceed (from the base case) so that the performance index was reduced.

Plant data were used to determine if simulation results were accurate. These data are recorded after all volatile matter (including a significant amount of water) is removed from the raw gas stream, while the ASPEN/SP simulation provides results that include all component flows in the raw gas. So the plant data were adjusted to be on the same basis (this was inadvertently omitted in previous optimization work (4)). For example, the mole fractions of non-condensible components in the raw gas stream (plant data) were each reduced to account for the condensible volatile flow. In addition, the weighting factors used to account for the relative importance of the various normalized error values for each response were changed to reflect a change in the opinion of Great Plains plant personnel as to which were really the important gasifier performance measures.

In the initial optimization, simulations were run for the three gasification rates (high, average, and low) using identical kinetic parameters to provide results for comparing to the three sets of plant data. The kinetic parameters were then adjusted for the next run. This was very time consuming since each series of runs required 50-70 minutes of computer time and a minimum of 100 runs (possibly many more) were required before a minimum performance index could be located.

The second optimization was accomplished by running simulations at only one gasification rate (the average) to reduce the required simulation time to 15-25 minutes per run. This was the only practical alternative, and any small inconsistency in the minimized performance index from plant data at one rate compared with that for all three rates was presumably offset by the ability to perform a more complete optimization.

Chapter V

MODEL PREDICTIONS

ASPEN/SP Simulation Results

The previous optimization results, using kinetic constants determined by work performed prior to input modifications, are given in Table 4. The simulation predicted mass flow rates reasonably well. Notice, however, that the predicted coal feed flow and the flow of water in the raw gas are slightly higher than the plant data. In addition, predicted mole fractions of the raw gas components, with the exception of methane, deviate from plant data by up 20%. When the volatile matter adjustments were made to reduce non-condensible volatile flows, the mole fractions deviated even more.

Initial Optimization

Significant improvements were seen after making the previously outlined modifications to the input (see Table 5). In particular, the predicted mole fractions of the raw gas components (on a dry basis) are within 2% of plant data. For example, the predicted mole fraction of hydrogen in the raw gas is predicted at 0.3889 (average rate) compared to 0.3888 for actual plant data.

TABLE 4. Predictions With Optimized Rate Constants; June 4, 1992 (4)

RESPONSE	Units	WT	Low Rate	Avg Rate	High Rate	Normalized Error
PLANT DATA			Aug.'90	July'90	Nov.'89	
COAL FEED FLOW RATE	LB/HR		100248	104666	108620	
FIXED CARBON CONVERTED	%		99.48	99.48	99.48	
CONC. OF H2 IN RAW GAS (DRY)	MOL%		0.3909	0.3888	0.3966	
CONC. OF CO IN RAW GAS (DRY)	MOL%		0.1536	0.1542	0.1527	
CONC. OF CO2 IN RAW GAS (DRY)	MOL%		0.3183	0.3165	0.3169	
CONC. OF CH4 IN RAW GAS (DRY)	MOL%		0.1155	0.1153	0.1121	
RAW GAS MASS FLOW RATE (DRY)	LB/HR		127399	130890	137361	
FLOW OF WATER IN RAW GAS	LB/HR		82515	88423	91763	
RAW GAS TEMPERATURE	F					
REACTOR STEAM UTILIZATION			0.5085	0.4852	0.5008	
SIMULATION						
COAL FEED FLOW RATE	LB/HR	10	106483	112423	118400	0.1782
FIXED CARBON CONVERTED	%	10	97.26	97.30	97.17	0.0152
CONC. OF H2 IN RAW GAS (DRY)	MOL%	1	0.3265	0.3275	0.3293	0.0809
CONC. OF CO IN RAW GAS (DRY)	MOL%	1	0.1184	0.1219	0.1255	0.1281
CONC. OF CO2 IN RAW GAS (DRY)	MOL%	3	0.3614	0.3586	0.3562	0.1544
CONC. OF CH4 IN RAW GAS (DRY)	MOL%	1	0.1163	0.1145	0.1131	0.0002
RAW GAS MASS FLOW RATE (DRY)	LB/HR	1	123637	129963	136594	0.0009
FLOW OF WATER IN RAW GAS	LB/HR	10	88159	92442	96937	0.0975
RAW GAS TEMPERATURE	F	10	409.2	407.6	407.5	0.7361
REACTOR STEAM UTILIZATION		3	0.4742	0.4776	0.4811	0.0196
PEAK TEMPERATURE	F	0	1886	1897	1906	
MASS FLOW OF STEAM PRODUCED	LB/HR	0	8457	9169	9575	
OUTLET STEAM TEMPERATURE	F	0	1344	1179	1102	
			Performance Index			1.4111

However, the predicted mass flow rate of water in the raw gas is 7,000 to 9,000 lb/hr (8-10%) too high while the raw gas mass flow on a dry basis and the coal feed flow rates are low. Improvements in the mole fraction predictions were made at the expense of the flow rate predictions. Increasing the reaction rate of fixed carbon and steam would provide better predictions by reducing raw gas water flow, increasing dry raw gas mass flow, and increasing the coal feed rate. Since the steam utilization depends on steam consumed in the gasifier, this prediction would also improve if more steam were consumed.

TABLE 5. Predictions With Optimized Rate Constants; April 1, 1993

RESPONSE	Units	WT	Low Rate	Avg Rate	High Rate	Normalized Error
PLANT DATA			Aug.'90	July '90	Nov.'89	
COAL FEED FLOW RATE	LB/HR		100248	104666	108620	
FIXED CARBON CONVERTED	%		99.48	99.48	99.48	
CONC. OF H2 IN RAW GAS (DRY)	MOL%		0.3909	0.3888	0.3966	
CONC. OF CO IN RAW GAS (DRY)	MOL%		0.1536	0.1542	0.1527	
CONC. OF CO2 IN RAW GAS (DRY)	MOL%		0.3183	0.3165	0.3169	
CONC. OF CH4 IN RAW GAS (DRY)	MOL%		0.1155	0.1153	0.1121	
RAW GAS MASS FLOW RATE (DRY)	LB/HR		127399	130890	137361	
FLOW OF WATER IN RAW GAS	LB/HR		82515	88423	91763	
RAW GAS TEMPERATURE	F					
REACTOR STEAM UTILIZATION			0.5085	0.4852	0.5008	
SIMULATION						
COAL FEED FLOW RATE	LB/HR	10	96972	102407	107947	0.0149
FIXED CARBON CONVERTED	%	10	96.97	97.30	97.22	0.0163
CONC. OF H2 IN RAW GAS (DRY)	MOL%	5	0.3871	0.3889	0.3911	0.0015
CONC. OF CO IN RAW GAS (DRY)	MOL%	5	0.1513	0.1532	0.1542	0.0018
CONC. OF CO2 IN RAW GAS (DRY)	MOL%	5	0.3181	0.3175	0.3165	6.1E-05
CONC. OF CH4 IN RAW GAS (DRY)	MOL%	5	0.1191	0.1150	0.1113	0.0052
RAW GAS MASS FLOW RATE (DRY)	LB/HR	1	112040	117595	123040	0.0355
FLOW OF WATER IN RAW GAS	LB/HR	3	90683	95566	100701	0.0773
RAW GAS TEMPERATURE	F	10	404.1	403.1	403.1	0.8294
REACTOR STEAM UTILIZATION		3	0.4080	0.4054	0.4035	0.3134
PEAK TEMPERATURE	F	0	1994	2005	2015	
MASS FLOW OF STEAM PRODUCED	LB/HR	0	8457	9115	9157	
OUTLET STEAM TEMPERATURE		0	578.9	460.0	460.0	
			Performance Index			1.2953

Optimization With Conversion to Wet Basis

It was thought that agreement of mass flow rates between predictions and plant data could be obtained and that high normalized errors for the raw gas temperature and steam utilization were affecting the optimization by shifting the location of the minimum. In an attempt to obtain a mass flow agreement, all predicted concentrations (including water) were converted to mole fractions on a wet basis and weighted at ten, and all other predictions were weighted at zero, except the coal feed which was also weighted at ten. Converting the raw gas component concentrations to a wet basis results in a much larger normalized error because of a large error in the water flow prediction. For example, the hydrogen mole fraction on a wet basis obtained from plant data is 0.2138 (Avg Rate) while the predicted value is 0.1964, an error of 7%.

Results obtained from this optimization (Table 6) were similar to those previously obtained in that the flow of raw gas was low while the flow of water in the raw gas washigh by a similar margin. However, some important improvements were noticed. The coal feed flow rate increased by 5% from the previous optimization (Table 5) while the flow of water in the raw gas increased by much less (1%). Since 36% of the feed coal is water, this means that more water and fixed carbon are being consumed.

TABLE 6. Predictions With Optimized Rate Constants (Wet Basis)

RESPONSE	Units	WT	Low Rate	Avg Rate	High Rate	Normalized Error
PLANT DATA			Aug.'90	July '90	Nov.'89	
COAL FEED FLOW RATE	LB/HR		100248	104666	108620	
FIXED CARBON CONVERTED	%		99.48	99.48	99.48	
CONC. OF H2 IN RAW GAS (WET)	MOL%		0.2192	0.2138	0.2199	
CONC. OF CO IN RAW GAS (WET)	MOL%		0.0861	0.0848	0.0847	
CONC. OF CO2 IN RAW GAS (WET)	MOL%		0.1785	0.174	0.1757	
CONC. OF CH4 IN RAW GAS (WET)	MOL%		0.0648	0.0634	0.0621	
RAW GAS MASS FLOW RATE (DRY)	LB/HR		127399	130890	137361	
FLOW OF WATER IN RAW GAS	LB/HR		82515	88423	91763	
CONC. OF H2O IN RAW GAS	MOL%		0.4352	0.446	0.4416	
RAW GAS TEMPERATURE	F					
REACTOR STEAM UTILIZATION			0.5085	0.4852	0.5008	
SIMULATION						
COAL FEED FLOW RATE	LB/HR	10	101424	107461	113260	0.0281
FIXED CARBON CONVERTED	%		97.28	97.27	97.24	0
CONC. OF H2 IN RAW GAS (WET)	MOL%	10	0.1955	0.1964	0.1972	0.2913
CONC. OF CO IN RAW GAS (WET)	MOL%	10	0.0787	0.0794	0.0796	0.1514
CONC. OF CO2 IN RAW GAS (WET)	MOL%	10	0.1630	0.1623	0.1613	0.1886
CONC. OF CH4 IN RAW GAS (WET)	MOL%	10	0.0650	0.0628	0.0605	0.0074
RAW GAS MASS FLOW RATE (DRY)	LB/HR	0	116279	122405	128051	0
FLOW OF WATER IN RAW GAS	LB/HR	0	90465	95535	100645	0
CONC. OF H2O IN RAW GAS	MOL%	10	0.4809	0.4752	0.4836	0.2641
RAW GAS TEMPERATURE	F	0	396.2	396.5	39604	0
REACTOR STEAM UTILIZATION		0	0.4282	0.4252	0.4239	0
PEAK TEMPERATURE	F		1858	1869	1878	
MASS FLOW OF STEAM PRODUCED	LB/HR		8457	8517	8536	
OUTLET STEAM TEMPERATURE	F		466.3	460.0	460.0	
			Performance Index			0.9309

Predictions With Specific Heat Adjustment

The energy balance from the simulation results in a very low predicted raw gas temperature. These results assume that the energy associated with devolatilization is neutral, while it is actually an exothermic process (this is explained in more detail in Chapter VI). This energy can be compensated for in the ASPEN/SP model by adjusting the specific heat of the volatile matter. Adjusting this value from 0.43862 + 1.5414(10^{-4})T to 0.17 resulted in more accurate predicted raw gas temperatures. This change had very little impact on the simulation results other than the raw gas temperature (see Table 7).

TABLE 7. Predictions With Optimized Rate Constants (Cp=0.17)

RESPONSE	Units	WT	Low Rate	Avg Rate	High Rate	Normalized Error
PLANT DATA			Aug.'90	July'90	Nov.'89	
COAL FEED FLOW RATE	LB/HR		100248	104666	108620	
FIXED CARBON CONVERTED	%		99.48	99.48	99.48	
CONC. OF H2 IN RAW GAS (DRY)	MOL%		0.3909	0.3888	0.3966	
CONC. OF CO IN RAW GAS (DRY)	MOL%		0.1536	0.1542	0.1527	
CONC. OF CO2 IN RAW GAS (DRY)	MOL%		0.3183	0.3165	0.3169	
CONC. OF CH4 IN RAW GAS (DRY)	MOL%		0.1155	0.1153	0.1121	
RAW GAS MASS FLOW RATE (DRY)	LB/HR		127399	130890	137361	
FLOW OF WATER IN RAW GAS	LB/HR		82515	88423	91763	
RAW GAS TEMPERATURE	F					
REACTOR STEAM UTILIZATION			0.5085	0.4852	0.5008	
SIMULATION						
COAL FEED FLOW RATE	LB/HR	10	95739	101743	107116	0.0285
FIXED CARBON CONVERTED	%	10	97.31	97.25	97.21	0.0150
CONC. OF H2 IN RAW GAS (DRY)	MOL%	5	0.3874	0.3891	0.3914	0.0013
CONC. OF CO IN RAW GAS (DRY)	MOL%	5	0.1488	0.1507	0.1517	0.0078
CONC. OF CO2 IN RAW GAS (DRY)	MOL%	5	0.3205	0.3197	0.3188	0.0009
CONC. OF CH4 IN RAW GAS (DRY)	MOL%	5	0.1189	0.1151	0.1112	0.0048
RAW GAS MASS FLOW RATE (DRY)	LB/HR	1	111262	116970	122341	0.0391
FLOW OF WATER IN RAW GAS	LB/HR	3	90461	95562	100631	0.0754
RAW GAS TEMPERATURE	F	10				0.0166
REACTOR STEAM UTILIZATION		3	0.4056	0.4029	0.4012	0.3299
PEAK TEMPERATURE	F	0	1993	2004	2015	
MASS FLOW OF STEAM PRODUCED	LB/HR	0	8457	9074	9117	
OUTLET STEAM TEMPERATURE	F	0	570.8	460.0	460.0	
				Performance Index		0.5193

The kinetic parameters for the Table 7 predictions were held at the same values as those obtained from the initial optimization (Table 5).

A comparison between the two predicted temperature profile cases in Figure 8 (the thermally neutral and exothermic heat of devolatilization) show that the temperatures are nearly identical throughout the reaction zone. This is reasonable since the axial temperature gradient is small within the gasification zone. The temperature increase when exothermic devolatilization reactions are considered is primarily due to the drop in energy needed to heat the volatile portion of the coal feed to gasification (and devolatilization) temperatures. In other words, the volatile specific heat adjustment has no significant affect on temperatures (and concentrations) in the

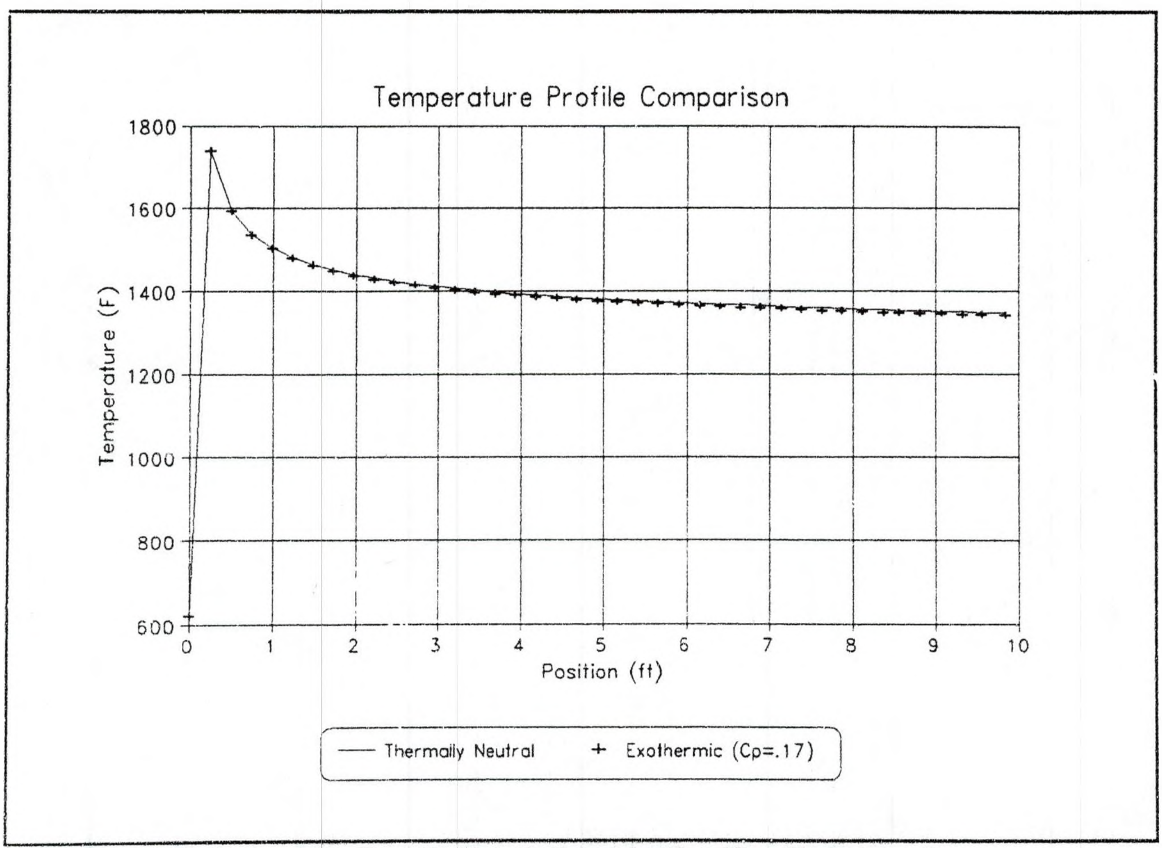

FIGURE 8. Temperature Profile Predictions In Gasifier Reaction Zone.

gasification/devolatilization zone but is accounted for in the drying zone. Consequently, the specific heat adjustment is not a good representation to the physical model since volatile reaction heat should be associated directly with devolatilization.

Table 8 gives the kinetic constants obtained from the optimization studies.

TABLE 8. Kinetic Rate Constants

	(Table 4)	(Table 5, 7)	(Table 6)
RC 1	3.02M	2.70M	3.00M
AE 1	27.0K	24.2K	27.0K
RC 2	525	610	325
AE 2	36.0K	39.0K	33.6K
RC 3	550	525	500
AE 3	74.0K	59.1K	63.0K
RC 4	4.90E-3	4.78E-3	5.35E-3
AE 4	17.1K	19.2K	18.8K
RC 5	20.7M	26.3M	25.0M
AE 5	14.9K	10.65K	12.4K

RC = Rate Constant; AE = Activation Energy

The first column gives the kinetic parameters for the simulation predictions of Table 4, the optimized predictions before the input adjustments were made. Column two gives the parameters for both Tables 5 and 7, the optimized predictions after input adjustment. The final column is the optimized parameters obtained after altering performance criteria in an attempt to achieve a mass flow agreement (Table 6).

Gasifier Model Equations

Data on a single gasifier were collected in 1988 (ERNIE tests) to correlate operating parameters to certain performance measures using a Box-Behnken design in three variables (oxygen flow, steam/oxygen ratio, and agent temperature) (20). To see if the ASPEN model with the optimized rate constants could predict the impact of these variable adjustments, the plant ERNIE test was repeated replacing the plant with the ASPEN model. The Box-Behnken test matrix (Table 9) consists of thirteen runs using scaled operating variables to represent high, average, and low values. The results of these ASPEN simulations were then fit to a quadratic equation in the three variables using regression analysis with coded variable rates (-1, 0, +1). The coefficients of the important quadratic equation terms (only significant terms were retained) are given in Table 10 along with the equations determined from the ERNIE tests. The coefficient of X_i for a particular response is the impact of changing the i^{th} operating variable from its average level to its high level. 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 nine responses listed in Table 9, are similar in comparison to the plant model. Both methane (CH_4) and hydrogen (H_2) mole fractions are correlated with oxygen flow (X_1) and steam/oxygen ratio (X_2) to nearly the same magnitude for both models (i.e., 0.33 versus 0.31 coefficients for H_2 mol% and variable X_1). Others are not so similar. The ASPEN model predicted the response of variable X_3, the agent temperature, in the same direction but with a significantly smaller magnitude for each of the seven responses that had significant plant model coefficients. On the other hand, a few of the trends were predicted in the opposite direction (i.e., 0.20 versus -0.23 coefficients for Equivalent SNG Rate and variable X_2).

TABLE 9. Box-Behnken Test Matrix

Box-Behnken design values (coded value)[1]			
O_2, % of design (X_1)	H_20/O_2 (X_2)	Temp, F (X_3)	Code Name[2]
100 (0)	(-1)	(-1)	F022
100 (0)	(-1)	(+1)	F021
100 (0)	(+1)	(+1)	F011
100 (0)	(+1)	(-1)	F012
92 (-1)	(+1)	(0)	F210
92 (-1)	(-1)	(0)	F220
108 (+1)	(-1)	(0)	F120
108 (+1)	(+1)	(0)	F110
92 (-1)	(0)	(-1)	F202
92 (-1)	(0)	(+1)	F201
108 (+1)	(0)	(+1)	F101
108 (+1)	(0)	(-1)	F102
100 (0)	(0)	(0)	F000

Definition of Coded Operating Variables:
X_1 = Oxygen Flow, % of design
X_2 = Steam/Oxygen Ratio, lbs/scf)
X_3 = Agent Temperature, °F

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[1] Actual design valus can be found in (4).

[2] Simulation predictions are given in Appendix C under these file codenames.

TABLE 10. Constants and Significant Coefficients of Gasifier Model Equations

Response	**Const.**	**X_1**	**X_2**	**X_3**	**X_1X_2**	**X_2X_3**	**X_1X_3**	**X_1^2**	**X_2^2**	**X_3^2**
Equiv. SNG Rate (kscfh)										
(P)	11.59	0.73	0.20	0.18	---	---	---	---	---	---
(A)	12.81	0.84	-0.23	0.09	---	---	---	---	---	---
Equiv. SNG Rate/Equiv. Gasification (kscfh/eq)										
(P)	11.6	-0.20	0.20	0.18	--	--	--	--	--	--
(A)	12.82	-0.18	-0.23	0.09	--	--	--	--	--	--
CO_2 in Raw Gas (mol%)										
(P)	32.30	--	0.31	-0.40	--	--	--	--	--	-0.37
(A)	31.89	-0.09	0.62	-0.13	--	--	--	--	-0.04	--
CH_4 in Raw Gas (mol%)										
(P)	10.90	-0.34	-0.22	0.22	--	--	--	--	-0.03	--
(A)	11.47	-0.27	-0.30	0.03	--	--	--	--	--	--
H_2 in Raw Gas (mol%)										
(P)	40.88	0.33	0.64	-0.25	--	--	--	--	-0.28	--
(A)	38.91	0.31	0.73	-0.04	--	--	--	-0.01	--	--
CO in Raw Gas (mol%)										
(P)	14.27	-0.20	-0.65	0.40	--	--	--	--	0.44	0.26
(A)	15.19	0.08	-1.01	0.14	--	--	--	--	0.05	--
H_2/CO										
(P)	2.90	0.06	0.17	-0.09	--	-0.01	--	--	-0.10	--
(A)	2.56	0.01	0.22	-0.03	--	--	--	--	0.01	--
Outlet Temperature (°F)										
(P)	482	--	13	--	--	--	--	--	--	--
(A)	484	9.91	19.7	-2.91	--	--	--	--	--	--
Gas Liquor/Equiv. Gasification (gal/day X 103))										
(P)	256	--	20	--	--	--	--	--	--	--
(A)	307	0.79	11.0	--	--	--	--	--	--	--

(P) = Plant model

(A) = ASPEN model (04/01/93)

X_1 = Coded Oxygen Flow X_2 = Coded Steam/Oxygen Ratio X_3 = Coded Agent Temperature

Discussion of Results

Ultimate Prediction Levels

Consider the combination of DENN kinetic reaction equations 3, 4, and 5:

$$3\ H_2O + 3\ C \rightleftharpoons CO_2 + CO + H_2 + CH_4$$

Increasing the forward reaction rate would provide better mass flow predictions. However, this reaction combination does not occur at an adequate rate with the optimized kinetic parameters. Possible explanations for this are:

1. We have not reached the minimum location in our optimization.
2. The reaction(s) are bounded by equilibrium constraints in the kinetic model.
3. The model for devolatilization is inappropriate.
4. The model for drying the feed coal is inappropriate.
5. FORTRAN code errors and undiscovered "bugs" still exist.

1. Local Minima

Each simulation requires 15-25 minutes of computing time when using the carbon conversion specification routine. The number of variables being considered in the kinetic optimization (ten), in addition to other variables that could be considered, creates a very time consuming route to the optimum. In an ideal situation (i.e., very short computing time), an exploratory search beginning at several different starting positions in the multi-variable plane would be done to see whether each case converged to the same point or if there were local minima (a "false" optimum). This was unrealistic in the time frame available for this study and the local minima hypothesis is believed to be an unlikely situation since the optimization with conversion to wet basis (Table 6) provided results similar to the initial optimization (Table 5).

2. Equilibrium Constraints

Equilibrium constants are documented in literature and should not be adjusted. If the kinetic optimization is being constrained by equilibrium, which depends only on temperature, then the temperature profile within the gasifier is inappropriate. Recall that the temperature within the reaction zone of the model does not fall below 1350°F with the optimized kinetic rate constants (see Figure 8). However, devolatilization and gasification reactions will occur at much lower temperatures; the reaction rates may or may not be reduced (remember kinetic rate constants depend on coal composition) but equilibrium concentrations will shift. Temperature limitations on gasification reactions and devolatilization can be removed by improving coal drying and devolatilization processes in the RGAS model. This is discussed further in the following paragraphs.

3. Inappropriate Devolatilization Model

Both gasification and devolatilization rates depend on temperature. Therefore, these two zones may overlap, causing the evolution of volatile products to affect the concentration of gasification reactants, and thus the reaction rates. The current devolatilization model is a simple linear temperature dependant evolution of volatile matter and does not reflect actual volatile evolution. In other words, the model assumes that devolatilization begins at a lower temperature limit and proceeds at a constant rate until the upper temperature limit is reached, so that all volatile species evolve consistently throughout the entire temperature range. The order and appearance of the volatile species when coal is heated at a constant rate is important. After drying, the sequence is chemical water, carbon dioxide, carbon monoxide, higher hydrocarbons (tars, etc.), ethane, methane, and finally hydrogen. The order in not precise, and substantial overlapping occurs (1).

The two assumptions made in order to simultaneously solve for the coal gas composition in Table 2 result in 359 lbmol/hr of methane being evolved during devolatilization. The methane in the raw gas flow from plant data is just 698 lbmol/hr. These assumptions result in 59% of the methane being produced during devolatilization. In addition, the flow of water from devolatilization makes up 14% of the raw gas water after excluding water resulting from drying of the feed coal. These are significant amounts and will have an effect on reaction rates. Using different criteria to solve for coal gas distributions and developing a more accurate devolatilization species sequence will affect ASPEN/RGAS predictions. It is possible that problems being encountered in obtaining accurate raw gas and water flows and temperatures can be explained by developing a better understanding of what is occurring in the devolatilization zone.

4. Inappropriate Model For Drying

The heating and drying of coal occurs after convergence of the gasifier reaction zone. Water released during drying consists of inherent and surface moisture contained in cracks and capillaries and also includes physically and chemically absorbed moisture. The percentage of raw gas water that originates from water in the feed coal is 43%. In the ASPEN model, this water is not available as a reactant but is added to the raw gas leaving the reaction zone. Yoon (26) estimated a heating and drying time of the order of 60 to 90 seconds for coal having 10% moisture and concluded that drying is instantaneous when compared to a solids residence time of one hour or more. However, North Dakota lignite contains 36% water. One could easily assume that at water saturation temperatures in the gasifier (460° F), with equilibrium favoring a forward reaction and coal providing a catalytic surface, the water-gas shift reaction would consume a portion of this water.

Consider the temperature profiles in Figure 6. The predicted temperature at the top of the gasification (and devolatilization) zone is ~1350°F (732°C). Between this temperature and the raw gas temperature (250°C) is the coal heating and drying zone. Within this broad temperature range (nearly 500°C) no reactions occur in the ASPEN model. In fact, coal drying, devolatilization, and char gasification are not independent processes in coal gasification. For example, coal gasification reactions for North Dakota lignite begin in the temperature range of 550-850°C for pulverized coal samples subjected to a wide range of hydrogen pressures (10-280 atm) and a high heating rate (~10^4°C/s) (8). In addition, there is evidence that devolatilization begins at 350-400°C and is a strong function of temperature after that (1).

During the ASPEN simulation, the final (lower) temperature for volatile matter release is reset to the gas outlet temperature. Since coal drying and devolatilization are handled separately in the RGAS model, devolatilization begins at temperatures exceeding 700°C after the coal is heated and dried. Because of this separation in zones both the devolatilization and gasification processes are being "cut off" from the temperatures and reactants (steam) available in the drying zone.

Gasification and devolatilization are currently modeled as concurrent processes. However, gasification, devolatilization, and drying are processes that depend on temperature. If drying were combined with the former two processes, free water would be available as a gasification reactant and devolatilization and gasification could occur at lower temperatures. Adding drying as an incremental process in the RGAS model would invalidate one assumption. The solid and gas temperatures are assumed to be equal at any one axial position within the bed of coal. During the heating and drying of coal this is an inadequate assumption and would need to be addressed when making changes to incorporate drying into the reaction zone.

5. Undiscovered Errors and "Bugs"

During the course of this investigation several "bugs" in the RGAS software were discovered which required programming adjustments. Some were minor and had little effect on simulation results while others were significant (i.e.,, carbon conversion design specification). It is believed that the simulation is now running properly. However, yet undiscovered programming inadequacies could become apparent. For example, during the final stages of this project (while deriving kinetic rate equations and comparing with FORTRAN routine equations), a programming error was discovered in the FORTRAN kinetic subroutine, DELKIN. This error affects the calculation of the rate of reaction 3.

Reaction 3: Bouduard reaction $CO_2 + C \rightleftharpoons 2CO$

To be more precise, the forward rate of the Bouduard reaction is given by:

$$R_3 = K_3\left(y_{CO_2} - \frac{P y_{CO}^2}{K_3^{eq}}\right)\left(\frac{P}{RT}\right)^2(1 - \epsilon_b)[C] \qquad \textbf{(3.19)}$$

where y is mole fraction and K_3 and K_3^{eq} are the kinetic and equilibrium coefficients from the Arrhenius equation. In the numerator of the second term is the squared mole fraction of carbon monoxide. Up until March of 1993 this term was $Py_{co}y_{H2} / K_3^{eq}$.

A preliminary investigation of the effect this change would have on ASPEN predictions was performed using the optimized rate constants and several input files from the Box-Behnken test matrix. Surprisingly, the results were unchanged (up to four significant figures) from those obtained from the original kinetic subroutine. However, it was noticed during optimization studies that the rate constant for reaction 3 had no effect on model predictions under particular kinetic conditions. This suggests that either the reaction is instantaneous or nonexistent. If this is the case, then changing a reactant variable in Equation 3.19 may not affect ASPEN predictions.

Impacts of Operating Variables

While the ASPEN model is predicting the ultimate response values more accurately, the ability to predict trends from adjustments to the three operating variables (Box-Behnken test matrix) have not improved much from previous optimization studies (some coefficients have improved, others are worse). However, some of the predicted trends are very good and most others are at least in the same direction (but different in magnitude). The three coefficients with an opposite sign (mol% CO and Equivalent SNG Rate) predict responses that directly involve carbon monoxide concentrations (and indirectly the Bouduard reaction). This reaction is believed to be occurring at an insignificant rate in the ASPEN model due to a low rate constant caused from optimization studies performed with a faulty reaction rate equation.

C. RGAS Convergence Scheme

The FORTRAN routine, which models the combustion and gasification zones in the gasifier (URE09), is a two point boundary value problem that requires an iterative approach for convergence. The composition, flow rate, and temperature of the reactants entering the bottom of the gasifier are specified. Also known are the coal feed flow and temperature at the top of the gasifier. It is neccessary, to solve this problem, to assume the amount of unreacted carbon in the ash. The differential mass and energy balance equations are integrated in the direction of the gas flow from the bottom to the top of the gasifier. If the correct amount of unreacted carbon has been assumed, the calculated amount entering the top will match the known value. If not, a new value of unreacted carbon is assumed and the integration is repeated (19).

The carbon conversion design specification routine added to the ASPEN/RGAS algorithm "guesses" (using a secant convergence scheme) the coal feed flow rate and calculates the carbon conversion. If the calculated carbon conversion does not match the specified value a new "guess" is made and the calculations are repeated. This design specification was added to prevent 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). A 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). In essence, the new algorithm contains a double-loop convergence scheme where it "guesses" a coal feed flow then "guesses" a carbon conversion (see Figure 9) This is a very inefficient algorithm because it makes unnecessary calculations and iterations. The solution could be found with just one iteration by making programming adjustments to the original FORTRAN routine (URE09).

For example, if the unreacted carbon flow (or carbon conversion) is specified along with the reactant characteristics entering the bottom of the gasifier, then everything is known at this boundary except the ash flow rate. This flow rate depends on the ash mass fraction from the proximate analysis and the coal feed flow rate. Once again, it becomes a two-point boundary value problem. However, since ash is not a reactant and contributes little to the mass and energy balances, it could be approximated using a correlation involving the three operating variables (oxygen flow, steam/oxygen ratio, and steam temperature) and allow the direct calculation of flow predictions at the top of the gasifier.

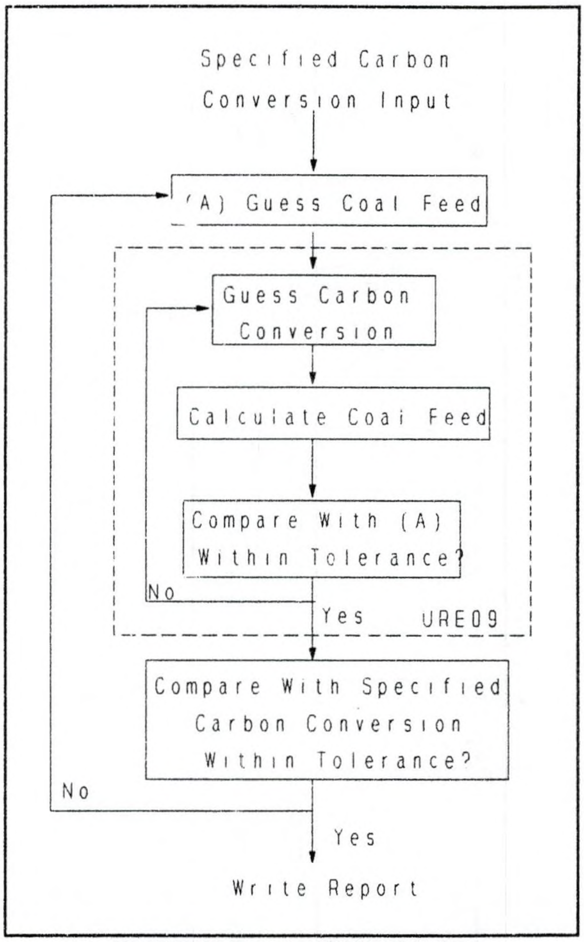

FIGURE 9. ASPEN/RGAS Convergence Scheme

Chapter VI

HEAT OF DEVOLATILIZATION

In the RGAS model of a coal gasifier, coal devolatilization is modeled using a linear temperature dependent evolution of an experimentally determined mixture of volatile components and assumed to be thermally neutral. With this assumption, using optimized kinetic parameters, a disappointing energy balance resulted that predicted a raw gas temperature significantly below plant data. However, it was reported by Om P. Mahajan (13) that the enthalpies associated with pyrolysis of differing coal types have a large variability and may either be positive or negative. This study was undertaken to better define the enthalpies associated with Great Plains lignite coal devolatilization.

Experimental

Five samples of North Dakota lignite were analyzed to determine enthalpies associated with devolatilization using a pressure differential scanning calorimeter (DSC). The samples were subjected to 900 psi in an inert atmosphere and energy was applied to create a temperature ramp of 10°C/min from ambient temperature to 570°C. Measurements of heat flow versus temperature and time were recorded at 6 second intervals. A sapphire sample was subjected to the same conditions and used as a standard. Thermo-gravimetric analyses (TGA) were performed using the same temperature ramp at ambient pressure to estimate the rate of volatile weight loss.

Energy Balance

An energy balance on the coal can be written as:

$$\frac{dQ_{coal}}{dt\,M} = \frac{dH_{coal}}{dt\,M} = \frac{1}{M\,dt}\sum_i\left[(\mu_i C_{p,i})\,dT + (\Delta H_i dm_i)_{vap} + (\Delta H_i dm_i)_{Rxn}\right] \qquad \textbf{(6.1)}$$

where M is the mass of the coal sample, μ_i is the mass of proximate component i, and m_i is the mass of vaporized component i. Therefore, μ_i/M represents the mass fraction of proximate component i (from the proximate analysis). Similarly, the enthalpy change in the sapphire can be written as:

$$\frac{dQ_{sap}}{dt\,M'} = \frac{dH_{sap}}{dt\,M'} = C_p'\frac{dT}{dt} \qquad \textbf{(6.2)}$$

where C_p' is a known experimental value represented by (8):

$$C_p'\ [J/g\,^\circ K] = -0.1224 + 0.004392\,T - 5.241\,(10^{-6})\,T^2 + 2.226(10^{-9})\,T^3 \qquad \textbf{(6.3)}$$

Taking the ratio of the two enthalpies and rearranging (i.e. multiplying by one) to reduce errors due to nonlinearities in the temperature calibration and control system (i.e., dQ/dt = $f\{T\}$) results in:

$$\begin{aligned}\begin{matrix}\text{Total Heat}\\ \text{(adjusted)}\end{matrix} &= \frac{dQ_{coal}/dt}{dQ_{sap}/dt}\frac{M'}{M}C_p'\frac{dT}{dt}\\ &= \frac{1}{M\,dt}\sum_i\left[(\mu_i C_{p,i})\,dT + (\Delta H_i dm_i)_{vap} + (\Delta H_i dm_i)_{Rxn}\right]\end{aligned} \qquad \textbf{(6.4)}$$

From DSC results and the heat capacity of sapphire the left-hand side of (4) can be evaluated. The sensible heat, latent heat, and heat of reaction terms are expanded using the proximate components: water (H_2O), fixed carbon (FC), volatiles (vol), and ash.

$$\sum_i (\mu C_p)_i = (\mu C_p)_{H_2O} + (\mu C_p)_{FC} + (\mu C_p)_{vol} + (\mu C_p)_{ash} \qquad \textbf{(6.5)}$$

Fixed carbon and ash remain in the solid state and so drop from the latent heat term.

$$\sum_i (\Delta H_{vap} dm)_i = (\Delta H_{vap} dm)_{H_2O} + (\Delta H_{vap} dm)_{vol} \qquad \textbf{(6.6)}$$

Similarly, ash is non- reactive and has no heat of reaction term:

$$\sum_i (\Delta H_{Rxn} dm)_i = (\Delta H_{Rxn} dm)_{WGS} + (\Delta H_{vap} dm)_{FC} + (\Delta H_{vap} dm)_{vol} \qquad \textbf{(6.7)}$$

where WGS represents the water-gas shift reaction.

$$H_2O \quad + \quad CO \quad \rightleftharpoons \quad CO_2 + \quad H_2 \qquad\qquad \Delta H = +2{,}853 \quad \text{KJ/Kg mol}$$

In order to simplify this analysis, the reaction with fixed carbon and the water-gas shift reaction were neglected. This is addressed further in the discussion section.

The heat of vaporization of water and the heat capacities of water (16), fixed carbon, and ash at 900 psi can be approximated using the Kirov correlations (9) by:

$$C_{p,FC} = 0.165 + 0.00068\,T - 4.2(10^{-7})\,T^2 \qquad \text{cal/g°C}$$

$$C_{p,ash} = 0.18 + 0.00014\,T \qquad T\ [=]\ \text{Celsius}$$

$$C_{p,H2O(l)} = 0.9909 + 1.582(10^{-4})\,T - 1.708(10^{-6})\,T^2 + 1.434(10^{-8})\,T^3 \qquad \text{cal/g°C}$$

$$\Delta H_{vap,H_2O} = 1558. \qquad \text{J/g}$$

The remaining sensible, latent, and reaction heat for the volatile matter ($C_{p,vol}$ + $\Delta H_{vap,vol}$ + ΔH_{Rxn} = heat of devolatilization) is brought to the left-hand side to produce an overall volatile enthalpy:

$$\text{Heat of Devolatilization} = \frac{1}{M}\int\left[\mu_{vol}C_p dT + (\Delta H dm)_{vap} + (\Delta H dm)_{Rxn}\right]_{vol} = \text{Total Heat (adjusted)} - \text{Non Volatile Enthalpy} \quad \textbf{(6.8)}$$

$$= \int \frac{dQ_{coal}/M}{dQ_{sap}/M'} C_p dT - \frac{1}{M}\int(\mu_{H_2O}C_p dT + \Delta H_{vap} dm)_{H_2O} - \frac{\mu_{FC}}{M}\int C_{p,FC} dT - \frac{\mu_{ash}}{M}\int C_{p,ash} dT$$

From the DSC and TGA analyses, the heat of devolatilization is approximated by substituting the change in mass, temperature, and energy supplied within each 6 second interval i and summing over the entire temperature range.

$$\text{Heat of Devolatilization} = \sum_{i=i_0}^{I}\left[\left(\frac{\Delta Q_{i,coal}/M}{\Delta Q_{i,sap}/M'} C_p' - \left(\frac{\mu}{M}C_p\right)_{FC} - \left(\frac{\mu}{M}C_p\right)_{ash} - \left(\frac{\mu}{M}C_p\right)_{H_2O}\right)\Delta T_i - \left(\Delta H_{vap}\frac{\Delta m_i}{\mu}\right)_{H_2O}\right] \quad \textbf{(6.9)}$$

Since the water and volatile matter undergo a change of phase, the instantaneous heat of vaporization and heat capacity within the **Δt** interval can be written as:

$$C_{p,H_2O} = C_{p,H_2O(l)}(1 - VF_{H_2O}) + C_{p,H_2O(v)}(VF_{H_2O}) \quad \textbf{(6.10a)}$$

$$C_{p,vol} = C_{p,vol(l)}(1 - VF_{vol}) + C_{p,vol(v)}(VF_{vol}) \quad \textbf{(6.10b)}$$

$$dH_{vap,H_2O} = 1558\ dm_{H_2O}\ \text{Joules} \quad \textbf{(6.11a)}$$

$$\Delta H_{vap,vol} = \text{Unknown} \quad \textbf{(6.11b)}$$

where VF is the vapor fraction.

To adjust for the weight loss during the DSC analyses we will assume that as matter is vaporized it leaves the system immediately and thus, maintains a constant pressure. Therefore, the gaseous matter does not absorb any further energy and the second term in Equations 6.10a and 6.10b vanish.

To account for the loss of volatile matter a TGA analysis with a 10°C/min temperature ramp was used (see Figure 10) to approximate the vapor fraction of volatile matter. As before, incremental intervals are summed:

$$VF_{vol} = \int_0^t \frac{dm_{vol}}{\mu_{vol}\, dt} \doteq \sum_{j=j_0}^{J} \frac{\Delta m_j}{\Delta t_j\, \mu_{vol}} \tag{6.12}$$

where j_0 and J are the Δt intervals at 20 and 56 minutes. The rate of vaporization of water, dm_{H_2O}/dt, can be approximated by a normal distribution:

$$\frac{dm_{H_2O}}{dt} = \frac{\mu_{H_2O}}{\sigma\sqrt{2\pi}} \exp\left(\frac{t-t_0}{2\sigma^2}\right). \tag{6.13}$$

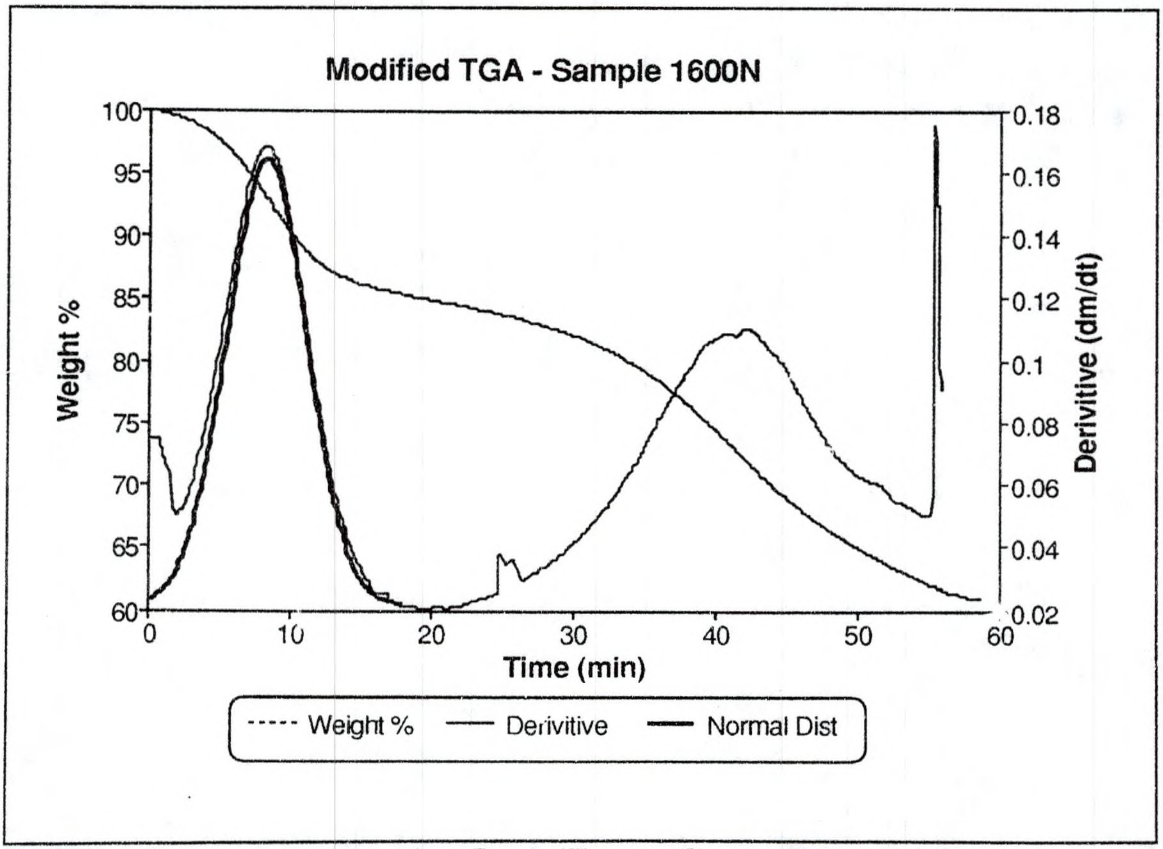

FIGURE 10. Linear Temperature Ramp Thermo-Gravimetric Analysis.

This is a reasonable since the left hand peak in Figure 10 (due to water vaporization) is a close approximation to the superimposed normal distribution. The vapor fraction of water is then:

$$VF_{H_2O} = \frac{1}{\mu_{H_2O}} \int_0^t \frac{dm_{H_2O}}{dt}\, dt = \int_0^t \frac{1}{\sigma\sqrt{2\pi}} \exp\left(\frac{t-t_0}{2\sigma^2}\right) dt \qquad \textbf{(6.14)}$$

where t_0 is the time of the peak temperature in the DSC curve, and σ was carefully chosen at 2.8 to match the width of the normal distribution with the width of the TGA water vaporization curve.

Results

Figure 11 is a graph of the raw data of heat flow versus temperature obtained during an experimental run using coal sample 1600N. The large peak is a result of the energy needed to vaporize water.

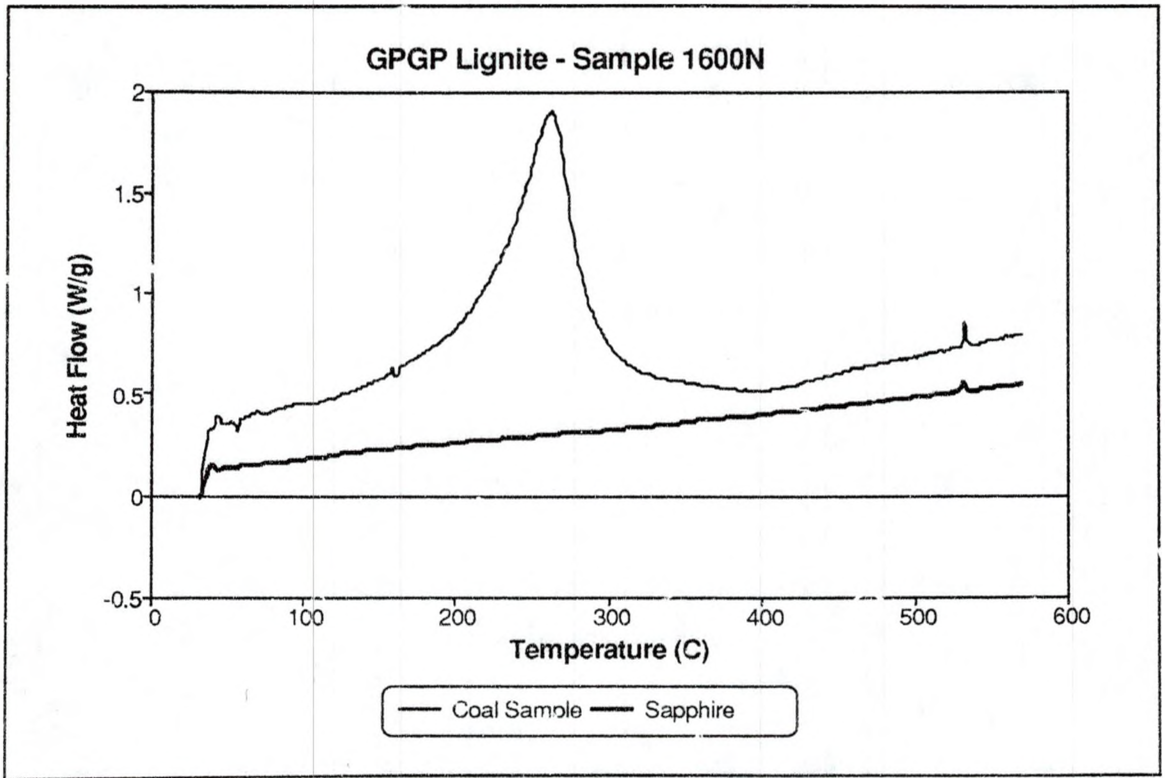

FIGURE 11. Raw Differential Scanning Calorimeter Results.

Figure 12 shows the adjusted heat flow data (Equation 6.4), the sum of the non-volatile enthalpies (negative terms in Equation 6.9), and the resultant net heat of devolatilization (Equation 6.9). The heat of devolatilization is the sum of the volatile specific heat, the heat of vaporization, plus any reactions that may be occurring. The volatile heat flow below 150°C is constant at 0.5 J/g; above 350°C it is 0.8 J/g and indicates that endothermic reactions and/or volatilization of heavy volatile matter are occurring since the proximate fixed carbon and ash has a much smaller sensible heat contribution. The large exothermic (negative heat flow) dip in the volatile enthalpy curve suggests that exothermic reactions are occurring concurrent with water vaporization.

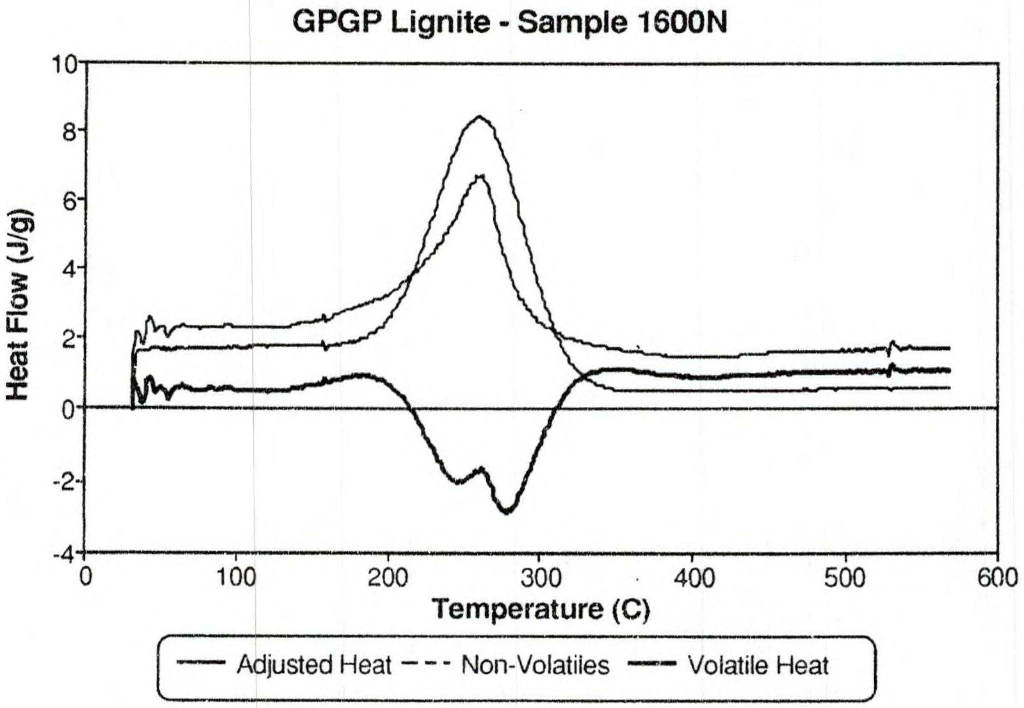

FIGURE 12. Adjusted Differential Scanning Calorimeter Results.

A proximate analysis of each blended coal sample was performed and is given in Table 11.

TABLE 11. Proximate Analyses of Coal Samples

Sample	(Wt%) Water	(Wt%) Volatiles	Fixed Carbon	(Wt%) Ash	(Wt% daf) Carbon
0200B	32.82	27.28	32.17	7.74	71.04
1000N	31.49	29.01	30.90	8.54	70.63
1600N	32.14	28.90	29.31	9.61	70.54
1400G	34.41	27.29	32.73	5.52	70.27
2200G	31.67	29.20	33.56	5.59	71.12

The summation of the enthalpies shown in Figure 12 are given in Table 12 for each coal sample over the temperature range of 100°C to 570°C along with an average volatile heat. The average volatile heat is calculated from:

$$\begin{array}{c}\text{Avg Volatile}\\\text{Heat}\end{array} = \frac{\text{Eqn 9}}{(570-100)^\circ C}\left(\frac{M}{\mu_{vol}}\right)(1\ cal/4.184\ J) \qquad \textbf{(6.15)}$$

and represents a specific heat value to be used for the ASPEN/RGAS simulation.

TABLE 12. DSC Net Enthalpies (J/g coal)

Sample	Adjusted	Non-Vol	Volatiles	(cal/g°C) Avg Heat
0200B	1191	1003	+188	+0.35
1000N	1027	982	+45	+0.07
1600N	1157	968	+189	+0.33
1400G	961	1049	-88	-0.14
2200G	1098	992	+107	+0.16

Discussion of Results

The specific heat for volatile matter is approximated in ASPEN\RGAS by 0.4386 + 1.5414(10^{-4})T, and devolatilization is considered thermally neutral. The values obtained in this analysis fall below this in a range of -0.14 to +0.35 which means that less energy is being absorbed by the volatile matter. In other words, more energy is being generated by cracking reactions than is required to vaporize the volatiles.

The specific heat value obtained from the RGAS optimization study (0.17) is well within this range. Even so, the coal samples in the present study were subjected to different concentrations of reactants since the countercurrent flow of coal and reactants in a gasifier is difficult to reproduce in a differential scanning calorimeter. Mahajan, et.al. performed experiments on dried coal which simplified calculations. However, this method would significantly reduce the presence of water vapor, which is involved in the water-gas shift reaction. The equilibrium of this reaction favors the formation of hydrogen gas at low temperatures ($K_p^{eq}>1$ when $T< 1100$ K). Water vapor and hydrogen gas are major reactants in the cracking and hydrogenation reactions that occur during devolatilization.

At atmospheric pressure, water is evolved separately from the volatile matter; this is not the case under pressurized conditions. Coal drying, devolatilization, and char gasification are not independent in coal gasification. Devolatilization is generally thought to result from chemical decomposition reactions. Elevated temperatures cause the aromatic clusters of organic polymers present in the coal to decompose. Some of the fragments are highly reactive free radicals subject to a variety of secondary reactions. "Hydrogen will react with devolatilizing coal several orders of magnitude faster than with the residual char. The short-lived rapid-rate carbon species is not clearly identified, though convincing evidence suggests that hydrogen interferes with the char forming secondary reactions presumably by hydrogenating reactive fragments sufficiently to stabilize them during their escape" (1).

In other words, the experimental conditions that coal is subjected to will affect the amount of decomposing volatiles that form char. For example, in an inert atmosphere Mahajan observed incomplete coal devolatilization. The ratio of total weight loss to proximate volatile matter ranged from 0.5 to 0.75. On the other hand, the hydrogenation of active carbon intermediates is apparent when coal is heated at high hydrogen gas pressures (10). The results of the DSC experiments indicate that exothermic reactions are occurring simultaneously with water vaporization and that steam may be a reactant in devolatilization.

In the derivation of the heat of devolatilization it was assumed that no char gasification reactions occurred. This is an important assumption since many researchers have reported total to proximate volatile weight loss in excess of one and indicates the occurance of char gasification. In the RGAS model this ratio can be specified. An elemental mole balance would then result in adjustments made to the coal gas volatile components only. Coal gas is evolved with no adjustment for reaction heat but adjustments can be made to account for the heat of devolatilization. These adjustments are redundant. A value for the heat of devolatilization with this ratio equal to one can theoretically be determined from the procedure used by Johnson (11):

$$\Delta H_{Rxn} = h_f \Delta F + h_v \Delta V \qquad \textbf{(6.16)}$$

where ΔF = fixed carbon gasified,

ΔV = Δm - ΔF = volatile matter gasified,

h_f, h_v = average heats of reaction for fixed carbon gasification and the heat of devolatilization.

Rearranging results in:

$$\frac{\Delta H_{Rxn}}{\Delta V} = h_f\left(\frac{\Delta m}{\Delta V} - 1\right) + h_v. \qquad \textbf{(6.17)}$$

Thus, a plot of ($\Delta H_{Rxn}/\Delta V$) versus ($\Delta m/\Delta V$ - 1) should give the heat of devolatilization at the intercept ($\Delta m = \Delta V$). This procedure may give adequate results for a single coal sample subjected to different hydrogen partial pressures but it is unknown how different coal samples will affect the variability of this intercept.

In this analysis we assumed that gaseous volatile matter does not absorb energy. In the gasifier model the volatile matter remains in the reactor to absorb heat and should be included in an energy balance to predict the heat of devolatilization. However, this is thought to be unimportant since Great Plains raw gas temperatures are only slightly above water saturation temperatures and most of the sensible heat absorbed by volatile matter is returned in the coal drying zone (in fact it is probable that heavy tars and oils are recondensed).

Although a specific value for the heat of devolatilization cannot be determined, it can be concluded that, since exothermic reactions occur, the specific heat for volatile matter in the ASPEN model should be adjusted to obtain more accurate raw gas temperatures. These results also indicate that drying and devolatilization under pressure are not independent processes and that "free" water may play an important role in these exothermic reactions.

At this point further DSC studies are not recommended. However, any future DSC experiments should be done using the following alterations to the current procedure.

- Reduce DSC pressure to more closely match Great Plains gasifier operating conditions (460 psi).

- Approximate the countercurrent gas-solid flow in a moving-bed gasifier by providing an environment containing raw gas components (perhaps a 1:1 ratio of H_2 and CO_2).
- Perform a constant temperature ramp TGA under pressurized conditions.[1]

These adjustments should allow the energy associated with devolatilization and gasification to be evaluated separately using linear regression (Equation 6.17).

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[1] Equipment to perform a pressurized linear temperature ramp thermo-gravimetric analysis with a capacity to achieve 600 psi and 900°C should be available at the Energy and Environmental Research Center, University of North Dakota, in May, 1993

Chapter VII

CONCLUSIONS AND RECOMMENDATIONS

Improvements in mole fraction predictions have been made at the expense of less accurate flow rate predictions. An elemental mole balance on the volatile matter in the coal has led to improved volatile flow predictions. Low raw gas temperature predictions have been determined to be the result of neglecting the exothermic nature of North Dakota lignite devolatilization, which was determined from differential scanning calorimeter experiments. An ASPEN/SP routine was used to estimate the heat transfer coefficient of the reactor wall. In addition, several ASPEN/RGAS simulation errors were defined and corrected.

Current predictions can be improved by defining parameters in the RGAS model that are constraining the approach to more accurate predictions (a "better" optimum). Increasing the consumption of steam (and carbon) would improve model predictions. However, because of the separation between the coal drying and gasification processes, gasification reactions and potential devolitilization reactants are being constrained by a temperature boundary. In addition, steam generated from drying coal is bounded from taking part in gasification reactions. Because reaction equilibria play no role at temperatures below that determined at the gasification/drying zone boundary (~ 1000°K), no further "tuning" of kinetic rate constants with the present model is recommended.

Rather, the model itself should be adjusted by developing improved RGAS algorithms for coal drying and devolatilization.

The following recommendations should provide improvement in future coal gasifier simulation studies.

- Perform an exploratory study using the kinetic parameters for the Bouduard reaction (Reaction 3) and the corrected kinetic FORTRAN code (DELKIN) to determine the effect this reaction has on predicted mole fractions (as compared to those obtained with the original DELKIN routine).
- Develop a more detailed model of North Dakota lignite devolatilization by determining coal gas distributions and the sequence of evolution of the non-condensible volatiles involved in gasification reactions.
- The heat of devolatilization appears to depend on coal composition. By considering the volatile specific heat to be an adjustable parameter, reactor temperatures can be more closely related to experimental data.
- Change the RGAS algorithm to use the carbon conversion as a boundary condition in its convergence scheme rather than the coal feed. This will simplify calculations and reduce the computing time by several factors. A correlation to predict the ash flow from the three operating variables will need to be developed.
- The RGAS model should be changed to achieve better temperature profile predictions and allow "free" water from coal drying to be available as a reactant. Since coal drying and volatile evolution are similar processes, they should be combined into a single process.

- The kinetic optimization procedure statistically compares predictions with test data for nine responses. The criteria used emphasized the importance of some responses. The importance and validity of these criteria should be verified prior to conducting further optimization studies.
- Since the reactor is modeled as a plug flow system, the reactor length is related to the extent of the reaction. Therefore, the entire bed depth should be accurately measured (including the heating and drying zone when combined with the reaction model).

These are some pronounced but necessary changes that will simplify calculations as well as produce a better representation of the physical gasifier and hopefully increase the accuracy of predicting both ultimate responses and trends from operating variables.

APPENDIX A

Updated RGAS Input File and FORTRAN Routines

```
;
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."
;
;--------------------------------------------------------------------------
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;                              Global Parameters
;--------------------------------------------------------------------------
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IN-UNITS SI
OUT-UNITS ENG
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HISTORY-UNITS SI
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SIM-OPTIONS RESULTS-PASS=1 HMB-RESULTS=2
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RUN-CONTROL MAX-TIME=10000
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;--------------------------------------------------------------------------
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;                               Report Options
;--------------------------------------------------------------------------
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;
REPORT FLOWSHEET PROPERTIES BLOCKS STREAMS
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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
;--------------------------------------------------------------------------
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;
;   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                     /
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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           /
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C9H14O    ISOPHORONE                    /
C10H8     NAPHTHALENE                   /
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           C10H14O2  P-TERT-BUTYLCATECHOL          /
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           C10H23N   N-DECYLAMINE                  /
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           C11H10-2  2-METHYLNAPHTHALENE           /
           C11H16O   P-TERT-AMYLPHENOL             /
           C11H24    N-UNDECANE                    /
           C12H9N    DIBENZOPYRROLE                /
           C12H10    DIPHENYL                      /
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           C12H10O   DIPHENYL-ETHER                /
           C12H11N   DIPHENYLAMINE                 /
           C13H10    FLUORENE                      /
           C13H10O   BENZOPHENONE                  /
           C13H12    DIPHENYLMETHANE               /
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           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
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;
ATTR-COMPS COAL PROXANAL ULTANAL SULFANAL
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;--------------------------------------------------------------------------
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-----
;
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
    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 /
```

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             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
;
;===========================================================================
====
;                            Design Specifications

;===========================================================================
====
;
Design-Spec Spec1
   Define FCCLFD Comp-Attr-Var Stream=COAL-TAR Subs=NC Comp=COAL &
                Attr=Proxanal Elem=2
   Define FCCHAR Comp-Attr-Var Stream=CHAR Subs=NC Comp=COAL Attr=Proxanal
&
                Elem=2
   Define FLCHAR Mass-Flow Stream=CHAR Subs=NC Comp=COAL
   Define FLCLFD Mass-Flow Stream=COAL-TAR Subs=NC Comp=COAL
F      CC=1-FCCHAR*FLCHAR/FCCLFD/FLCLFD
   Spec 'CC' To '.975'
   Tol-Spec .0005
   Vary Substream-Var Stream=COAL-FD Subs=NC Var=Mass-Flow
   Limits Lower=11.5 Upper=13.1
;
;--------------------------------------------------------------------------
-----
;                        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 /
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         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 2.700E+06    & ; Rate Constant for Reaction #1
        24200        & ; Activation Energy for Reaction #1
        610          & ; Rate Constant for Reaction #2
        39000        & ; Activation Energy for Reaction #2
        525          & ; Rate Constant for Reaction #3
        59100        & ; Activation Energy for Reaction #3
        4.780E-03    & ; Rate Constant for Reaction #4
        19200        & ; Activation Energy for Reaction #4
        2.630E+07    & ; Rate Constant for Reaction #5
        10650        & ; Activation Energy for Reaction #5
        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
        0.0          & ; 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)
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        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
        750.0        & ; Final Temperature for Volatile Matter Release
        1205.3822    & ; 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
        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
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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-10in Rectisol Naphth
4.12553E-03   & ;  Mass Fraction of C7H16-1   in Rectisol Naphth
0.00000E+00   & ;  Mass Fraction of C8H8O2    in Rectisol Naphth
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
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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
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  in 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-10in Crude Phenol
0.00000E+00   & ;  Mass Fraction of C7H16-1   in Crude Phenol
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```
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
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
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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
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-10in 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
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        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
        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
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
        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
```

```
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          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
C*    DABS(X) = ABS(X)
C*    DMIN1(X,Y) = AMIN1(X,Y)
C** DOUBLE PRECISION
C*    DABS(X) = ABS(X)
      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  ,IMISC  ,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: BWE    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
C       INITIALIZATION SECTION
C
      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 1000 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)
 1000 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,JDS,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)
C
      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
C
C     BEGIN ITERATION LOOP
C
      NIT=INT1(1)
      DO 4900 IT=1,NIT
      IF(IT.EQ.1.AND.LODIAG.GE.6) WRITE(NH,9000)
      IF(IT-2) 2800,2900,3000
 2800 WTCHAR=REAL1(LRK3+4)*WTCHRF
      WK2(1)=WTCHAR
      GO TO 3200
 2900 WTCHAR=REAL1(LRK3+5)*WTCHRF
      WK2(3)=WTCHAR
      GO TO 3200
 3000 WTCHAR=WK2(3)+(WK2(3)-WK2(1))*(WTCHRF-WK2(4))/(WK2(4)-WK2(2))
C
C     CHECK FOR NEGATIVE GUESS OF OUTLET FIXED CARBON
C
      IF(WTCHAR.GE.WK2(1).AND.WTCHAR.LE.WK2(3)) GO TO 3200
 3100 CONTINUE
      IF(MERRPT(IPROG,IDS,2,8684107,LODIAG,KPFLG3).EQ.0) GO TO 3150
      WRITE(NH,9350)
 3150 CALL ERROR(2,ICLASS)
      ISCP(5)=-7
C     GO TO 5000
 3200 WTTTL=WTASH+WTCHAR
      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(NH,9500) 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(NH,9600)
 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
      IF(IT.EQ.1.AND.DLTCHR.LT.0.D+00) GO TO 3100
      ADC=DABS(DLTCHR)
      IF(ADC.LE.1.E-02) GO TO 5000
      IF(IT-2) 4500,4600,4700
 4500 WK2(2)=TPCHRF
      GO TO 4800
 4600 WK2(4)=TPCHRF
      GO TO 4800
 4700 IF(DLTCHR.GT.0.D+00) WK2(1)=WTCHAR
      IF(DLTCHR.GT.0.D+00) WK2(2)=TPCHRF
      IF(DLTCHR.LT.0.D+00) WK2(3)=WTCHAR
      IF(DLTCHR.LT.0.D+00) WK2(4)=TPCHRF
 4800 CONTINUE
      IF(LODIAG.GE.5) THEN
```

```
          WRITE(NH,9900) B(LVRO3+IDXSUB(2)+NNCC+9),WTCHAR,WTTTL,
     1                   B(LVROUT+IDXSUB(2)+NNCC+9),
     2                   B(LVROUT+IDXSUB(2)+NNCC-1),TPCHRF,DLTCHR
        END IF
C
C       RESET DEVOLATILIZATION LOW TEMPERATURE TO GAS OUTLET TEMPERATURE
C
        REAL1(LRK3+2)=B(LVROUT+IDXSUB(1)+NCC)
  4900  CONTINUE
        IF(MERRPT(IPROG,IDS,2,8684108,LODIAG,KPFLG3).EQ.0) GO TO 4950
        WRITE(NH,9700) NIT
  4950  CALL ERROR(2,ICLASS)
        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
      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.)
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)
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',
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    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$ #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          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
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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     )
      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$ #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   ,
     1                    INT    ,NREAL  ,REAL   ,NPO    ,NBOPST ,
     2                    NIDS   ,IDS    ,NISCP  ,ISCP   ,NIREP  ,
     3                    IREP   ,NB     )
C
C-----------------------------------------------------------------------
C
C *--------------------------------------------------------------------*
C *                          **** NOTICE ****                          *
C *--------------------------------------------------------------------*
C
C %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
C
C                           COPYRIGHT (C) 1991
C                        SIMULATION SCIENCES INC.
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
      DIMENSICN 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)
      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        RETRIEVE THE HEADER
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)
```

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         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
C
C        PERCENTAGE OF FIXED CARBON CONVERTED
C
      IOFF = INT(59)
      WRITE(NR,1460) REAL(IOFF+4)
      IF (NSUM.NE.0) WRITE(NSUM,1460) REAL(IOFF+4)
C
C        PEAK TEMPERATURE
C
      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 )
      WRITE(NR,1470) (LABEL1(I),I=1,4), RVAL1
      IF (NSUM.NE.0) WRITE(NSUM,1470) (LABEL1(I),I=1,4), RVAL1
C
C        FIND THE KEY COMPONENTS
C
      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
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  250 CONTINUE
      IF ( ICOMP(6) .EQ. 0 ) GO TO 9999
C
C        DRY RAW GAS COMPOSITION AND FLOW RATE, WATER FLOW RATE, &
C        RAW GAS TEMPERATURE
C
      CALL LOCATS ( NBSOUT(1), LVIO, LVRO, LDO, NBSO )
      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
               WRITE(NR,1480) IDSCC(1,J), IDSCC(2,J), RVAL1
               IF (NSUM.NE.0) WRITE(NSUM,1480) IDSCC(1,J), IDSCC(2,J),
     1                                         RVAL1
  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 )
            WRITE(NR,1490) (LABEL1(I),I=1,4), RVAL1
            IF (NSUM.NE.0) WRITE(NSUM,1490) (LABEL1(I),I=1,4), RVAL1
            RVAL0 = DRYFLO * RGAS * 273.15D0 / PREF
            CALL RCONV1 ( 50, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
            WRITE(NR,1500) (LABEL1(I),I=1,4), RVAL1
            IF (NSUM.NE.0) WRITE(NSUM,1500) (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 )
         WRITE(NR,1510) (LABEL1(I),I=1,4), RVAL1
         IF (NSUM.NE.0) WRITE(NSUM,1510) (LABEL1(I),I=1,4), RVAL1
         RVAL0 = B(IOFF+NCC+1)
         CALL RCONV1 ( 22, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
         WRITE(NR,1520) (LABEL1(I),I=1,4), RVAL1
         IF (NSUM.NE.0) WRITE(NSUM,1520) (LABEL1(I),I=1,4), RVAL1
      END IF
C
C        STEAM JACKET DUTY, STEAM FLOW RATE, & STEAM TEMPERATURE
C
      CALL LOCATS ( NBSIN(3) , LVII, LVRI, LDI, NBSI )
      CALL LOCATS ( NBSOUT(3), LVIO, LVRO, LDO, NBSO )
      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(NR,1530) (LABEL1(I),I=1,4), RVAL1
         IF (NSUM.NE.0) WRITE(NSUM,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 )
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         WRITE(NR,1540) (LABEL1(I),I=1,4), RVAL1
         IF (NSUM.NE.0) WRITE(NSUM,1540) (LABEL1(I),I=1,4), RVAL1
         RVAL0 = B(IOFFO+NCC+1)
         CALL RCONV1 ( 22, RVAL0, RVAL1, LABEL1, IFM, IPR, STRNG1 )
         WRITE(NR,1550) (LABEL1(I),I=1,4), RVAL1
         IF (NSUM.NE.0) WRITE(NSUM,1550) (LABEL1(I),I=1,4), RVAL1
      END IF
C
C        STEAM UTILIZATION WITHIN REACTOR
C
      CALL LOCATS ( NBSIN(1) , LVII1, LVRI1, LDI1, NBSI1 )
      CALL LOCATS ( NBSIN(2) , LVII2, LVRI2, LDI2, NBSI2 )
      CALL LOCATS ( NBSOUT(1), LVIO1, LVRO1, LDO1, NBSO1 )
      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
         WRITE(NR,1560) STUTIL
         IF (NSUM.NE.0) WRITE(NSUM,1560) STUTIL
      END IF
C
C        RETURN
C
 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)
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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:')
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,
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    9       /5X,'UNUSED                                    ',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)
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)
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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$ #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
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          CAMBRIDGE, MA
C----------------------------------------------------------------------
      SUBROUTINE FLASHA(B      ,NPH    ,LPB    ,IPHASE ,NBOPST ,
     1                  NCPM   ,NCPCS  ,SCS    ,NCPNCS ,SNCS   ,
     2                  HM     ,NPKODE ,KPHASE ,LCPDIA ,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 (SUBROUTIN'
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
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 = JWORK(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          COPYRIGHT (C) 1981-85
C          JAY S. DWECK, CONSULTANT, INC.
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/NCPMCO,NCPCSO,NCPNCO,NTRIAL,KRSTRT,IDUMY,
     1 TCALC,PCALC,VCALC,HCALC,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.D+04,1222.D+06,1472.D-09,0.0265D0/
       DATA HKEQ/0.,3[illegible]457D0,40300D0,-21854D0,-7860D0/
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
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
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      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
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)
      AKI(1)=REAL1(LRK1+1)
      EKI(1)=REAL1(LRK1+2)
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      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)
      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
      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
      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))
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      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
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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
C     OBTAIN DEVOLATILIZATION TERM OF RHS
C
      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.)
      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
```

Heat Transfer Coefficient Design Specification

```
;------------------------------------------------------------
Design-Spec UCP
     Define WTEMP Stream-Var Stream=Cool-Out Var=Temp
     Spec 'WTEMP' to '512'
     Tol-Spec=5
     Vary Block-Var Block=Gasifier Sent=Param Var=UCP
     Limits Lower=0 Upper=200
;------------------------------------------------------------
```

*Note: This ASPEN routine will vary the heat tansfer coefficient (UCP) of the reactor wall until the resultant cooling water temperature is 512 K with a tolerance of +/- 5 K. The gasifier block calculations will be iterated until convergence using a secant method. The heat transfer coefficient is bounded by limits of 0 and 200 Watts/m^2 K.

APPENDIX B

Hooke-Jeeves Searches

TABLE 13. Hooke-Jeeves Searches - Initial Optimization

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

Normalized Errors Normalized Errors Normalized Errors

(Place Cursor in A# and type ALT-Z)

RC #1	AE #1	RC #2	AE #2	RC #3	AE #3	RC #4	AE #4	RC#5/10	AE #5	Coal FD	C Co	H2	CO	CO2	CH4	RG Mas	RG H2	RG Te	Stm Util	P Index	
3019000	26999	524.9	36012	550	74000	0.0049	17114	20670.5	14900	0	0.0379	0.0456	0.0018	0.0002	0.4266	0.0024	0.1119	1.2797	0.0437	1.9498	
3019000	27000	525	36012	550	74000	0.0049	17114	20670.5	14900	0.396	0.0164	211	0.0165	0.0165	2.8056	0.0016	0.1562	1.1064	0.1041	4.8304	NEW WT ADL.CL FL
2500000	30000	600	42000	550	60000	0.004	20204	24000	12200	0.396	0.9188	0.0162	0.0609	0.0647	0.0166	0.035	0.5107	0.9122	0.8267	3.758	First Change over stage
2000000	33000	715	48000	550	46000	0.0031	23290	27300	9500	0.396	2.1297	0.0302	0.0062	0.0895	0.1076	0.1324	0.9956	0.6194	2.046	6.5526	Pattern Move
2500000	30000	600	42000	550	60000	0.004	20204	24000	12200	0.396	1.0947	0.0145	0.0562	0.0796	0.0344	0.0291	0.5881	0.9371	0.8351	4.0648	New coal flow rts
2500000	30000	600	42000	550	60000	0.004	20204	24000	12200	0.396	0.7478	0.0178	0.0664	0.0542	0.0086	0.0403	0.4416	0.8701	0.8257	3.4684	
2500000	30000	600	42000	550	60000	0.004	20204	24000	12200	0.8397	0.0043	0.0331	0.1009	0.0042	0.116	0.0932	0.1111	0.0117	0.7882	2.1023	10.4, 11.0, 11.5
3000000	30000	600	42000	550	60000	0.004	20204	24000	12200	0.8397	0.0048	0.0335	0.1012	0.0037	0.1223	0.0941	0.1095	0.006	0.7803	2.095	
3000000	33000	600	42000	550	60000	0.004	20204	24000	12200	0.8397	0.1716	0.0389	0.0603	0.0153	0.1303	0.0883	0.1237	0.1905	0.8492	2.5077	
3000000	27000	660	42000	550	60000	0.004	20204	24000	12200	0.8397	0.0015	0.034	0.1029	0.0034	0.115	0.1093	0.0897	0.3889	0.6826	2.367	
3000000	27000	540	42000	550	60000	0.004	20204	24000	12200	0.8397	0.0069	0.03	0.1056	0.0025	0.1133	0.0972	0.1146	0.0023	0.805	2.1172	
3000000	27000	600	42000	550	60000	0.004	20204	24000	12200	0.9839	6.8E-05	0.0191	[illegible]	0.0182	0.4381	0.0938	0.0967	0.0006	0.7711	2.5166	Base B1 DES-SPE
3000000	27000	600	38000	550	60000	0.004	20204	24000	12200	0.5548	0.0002	0.0694	0.1154	0.0017	0.6271	0.046	0.0665	0.2851	0.4501	2.2164	
2700000	27000	600	38000	550	60000	0.004	20204	24000	12200	0.5546	0.0002	0.07	0.1153	0.0019	0.6359	0.0461	0.0666	0.282	0.45	2.2226	
3300000	27000	600	38000	550	60000	0.004	20204	24000	12200	0.5561	0.0002	0.0699	0.1155	0.0019	0.6357	0.0461	0.0665	0.2874	0.4497	2.2289	
2700000	30000	600	38000	550	60000	0.004	20204	24000	12200	0.5828	0.0002	0.0762	0.1075	0.0014	0.6945	0.0474	0.0649	0.2595	0.4537	2.2881	
2700000	24000	600	38000	550	60000	0.004	20204	24000	12200	0.5532	0.0001	0.0685	0.1165	0.0018	0.618	0.0457	0.0667	0.274	0.4501	2.1945	
2700000	24000	540	38000	550	60000	0.004	20204	24000	12200	0.5513	0.0002	0.0665	0.1181	0.0021	0.6067	0.0462	0.0672	0.2936	0.4517	2.2035	
2700000	24000	660	38000	550	60000	0.004	20204	24000	12200	0.5472	0.0003	0.071	0.1142	0.0017	0.6414	0.0455	0.0669	0.273	0.4491	2.2104	
3000000	24000	600	38000	600	60000	0.004	20204	24000	12200	0.5506	0.0002	0.0689	0.1163	0.0019	0.6235	0.0463	0.0665	0.3156	0.4483	2.2381	
3000000	24000	600	38000	500	60000	0.004	20204	24000	12200	0.5506	0.0002	0.0689	0.1163	0.0019	0.6235	0.0463	0.0665	0.3155	0.4483	2.238	
3000000	24000	600	38000	550	54000	0.004	20204	24000	12200	0.553	0.0001	0.0688	0.1166	0.0019	0.622	0.0463	0.0664	0.3089	0.4487	2.2327	
3000000	24000	600	38000	550	66000	0.004	20204	24000	12200	0.5506	0.0002	0.0689	0.1163	0.0019	0.6234	0.0463	0.0665	0.3152	0.4484	2.2376	
3000000	24000	600	38000	550	54000	0.0036	20204	24000	12200	0.6119	0.0002	0.0879	0.1223	0.0017	0.7794	0.0498	0.0648	0.2573	0.4644	2.4397	
3000000	24000	600	38000	550	54000	0.0044	20204	24000	12200	0.4847	0.0003	0.0524	0.1107	0.0021	0.4867	0.0425	0.0691	0.3537	0.4341	2.0363	
3000000	24000	600	38000	550	54000	0.0044	22224	24000	12200	1.007	0.0001	0.2333	0.1529	0.0005	1.9376	0.0725	0.0537	0.1186	0.5428	4.1191	
3000000	24000	600	38000	550	54000	0.0044	20204	26000	12200	0.4843	0.0003	0.0524	0.1108	0.0021	0.4864	0.0425	0.0691	0.3549	0.4339	2.0367	
3000000	24000	600	38000	550	54000	0.0044	20204	26000	11000	0.4824	0.0003	0.0521	0.1113	0.0021	0.4815	0.0423	0.0691	0.3553	0.4333	2.0297	Base B2
3000000	21000	600	34000	550	48000	0.0048	20204	24000	9800	Error; cannot make pattern move. Use smaller variable adjustments (5%).											Pattern Move
2850000	24000	600	38000	550	54000	0.0044	20204	26000	11000	0.5016	4.1E-05	0.0525	0.1118	0.0022	0.4867	0.0421	0.0678	0.2925	0.4348	1.992	+/-0.0005 tol; not converge; 5
2850000	24000	600	38000	550	54000	0.0044	20204	26000	11000	0.4899	0.0002	0.0522	0.1116	0.0022	0.4828	0.0419	0.0687	0.3083	0.4346	1.9924	+/-0.002 tol; 53.8 min run tim
2850000	22800	600	38000	550	54000	0.0044	20204	26000	11000	0.489	0.0002	0.0524	0.1117	0.0023	0.4873	0.0422	0.0686	0.326	0.4338	2.0135	
2850000	25200	600	38000	550	54000	0.0044	20204	26000	11000	0.4906	0.0002	0.0532	0.1112	0.0023	0.4972	0.0424	0.0685	0.3345	0.4336	2.0336	
2850000	24000	570	38000	550	54000	0.0044	20204	26000	11000	0.4894	0.0002	0.0518	0.1121	0.0025	0.4869	0.0425	0.0687	0.3375	0.4342	2.0259	
2850000	24000	630	38000	550	54000	0.0044	20204	26000	11000	0.4902	0.0002	0.0534	0.1106	0.0021	0.4949	0.0424	0.0683	0.3426	0.4326	2.0373	

TABLE 13 (cont). Hooke-Jeeves Searches - Initial Optimization

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

											Normalized Errors			Normalized Errors			Normalized Errors				
RC #1	AE #1	RC #2	AE #2	RC #3	AE #3	RC #4	AE #4	RC#5/10	AE #5	Coal FD	C Conv	H2	CO	CO2	CH4	RG Mas	RG H2	RG Te	Stm Util	P Index	
2850000	24000	600	36100	550	54000	0.0044	20204	26000	11000	0.5173	0.0002	0.0639	0.0903	0.0008	0.5944	0.0435	0.0679	0.2498	0.4418	2.0699	
2850000	24000	600	39900	550	54000	0.0044	20204	26000	11000	0.5559	0.0001	0.0305	0.106	0.0063	0.3746	0.0532	0.0782	0.2489	0.5111	1.965	
2850000	24000	600	39900	575	54000	0.0044	20204	26000	11000	0.5559	0.0001	0.0305	0.1061	0.0063	0.3746	0.0532	0.0782	0.2492	0.5111	1.9654	
2850000	24000	600	39900	525	54000	0.0044	20204	26000	11000	0.5559	0.0001	0.0305	0.106	0.0063	0.3745	0.0532	0.0783	0.2486	0.5112	1.9647	
2850000	24000	600	39900	525	56700	0.0044	20204	26000	11000	0.5559	0.0001	0.0305	0.1059	0.0063	0.3737	0.0531	0.0783	0.2445	0.5114	1.9598	
2850000	24000	600	39900	525	56700	0.00462	20204	26000	11000	0.5263	0.0001	0.0245	0.102	0.0065	0.3167	0.0512	0.0796	0.2532	0.5048	1.8649	
2850000	24000	600	39900	525	56700	0.00462	21214	26000	11000	0.8121	0.0002	0.1008	0.1371	0.0046	0.9863	0.0684	0.0686	0.1534	0.5637	2.8953	
2850000	24000	600	39900	525	56700	0.00462	19194	26000	11000	1.488	1.9E-05	0.0011	0.052	0.0366	0.1016	0.0678	0.0121	0.7549	0.3122	2.8263	error
2850000	24000	600	39900	525	56700	0.00462	19200	26000	11000	0.2474	0.0002	0.0027	0.0678	0.0096	0.0059	0.0331	0.0937	0.4586	0.4281	1.3472	
2850000	24000	600	39900	525	56700	0.00462	19200	24700	11000	0.2476	0.0002	0.0027	0.0678	0.0096	0.006	0.0331	0.0937	0.4577	0.4282	1.3466	
2850000	24000	600	39900	525	56700	0.00462	19200	24700	10450	0.2434	0.0002	0.0027	0.0666	0.0093	0.0057	0.033	0.094	0.4719	0.4268	1.3536	
2850000	24000	600	39900	525	56700	0.00462	19200	24700	11450	0.2473	0.0002	0.003	0.0685	0.0082	0.0058	0.0322	0.0951	0.3973	0.4331	1.2906	Base B3
2700000	24000	600	41800	500	59400	0.00484	18200	23400	11900	0.34	0.0001	0.0402	0.0517	0.0273	0.0661	0.0506	0.1203	0.1794	0.5887	1.4646	PATTERN MOVE
2780000	24000	600	41800	500	59400	0.00484	18200	23400	11900	0.3434	0.0001	0.0403	0.0517	0.0275	0.0658	0.0507	0.1198	0.1758	0.5884	1.4636	
2780000	24720	600	41800	500	59400	0.00484	18200	23400	11900	0.3348	0.0003	0.0402	0.0514	0.0268	0.0673	0.0506	0.1211	0.1914	0.589	1.4727	
2780000	23280	600	41800	500	59400	0.00484	18200	23400	11900	0.3291	0.0003	0.0403	0.0517	0.0264	0.0689	0.05	0.1224	0.1746	0.5905	1.4543	
2780000	23280	618	41800	500	59400	0.00484	18200	23400	11900	0.3226	0.0002	0.0414	0.0512	0.0265	0.0734	0.0487	0.1204	0.1865	0.5786	1.4497	
2780000	23280	618	39700	500	59400	0.00484	18200	23400	11900	1.7497	1.9E-05	0.0625	0.0253	0.0515	0.1121	0.0417	0.0055	0.4982	0.193	2.7395	error
2780000	23280	618	43054	500	59400	0.00484	18200	23400	11900	0.7079	0.0002	0.0216	0.0626	0.0405	0.0049	0.0874	0.1282	0.0009	0.8137	1.8679	
2780000	23280	618	39900	500	59400	0.00484	18200	23400	11900	0.0496	0.0002	0.0656	0.0398	0.0126	0.292	0.0154	0.1102	0.6557	0.3359	1.5769	
2780000	23280	618	41800	475	59400	0.00484	18200	23400	11900	0.3237	0.0002	0.0415	0.0511	0.0265	0.0735	0.0491	0.1197	0.2073	0.5765	1.469	
2780000	23280	618	41800	525	59400	0.00484	18200	23400	11900	0.3237	0.0002	0.0415	0.0511	0.0265	0.0735	0.0491	0.1197	0.2074	0.5765	1.4691	
2780000	23280	618	41800	500	56700	0.00484	18200	23400	11900	0.3233	0.0002	0.0415	0.0512	0.0265	0.0734	0.0487	0.1203	0.1861	0.5785	1.4497	
2780000	23280	618	41800	500	62100	0.00484	18200	23400	11900	0.3231	0.0002	0.0415	0.0511	0.0265	0.0735	0.0491	0.1198	0.208	0.5765	1.4692	
2780000	23280	618	41800	500	59400	0.00462	18200	23400	11900	0.3337	0.0003	0.037	0.0524	0.0251	0.0604	0.0496	0.1207	0.1676	0.5864	1.4332	
2780000	23280	618	41800	500	59400	0.00462	17290	23400	11900	0.1824	0.0049	0.0805	0.0428	0.0293	0.2378	0.0387	0.1371	0.326	0.5408	1.6203	
2780000	23280	618	41800	500	59400	0.00462	19200	23400	11900	0.5309	0.0003	0.0042	0.0683	0.0214	0.0198	0.064	0.1104	0.0795	0.6475	1.5464	
2780000	23280	618	41800	500	59400	0.00462	18200	24700	11900	0.3402	0.0001	0.037	0.0525	0.0263	0.0578	0.0501	0.1192	0.1777	0.5839	1.4449	
2780000	23280	618	41800	500	59400	0.00462	18200	24700	11450	0.3451	0.0001	0.037	0.0529	0.0264	0.0579	0.0499	0.1187	0.1586	0.5848	1.4313	
P. Index too large. Will not make pattern move. Collapse back to old base B3.																					
+/-30000	+/-500	+/-10	+/-400	+/-10	+/-600	+/-4E-5	+/-200	+/-300	+/-100	Choose new increments.											
2850000	24000	600	39900	525	56700	0.00462	19200	24700	11450	0.2473	0.0002	0.003	0.0685	0.0082	0.0058	0.0322	0.0951	0.3973	0.4331	1.2906	Base B3
2800000	24000	600	39900	525	56700	0.00462	19200	24700	11450	0.251	0.0001	0.0027	0.0678	0.0094	0.0057	0.033	0.0936	0.4375	0.4293	1.3301	
2900000	24000	600	39900	525	56700	0.00462	19200	24700	11450	0.2525	0.0001	0.0027	0.0678	0.0095	0.0058	0.0331	0.0932	0.4432	0.4288	1.3368	
2850000	24500	600	39900	525	56700	0.00462	19200	24700	11450	0.25565	7.7E-05	0.00268	0.0678	0.00954	0.00614	0.03305	0.09307	0.42244	0.42986	1.3203	
2850000	23500	600	39900	525	56700	0.00462	19200	24700	11450	0.25033	0.00015	0.00271	0.06782	0.00953	0.00607	0.03301	0.09368	0.44387	0.42901	1.3362	
2850000	24000	600	39900	525	56700	0.00462	19200	24700	11450	0.23939	0.00041	0.00274	0.0675	0.00929	0.00587	0.0327	0.09541	0.45389	0.42964	1.33685	Base B3
2820000	24500	600	39900	525	56700	0.00462	19200	24700	11450	0.2576	6.1E-05	0.00269	0.06801	0.00921	0.00561	0.03294	0.09288	0.40965	0.43048	1.30914	
2820000	24500	590	39900	525	56700	0.00462	19200	24700	11450	0.25788	8.4E-05	0.00284	0.06805	0.00916	0.00592	0.03311	0.09383	0.40039	0.43431	1.30556	

TABLE 13 (cont). Hooke-Jeeves Searches - Initial Optimization

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

RC #1	AE #1	RC #2	AE #2	RC #3	AE #3	RC #4	AE #4	RC#5/10	AE #5	Coal FD	C Conv	H2	CO	CO2	CH4	RG Mas	RG H2	RG Te	Stm Util	P Index	
										Normalized Errors				Normalized Errors			Normalized Errors				
2820000	24500	610	39900	525	56700	0.00462	19200	24700	11450	0.25805	8E-05	0.00259	0.06776	0.00951	0.00588	0.03281	0.09296	0.44363	0.42628	1.33956	
2820000	24500	590	39500	525	56700	0.00462	19200	24700	11450	0.22466	7.2E-05	0.00212	0.06841	0.00802	0.00581	0.02941	0.09059	0.47699	0.40208	1.30815	
2820000	24500	590	41300	525	56700	0.00462	19200	24700	11450	0.46153	6.5E-05	0.0042	0.0683	0.01814	0.01336	0.05484	0.10565	0.1123	0.592	1.43039	wrong value
2820000	24500	590	40300	525	56700	0.00462	19200	24700	11450	0.30159	6.9E-05	0.00328	0.06722	0.01198	0.00694	0.03878	0.09608	0.37252	0.46792	1.36638	
2820000	24500	590	39900	530	56700	0.00462	19200	24700	11450	0.25788	8.4E-05	0.00284	0.06805	0.00916	0.00592	0.03311	0.09383	0.40042	0.43431	1.3056	
2820000	24500	590	39900	515	56700	0.00462	19200	24700	11450	0.25788	8.4E-05	0.00284	0.06805	0.00916	0.00592	0.03311	0.09383	0.40033	0.43432	1.30552	
2820000	24500	590	39900	515	56100	0.00462	19200	24700	11450	0.25786	8.4E-05	0.00284	0.06806	0.00917	0.00593	0.03312	0.09382	0.40107	0.43428	1.30622	
2820000	24500	590	39900	515	57300	0.00462	19200	24700	11450	0.25789	8.4E-05	0.00284	0.06805	0.00915	0.00592	0.0331	0.09383	0.39975	0.43435	1.30497	
2820000	24500	590	39900	515	57300	0.00466	19200	24700	11450	0.25369	8.2E-05	0.00316	0.06753	0.0092	0.0053	0.03276	0.09411	0.40049	0.43301	1.29932	
2820000	24500	590	39900	515	57300	0.00466	19000	24700	11450	0.20932	5.2E-05	0.00819	0.06137	0.01054	0.00902	0.02982	0.0962	0.46929	0.41447	1.30829	
2820000	24500	590	39900	515	57300	0.00466	19400	24700	11450	0.30548	6.3E-05	0.00102	0.07344	0.00932	0.02479	0.03696	0.09024	0.39894	0.44602	1.38628	
2820000	24500	590	39900	515	57300	0.00466	19200	24400	11450	0.25372	7.5E-05	0.00306	0.06733	0.00951	0.00527	0.03302	0.09382	0.41708	0.43183	1.3147	
2820000	24500	590	39900	515	57300	0.00466	19200	25000	11450	0.25323	7.4E-05	0.00306	0.06738	0.0095	0.00527	0.03293	0.09398	0.41108	0.43217	1.30868	
2820000	24500	590	39900	515	57300	0.00466	19200	24700	11350	0.25662	5.7E-05	0.00308	0.06809	0.00917	0.00398	0.0322	0.09438	0.33812	0.43551	1.2412	Base B4
2760000	24500	590	39900	515	57300	0.00466	19200	24700	11350	0.25654	5.3E-05	0.003	0.06733	0.00988	0.00516	0.03324	0.09315	0.42203	0.43075	1.32112	Pattern move
2880000	24500	590	39900	515	57300	0.00466	19200	24700	11350	0.25664	5.9E-05	0.00308	0.0681	0.00915	0.00391	0.03222	0.09433	0.34007	0.43541	1.24296	
2820000	25500	590	39900	515	57300	0.00466	19200	24700	11350	0.25766	5.7E-05	0.00299	0.06733	0.00962	0.00515	0.03308	0.09343	0.40258	0.43236	1.30425	
2820000	23500	590	39900	515	57300	0.00466	19200	24700	11350	0.25521	7E-05	0.00307	0.06789	0.00963	0.00433	0.03276	0.09371	0.39201	0.43216	1.29084	
2820000	24500	580	39900	515	57300	0.00466	19200	24700	11350	0.25655	7.4E-05	0.0031	0.06718	0.00986	0.0054	0.0337	0.09378	0.43621	0.43337	1.33923	
2820000	24500	610	39900	515	57300	0.00466	19200	24700	11350	0.24493	6E-05	0.0029	0.06338	0.00964	0.00554	0.03346	0.09238	0.51701	0.42108	1.39039	
2820000	24500	590	39900	535	57300	0.00466	19200	24700	11350	0.24684	0.00023	0.00307	0.06761	0.00936	0.004	0.03248	0.09515	0.39366	0.43311	1.28552	
2820000	24500	590	39900	495	57300	0.00466	19200	24700	11350	0.24684	0.00023	0.00307	0.06761	0.00936	0.004	0.03248	0.09516	0.3935	0.43311	1.28537	
2820000	24500	590	39900	515	58500	0.00466	19200	24700	11350	0.24687	0.00023	0.00307	0.06761	0.00935	0.004	0.03247	0.09516	0.39276	0.43315	1.28468	
2820000	24500	590	39900	515	56100	0.00466	19200	24700	11350	0.24679	0.00023	0.00307	0.06762	0.00937	0.00401	0.03249	0.09514	0.39493	0.43304	1.2867	
2820000	24500	590	39900	515	57300	0.00462	19200	24700	11350	0.25159	0.00025	0.00272	0.06809	0.00951	0.00475	0.03303	0.09455	0.40826	0.43356	1.30631	
2820000	24500	590	39900	515	57300	0.0047	19200	24700	11350	0.24364	0.0002	0.00341	0.06722	0.00933	0.00348	0.0321	0.09544	0.38999	0.43207	1.27688	
2820000	24500	590	39900	515	57300	0.00466	19200	24700	11150	0.24761	0.00018	0.00398	0.06953	0.00691	0.00834	0.03077	0.09731	0.3304	0.44237	1.23741	
2820000	24500	590	39900	515	57300	0.00466	19200	24700	11350	0.24684	0.00023	0.00307	0.06761	0.00936	0.004	0.03248	0.09516	0.39358	0.43311	1.28544	B4 (Diff Tol Spec)
2820000	24500	590	39900	495	58500	0.0047	19200	24700	11150	0.24207	0.00028	0.00314	0.06049	0.01054	0.0045	0.03561	0.09327	0.58524	0.4226	1.45775	
2820000	24500	590	39900	495	58500	0.00466	19200	24700	11350	0.24687	0.00023	0.00307	0.06761	0.00935	0.004	0.03247	0.09516	0.39271	0.43316	1.28463	
2820000	24500	590	39900	495	58500	0.00462	19200	24700	11350	0.25162	0.00025	0.00271	0.06806	0.00958	0.00477	0.03307	0.0945	0.41079	0.43336	1.30871	
2820000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.24768	0.00018	0.00398	0.06953	0.0069	0.00835	0.03076	0.09732	0.32953	0.44243	1.23666	Base B5
+/-30000	+/-500	+/-10	+/-400	+/-10	+/-600	+/-4E-5	+/-200	+/-300	+/-100												
																					HOOKE
2820000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.25783	0.00019	0.00333	0.0690	0.01013	0.00516	0.0344	0.09263	0.40283	0.43074	1.30715	Base B5
2850000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.26172	0.00013	0.00333	0.07073	0.01013	0.00512	0.03328	0.09364	0.29615	0.43655	1.21078	Base B6
2850000	24000	590	39900	495	58500	0.00466	19200	24700	11150	0.26254	0.00024	0.00431	0.07248	0.00742	0.00812	0.0318	0.09477	0.29366	0.4429	1.21823	
2850000	25000	590	39900	495	58500	0.00466	19200	24700	11150	0.25763	0.0002	0.00426	0.07197	0.00746	0.00839	0.03218	0.0952	0.31847	0.44184	1.23762	
2850000	24500	580	39900	495	58500	0.00466	19200	24700	11150	0.26552	9.7E-05	0.00334	0.0702	0.01062	0.00537	0.03494	0.09229	0.38788	0.43359	1.30385	

TABLE 13 (cont). Hooke-Jeeves Searches - Initial Optimization

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

											Normalized Errors			Normalized Errors			Normalized Errors				
RC #1	AE #1	RC #2	AE #2	RC #3	AE #3	RC #4	AE #4	RC#5/10	AE #5	Coal FD	C Conv	H2	CO	CO2	CH4	RG Mas	RG H2	RG Te	Stm Util	P Index	
2850000	24500	600	39900	495	58500	0.00466	19200	24700	11150	0.25686	0.00017	0.00326	0.06988	0.01019	0.00563	0.03449	0.09146	0.44168	0.42571	1.33932	
2850000	24500	590	39500	495	58500	0.00466	19200	24700	11150	0.221	0.00027	0.00264	0.07054	0.0086	0.00509	0.03022	0.09034	0.46271	0.40006	1.29145	
2850000	24500	590	40300	495	58500	0.00466	19200	24700	11150	0.30954	7.1E-05	0.0039	0.06951	0.01279	0.00593	0.03995	0.0943	0.33478	0.46613	1.3369	
2850000	24500	590	39900	485	58500	0.00466	19200	24700	11150	0.25785	0.0002	0.00337	0.07063	0.00995	0.00517	0.03318	0.09419	0.30217	0.43661	1.21333	
2850000	24500	590	39900	505	58500	0.00466	19200	24700	11150	0.25785	0.0002	0.00337	0.07063	0.00995	0.00518	0.03318	0.09419	0.3022	0.43661	1.21336	
2850000	24500	590	39900	495	57900	0.00466	19200	24700	11150	0.25785	0.0002	0.00337	0.07063	0.00995	0.00517	0.03318	0.09419	0.30211	0.43661	1.21326	
2850000	24500	590	39900	495	59100	0.00466	19200	24700	11150	0.25703	0.00022	0.00337	0.07058	0.00999	0.00517	0.03321	0.09426	0.30003	0.43641	1.21626	
2850000	24500	590	39900	495	58500	0.00462	19200	24700	11150	0.26308	0.0002	0.00304	0.07058	0.01002	0.00592	0.03473	0.0923	0.39561	0.43215	1.30763	
2850000	24500	590	39900	495	58500	0.0047	19200	24700	11150	0.25223	0.00024	0.00372	0.06934	0.01003	0.00485	0.03391	0.09318	0.39715	0.42995	1.2946	
2850000	24500	590	39900	495	58500	0.00466	19400	24700	11150	0.30935	0.00021	0.00116	0.07629	0.00936	0.02231	0.03797	0.03965	0.35449	0.44696	1.34775	
2850000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.26172	0.00013	0.00333	0.07073	0.01013	0.00512	0.03328	0.09364	0.29615	0.43655	1.21078	Base B6 Hooke
2850000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.24358	0.0004	0.00404	0.0693	0.00674	0.00864	0.03067	0.09773	0.35459	0.44207	1.25775	Case-Study
2880000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.24568	0.00033	0.00404	0.0694	0.00673	0.00868	0.03067	0.09747	0.3506	0.44231	1.25591	Temporary Head
2910000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.24361	0.0004	0.00404	0.0694	0.00679	0.00872	0.0304	0.09806	0.33211	0.44337	1.23689	
										Temperatures are abnormal??											
2850000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.26362	9.7E-05	0.00333	0.07085	0.0101	0.00508	0.03316	0.09356	0.28082	0.43736	1.19799	Hooke
2850000	24500	590	39900	495	58500	0.00466	19200	24700	11150	0.24467	0.00038	0.00404	0.06949	0.00672	0.00862	0.03027	0.09813	0.31691	0.44409	1.22329	Case

TABLE 13 (cont). Hooke-Jeeves Searches - Initial Optimization

*These runs were made after adjusting plant data.

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

Weighted Fractional Errors Weighted Fractional Errors

RC #1	AE #1	RC #2	AE #2	RC #3	AE #3	RC #4	AE #4	RC#5/10	AE #5	Coal FD	C Conv	H2	CO	CO2	CH4	RG Mas	RG H2	RG Te	Stm Util	P Index	
+/-90000	+/-500	+/-20	+/-600	+/-15	+/-1000	+/-14E-5	+/-400	+/-900	+/-250												
2850000	24500	590	39900	495	58500	0.00466	19200	24700	11150	-0.7457	-0.0053	-0.0077	-0.1126	0.0745	-0.0389	-0.1219	0.21235	-1.0948	-0.567	2.98162	Base B6
2850000	24500	590	39900	495	58500	0.00466	19200	25000	11150	-0.7467	-0.0053	-0.0083	-0.1106	0.07389	-0.038	-0.1219	0.21255	-1.0923	-0.5674	2.97691	
2850000	24500	590	39900	495	58500	0.0047	19200	25000	11150	-0.7027	-0.0086	-0.0125	-0.0638	0.05434	-0.0331	-0.1194	0.21484	-1.0913	-0.5609	2.86147	
2850000	24500	590	39900	510	58500	0.0047	19200	25000	11150	-0.7027	-0.0086	-0.0125	-0.0638	0.05434	-0.0331	-0.1194	0.21484	-1.0914	-0.5609	2.86153	
2850000	24500	600	39900	510	58500	0.0047	19200	25000	11150	-0.6858	-0.0083	-0.0114	-0.0413	0.04411	-0.0376	-0.118	0.21422	-1.098	-0.5554	2.81433	
2950000	24500	600	39900	510	58500	0.0047	19200	25000	11150	-0.6815	-0.0125	-0.0113	-0.0407	0.04487	-0.0395	-0.1182	0.21428	-1.1327	-0.5545	2.85004	
2750000	24500	600	39900	510	58500	0.0047	19200	25000	11150	-0.6865	-0.0088	-0.0117	-0.0417	0.04325	-0.0355	-0.1177	0.21452	-1.0723	-0.5562	2.78804	
2650000	24500	610	39900	525	58500	0.00474	19200	25300	11150	-0.6789	-0.0038	-0.015	-0.0411	0.04302	-0.0245	-0.1167	0.21373	-1.0783	-0.5527	2.7677	Base B7
2650000	24500	610	39900	525	58500	0.00474	19200	25800	11150	-0.659	-0.0087	-0.0149	-0.018	0.03324	-0.0285	-0.1157	0.21469	-1.0876	-0.5496	2.7299	
2650000	24500	610	39900	525	58500	0.00474	19200	25800	11400	-0.6551	-0.0125	-0.0146	-0.0171	0.03392	-0.0308	-0.116	0.21477	-1.1225	-0.5488	2.76618	
2650000	24500	610	39900	525	58500	0.00474	19200	25800	10900	-0.6632	-0.0047	-0.0149	-0.0185	0.03327	-0.0281	-0.1157	0.21422	-1.0729	-0.5498	2.71528	
2650000	24500	610	39900	525	58500	0.00474	19000	25800	10900	-0.5877	0.00367	-0.061	0.01077	0.0342	0.08734	-0.1105	0.21365	-1.1879	-0.5298	2.82647	
2650000	24500	610	39900	525	58500	0.00474	19400	25800	10900	-0.7501	-0.0048	0.03311	-0.0329	0.03038	-0.1565	-0.1215	0.20961	-1.027	-0.5625	2.9285	
2650000	24500	610	39900	525	58800	0.00474	19200	25800	10900	-0.6632	-0.0047	-0.0149	-0.0185	0.03327	-0.0281	-0.1157	0.21422	-1.0726	-0.5498	2.71507	
2650000	24500	610	39600	525	58800	0.00474	19200	25800	10900	-0.6129	-0.0049	-0.0088	-0.0229	0.02498	-0.0219	-0.1104	0.21157	-1.1185	-0.532	2.66887	Base B8
2650000	24800	610	39600	525	58800	0.00474	19200	25800	10900	-0.6074	-0.0081	-0.0074	-0.0203	0.02949	-0.0343	-0.1121	0.21009	-1.2577	-0.5278	2.81467	
2650000	24200	610	39600	525	58800	0.00474	19200	25800	10900	-0.6153	-0.0049	-0.0078	-0.021	0.02904	-0.0319	-0.1118	0.20936	-1.2248	-0.5283	2.78413	
2650000	24200	610	39300	525	59100	0.00474	19200	26300	10650	-0.5689	-0.0072	-0.0004	-0.0251	0.02216	-0.0325	-0.1074	0.20673	-1.2867	-0.5115	2.76868	T. Head
2650000	24200	610	39300	525	59100	0.00474	19200	26800	10650	-0.5599	-0.0134	9E-05	-0.0309	0.02597	-0.0346	-0.1079	0.20713	-1.3456	-0.5101	2.83565	
2650000	24200	610	39300	525	59100	0.00474	19200	25800	10650	-0.5769	-0.0048	0.00022	-0.0377	0.02874	-0.0338	-0.1082	0.20556	-1.3201	-0.5112	2.82736	
2650000	24200	610	39300	525	59100	0.00478	19200	26300	10650	-0.5785	-0.0061	-0.0057	-0.0474	0.03024	-0.0114	-0.1071	0.20729	-1.2389	-0.515	2.74778	
2650000	24200	610	39000	525	59100	0.00478	19200	26300	10650	-0.5463	-0.0041	0.00324	-0.0408	0.02068	-0.0218	-0.1032	0.20227	-1.299	-0.4972	2.73851	
2650000	23900	610	39000	525	59100	0.00478	19200	26300	10650	-0.5368	-0.0101	0.00381	-0.0391	0.02305	-0.0278	-0.1041	0.20219	-1.3764	-0.4946	2.81798	
2650000	24500	610	39000	525	59100	0.00478	19200	26300	10650	-0.5468	-0.0047	0.00428	-0.0499	0.02701	-0.0271	-0.1046	0.20253	-1.3574	-0.4978	2.82213	
2700000	24200	610	39000	525	59100	0.00478	19200	26300	10650	-0.5455	-0.0041	0.00213	-0.0523	0.02126	-0.0111	-0.1024	0.20529	-1.2147	-0.5029	2.66181	Base B9
2700000	24200	620	39000	525	59100	0.00478	19200	26300	10650	-0.5332	-0.0106	0.0045	-0.0502	0.02488	-0.0239	-0.1037	0.20396	-1.3512	-0.4972	2.80334	
2700000	24200	600	39000	525	59100	0.00478	19200	26300	10650	-0.5199	-0.0119	0.00085	-0.052	0.02109	-0.008	-0.1025	0.20948	-1.2478	-0.5047	2.6781	
2700000	24200	610	39000	535	59100	0.00478	19200	26300	10650	-0.5455	-0.0041	0.00213	-0.0523	0.02126	-0.0111	-0.1024	0.20529	-1.2147	-0.5029	2.66179	
2700000	24200	610	39000	525	59300	0.00478	19200	26300	10650	-0.5455	-0.0041	0.00213	-0.0523	0.02126	-0.0111	-0.1024	0.20529	-1.2146	-0.5029	2.66174	
2700000	24200	610	39000	525	59100	0.00478	19400	26300	10650	-0.65	0.00559	0.05702	-0.0584	0.01746	-0.1647	-0.1098	0.19707	-1.2285	-0.5129	3.00141	
2700000	24200	610	39000	525	59100	0.00478	19100	26300	10650	-0.4934	-0.0048	-0.0236	-0.0317	0.02256	0.049	-0.1	0.20475	-1.3396	-0.4888	2.75823	
2700000	24200	610	39000	525	59100	0.00478	19200	26300	10800	-0.5373	-0.0101	0.00216	-0.0517	0.02141	-0.0118	-0.1025	0.20612	-1.2412	-0.5025	2.68681	
2700000	24200	610	39000	525	59100	0.00478	19200	26300	10500	-0.5441	0.00172	0.00251	-0.0523	0.02288	-0.0144	-0.103	0.20493	-1.2512	-0.5018	2.69887	

TABLE 14. Hooke-Jeeves Searches - Weight Adjustments

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

Normalized Errors Normalized Errors Normalized Errors

RC #1	AE #1	RC #	AE #2	RC #	AE #3	RC #4	AE #4	RC#5/1	AE #5	Coal F	C Con	H2	CO	CO2	CH4	RG Ma	RG H2	RG Te	Stm Util	P Index	
+/-5000	+/-500	+/-10	+/-800	+/-10	+/-1000	+/-5E-5	+/-400	+/-500	+/-200	10	10	10	10	10	10	10	10				
2800000	25000	600	40000	520	57000	0.00465	19200	24500	11400	0.25927	0.00013	0.00606	0.13376	0.02645	0.01206	0.34409	0.31292	0	0	1.08875	Base A1
2850000	25000	600	40000	520	57000	0.00465	19200	24500	11400	0.25779	0.00017	0.00617	0.13395	0.0196	0.01114	0.34212	0.31413	0	0	1.08506	
2850000	25500	600	40000	520	57000	0.00465	19200	24500	11400	0.25181	0.00027	0.00601	0.13396	0.01976	0.01046	0.33748	0.31886	0	0	1.07864	
2850000	25500	590	40000	520	57000	0.00465	19200	24500	11400	0.25686	0.00028	0.00614	0.1343	0.01989	0.00979	0.34003	0.31955	0	0	1.08683	
2850000	25500	610	40000	520	57000	0.00465	19200	24500	11400	0.25735	0.00011	0.00592	0.13403	0.01972	0.01188	0.33746	0.31302	0	0	1.0795	
2850000	25500	600	39200	520	57000	0.00465	19200	24500	11400	0.19675	0.0002	0.00371	0.1364	0.01342	0.01121	0.26353	0.29808	0	0	0.92328	
2850000	25500	600	39200	530	57000	0.00465	19200	24500	11400	0.19675	0.0002	0.00371	0.1364	0.01342	0.01121	0.26354	0.29807	0	0	0.9233	
2850000	25500	600	39200	510	57000	0.00465	19200	24500	11400	0.19675	0.0002	0.00371	0.1364	0.01341	0.0112	0.26353	0.29808	0	0	0.92328	
2850000	25500	600	39200	510	56000	0.00465	19200	24500	11400	0.19674	0.0002	0.00346	0.1357	0.01517	0.01223	0.27032	0.29546	0	0	0.92928	
2850000	25500	600	39200	510	58000	0.00465	19200	24500	11400	0.19675	0.0002	0.00371	0.13639	0.0134	0.0112	0.26344	0.2981	0	0	0.92318	
2850000	25500	600	39200	510	58000	0.0047	19200	24500	11400	0.19283	0.00014	0.00424	0.13498	0.01421	0.00946	0.26246	0.29747	0	0	0.91578	
2850000	25500	600	39200	510	58000	0.0047	19600	24500	11400	0.29537	0.00013	0.00757	0.16279	0.01269	0.14908	0.33921	0.27574	0	0	1.24256	
2850000	25500	600	39200	510	58000	0.0047	18800	24500	11400	0.10948	0.00013	0.03097	0.10924	0.01623	0.09036	0.19454	0.31853	0	0	0.86949	
2850000	25500	600	39200	510	58000	0.0047	18800	25000	11400	0.10401	0.0003	0.03052	0.09389	0.01466	0.08092	0.1962	0.32227	0	0	0.84275	
2850000	25500	600	39200	510	58000	0.0047	18800	25000	11200	0.10645	0.0002	0.02816	0.07645	0.01274	0.04748	0.21282	0.31745	0	0	0.80177	Base A2
2900000	26000	600	38400	500	59000	0.00475	18400	25500	11000	0.02194	0.00016	0.08759	0.08403	0.01282	0.45234	0.08899	0.33124	0	0	1.07912	Temporary Head
2950000	26000	600	38400	500	59000	0.00475	18400	25500	11000	0.02121	0.0002	0.08752	0.0836	0.01358	0.44431	0.09069	0.33052	0	0	1.07162	
2950000	26500	600	38400	500	59000	0.00475	18400	25500	11000	0.02197	0.00023	0.08678	0.08328	0.01383	0.43683	0.09044	0.33114	0	0	1.06448	
2950000	26500	610	38400	500	59000	0.00475	18400	25500	11000	0.02223	0.00013	0.08679	0.08284	0.0131	0.44324	0.08991	0.32819	0	0	1.06643	
2950000	26500	590	38400	500	59000	0.00475	18400	25500	11000	0.02367	0,00012	0.0872	0.08304	0.01351	0.44133	0.09314	0.32843	0	0	1.07044	
2950000	26500	600	37600	500	59000	0.00475	18400	25500	11000	0.01466	8.9E-05	0.08043	0.08143	0.01039	0.43348	0.06948	0.31979	0	0	1.00974	
2950000	26500	600	37600	510	59000	0.00475	18400	25500	11000	0.01466	8.9E-05	0.08043	0.08143	0.01039	0.43347	0.06947	0.31978	0	0	1.00972	
2950000	26500	600	37600	500	60000	0.00475	18400	25500	11000	0.01467	8.7E-05	0.08043	0.08143	0.01039	0.43355	0.06937	0.31989	0	0	1.0098	
2950000	26500	600	37600	510	60000	0.00475	18400	25500	11000	0.01467	8.8E-05	0.08043	0.08143	0.01039	0.43353	0.06937	0.31988	0	0	1.00978	
2950000	26500	600	37600	500	58000	0.00475	18400	25500	11000	0.01464	9.1E-05	0.08044	0.08147	0.01034	0.43414	0.06939	0.3199	0	0	1.01042	
2950000	26500	600	37600	500	59000	0.0048	18400	25500	11000	0.01292	0.00013	0.08455	0.0795	0.01063	0.45743	0.0683	0.32074	0	0	1.03419	
2950000	26500	600	37600	500	59000	0.0047	18400	25500	11000	0.01605	0.00013	0.07663	0.08285	0.00961	0.41643	0.07088	0.3208	0	0	0.99339	
2950000	26500	600	37600	500	59000	0.0047	18000	25500	11000	0.0038	0.00017	0.17076	0.06027	0.01251	1.02119	0.0313	0.34455	0	0	1.64456	
2950000	26500	600	37600	500	59000	0.0047	18800	25500	11000	0.06793	0.00015	0.01986	0.10753	0.00878	0.0707	0.13285	0.29589	0	0	0.70369	
2950000	26500	600	37600	500	59000	0.0047	18800	25000	11000	0.06732	0.00019	0.01996	0.10816	0.00828	0.07387	0.13024	0.29793	0	0	0.70596	
2950000	26500	600	37600	500	59000	0.0047	18800	26000	11000	0.06754	0.00016	0.0199	0.10789	0.00868	0.07136	0.12975	0.29805	0	0	0.70333	
2950000	26500	600	37600	500	59000	0.0047	18800	26000	11200	0.06718	0.00018	0.01972	0.10749	0.00906	0.06885	0.13282	0.29672	0	0	0.70202	Base A3
3050000	27500	600	36000	490	60000	0.0047	18800	27000	11200	0.06999	0.00026	0.01189	0.10276	0.00598	0.03645	0.12785	0.28954	0	0	0.64473	Temporary Head
3100000	27500	600	36000	490	60000	0.0047	18800	27000	11200	0.07232	0.00012	0.0119	0.10246	0.00563	0.03818	0.13274	0.28583	0	0	0.64918	
3000000	27500	600	36000	490	60000	0.0047	18800	27000	11200	0.07304	0.00014	0.01184	0.10284	0.00589	0.03689	0.12947	0.28674	0	0	0.64685	
3050000	28000	600	36000	490	60000	0.0047	18800	27000	11200	0.07485	0.00013	0.01154	0.10265	0.00554	0.036	0.12715	0.2872	0	0	0.64507	
3050000	27000	600	36000	490	60000	0.0047	18800	27000	11200	0.07334	0.00012	0.0121	0.10389	0.00592	0.03843	0.1273	0.28714	0	0	0.64823	

TABLE 14 (cont). Hooke-Jeeves Searches - Weight Adjustments

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

Normalized Errors Normalized Errors Normalized Errors

RC #1	AE #1	RC #	AE #2	RC #	AE #3	RC #4	AE #4	RC#5/1	AE #5	Coal F	C Con	H2	CO	CO2	CH4	RG Ma	RG H2	RG Te	Stm Util	P Index	
+/-5000	+/-500	+/-10	+/-800	+/-10	+/-1000	+/-5E-5	+/-400	+/-500	+/-200	10	10	10	10	10	10	10	10				
3050000	27500	610	36000	490	60000	0.0047	18800	27000	11200	0.07296	0.00018	0.01204	0.10386	0.00512	0.0411	0.12273	0.29058	0	0	0.64857	
3050000	27500	590	36000	490	60000	0.0047	18800	27000	11200	0.07407	0.00013	0.01183	0.10318	0.00594	0.03648	0.12854	0.28609	0	0	0.64625	
3050000	27500	600	35200	490	60000	0.0047	18800	27000	11200	0.07602	0.00019	0.00966	0.1008	0.00507	0.02744	0.13047	0.28701	0	0	0.63665	A3b
3050000	27500	600	35200	500	60000	0.0047	18800	27000	11200	0.07602	0.00019	0.00966	0.1008	0.00507	0.02744	0.13047	0.28701	0	0	0.63665	
3050000	27500	600	35200	510	60000	0.0047	18800	27000	11200	0.07602	0.00019	0.00966	0.1308	0.00507	0.02744	0.13047	0.28701	0	0	0.63665	
3050000	27500	600	35200	550	60000	0.0047	18800	27000	11200	0.07602	0.00019	0.00966	0.1008	0.00507	0.02744	0.13048	0.287	0	0	0.63666	
3050000	27500	600	35200	700	60000	0.0047	18800	27000	11200	0.07602	0.00019	0.00966	0.10081	0.00507	0.02743	0.13048	0.287	0	0	0.63666	
3050000	27500	600	35200	350	60000	0.0047	18800	27000	11200	0.07602	0.00019	0.00966	0.10079	0.00507	0.02744	0.13045	0.28701	0	0	0.63662	
3050000	27500	600	35200	100	60000	0.0047	18800	27000	11200	0.07601	0.00019	0.00966	0.10078	0.00507	0.02744	0.13045	0.28701	0	0	0.6366	
3050000	27500	600	35200	490	60000	0.0047	18800	28000	11200	0.07639	0.00019	0.00954	0.10083	0.00521	0.02615	0.12999	0.28718	0	0	0.6355	
3050000	27500	600	35200	490	60000	0.0047	18800	28000	10800	0.07727	0.00014	0.00976	0.10116	0.00504	0.02801	0.12949	0.28642	0	0	0.63729	
3050000	27500	600	35200	490	60000	0.0047	18800	28000	11400	0.07528	0.0002	0.00965	0.10078	0.00521	0.02692	0.12966	0.28822	0	0	0.63591	
3050000	27500	600	35200	490	61000	0.0047	18800	28000	11200	0.07639	0.00019	0.00954	0.10063	0.00521	0.02615	0.12996	0.28719	0	0	0.63547	
3050000	27500	600	35200	490	61000	0.00475	18800	28000	11200	0.07219	0.00018	0.01092	0.09955	0.00514	0.0329	0.12481	0.28888	0	0	0.63457	Base A4
3050000	27500	600	35200	490	61000	0.00475	19200	28000	11200	0.17217	0.00013	0.00394	0.12655	0.00433	0.05728	0.2092	0.26609	0	0	0.83966	
3050000	27500	600	35200	490	61000	0.00475	18400	28000	11200	**error** Does not complete simulation. No errors reported. See Runid FAULT.											
3150000	28500	600	32800	480	63000	0.0048	18800	30000	11200	0.01505	0.00024	0.02038	0.03637	0.48826	2.35165	1.80626	0.07083	0	0	4.78904	Temporary Head
Severe Error Tempeerature Too Low for Devolatilization. RG Temp = 345 F.									**Severe Error** Tempeerature Too Low for Devolatilization. RG Temp = 345 F.										Decrease Increments.		
+/-20000	+/-200	+/-5	+/-600	+/-5	+/-500	+/-2E-5	+/-200	+/-200	+/-100												
3100000	28000	600	34000	485	62000	0.00477	18800	29000	11200	0.07837	0.00013	0.00876	0.09448	0.0043	0.02316	0.12929	0.28424	0	0	0.62271	Temporary Head
3100000	28000	600	34000	485	62000	0.00477	18800	29000	11200	0.07837	0.00013	0.00876	0.09448	0.0043	0.02316	0.12929	0.28424	0	0	0.62271	Temp Head(tol=.001)
3120000	28000	600	34000	485	62000	0.00477	18800	29000	11200	0.07936	9.2E-05	0.00878	0.09434	0.00436	0.02324	0.13142	0.28211	0	0	0.62371	
3080000	28000	600	34000	485	62000	0.00477	18800	29000	11200	0.07882	0.00012	0.00868	0.09434	0.00429	0.02286	0.13028	0.28298	0	0	0.62238	
3080000	27800	600	34000	485	62000	0.00477	18800	29000	11200	0.07875	9.7E-05	0.00879	0.09471	0.00454	0.02254	0.12992	0.28347	0	0	0.62281	
3080000	28200	600	34000	485	62000	0.00477	18800	29000	11200	0.07639	0.0002	0.00875	0.09416	0.00403	0.02379	0.12873	0.28544	0	0	0.62199	
3080000	28200	595	34000	485	62000	0.00477	18800	29000	11200	0.07814	0.00015	0.00869	0.09431	0.00414	0.02309	0.12813	0.28483	0	0	0.62148	
3080000	28200	595	34600	485	62000	0.00477	18800	29000	11200	0.07785	0.0001	0.00976	0.09617	0.00448	0.02829	0.12917	0.2834	0	0	0.62921	
3080000	28200	595	33400	485	62000	0.00477	18800	29000	11200	0.0308	0.00017	0.01971	0.04534	0.4911	2.33491	1.22813	0.14456	0	0	4.29471	
3080000	28200	595	34000	480	62000	0.00477	18800	29000	11200	0.07814	0.00015	0.00869	0.09431	0.00414	0.02309	0.12813	0.28483	0	0	0.62148	
3080000	28200	595	34000	480	62500	0.00477	18800	29000	11200	0.07814	0.00015	0.00869	0.09431	0.00414	0.02309	0.12813	0.28483	0	0	0.62149	
3080000	28200	595	34000	480	61500	0.00477	18800	29000	11200	0.07814	0.00015	0.00869	0.09432	0.00414	0.02309	0.12814	0.28483	0	0	0.6215	
3080000	28200	595	34000	480	62000	0.00479	18800	29000	11200	0.07714	0.00012	0.00921	0.09368	0.00408	0.02587	0.12797	0.28389	0	0	0.62197	
3080000	28200	595	34000	480	62000	0.00475	18800	29000	11200	0.0817	0.0001	0.00792	0.09472	0.00443	0.01886	0.13234	0.28213	0	0	0.62222	
3080000	28200	595	34000	480	62000	0.00477	19000	29000	11200	0.12607	0.00013	0.00227	0.10709	0.00391	0.0133	0.16986	0.27393	0	0	0.69655	
3080000	28200	595	34000	480	62000	0.00477	18600	29000	11200	0.04244	8.8E-05	0.02516	0.0815	0.00452	0.11042	0.09365	0.29329	0	0	0.65107	
3080000	28200	595	34000	480	62000	0.00477	18800	29200	11200	0.0793	0.00012	0.00872	0.0941	0.00406	0.02357	0.12931	0.2834	0	0	0.62258	
3080000	28200	595	34000	480	62000	0.00477	18800	28800	11200	0.08009	9.8E-05	0.0087	0.09407	0.00417	0.02314	0.12932	0.28296	0	0	0.62254	
3080000	28200	595	34000	480	62000	0.00477	18800	29000	11100	0.07731	0.00017	0.00877	0.09409	0.00409	0.02359	0.12954	0.28456	0	0	0.62212	
3080000	28200	595	34000	480	62000	0.00477	18800	29000	11300	0.08052	8.8E-05	0.00868	0.09417	0.004	0.02361	0.12853	0.28339	0	0	0.62298	
3080000	28200	595	34000	480	62000	0.00477	18800	29000	11200	0.07814	0.00015	0.00869	0.09431	0.00414	0.02309	0.12813	0.28483	0	0	0.62148	Base A5

TABLE 14 (cont). Hooke-Jeeves Searches - Weight Adjustments, Wet Basis

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

											Percentage Error			Percentage Error		Percentage Error						
RC #1	AE #1	RC #	AE #2	RC #	AE #3	RC #4	AE #4	RC#5/1	AE #5	Coal F	C Con	H2	CO	CO2	CH4	RG Ma	RG H2	RG Te	Stm Util	Index		
3000000	27000	605	33600	475	63000	0.00479	18800	20500	12400	-4.2654	0.12825	-7.3131	-10.602	-5.7164	-5.7696	-9.4087	8.79324	-7.1149	-14.409	42.4592	Base C1	38.1938
3000000	27000	605	33600	475	63000	0.00479	18800	21500	12400	-4.2577	0.12815	-7.316	-10.602	-5.7137	-5.7688	-9.4117	8.79422	-7.1878	-14.4	42.4528		
3000000	27000	605	33600	475	63000	0.0048	18800	21500	12400	-4.187	0.0972	-7.3602	-10.578	-5.6918	-6.0313	-9.5767	8.86363	-9.1211	-14.223	42.7119		
3000000	27000	605	33600	475	63000	0.00465	18800	21500	12400	-4.7587	0.18997	-6.466	-9.8735	-6.2859	-6.082	-8.6019	8.4053	3.80475	-15.209	41.8713		
3000000	27000	625	33600	475	63000	0.00465	18800	21500	12400	-4.6426	0.07026	-6.4882	-9.877	-6.3008	-6.2492	-8.6768	8.45725	2.60847	-15.136	42.0151		
3000000	27000	585	33600	475	63000	0.00465	18800	21500	12400	-4.7737	0.1964	-6.4762	-9.8641	-6.2734	-6.0668	-8.6133	8.40328	3.67045	-15.188	41.8574		
3000000	27000	585	33600	500	63000	0.00465	18800	21500	12400	-4.7737	0.1964	-6.4762	-9.8641	-6.2734	-6.0668	-8.6133	8.40328	3.67045	-15.188	41.8574	No Effect	
3100000	27000	585	33600	500	63000	0.00465	18800	21500	12400	-4.7765	0.24163	-6.4636	-9.8718	-6.2846	-5.8997	-8.5163	8.36673	4.74773	-15.274	41.6629	Base C2	36.88636
3200000	27000	565	33600	475	63000	0.00451	18800	22500	12400	-5.3599	0.20545	-6.2925	-10.454	-6.3345	-6.655	-8.7486	8.51005	6.80103	-15.768	43.6062	T.Head	
3200000	27000	565	33600	475	63000	0.00451	18800	23500	12400	-5.3533	0.20404	-6.2965	-10.455	-6.3308	-6.6787	-8.7646	8.51625	6.59545	-15.749	43.6304		
3200000	27000	565	33600	475	63000	0.00451	18800	21500	12400	-5.3669	0.20696	-6.3206	-10.457	-6.3127	-7.1237	-9.0091	8.61442	4.16054	-15.571	44.1957		
3200000	27000	565	33600	475	63000	0.00437	18800	22500	12400	-5.6042	0.10564	-6.1096	-10.66	-6.477	-8.216	-9.2727	8.78039	4.01446	-15.787	45.8468		
3200000	27000	565	33600	475	63000	0.00465	18800	22500	12400	-4.9342	0.18012	-6.5701	-10.266	-6.1693	-6.0846	-8.7646	8.49047	3.36901	-15.304	42.5152		
3200000	27000	565	33600	490	63000	0.00465	18800	22500	12400	-4.9342	0.18012	-6.5701	-10.266	-6.1693	-6.0846	-8.7646	8.49047	3.36901	-15.304	42.5152		
3200000	27000	545	33600	475	63000	0.00465	18800	22500	12400	-4.9048	0.16927	-6.581	-10.263	-6.1712	-5.9497	-8.7058	8.47015	3.84504	-15.337	42.3398		
3300000	27000	545	33600	475	63000	0.00465	18800	22500	12400	-4.5828	0.09137	-6.7517	-10.232	-6.124	-7.9596	-9.7868	8.95619	-8.2157	-14.417	44.6065		
3100000	27000	545	33600	475	63000	0.00465	18800	22500	12400	-4.8598	0.11237	-6.5871	-10.255	-6.1784	-5.9098	-8.6821	8.46693	3.86777	-15.341	42.2574	Base C3	37.3976
3100000	27000	505	33600	475	63000	0.00465	18800	23500	12400	-4.7976	0.13016	-6.6227	-10.246	-6.1684	-5.7709	-8.6454	8.45648	3.92025	-15.333	42.062	T.HEAD	
3100000	27000	505	33600	475	63000	0.00465	18800	24500	12400	-4.7924	0.12956	-6.6247	-10.246	-6.1652	-5.7731	-8.6485	8.45715	3.84256	-15.324	42.0582		
3100000	27000	505	33600	490	63000	0.00465	18800	24500	12400	-4.7924	0.12956	-6.6247	-10.246	-6.1652	-5.7731	-8.6485	8.45715	3.84256	-15.324	42.0582		
3100000	27000	505	33600	460	63000	0.00465	18800	24500	12400	-4.7924	0.12956	-6.6247	-10.246	-6.1652	-5.7731	-8.6485	8.45715	3.84256	-15.324	42.0582		
3100000	27000	525	33600	475	63000	0.00465	18800	24500	12400	-4.7785	0.11438	-6.6171	-10.256	-6.1757	-5.8758	-8.6829	8.47775	3.51777	-15.312	42.1809		
3100000	27000	485	33600	475	63000	0.00465	18800	24500	12400	-4.7504	0.10996	-6.6347	-10.237	-6.1712	-5.5312	-8.5339	8.41524	4.80723	-15.393	41.7392		
2100000	27000	485	33600	475	63000	0.00465	18800	24500	12400	-4.8281	0.18977	-6.6364	-10.245	-6.1516	-6.1302	-8.841	8.53086	2.06632	-15.193	42.5218		
3000000	27000	485	33600	475	63000	0.00465	18800	24500	12400	-4.8129	0.16856	-6.624	-10.238	-6.1616	-5.5834	-8.5629	8.41651	4.76446	-15.384	41.8367		
3200000	27000	485	33600	475	63000	0.00465	18800	24500	12400	-4.8743	0.20213	-6.6494	-10.237	-6.1201	-6.076	-8.8509	8.51779	1.95785	-15.16	42.4746		
3100000	27000	485	33600	475	63000	0.00451	18800	24500	12400	-5.2572	0.19359	-6.3864	-10.429	-6.286	-6.8043	-8.9166	8.5784	4.40909	-15.556	43.741		
3100000	27000	485	33600	475	63000	0.00479	18800	24500	12400	-4.2119	0.21047	-6.9118	-10.09	-6.0506	-4.7782	-8.4208	8.37802	2.625	-15.061	40.4206	Base C4	36.20867
3100000	27000	425	33600	475	63000	0.00493	18800	24500	12400	-3.8518	0.06001	-7.1726	-9.8292	-5.881	-3.146	-7.9303	8.12403	4.18388	-14.92	38.0046	T.Head	
3100000	27000	425	33600	475	63000	0.00493	18800	25500	12400	-3.8365	0.051[illegible]6	-7.1837	-9.8302	-5.8739	-3.242	-7.9884	8.14819	3.50599	-14.866	38.1145		
3100000	27000	425	33600	475	63000	0.00493	18800	23500	12400	-3.9568	0.12[illegible]63	-7.1657	-9.8254	-5.8568	-3.3246	-8.038	8.14769	3.45331	-14.853	38.277		
3100000	27000	425	33600	475	63000	0.00507	18800	24500	12400	-3.5461	0.09921	-7.4057	-9.6413	-5.7211	-2.3305	-7.8043	8.03017	2.71674	-14.598	36.6749		
3100000	27000	425	33600	500	63000	0.00507	18800	24500	12400	-3.5461	0.09921	-7.4057	-9.6413	-5.7211	-2.3305	-7.8043	8.03017	2.71674	-14.598	36.6749	No Effect	
3100000	27000	405	33600	475	63000	0.00507	18800	24500	12400	-3.6101	0.16906	7.4063	9.6296	-5.7039	-2.1516	-7.7378	7.98777	3.5593	-14.643	36.4893	Base C5	32.87918
3150000	27000	405	33600	475	63000	0.00507	18800	24500	12400	-3.4611	0.11227	-7.4383	-9.6409	-5.7236	-2.2171	-7.7653	8.02773	2.7876	-14.606	36.5087		
3050000	27000	405	33600	475	63000	0.00507	18800	24500	12400	-3.2796	0.10423	-7.5935	-9.5862	-5.6426	-4.1886	-8.8632	8.48346	-8.8756	-13.676	38.7739	Low Temp?	
3100000	27000	325	33600	475	63000	0.00535	18800	24500	12400	-2.6749	0.17891	-8.0013	-9.2207	-5.4013	0.22847	-7.1877	7.72686	2.29132	-14.121	33.2535	T.Head	
3100000	27000	325	33600	475	63000	0.00535	18800	25000	12400	-2.4829	0.16783	-7.9122	-8.8104	-5.5178	0.55036	-6.8798	7.58378	4.02996	-14.113	32.8574		
3100000	27000	325	33600	475	63000	0.00549	18800	25000	12400	-2.0291	0.10252	-8.1603	-8.6337	-5.3962	1.40619	-6.7041	7.50354	2.63264	-13.826	33.129		
3100000	27000	325	33600	475	63000	0.00521	18800	25000	12400	-2.8879	0.20002	-7.7192	-8.9818	-5.6078	-0.8987	-7.4024	7.80552	1.6531	-14.112	33.9009		
3100000	27000	325	33600	0	63000	0.00535	18800	25000	12400	-2.4103	0.12001	-7.9833	-8.7984	-5.4773	-0.1126	-7.2771	7.74552	-0.4107	-13.771	32.5274		
3100000	27000	305	33600	0	63000	0.00535	18800	25000	12400	-2.032	0.05207	-8.1767	-8.7292	-5.435	-1.4311	-8.0541	8.10272	-9.4045	-13.045	33.9067		
3100000	27000	345	33600	0	63000	0.00535	18800	25000	12400	-2.672	0.25661	-7.8463	-8.8228	-5.5088	0.40796	-6.9203	7.572	4.40723	-14.137	32.8299		
3000000	27000	325	33600	0	63000	0.00535	18800	25000	12400	-2.4284	0.08614	-7.9763	-8.7893	-5.4761	-0.07	-7.2534	7.73111	-0.163	-13.785	32.4712	Base C6	30.04276
2900000	27000	285	33600	0	63000	0.00553	18800	25500	12400	-1.883	0.13348	-8.2806	-8.5495	-5.3447	2.20946	-6.4367	7.38771	4.20599	-13.866	33.6548	T.Head	31.77186
2900000	27000	285	33600	100	63000	0.00553	18800	25500	12400	-1.883	0.13348	-8.2806	-8.5495	-5.3447	2.20941	-6.4367	7.38777	4.20661	-13.866	33.655		
2900000	27000	285	33600	100	58000	0.00553	18800	25500	12400	-1.883	0.13358	-8.2804	-8.5499	-5.3448	2.21129	-6.4359	7.38749	4.21736	-13.867	33.6568		
2900000	27000	285	33600	500	70000	0.00553	18800	25500	12400	-1.883	0.13348	-8.2806	-8.5495	-5.3447	2.20946	-6.4367	7.38771	4.20599	-13.866	33.6548		
2900000	27000	285	33600	500	70000	0.00553	18800	26000	12400	-1.8782	0.13187	-8.2834	-8.5487	-5.3424	2.19249	-6.4482	7.39208	4.05909	-13.853	33.6372		

TABLE 14 (cont). Hooke-Jeeves Searches - Weight Adjustments, Wet Basis

Kinetic Parameters

AE = Activation Energy RC = Rate Constant

											Percentage Error			Percentage Error		Percentage Error					
RC #1	AE #1	RC #	AE #2	RC #	AE #3	RC #4	AE #4	RC#5/1	AE #5	Coal F	C Con	H2	CO	CO2	CH4	RG Ma	RG H2	RG Te	Stm Util	Index	
2900000	27000	285	33600	500	70000	0.00567	18800	26000	12400	2.57615	-2.5583	-9.0933	-8.4602	-5.971	3.52144	-5.5512	7.79213	-3.586	-13.646	37.4143	Did Not Converge
2900000	27000	285	33600	500	70000	0.00567	18800	26000	12400	-1.4617	0.08745	-8.5562	-8.3652	-5.1882	2.66797	-6.5032	7.39228	0.39711	-13.384	33.6315	
2900000	27000	285	33600	500	80000	0.00567	18800	26000	12400	-1.4617	0.08745	-8.5562	-8.3652	-5.1882	2.66797	-6.5032	7.39228	0.39711	-13.384	33.6315	
2900000	27000	285	33600	500	40000	0.00567	18800	26000	12400	-2.8143	-3.1055	-11.726	-21.456	-3.3701	1.99325	-10.197	10.7574	-4.7903	-18.756	52.1177	
2900000	27000	285	33600	500	50000	0.00567	18800	26000	12400	-1.4865	0.07559	-8.5977	-8.4733	-5.1497	2.47797	-6.6522	7.45959	-0.8756	-13.326	33.6448	
2900000	27000	265	33600	500	70000	0.00567	18800	26000	12400	-1.5381	0.22555	-8.5789	-8.3521	-5.1623	2.88486	-6.4451	7.35207	1.2376	-13.427	33.8683	
2900000	27000	305	33600	500	70000	0.00567	18800	26000	12400	-1.5897	0.19801	-8.5001	-8.3956	-5.1859	2.38897	-6.6048	7.41845	0.00847	-13.363	33.4788	
2950000	27000	305	33600	500	70000	0.00567	18800	26000	12400	-1.2668	0.16846	-8.5965	-8.4276	-5.206	1.92041	-6.86	7.58089	-3.5269	-13.134	32.9983	Base C7
2950000	27000	305	33600	500	70000	0.00567	18800	26000	12400	-2.2154	0.11318	-8.9022	-10.111	-4.7622	0.60048	-8.0602	8.13955	10.3002	-13.322	34.7303	Set Cp(vol)=0
2900000	27000	285	33600	500	70000	0.00599	18800	27000	12400	-0.8312	0.09328	-9.0804	-8.333	-4.8357	4.91984	-5.9989	7.15605	0.0405	-13.092	35.1562	T.Head
2900000	27000	285	33600	500	70000	0.00599	18800	27500	12400	-0.8293	0.09338	-9.0803	-8.3326	-4.8346	4.92429	-5.9966	7.15476	0.04236	-13.091	35.1559	
2900000	27000	285	33600	500	70000	0.00599	18800	26500	12400	-0.8341	0.09378	-9.0784	-8.3347	-4.8364	4.9207	-5.9966	7.15511	0.08161	-13.096	35.1594	
2900000	27000	285	33600	500	70000	0.0061	18800	27000	12400	-0.6583	0.18484	-9.2158	-8.2117	-4.7395	5.68821	-5.7842	7.03991	0.55062	-12.987	35.5534	
2900000	27000	285	33600	500	70000	0.0059	18800	27000	12400	-1.0261	0.0791	-8.9688	-8.4337	-4.8987	4.1537	-6.2556	7.27352	-0.9969	-13.126	34.7545	
2900000	27000	305	33600	500	70000	0.0059	18800	27000	12400	-1.2028	0.22113	-8.8544	-8.4788	-4.9371	4.381	-6.0425	7.17722	2.14483	-13.384	35.0314	
2900000	27000	265	33600	500	70000	0.0059	18800	27000	12400	-1.0892	0.21178	-9.0075	-8.4189	-4.8617	4.22971	-6.2847	7.26762	-1.13	-13.092	34.8746	
2950000	27000	285	33600	500	70000	0.0059	18800	27000	12400	-1.0538	0.08182	-8.9851	-8.4228	-4.8742	3.95767	-6.384	7.31374	-2.2835	-13.015	34.6074	
2950000	27000	285	33600	500	60000	0.0059	18800	27000	12400	-1.0538	0.08182	-8.9854	-8.4237	-4.8742	3.9565	-6.3848	7.31414	-2.288	-13.015	34.6079	
2950000	27000	285	33600	500	80000	0.0059	18800	27000	12400	-1.0538	0.08182	-8.9851	-8.4228	-4.8742	3.95767	-6.384	7.31374	-2.2833	-13.015	34.6074	
2950000	27000	285	33600	500	80000	0.0059	18800	27000	12800	-1.0796	0.08825	-8.9721	-8.4236	-4.8917	3.98851	-6.3511	7.30416	-1.7428	-13.074	34.6597	
2950000	27000	285	33600	500	80000	0.0059	18800	27000	12000	-1.0032	0.06131	-9.0168	-8.419	-4.8495	3.77265	-6.5093	7.36284	-3.7967	-12.879	34.424	
2950000	27000	285	33600	500	80000	0.0059	18200	27000	12000	6.28349	0.44175	-15.177	-4.8204	-0.7935	-2.8498	-15.809	10.7464	-29.276	2.08759	40.6702	Did Not Converge
2950000	27000	285	33600	500	80000	0.0059	18800	27000	12000	-2.1256	0.12454	-9.2283	-10.577	-4.472	4.17511	-6.7683	7.60806	24.6521	-14.155	38.1858	Set Cp(vol)=-.1
2950000	27000	285	3360C	500	80000	0.0059	18800	27000	12000	-0.8303	0.09951	-9.2955	-8.6888	-4.6866	2.75799	-7.3	7.72409	-12.713	-12.323	33.9832	Selectivity=2
2950000	27000	285	33600	500	80000	0.0059	18800	27000	12000	-0.7051	0.05769	-9.3982	-8.68	-4.6066	3.46425	-7.0815	7.622	-11.92	-12.326	34.4762	Selectivity=1
1790000	27000	613	40000	367.8	42000	0.008356	16046	30000	14400	13.8653	-3.3764	-19.491	-5.1748	-2.7635	32.7902	-1.1483	6.66842	-17.141	-9.6519	80.7529	
3000000	27000	325	33600	500	63000	0.00535	18800	25000	12400	-2.8143	-2.5181	-10.468	-7.7823	-3.7937	2.99673	-11.67	7.57311	-16.351	-3.6859	35.4282	No convergence
3000000	27000	325	33600	500	63000	0.00535	18800	25000	12400	-6.5898	0.07187	-9.8793	-7.9642	-3.0287	2.4507	-12.253	7.13264	-13.044	-3.9901	37.0453	
3000000	27000	325	33600	0	63000	0.00535	18800	25000	12400	2.4284	0.08614	-7.9763	-8.7893	5.4761	-0.07	-7.2534	7.73411	-0.163	-13.785	32.4712	Base C6

APPENDIX C

Box-Behnken Simulation Predictions

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PERFORMANCE SUMMARY:  F022

  COAL FEED FLOW RATE                          LB/HR                    104136.
  FIXED CARBON CONVERTED                       %                        97.2492
  PEAK TEMPERATURE                             F                        2039.49
  CONC. OF O2         IN RAW GAS (DRY)  MOL%                     .152328E-97
  CONC. OF H2         IN RAW GAS (DRY)  MOL%                     .382128
  CONC. OF CO         IN RAW GAS (DRY)  MOL%                     .162457
  CONC. OF CO2        IN RAW GAS (DRY)  MOL%                     .312527
  CONC. OF CH4        IN RAW GAS (DRY)  MOL%                     .117244
  RAW GAS MASS FLOW RATE (DRY)                 LB/HR                    118822.
  RAW GAS VOLUME FLOW RATE (DRY)               STD-CUFT/HR              .188014E+07
  FLOW OF WATER IN RAW GAS                     LB/HR                    92677.9
  RAW GAS TEMPERATURE                          F                        420.342
  HEAT TRANSFERRED TO STEAM JACKET             BTU/HR                   .718234E+07
  MASS FLOW OF STEAM PRODUCED                  LB/HR                    9169.00
  OUTLET STEAM TEMPERATURE                     F                        463.526
  REACTOR STEAM UTILIZATION                                             .420231


PERFORMANCE SUMMARY:  F021

  COAL FEED FLOW RATE                          LB/HR                    105508.
  FIXED CARBON CONVERTED                       %                        97.2679
  PEAK TEMPERATURE                             F                        2050.91
  CONC. OF O2         IN RAW GAS (DRY)  MOL%                     .327221E-97
  CONC. OF H2         IN RAW GAS (DRY)  MOL%                     .381479
  CONC. OF CO         IN RAW GAS (DRY)  MOL%                     .165399
  CONC. OF CO2        IN RAW GAS (DRY)  MOL%                     .309854
  CONC. OF CH4        IN RAW GAS (DRY)  MOL%                     .117672
  RAW GAS MASS FLOW RATE (DRY)                 LB/HR                    119941.
  RAW GAS VOLUME FLOW RATE (DRY)               STD-CUFT/HR              .190068E+07
  FLOW OF WATER IN RAW GAS                     LB/HR                    92726.5
  RAW GAS TEMPERATURE                          F                        416.408
  HEAT TRANSFERRED TO STEAM JACKET             BTU/HR                   .721221E+07
  MASS FLOW OF STEAM PRODUCED                  LB/HR                    9169.00
  OUTLET STEAM TEMPERATURE                     F                        470.470
  REACTOR STEAM UTILIZATION                                             .425209


PERFORMANCE SUMMARY:  F011

  COAL FEED FLOW RATE                          LB/HR                    103173.
  FIXED CARBON CONVERTED                       %                        97.2511
  PEAK TEMPERATURE                             F                        1981.12
  CONC. OF O2         IN RAW GAS (DRY)  MOL%                     .246535E-93
  CONC. OF H2         IN RAW GAS (DRY)  MOL%                     .395810
  CONC. OF CO         IN RAW GAS (DRY)  MOL%                     .144623
  CONC. OF CO2        IN RAW GAS (DRY)  MOL%                     .322456
  CONC. OF CH4        IN RAW GAS (DRY)  MOL%                     .112020
  RAW GAS MASS FLOW RATE (DRY)                 LB/HR                    119433.
  RAW GAS VOLUME FLOW RATE (DRY)               STD-CUFT/HR              .190285E+07
  FLOW OF WATER IN RAW GAS                     LB/HR                    100891.
  RAW GAS TEMPERATURE                          F                        453.169
  HEAT TRANSFERRED TO STEAM JACKET             BTU/HR                   .707319E+07
  MASS FLOW OF STEAM PRODUCED                  LB/HR                    9049.02
  OUTLET STEAM TEMPERATURE                     F                        459.950
  REACTOR STEAM UTILIZATION                                             .391232
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PERFORMANCE SUMMARY:  F012

  COAL FEED FLOW RATE                          LB/HR                  101797.
  FIXED CARBON CONVERTED                       %                      97.2078
  PEAK TEMPERATURE                             F                      1968.96
  CONC. OF O2        IN RAW GAS  (DRY)  MOL%                  .253852E-93
  CONC. OF H2        IN RAW GAS  (DRY)  MOL%                  .396618
  CONC. OF CO        IN RAW GAS  (DRY)  MOL%                  .141837
  CONC. OF CO2       IN RAW GAS  (DRY)  MOL%                  .325105
  CONC. OF CH4       IN RAW GAS  (DRY)  MOL%                  .111325
  RAW GAS MASS FLOW RATE  (DRY)            LB/HR                  118121.
  RAW GAS VOLUME FLOW RATE  (DRY)          STD-CUFT/HR            .187931E+07
  FLOW OF WATER IN RAW GAS                 LB/HR                  100919.
  RAW GAS TEMPERATURE                          F                      456.623
  HEAT TRANSFERRED TO STEAM JACKET         BTU/HR                 .704469E+07
  MASS FLOW OF STEAM PRODUCED              LB/HR                  9012.56
  OUTLET STEAM TEMPERATURE                     F                      459.950
  REACTOR STEAM UTILIZATION                                           .385961
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PERFORMANCE SUMMARY:  F210

  COAL FEED FLOW RATE                          LB/HR                  95101.0
  FIXED CARBON CONVERTED                       %                      97.2264
  PEAK TEMPERATURE                             F                      1971.33
  CONC. OF O2        IN RAW GAS  (DRY)  MOL%                  .454034E-97
  CONC. OF H2        IN RAW GAS  (DRY)  MOL%                  .393031
  CONC. OF CO        IN RAW GAS  (DRY)  MOL%                  .142364
  CONC. OF CO2       IN RAW GAS  (DRY)  MOL%                  .324789
  CONC. OF CH4       IN RAW GAS  (DRY)  MOL%                  .114384
  RAW GAS MASS FLOW RATE  (DRY)            LB/HR                  110060.
  RAW GAS VOLUME FLOW RATE  (DRY)          STD-CUFT/HR            .174567E+07
  FLOW OF WATER IN RAW GAS                 LB/HR                  93145.6
  RAW GAS TEMPERATURE                          F                      443.478
  HEAT TRANSFERRED TO STEAM JACKET         BTU/HR                 .701833E+07
  MASS FLOW OF STEAM PRODUCED              LB/HR                  8978.83
  OUTLET STEAM TEMPERATURE                     F                      459.950
  REACTOR STEAM UTILIZATION                                           .391345
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PERFORMANCE SUMMARY:  F220

  COAL FEED FLOW RATE                          LB/HR                  97292.1
  FIXED CARBON CONVERTED                       %                      97.1397
  PEAK TEMPERATURE                             F                      2040.92
  CONC. OF O2        IN RAW GAS  (DRY)  MOL%                  .197304-101
  CONC. OF H2        IN RAW GAS  (DRY)  MOL%                  .378463
  CONC. OF CO        IN RAW GAS  (DRY)  MOL%                  .162801
  CONC. OF CO2       IN RAW GAS  (DRY)  MOL%                  .312376
  CONC. OF CH4       IN RAW GAS  (DRY)  MOL%                  .120335
  RAW GAS MASS FLOW RATE  (DRY)            LB/HR                  110582.
  RAW GAS VOLUME FLOW RATE  (DRY)          STD-CUFT/HR            .174390E+07
  FLOW OF WATER IN RAW GAS                 LB/HR                  85685.4
  RAW GAS TEMPERATURE                          F                      412.162
  HEAT TRANSFERRED TO STEAM JACKET         BTU/HR                 .715690E+07
  MASS FLOW OF STEAM PRODUCED              LB/HR                  9156.11
  OUTLET STEAM TEMPERATURE                     F                      459.950
  REACTOR STEAM UTILIZATION                                           .424898
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PERFORMANCE SUMMARY:  F120

  COAL FEED FLOW RATE                LB/HR                   112382.
  FIXED CARBON CONVERTED             %                       97.2085
  PEAK TEMPERATURE                   F                       2049.39
  CONC. OF O2       IN RAW GAS (DRY) MOL%                    .959069E-94
  CONC. OF H2       IN RAW GAS (DRY) MOL%                    .384768
  CONC. OF CO       IN RAW GAS (DRY) MOL%                    .164441
  CONC. OF CO2      IN RAW GAS (DRY) MOL%                    .310654
  CONC. OF CH4      IN RAW GAS (DRY) MOL%                    .114893
  RAW GAS MASS FLOW RATE (DRY)       LB/HR                   127955.
  RAW GAS VOLUME FLOW RATE (DRY)     STD-CUFT/HR             .203285E+07
  FLOW OF WATER IN RAW GAS           LB/HR                   99785.1
  RAW GAS TEMPERATURE                F                       421.827
  HEAT TRANSFERRED TO STEAM JACKET   BTU/HR                  .722778E+07
  MASS FLOW OF STEAM PRODUCED        LB/HR                   9169.00
  OUTLET STEAM TEMPERATURE           F                       474.088
  REACTOR STEAM UTILIZATION                                  .420293
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PERFORMANCE SUMMARY:  F110

  COAL FEED FLOW RATE                LB/HR                   109750.
  FIXED CARBON CONVERTED             %                       97.2722
  PEAK TEMPERATURE                   F                       1978.55
  CONC. OF O2       IN RAW GAS (DRY) MOL%                    .189723E-90
  CONC. OF H2       IN RAW GAS (DRY) MOL%                    .399051
  CONC. OF CO       IN RAW GAS (DRY) MOL%                    .143983
  CONC. OF CO2      IN RAW GAS (DRY) MOL%                    .322995
  CONC. OF CH4      IN RAW GAS (DRY) MOL%                    .109196
  RAW GAS MASS FLOW RATE (DRY)       LB/HR                   127375.
  RAW GAS VOLUME FLOW RATE (DRY)     STD-CUFT/HR             .203468E+07
  FLOW OF WATER IN RAW GAS           LB/HR                   108632.
  RAW GAS TEMPERATURE                F                       464.303
  HEAT TRANSFERRED TO STEAM JACKET   BTU/HR                  .709732E+07
  MASS FLOW OF STEAM PRODUCED        LB/HR                   9079.89
  OUTLET STEAM TEMPERATURE           F                       459.950
  REACTOR STEAM UTILIZATION                                  .386163
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PERFORMANCE SUMMARY:  F202

  COAL FEED FLOW RATE                LB/HR                   95764.6
  FIXED CARBON CONVERTED             %                       97.2180
  PEAK TEMPERATURE                   F                       1999.26
  CONC. OF O2       IN RAW GAS (DRY) MOL%                    .827046E-99
  CONC. OF H2       IN RAW GAS (DRY) MOL%                    .386076
  CONC. OF CO       IN RAW GAS (DRY) MOL%                    .151118
  CONC. OF CO2      IN RAW GAS (DRY) MOL%                    .319683
  CONC. OF CH4      IN RAW GAS (DRY) MOL%                    .117322
  RAW GAS MASS FLOW RATE (DRY)       LB/HR                   110068.
  RAW GAS VOLUME FLOW RATE (DRY)     STD-CUFT/HR             .173983E+07
  FLOW OF WATER IN RAW GAS           LB/HR                   89392.3
  RAW GAS TEMPERATURE                F                       430.140
  HEAT TRANSFERRED TO STEAM JACKET   BTU/HR                  .707683E+07
  MASS FLOW OF STEAM PRODUCED        LB/HR                   9053.68
  OUTLET STEAM TEMPERATURE           F                       459.950
  REACTOR STEAM UTILIZATION                                  .405727
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PERFORMANCE SUMMARY:  F201

  COAL FEED FLOW RATE                        LB/HR                       96971.0
  FIXED CARBON CONVERTED                     %                           97.2178
  PEAK TEMPERATURE                           F                           2010.91
  CONC. OF O2        IN RAW GAS (DRY)  MOL%                        .171315E-99
  CONC. OF H2        IN RAW GAS (DRY)  MOL%                        .385354
  CONC. OF CO        IN RAW GAS (DRY)  MOL%                        .153473
  CONC. OF CO2       IN RAW GAS (DRY)  MOL%                        .317539
  CONC. OF CH4       IN RAW GAS (DRY)  MOL%                        .117880
  RAW GAS MASS FLOW RATE (DRY)               LB/HR                       111027.
  RAW GAS VOLUME FLOW RATE (DRY)             STD-CUFT/HR                 .175692E+07
  FLOW OF WATER IN RAW GAS                   LB/HR                       89431.1
  RAW GAS TEMPERATURE                        F                           425.011
  HEAT TRANSFERRED TO STEAM JACKET           BTU/HR                      .709790E+07
  MASS FLOW OF STEAM PRODUCED                LB/HR                       9080.63
  OUTLET STEAM TEMPERATURE                   F                           459.950
  REACTOR STEAM UTILIZATION                                              .410280


PERFORMANCE SUMMARY:  F101

  COAL FEED FLOW RATE                        LB/HR                       111954.
  FIXED CARBON CONVERTED                     %                           97.1994
  PEAK TEMPERATURE                           F                           2018.94
  CONC. OF O2        IN RAW GAS (DRY)  MOL%                        .579175E-92
  CONC. OF H2        IN RAW GAS (DRY)  MOL%                        .391591
  CONC. OF CO        IN RAW GAS (DRY)  MOL%                        .155164
  CONC. OF CO2       IN RAW GAS (DRY)  MOL%                        .315681
  CONC. OF CH4       IN RAW GAS (DRY)  MOL%                        .112519
  RAW GAS MASS FLOW RATE (DRY)               LB/HR                       128510.
  RAW GAS VOLUME FLOW RATE (DRY)             STD-CUFT/HR                 .204859E+07
  FLOW OF WATER IN RAW GAS                   LB/HR                       104219.
  RAW GAS TEMPERATURE                        F                           441.360
  HEAT TRANSFERRED TO STEAM JACKET           BTU/HR                      .717352E+07
  MASS FLOW OF STEAM PRODUCED                LB/HR                       9169.00
  OUTLET STEAM TEMPERATURE                   F                           461.474
  REACTOR STEAM UTILIZATION                                              .405373


PERFORMANCE SUMMARY:  F102

  COAL FEED FLOW RATE                        LB/HR                       110579.
  FIXED CARBON CONVERTED                     %                           97.2784
  PEAK TEMPERATURE                           F                           2006.99
  CONC. OF O2        IN RAW GAS (DRY)  MOL%                        .491504E-92
  CONC. OF H2        IN RAW GAS (DRY)  MOL%                        .392323
  CONC. OF CO        IN RAW GAS (DRY)  MOL%                        .152866
  CONC. OF CO2       IN RAW GAS (DRY)  MOL%                        .317986
  CONC. OF CH4       IN RAW GAS (DRY)  MOL%                        .111838
  RAW GAS MASS FLOW RATE (DRY)               LB/HR                       127270.
  RAW GAS VOLUME FLOW RATE (DRY)             STD-CUFT/HR                 .202660E+07
  FLOW OF WATER IN RAW GAS                   LB/HR                       104147.
  RAW GAS TEMPERATURE                        F                           443.185
  HEAT TRANSFERRED TO STEAM JACKET           BTU/HR                      .715284E+07
  MASS FLOW OF STEAM PRODUCED                LB/HR                       9150.91
  OUTLET STEAM TEMPERATURE                   F                           459.950
  REACTOR STEAM UTILIZATION                                              .401228
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PERFORMANCE SUMMARY:  F000

  COAL FEED FLOW RATE                           LB/HR                       103770.
  FIXED CARBON CONVERTED                        %                           97.1999
  PEAK TEMPERATURE                              F                           2009.22
  CONC. OF O2        IN RAW GAS (DRY)           MOL%                        .322287E-95
  CONC. OF H2        IN RAW GAS (DRY)           MOL%                        .389076
  CONC. OF CO        IN RAW GAS (DRY)           MOL%                        .153027
  CONC. OF CO2       IN RAW GAS (DRY)           MOL%                        .317904
  CONC. OF CH4       IN RAW GAS (DRY)           MOL%                        .114663
  RAW GAS MASS FLOW RATE (DRY)                  LB/HR                       119129.
  RAW GAS VOLUME FLOW RATE (DRY)                STD-CUFT/HR                 .189131E+07
  FLOW OF WATER IN RAW GAS                      LB/HR                       96780.6
  RAW GAS TEMPERATURE                           F                           433.397
  HEAT TRANSFERRED TO STEAM JACKET              BTU/HR                      .712296E+07
  MASS FLOW OF STEAM PRODUCED                   LB/HR                       9112.69
  OUTLET STEAM TEMPERATURE                      F                           459.950
  REACTOR STEAM UTILIZATION                                                 .405459
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APPENDIX D

Elemental Mole Balance on Volatile Matter

Elemental Mole Balance UND Case Average

Coal Flow = 13.2

Proxanal = 35.96 46.3 44.2 9.5

Ultanal = 9.52 65.7 4.52 0.88 0 0.96 18.4

UND Case Average

Tar-rec Coal Flow = 0.019

Proxanal 13.58 12.96 12.35 74.69

Ultanal = 74.69 18.37 1.27 0.25 0 0.27 5.15

Fraction Volatile Matter Released by Pyrolysis =	1	Total Mass Flow =	3.732	Kg/s
Mass Fraction of Phenol in Volatile Matter =	0.039	Phenol	0.144	Kg/s
Mass Fraction of Naphtha in Volatile Matter =	0.019	Naphtha	0.07	Kg/s
Mass Fraction of Tar Oils in Volatile Matter =	0.122	Tar Oils	0.454	Kg/s

Table 1 -- Composition of Volatiles
Actual Compositions

		Weight %			Elements					Molecular	Phenol	Naphth	Tar oils	Phenol	Naphth	Tar oil	MOLAR FLOWS			(Kg mol/sec)	
COMPONENT	ALIAS	Phen	Naph	Tar	C	H	O	S	N	Weight	Weight	Weight	Weight	mol%	mol%	mol%	C	H	O	S	N
methyl-mercaptan	CH4S	0	0.17	0	1	4		1		48.103	0	3.5E-05	0	0.000	0.287	0.000	2.5E-06	1E-05	0	2.5E-06	0
methanol	CH4O	0	0.15	0	1	4	1			32.042	0	4.7E-05	0	0.000	0.381	0.000	3.3E-06	1.3E-05	3.3E-06	0	0
acetonitrile	C2H3N	0	0.11	0.01	2	3			1	41.052	0	2.7E-05	2.4E-06	0.000	0.218	0.032	6E-06	9E-06	0	0	3E-06
ethylene	C2H4	0	0	0	2	4				28.054	0	0	0	0.000	0.000	0.000	0	0	0	0	0
thiirane	* C2H4	0	0.15		2	4		1		60.114	0	2.5E-05	0	0.000	0.203	0.000	3.5E-06	7E-06	0	1.8E-06	0
acetaldehyde	C2H4O-1	0	0.2	0	2	4	1			44.053	0	4.5E-05	0	0.000	0.369	0.000	6.4E-06	1.3E-05	3.2E-06	0	0
ethyl-mercaptan	C2H6S-1	0	0.28	0	2	6		1		62.129	0	4.5E-05	0	0.000	0.367	0.000	6.4E-06	1.9E-05	0	3.2E-06	0
propyl-mercaptan	* C2H6S-1	0	0.05	0.5	3	8		1		76.156	0	6.6E-06	6.6E-05	0.000	0.053	0.861	9.1E-05	0.0002	0	3E-05	0
di-methyl-sulfide	C2H6S-2	0	0	0	2	6		1		62.129	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-methyl-mercaptan	* C2H6S-2	0	0.11		2	7		1		63.137	0	1.7E-05	0	0.000	0.142	0.000	2.5E-06	8.6E-06	0	1.2E-06	0
propionitrile	C3H5N	0	0.2	0	3	5			1	55.079	0	3.6E-05	0	0.000	0.295	0.000	7.7E-06	1.3E-05	0	0	2.6E-06
acetone	C3H6O-1	0.07	3.96	0.06	3	6	1			58.08	1.2E-05	0.0007	1E-05	0.111	5.545	0.136	0.0002	0.0003	5.4E-05	0	0
thiophene	C4H4S	0	0.64	0	4	4		1		84.136	0	7.6E-05	0	0.000	0.619	0.000	2.1E-05	2.1E-05	0	5.4E-06	0
pyrrole	C4H5N-2	0.1	0.08	0.1	4	5			1	67.09	1.5E-05	1.2E-05	1.5E-05	0.137	0.097	0.196	3.9E-05	4.9E-05	0	0	9.8E-06
methyl-ethyl-ketone	C4H8O-3	0.02	4.53	0.1	4	8	1			72.107	2.8E-06	0.0006	1.4E-05	0.025	5.109	0.182	0.0002	0.0004	5.1E-05	0	0
pyridine	C5H5N	0.3	0.03	0.02	5	5			1	79.101	3.8E-05	3.8E-0[illegible]	2.5E-06	0.348	0.031	0.033	3.4E-05	3.4E-05	0	0	6.9E-06
cyclopentadiene	C5H6	0	0.2	0	5	6				66.102	0	3E-05	0	0.000	0.246	0.000	1.1E-05	1.3E-05	0	0	0
cyclopentene	C5H8-1	0	0.1	0	5	8				68.118	0	1.5E-05	0	0.000	0.119	0.000	5.2E-06	8.3E-06	0	0	0
1,4-pentadiene	C5H8-4 0.	0	0.2	0	5	8				68.118	0	2.9E-05	0	0.000	0.239	0.000	1E-05	1.7E-05	0	0	0
cyclopentanone	C5H8O	0	0.5	0	5	8	1			84.118	0	5.9E-05	0	0.000	0.483	0.000	2.1E-05	3.4E-05	4.2E-06	0	0
methyl-furan	* C5H8O	0	1	0.1	5	6		1		98.162	0	0.0001	1E-05	0.000	0.829	0.134	5.9E-05	7.1E-05	0	1.2E-05	0
methyl-n-propyl-ketone	C5H10O-2	0.09	0.6	0.1	5	10	1			86.133	1E-05	7E-05	1.2E-05	0.096	0.567	0.152	5.8E-05	0.0001	1.2E-05	0	0
methyl-iso-propyl-ketone	C5H10O-3	0	0	0	5	10	1			86.133	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-butanone	* C5H10O-3	0	0.2	0.1	5	10	1			86.133	0	2.3E-05	1.2E-05	0.000	0.189	0.152	3.5E-05	6.9E-05	6.9E-06	0	0
1-pentanethiol	C5H12S	0	0	0	5	12		1		104.21	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-thiophene	* C5H12S	0	0.55	0.5	5	5		1		97.155	0	5.7E-05	5.1E-05	0.000	0.460	0.675	0.0001	0.0001	0	2.7E-05	0
benzene	C6H6	0	43.7	0.5	6	6				78.113	0	0.0056	6.4E-05	0.000	45.499	0.840	0.0025	0.0025	0	0	0
cyclohexadiene	* C6H6	0	0.3		6	8				80.129	0	3.7E-05	0	0.000	0.304	0.000	1.6E-05	2.1E-05	0	0	0

Elemental Mole Balance

UND Case Average

		Weight %			Elements					Molecular	Phenol	Naphth	Tar oils	Phenol	Naphth	Tar oil	MOLAR FLOWS			(Kg mol/sec)	
COMPONENT	ALIAS	Phen	Naph	Tar	C	H	O	S	N	Weight	Weight	Weight	Weight	mol%	mol%	mol%	C	H	O	S	N
phenyl-mercaptan	C6H6S	0	0	0	6	6		1		110.17	0	0	0	0.000	0.000	0.000	0	0	0	0	0
ethyl-thiophene	* C6H6S	0.12	0.07	0.1	6	7		1		111.18	1.1E-05	6.3E-06	9E-06	0.099	0.051	0.118	3.6E-05	4.3E-05	0	6.1E-06	0
di-methyl-thiophene	* C6H6S	0.12	0.05	0.01	6	8		1		112.19	1.1E-05	5.3E-06	8.9E-07	0.098	0.043	0.012	1.4E-05	1.9E-05	0	2.3E-06	0
phenol	C6H6O	34.47	0	1.6	6	6	1			94.113	0.0037	0	0.0002	33.607	0.000	2.230	0.0036	0.0036	0.0006	0	0
p-hydroquinone	C6H6O2	0	0	0	6	6	2			110.11	0	0	0	0.000	0.000	0.000	0	0	0	0	0
catechol	* C6H6O2	2	0	0.01	6	6	2			110.11	0.0002	0	9.1E-07	1.667	0.000	0.012	0.0002	0.0002	5.3E-05	0	0
aniline	C6H7N-1	0.05	0	0.1	6	7			1	93.128	5.4E-06	0	1.1E-05	0.049	0.000	0.141	3.4E-05	4E-05	0	0	5.6E-06
4-methyl-pyridine	C6H7N-2	0.4	0.5	0.17	6	7			1	93.126	4.3E-05	5.4E-05	1.8E-05	0.394	0.437	0.239	0.0001	0.0001	0	0	1.8E-05
cyclohexene	C6H10-2	0	0	0	6	10				82.145	0	0	0	0.000	0.000	0.000	0	0	0	0	0
hexadiene	* C6H10-2	0	0.5		6	10				82.145	0	6.1E-05	0	0.000	0.495	0.000	2.6E-05	4.3E-05	0	0	0
cyclohexanone	C6H10O	0	0	0	6	10	1			98.144	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-methyl-furan	* C6H10O	0	0.5		6	8	1			96.129	0	5.2E-05	0	0.000	0.423	0.000	2.2E-05	2.9E-05	3.7E-06	0	0
1-hexene	C6H12-3	0	2.3	0	6	12				84.161	0	0.0003	0	0.000	2.223	0.000	0.0001	0.0002	0	0	0
n-hexane	C6H14-1	0	1.9	0	6	14				86.177	0	0.0002	0	0.000	1.793	0.000	9.3E-05	0.0002	0	0	0
toluene	C7H8	0.07	17.1	1.4	7	8				92.14	7.6E-06	0.0019	0.0002	0.070	15.094	1.993	0.0014	0.0016	0	0	0
methyl-cyclohexadiene	* C7H8	0	0.5		7	10				94.156	0	5.3E-05	0	0.000	0.432	0.000	2.6E-05	3.7E-05	0	0	0
methyl-cyclohexene	* C7H8	0	0.6		7	12				96.172	0	6.2E-05	0	0.000	0.507	0.000	3.1E-05	5.3E-05	0	0	0
methyl-hexadiene	* C7H8	0	0.5		7	12				96.172	0	5.2E-05	0	0.000	0.423	0.000	2.6E-05	4.4E-05	0	0	0
methyl-phenyl-ether	C7H8O-1	0	0	0	7	8	1			108.14	0	0	0	0.000	0.000	0.000	0	0	0	0	0
anisole	* C7H8O-1	0.07	0.2	0.01	7	8	1			108.14	6.5E-06	1.8E-05	9.2E-07	0.059	0.150	0.012	1.9E-05	2.1E-05	2.7E-06	0	0
p-cresol	C7H8O-5	21.3		3.8	7	8	1			108.14	0.002	0	0.0004	18.073	0.000	4.609	0.0031	0.0035	0.0004	0	0
p-methoxy-phenol	C7H8O2	0	0	0	7	8	1			108.14	0	0	0	0.000	0.000	0.000	0	0	0	0	0
guaiacol	* C7H8O2	1.35	0	0.21	7	8	2			124.14	0.0001	0	1.7E-05	0.998	0.000	0.222	0.0002	0.0002	4.7E-05	0	0
methyl-catechol	* C7H8O2	9.5	0	1.1	7	8	2			124.14	0.0008	0	8.9E-05	7.022	0.000	1.162	0.0011	0.0012	0.0003	0	0
methyl-phenyl-amine	C7H9N-5	0	0	0.14	7	9			1	107.15	0	0	1.3E-05	0.000	0.000	0.171	4.2E-05	5.3E-05	0	0	5.9E-06
di-methyl-pyridine	* C7H9N-5	0	0.2	0.21	7	9			1	107.15	0	1.9E-05	2E-05	0.000	0.152	0.257	7.1E-05	9.2E-05	0	0	1E-05
2,6-di-methyl-pyridine	C7H9N-10	1	0	0	7	9			1	107.15	9.3E-05	0	0	0.856	0.000	0.000	9.4E-05	0.0001	0	0	1.3E-05
ethyl-pyridine	* C7H9N-10	0	0	0.1	7	9			1	107.15	0	0	9.3E-06	0.000	0.000	0.122	3E-05	3.8E-05	0	0	4.2E-06
methyl-cyclohexane	C7H14-6	0	1.1	0	7	14				98.188	0	0.0001	0	0.000	0.911	0.000	5.5E-05	0.0001	0	0	0
1-heptene	C7H14-7	0	1.4	0	7	14				98.188	0	0.0001	0	0.000	1.160	0.000	7E-05	0.0001	0	0	0
heptadiene	* C7H14-7	0	0.21		7	12				96.172	0	2.2E-05	0	0.000	0.178	0.000	1.1E-05	1.8E-05	0	0	0
5-methyl-2-hexanone	C7H14O-10	0	0.9	0.1	7	14	1			114.19	0	7.9E-05	8.8E-06	0.000	0.641	0.115	6.7E-05	0.0001	9.5E-06	0	0
n-heptane	C7H16-1	0	2.3	0	7	16				100.2	0	0.0002	0	0.000	1.867	0.000	0.0001	0.0003	0	0	0
di-methoxy-benzoate	C8H8O2	0	0	0	8	8	2			136.15	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-methoxy-benzene	* C8H8O2	0	0	1	8	10	2			138.17	0	0	7.2E-05	0.000	0.000	0.949	0.0003	0.0003	6.6E-05	0	0
p-toluic acid	C8H8O2-3	0	0	0	8	8	2			136.15	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-methyl-catechol	* C8H8O2-3	9.8			8	10	2			138.17	0.0007	0	0	6.508	0.000	0.000	0.0008	0.001	0.0002	0	0

Elemental Mole Balance

UND Case Average

COMPONENT	ALIAS	Weight % Phen	Weight % Naph	Weight % Tar	Elements C	Elements H	Elements O	Elements S	Elements N	Molecular Weight	Phenol Weight	Naphth Weight	Tar oils Weight	Phenol mol%	Naphth mol%	Tar oil mol%	MOLAR FLOWS (Kg mol/sec) C	H	O	S	N
xylene	C8H10-2	0.14	1.9	1.5	8	10				106.17	1.3E-05	0.0002	0.0001	0.121	1.455	1.853	0.0006	0.0008	0	0	0
ethyl-benzene	C8H10-4	0.07	4.34	0.7	8	10				106.17	6.6E-06	0.0004	6.6E-05	0.060	3.325	0.865	0.0005	0.0006	0	0	0
p-ethyl-phenol	C8H10O-3	2.6	0	0.8	8	10	1			122.17	0.0002	0	6.5E-05	1.953	0.000	0.859	0.0005	0.0006	6E-05	0	0
2,3-xylenol	C8H10O-5	7.4	0	3.18	8	10	1			122.17	0.0006	0	0.0003	5.558	0.000	3.414	0.0016	0.0021	0.0002	0	0
n,n-di-methyl-aniline	C8H11N	0	0	0	8	11			1	121.18	0	0	0	0.000	0.000	0.000	0	0	0	0	0
C3-pyridines	*C8H11N	0	0.2	0.3	8	11			1	121.18	0	1.7E-05	2.5E-05	0.000	0.134	0.325	9.9E-05	0.0001	0	0	1.2E-05
ethyl-aniline	*C8H11N	0	0	0.14	8	11			1	121.18	0	0	1.2E-05	0.000	0.000	0.152	4.2E-05	5.8E-05	0	0	5.2E-06
di-methyl-cyclohexane	C8H16-3	0	0.3	0	8	16				112.21	0	2.7E-05	0	0.000	0.217	0.000	1.5E-05	3E-05	0	0	0
n-octane	C8H18-1	0	1	0	8	18				114.23	0	8.8E-05	0	0.000	0.712	0.000	4.9E-05	0.0001	0	0	0
3-methyl-heptane	C8H18-3	0	0.2	0	8	18				114.23	0	1.8E-05	0	0.000	0.142	0.000	9.9E-06	2.2E-05	0	0	0
2,5-di-methyl-hexadiene	C8H18-5	0	0.5	0	8	18				114.23	0	4.4E-05	0	0.000	0.356	0.000	2.5E-05	5.6E-05	0	0	0
2,2-di-methyl-hexane	C8H18-8	0	0.3	0	8	18				114.23	0	2.6E-05	0	0.000	0.214	0.000	1.5E-05	3.3E-05	0	0	0
iso-quinoline	C9H7N-1	0	0	0	9	7			1	129.16	0	0	0	0.000	0.000	0.000	0	0	0	0	0
C4-pyridines	*C9H7N-1	0	0	0.63	9	13			1	135.21	0	0	4.7E-05	0.000	0.000	0.611	0.0002	0.0003	0	0	2.1E-05
tetra-hydro-quinone	*C9H7N-1	0	0	0.1	9	11			1	133.19	0	0	7.5E-06	0.000	0.000	0.098	3.1E-05	3.7E-05	0	0	3.4E-06
quinoline	C9H7N-2	0	0	1.42	9	7			1	129.16	0	0	0.0001	0.000	0.000	1.442	0.0004	0.0003	0	0	5E-05
alpha-methyl-styrene	C9H10	0	0	0	9	10				118.18	0	0	0	0.000	0.000	0.000	0	0	0	0	0
indan	*C9H10	0	0	0.3	9	10				118.18	0	0	2.5E-05	0.000	0.000	0.333	0.0001	0.0001	0	0	0
ethyl-benzoate	C9H10O2	0	0	0	9	10	2			150.18	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-methyl-guaiacol	*C9H10O2	0	0	0.1	9	12	2			152.19	0	0	6.6E-06	0.000	0.000	0.086	2.7E-05	3.6E-05	6E-06	0	0
n-propyl-benzene	C9H12-1	0	0.5	0	9	12				120.19	0	4.2E-05	0	0.000	0.338	0.000	2.6E-05	3.5E-05	0	0	0
1-methyl-2-ethyl-benzene	C9H12-3	0	0.5	0.43	9	12				120.19	0	4.2E-05	3.6E-05	0.000	0.338	0.469	0.0002	0.0002	0	0	0
1,2,4-tri-methyl-benzene	C9H12-7	0.1	0.4	0.2	9	12				120.19	8.3E-06	3.3E-05	1.7E-05	0.076	0.271	0.218	1E-04	0.0001	0	0	0
iso-phorone	C9H14O	0	0	0	9	14	1			136.21	0	0	0	0.000	0.000	0.000	0	0	0	0	0
C3-phenols	*C9H14O	1.5	0	2.1	9	12	1			136.19	0.0001	0	0.0002	1.011	0.000	2.023	0.0008	0.001	8.6E-05	0	0
naphthalene	C10H8	0.01	0.03	2.53	10	8				128.17	7.8E-07	2.3E-06	0.0002	0.007	0.019	2.589	0.0009	0.0007	0	0	0
m-divinyl-benzene	C10H10-1	0	0	0	10	10				130.19	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-methyl-benzo-furan	*C10H10-1	0	0	0.1	10	10	1			146.19	0	0	6.8E-06	0.000	0.000	0.090	3.1E-05	3.1E-05	3.1E-06	0	0
tetra-hydro-naphthalene	C10H12	0	0	0	10	12				132.2	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-indan	*C10H12	0	0	0.4	10	12				132.2	0	0	3E-05	0.000	0.000	0.397	0.0001	0.0002	0	0	0
tetralin	*C10H12	0	0	0.8	10	12				132.2	0	0	6.1E-05	0.000	0.000	0.794	0.0003	0.0003	0	0	0
sec-butyl-benzene	C10H14-3	0.1	0	0	10	14				134.22	7.5E-06	0	0	0.068	0.000	0.000	1.1E-05	1.5E-05	0	0	0
C4-benzene	*C10H14-3	0	0	1	10	14				134.22	0	0	7.5E-05	0.000	0.000	0.977	0.0003	0.0005	0	0	0
p-tert-butyl-phenol	C10H14O	0	0	0	10	14				134.22	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-benzo-furan	*C10H14O	0	0	0.3	9	8	1			132.16	0	0	2.3E-05	0.000	0.000	0.298	9.3E-05	8.2E-05	1E-05	0	0
C4-phenols	*C10H14O	0	0	0.7	10	14	1			150.22	0	0	4.7E-05	0.000	0.000	0.611	0.0002	0.0003	2.1E-05	0	0
p-tert-butyl-catechol	C10H14O2	0	0	0	10	14	2			166.22	0	0	0	0.000	0.000	0.000	0	0	0	0	0

Elemental Mole Balance

UND Case Average

		Weight %			Elements					Molecular	Phenol	Naphth	Tar oils	Phenol	Naphth	Tar oil	MOLAR FLOWS			(Kg mol/sec)	
COMPONENT	ALIAS	Phen	Naph	Tar	C	H	O	S	N	Weight	Weight	Weight	Weight	mol%	mol%	mol%	C	H	O	S	N
naphthol	*C10H14O2	1.1	0	0.5	10	8	1			144.17	7.6E-05	0	3.5E-05	0.700	0.000	0.455	0.0003	0.0002	2.7E-05	0	0
methyl-naphthol	*C10H14O2	1.1			11	10	1			158.2	7E-05	0	0	0.638	0.000	0.000	0.0001	0.0001	1E-05	0	0
n-decane	C10H22-1	0	0.4	0	10	22				142.28	0	2.8E-05	0	0.000	0.229	0.000	2E-05	4.4E-05	0	0	0
n-decyl-amine	C10H23N	0	0	0	10	23			1	157.3	0	0	0	0.000	0.000	0.000	0	0	0	0	0
C5-pyridine	*C10H23N	0	0	0.16	10	15			1	149.24	0	0	1.1E-05	0.000	0.000	0.141	4.9E-05	7.3E-05	0	0	4.9E-06
methyl-quinoline	*C10H23N	0	0	1.03	9	7			1	129.16	0	0	8E-05	0.000	0.000	1.046	0.0003	0.0003	0	0	3.6E-05
1-methyl-naphthalene	C11H10-1	0.1	0	0	11	10				142.2	7E-06	0	0	0.065	0.000	0.000	1.1E-05	1E-05	0	0	0
2-methyl-naphthalene	C11H10-2	0	0	5	11	10				142.2	0	0	0.0004	0.000	0.000	4.612	0.0018	0.0016	0	0	0
p-tert-amyl-phenol	C11H16O	0	0	0	11	16	1			164.25	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-naphthol	*C11H16O	0	0	0.4	11	10	1			158.2	0	0	2.5E-05	0.000	0.000	0.332	0.0001	0.0001	1.1E-05	0	0
hydroxy-C1-naphthalene	*C11H16O	0	0	3.21	11	10	1			158.2	0	0	0.0002	0.000	0.000	2.662	0.001	0.0009	9.2E-05	0	0
n-undecane	C11H24	0	0	0	11	24				156.31	0	0	0	0.000	0.000	0.000	0	0	0	0	0
C5-benzene	*C11H24	0	0	0.2	11	16				148.25	0	0	1.3E-05	0.000	0.000	0.177	6.7E-05	9.8E-05	0	0	0
di-benzo-pyrole	C12H9N	0	0	0	12	9			1	167.21	0	0	0	0.000	0.000	0.000	0	0	0	0	0
tri-methyl-quinoline	*C12H9N	0	0	0.5	12	13			1	171.24	0	0	2.9E-05	0.000	0.000	0.383	0.0002	0.0002	0	0	1.3E-05
indeno-pyridine	*C12H9N	0	0	0.1	12	9			1	167.21	0	0	6E-06	0.000	0.000	0.078	3.3E-05	2.4E-05	0	0	2.7E-06
di-phenyl	C12H10	0	0	1	12	10				154.21	0	0	6.5E-05	0.000	0.000	0.851	0.0004	0.0003	0	0	0
ace-naphthene	C12H10-2	0	0	0.95	12	10				154.21	0	0	6.2E-05	0.000	0.000	0.808	0.0003	0.0003	0	0	0
C2-naphthene	*C12H10-2	0	0	4.7	12	12				156.23	0	0	0.0003	0.000	0.000	3.946	0.0016	0.0016	0	0	0
di-phenyl-ether	C12H10O	0	0	0	12	10	1			170.21	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-benzo-furan	*C12H10O	0	0	2	12	8	1			168.19	0	0	0.0001	0.000	0.000	1.560	0.0006	0.0004	5.4E-05	0	0
di-phenyl-amine	C12H11N	0	0	0.16	12	11			1	169.23	0	0	9.5E-06	0.000	0.000	0.124	5.2E-05	4.7E-05	0	0	4.3E-06
di-methyl-quinoline	*C12H11N	0	0	0.6	11	11			1	157.21	0	0	3.8E-05	0.000	0.000	0.501	0.0002	0.0002	0	0	1.7E-05
phenyl-pyridine	*C12H11N	0	0	0.1	11	9			1	155.2	0	0	6.4E-06	0.000	0.000	0.085	3.2E-05	2.6E-05	0	0	2.9E-06
fluorene	C13H10	1	0	2	13	10				166.22	6E-05	0	0.0001	0.552	0.000	1.578	0.0008	0.0006	0	0	0
C1-aza-fluorene	*C13H10	0	0	0.1	13	11			1	181.24	0	0	5.5E-06	0.000	0.000	0.072	3.3E-05	2.8E-05	0	0	2.5E-06
di-hydro-fluorene	*C13H10	0	0	3	13	16				172.27	0	0	0.0002	0.000	0.000	2.284	0.001	0.0013	0	0	0
benzo-phenone	C13H10O	0	0	0	13	10	1			182.22	0	0	0	0.000	0.000	0.000	0	0	0	0	0
hydroxy-fluorene	*C13H10O	0	0	2.9	13	10	1			182.22	0	0	0.0002	0.000	0.000	2.088	0.0009	0.0007	7.2E-05	0	0
methyl-di-benzo-furan	*C13H10O	0	0	0.4	13	10	1			182.22	0	0	2.2E-05	0.000	0.000	0.288	0.0001	1E-04	1E-05	0	0
hydroxy-C2-naphthalene	*C13H10O	0	0	1.9	12	12	1			172.23	0	0	0.0001	0.000	0.000	1.447	0.0006	0.0006	5E-05	0	0
di-phenyl-methane	C13H12	0	0	0	13	12				168.24	0	0	0	0.000	0.000	0.000	0	0	0	0	0
tri-methyl-naphthalene	*C13H12	0	0	2.74	13	14				170.25	0	0	0.0002	0.000	0.000	2.111	0.0009	0.001	0	0	0
anthracene	C14H10-1	0.1	0	0.5	14	10				178.23	5.6E-06	0	2.8E-05	0.051	0.000	0.368	0.0002	0.0001	0	0	0
phen-anthrene	C14H10-2	0.1	0	2.1	14	10				178.23	5.6E-06	0	0.0001	0.051	0.000	1.546	0.0008	0.0005	0	0	0
trans-stilbene	C14H12-2	0	0	0	14	12				180.25	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-fluorene	*C14H12-2	0	0	3.6	14	12				180.25	0	0	0.0002	0.000	0.000	2.620	0.0013	0.0011	0	0	0

Elemental Mole Balance

UND Case Average

COMPONENT	ALIAS			Weight %					Elements			Molecular	Phenol	Naphth	Tar oils	Phenol	Naphth	Tar oil	MOLAR FLOWS			(Kg mol/sec)	
				Phen	Naph	Tar	C	H	O	S	N	Weight	Weight	Weight	Weight	mol%	mol%	mol%	C	H	O	S	N
n-tetradecane	C14H30			0	0	0.14	14	30				198.39	0	0	7.1E-06	0.000	0.000	0.093	4.5E-05	9.6E-05	0	0	0
p-cumo-phenol	C15H16O			0	0	0	15	16	1			212.29	0	0	0	0.000	0.000	0.000	0	0	0	0	0
benzo-quinoline	* C15H16O			0	0	0.34	13	9			1	179.22	0	0	1.9E-05	0.000	0.000	0.249	0.0001	7.8E-05	0	0	8.6E-06
n-pentadecane	C15H32			0	0	1	15	32				212.42	0	0	4.7E-05	0.000	0.000	0.618	0.0003	0.0007	0	0	0
methyl-phenanthrene	* C15H32			0.05	0	2.9	15	12				192.26	2.6E-06	0	0.0002	0.024	0.000	1.979	0.001	0.0008	0	0	0
fluor-anthene	C16H10-1			0	0	1	16	10				202.26	0	0	4.9E-05	0.000	0.000	0.649	0.0004	0.0002	0	0	0
hene-icosane	* C16H10-1			0	0	0.63	21	44				296.58	0	0	2.1E-05	0.000	0.000	0.279	0.0002	0.0004	0	0	0
pyrene	C16H10-2			0	0	0.1	16	10				202.26	0	0	4.9E-06	0.000	0.000	0.065	3.6E-05	2.2E-05	0	0	0
n-decyl-benzene	C16H26			0	0	0	16	26				218.38	0	0	0	0.000	0.000	0.000	0	0	0	0	0
di-hydro-pyrene	* C16H26			0	0	1.4	16	12				204.27	0	0	6.9E-05	0.000	0.000	0.899	0.0005	0.0004	0	0	0
n-hexadecane	C16H34			0	0	0.5	16	34				226.44	0	0	2.2E-05	0.000	0.000	0.290	0.0002	0.0003	0	0	0
crysene	C18H12			0	0	0.1	18	12				228.29	0	0	4.4E-06	0.000	0.000	0.057	3.6E-05	2.4E-05	0	0	0
methyl-crysene	* C18H12			0	0	0.6	19	14				242.32	0	0	2.5E-05	0.000	0.000	0.325	0.0002	0.0002	0	0	0
o-terphenyl	C18H14-1			0	0	0	18	14				230.31	0	0	0	0.000	0.000	0.000	0	0	0	0	0
benzo-anthracene	* C18H14-1			0	0	0.1	18	12				228.29	0	0	4.4E-06	0.000	0.000	0.057	3.6E-05	2.4E-05	0	0	0
benzo-pyrene	* C18H14-1			0	0	0.2	20	12				252.31	0	0	7.9E-06	0.000	0.000	0.104	7.2E-05	4.3E-05	0	0	0
benzo-fluor-anthene	* C18H14-1			0	0	0.1	20	12				252.31	0	0	4E-06	0.000	0.000	0.052	3.6E-05	2.2E-05	0	0	0
m-terphenyl	C18H14-2			0	0	0	18	14				230.31	0	0	0	0.000	0.000	0.000	0	0	0	0	0
methyl-fluor-anthene	* C18H14-2			0	0	2.1	17	12				217.72	0	0	9.6E-05	0.000	0.000	1.265	0.0007	0.0005	0	0	0
docosane	* C18H14-2			0	0	12	22	46				310.61	0	0	0.0004	0.000	0.000	5.068	0.0039	0.0081	0	0	0
tricosane	* C18H14-2			0	0	0.55	23	48				324.63	0	0	1.7E-05	0.000	0.000	0.222	0.0002	0.0004	0	0	0
tetracosane	* C18H14-2			0	0	0.45	24	50				338.66	0	0	1.3E-05	0.000	0.000	0.174	0.0001	0.0003	0	0	0
n-octadecane	C18H38			0	0	0.64	18	38				254.5	0	0	2.5E-05	0.000	0.000	0.330	0.0002	0.0004	0	0	0
n-nonadecane	C19H40			0	0	0.47	19	40				268.53	0	0	1.8E-05	0.000	0.000	0.230	0.0002	0.0003	0	0	0
n-eicosane	C20H42			0	0	0.46	20	42				282.55	0	0	1.6E-05	0.000	0.000	0.214	0.0001	0.0003	0	0	0
tetra-phenyl-ethylene	C26H20			0	0	0	26	20				332.44	0	0	0	0.000	0.000	0.000	0	0	0	0	0
pentacosane	* C26H20			0	0	0.48	25	52				352.69	0	0	1.4E-05	0.000	0.000	0.179	0.0002	0.0003	0	0	0
hexacosane	* C26H20			0	0	0.33	26	54				366.71	0	0	9E-06	0.000	0.000	0.118	0.0001	0.0002	0	0	0
heptacosane	* C26H20			0	0	0.61	27	56				380.74	0	0	1.6E-05	0.000	0.000	0.210	0.0002	0.0004	0	0	0
octacosane	* C26H20			0	0	0.35	28	58				394.77	0	0	8.9E-06	0.000	0.000	0.116	0.0001	0.0002	0	0	0
nonacosane	* C26H20			0	0	0.01	29	60				408.79	0	0	2.4E-07	0.000	0.000	0.003	3.2E-06	6.7E-06	0	0	0
TOTAL DRY		96.30	99.	96.3	99.42	97.29																	
WATER	H2O	3.70	0.	3.7	0.58	2.71		2	1			18.015	0.0021	0.0003	0.0015	18.845	2.618	19.732	0	0.002	0.001	0	0
TOTAL WET		100.00	10	100	100	100						Average Molecular Weight =	91.758	81.329	131.17	100	100	100					

RESULTS

	MOLAR FLOWS			(Kg mol/sec)	
	C	H	O	S	N
Condensable Volatile Molar Flows(Kg mol/s	0.046	0.056	0.0036	9E-05	0.000
Total Volatile Molar Flows (Kg mol/s)	0.136	0.379	0.0972	0.003	0.005
Non-Condesable Volatile Flows (Kgmol/s)	0.09	0.323	0.0937	0.002	0.005
LB MOL/HR	717.4	2563	743.33	19.36	40.04

* NOTE: The molecular formulas indicated with an asterisk (*) are DIPPR alias' available in ASPEN/SP. The actual molecular formula can be determined from the Elements column.

Component	Mass Flow LB/HR	WT %	Mol Flow LB MOL/HR
CH4	5754	19.451%	358.6
CO	5667	19.157%	202.3
CO2	2968	10.033%	67.43
C2H6	857.2	2.898%	28.51
C3H8	153.9	0.520%	3.491
H2	35.34	0.119%	17.53
H2S	659.6	2.230%	19.36
N2	560.9	1.896%	20.02
C2H4	130.6	0.441%	4.654
C3H6	171.4	0.579%	4.073
H2O	7317	24.737%	406.2
Coal gas (dry)	16957	57.326%	726
Phenol	1144	3.866%	
Naphtha	559.5	1.891%	
Tar Oil	3603	12.180%	
TOTAL Volatiles (wet	29579	100%	

Elemental Mole Balance **UND Case Low**

Coal Flow = 12.63
Proxanal = 35.65 46.28 44.19 9.53
Ultanal = 9.55 65.86 4.51 0.95 0 0.99 18

UND Case Low
Tar-rec Coal Flow = 0.0183
Proxanal 11.69 11.05 10.55 78.4
Ultanal = 78.4 15.72 1.08 0.23 0 0.24 4.33

Fraction Volatile Matter Released by Pyrolysis =	1	Total Mass Flow =	3.5932 Kg/s
Mass Fraction of Phenol in Volatile Matter =	0.046	Phenol	0.1654 Kg/s
Mass Fraction of Naphtha in Volatile Matter =	0.0183	Naphtha	0.0658 Kg/s
Mass Fraction of Tar Oils in Volatile Matter =	0.1039	Tar Oils	0.3733 Kg/s

Table 1 -- Composition of Volatiles
Actual Compositions

COMPONENT	DIPPR ALIAS	Phenol %wt	Naphtha %wt	Weight % Phen	Weight % Naph	Tar	C	H	O	S	N		Phenol Weight	Naphth Weight	Tar oils Weight	Phenol mol%	Naphth mol%	Tar oil mol%	MOLAR FLOWS (Kg mol/sec) C	H	O	S	N
methyl-mercaptan	CH4S		0.1	0	0.17	0	1	4		1		48.103	0	3.5E-05	0	0.000	0.287	0.000	2.3E-06	9.3E-06	0	2.3E-06	0
methanol	CH4O		0.15	0	0.15	0	1	4	1			32.042	0	4.7E-05	0	0.000	0.381	0.000	3.1E-06	1.2E-05	3.1E-06	0	0
acetonitrile	C2H3N		0.11	0	0.11	0.01	2	3			1	41.052	0	2.7E-05	2.4E-06	0.000	0.218	0.032	5.3E-06	8E-06	0	0	2.7E-06
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"
heptacosane	* C26H20			0	0	0.61	27	56				380.74	0	0	1.6E-05	0.000	0.000	0.210	0.0002	0.0003	0	0	0
octacosane	* C26H20			0	0	0.35	28	58				394.77	0	0	8.9E-06	0.000	0.000	0.116	9.3E-05	0.0002	0	0	0
nonacosane	* C26H20			0	0	0.01	29	60				408.79	0	0	2.4E-07	0.000	0.000	0.003	2.6E-06	5.5E-06	0	0	0
TOTAL DRY		96.30	99.42	96.3	99.4	97.3																	
WATER	H2O	3.70	0.58	3.7	0.58	2.71		2	1			18.015	0.0021	0.0003	0.0015	18.845	2.618	19.732	0	0.0018	0.0009	0	0
TOTAL WET		100.00	100.	100	100	100						Average Molecular Weight	91.758	81.329	131.17	100	100	100					

	MOLAR FLOWS C	H	O	(Kg mol/sec) S	N
Condensable Volatile Molar Flows(Kg mol/s)	0.0409	0.0502	0.0035	7.9E-05	0.0002
Total Volatile Molar Flows (Kg mol/s)	0.1323	0.3638	0.0922	0.0025	0.0055
Non-Condesable Volatile Flows (Kgmol/s)	0.0914	0.3136	0.0886	0.0024	0.0053
LB MOL/HR	725.64	2489.3	703.55	19.298	41.96

* NOTE: The molecular formulas indicated with an asterisk (*) are DIPPR alias' available in ASPEN/SP. The actual molecular formula can be determined from the Elements column.

Component	Mass Flow LB/HR	WT %	LB MOL/HR
CH4	5888.3	20.672%	367.04
CO	5802.3	20.370%	207.15
CO2	3038.9	10.668%	69.05
C2H6	837.3	2.939%	27.846
C3H8	150.35	0.528%	3.4097
H2	38.926	0.137%	19.311
H2S	657.59	2.309%	19.298
N2	587.73	2.063%	20.98
C2H4	111.6	0.392%	3.9779
C3H6	119.57	0.420%	2.8414
H2O	6454.9	22.661%	358.3
Coal gas (dry)	17233	60.498%	740.9
Phenol	1312.5	4.608%	
Naphtha	521.93	1.832%	
Tar Oil	2962.7	10.401%	
TOTAL Volatiles (wet)	28485	100.00%	

Elemental Mole Balance **UND Case High**

Coal Flow = 13.389
Proxanal = 36.2 46.67 43.75 9.58
Ultanal = 9.62 65.65 4.53 1 0 1.08 18

UND Case High
Tar-rec Coal Flow = 0.0198
Proxanal 13.71 13.06 12.24 74.7
Ultanal = 74.7 18.37 1.27 0.28 0 0.3 5.07

Fraction Volatile Matter Released by Pyrolysis =	1	Total Mass Flow =	3.7392 Kg/s we
Mass Fraction of Phenol in Volatile Matter =	0.0375	Phenol	0.1403 Kg/s we
Mass Fraction of Naphtha in Volatile Matter =	0.0201	Naphtha	0.075 Kg/s we
Mass Fraction of Tar Oils in Volatile Matter =	0.1333	Tar Oils	0.4983 Kg/s we

Table 1 -- Composition of Volatiles
Actual Compositions

COMPONENT	DIPPR ALIAS	Phenol %wt	Naphtha %wt	Weight % Phen	Weight % Naph	Weight % Tar	C	H	O	S	N		Phenol Weight	Naphth Weight	Tar oils Weight	Phenol mol%	Naphth mol%	Tar oil mol%	MOLAR FLOWS (Kg mol/sec) C	H	O	S	N
methyl-mercaptan	CH4S		0.1	0	0.17	0	1	4		1		48.103	0	3.5E-05	0	0.000	0.287	0.000	2.6E-06	1.1E-05	0	2.6E-06	0
methanol	CH4O		0.15	0	0.15	0	1	4	1			32.042	0	4.7E-05	0	0.000	0.381	0.000	3.5E-06	1.4E-05	3.5E-06	0	0
acetonitrile	C2H3N		0.11	0	0.11	0.01	2	3			1	41.052	0	2.7E-05	2.4E-06	0.000	0.218	0.032	6.4E-06	9.7E-06	0	0	3.2E-06
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	"
heptacosane	* C26H20			0	0	0.61	27	56				380.74	0	0	1.6E-05	0.000	0.000	0.210	0.0002	0.0004	0	0	0
octacosane	* C26H20			0	0	0.35	28	58				394.77	0	0	8.9E-06	0.000	0.000	0.116	0.0001	0.0003	0	0	0
nonacosane	* C26H20			0	0	0.01	29	60				408.79	0	0	2.4E-07	0.000	0.000	0.003	3.5E-06	7.3E-06	0	0	0
TOTAL DRY		96.30	99.42	96.3	99.4	97.3																	
WATER	H2O	3.70	0.58	3.7	0.58	2.71		2	1			18.015	0.0021	0.0003	0.0015	18.845	2.618	19.732	0	0.0021	0.0011	0	0
TOTAL WET		100.00	100.	100	100	100						Average Molecular Weight	91.758	81.329	131.17	100	100	100					

	MOLAR FLOWS (Kg mol/sec) C	H	O	S	N
Condensable Volatile Molar Flows(Kg mol/s)	0.0488	0.0601	0.0037	1E-04	0.0003
Total Volatile Molar Flows (Kg mol/s)	0.1348	0.3841	0.0968	0.0029	0.0061
Non-Condesable Volatile Flows (Kgmol/s)	0.086	0.324	0.0931	0.0028	0.0058
LB MOL/HR	682.74	2571.6	738.73	22.06	46.153

* NOTE: The molecular formulas indicated with an asterisk (*) are DIPPR alias' available in ASPEN/SP. The actual molecular formula can be determined from the Elements column.

Component	Mass Flow LB/HR	WT %	LB MOL/HR
CH4	5447.3	18.385%	339.55
CO	5117.5	17.272%	182.7
CO2	2680.2	9.046%	60.9
C2H6	905.79	3.057%	30.123
C3H8	243.98	0.823%	5.5329
H2	30.558	0.103%	15.159
H2S	751.71	2.537%	22.06
N2	646.47	2.182%	23.077
C2H4	137.97	0.466%	4.9181
C3H6	181.09	0.611%	4.3033
H2O	7822.8	26.403%	434.23
Coal gas (dry)	16142	54.484%	688.32
Phenol	1113.3	3.758%	
Naphtha	595.04	2.008%	
Tar Oil	3954.5	13.347%	
TOTAL Volatiles (wet)	29628	100.00%	

APPENDIX E

Differental Scanning Calorimeter Data Sets

To: Dr. J. Erjavec September 14, 1992

From: R. Timpe

RE: PDSC of GPGP lignite samples

Pressure Differential Scanning Calorimetry (PDSC) of GPGP Lignite

The samples of lignite analyzed (0200B, 1400G, 2200G, 1000N) were from a suite of six grab samples of lignite selected for a previous feed characterization study.

Method:

The tests were carried out in a DuPont PDSC cell under nitrogen gas at 900 psig. The temperature ramp was 10°C/min to 550°C (maximum temperature recommended for cell).

Data was collected from a blank, standard sapphire, and lignite.

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DSC Standard                                        09/02/92 16:35:43  Page  1

File:  A:ERJAV.005         Run Date:  27-Aug-92 09:03
Program:  DSC V4.0B        Run Number:  95

DuPont 2100 Thermal Analysis -- DSC

Sample:      SAPPHIRE FOR ERJAVEC'S PDSC
Size:       21.2000 mg
Cell Constant:   1.2013
Operator:    KULAS
Method:      DSC
Comment:     SAPPHIRE  FOR GREAT PLAIN COAL STUDY; A#4886

Peak  Start    Onset     Max     Stop       Area
        °C       °C       °C       °C
      31.36    32.07    38.92   570.59    164.9 J/g
      37.06            529.78   566.52    23.15 J/g
     110.72   111.72   143.89   330.80    7.446 J/g
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DSC Standard                                      09/04/92 10:57:58  Page  1

File:  A:ERJAV.105          Run Date:  4-Sep-92  08:29
Program:  DSC V4.0B         Run Number:  102

DuPont 2100 Thermal Analysis -- DSC

Sample:      PDSC OF GP 0200BAD 9/4/93
Size:       11.1000 mg
Cell Constant:   1.2013
Operator:    KULAS
Method:      DSC
Comment:     PDSC OF GP 0200BAD - ERJAVEC'S PDSC STUDY; A#4886

Peak   Start    Onset     Max     Stop       Area
         °C       °C       °C       °C
       21.96    21.97   261.74   579.65   1190. J/g
       26.40   206.25   262.76   566.52   524.3 J/g
      110.72   208.10   262.76   330.80   534.7 J/g
```

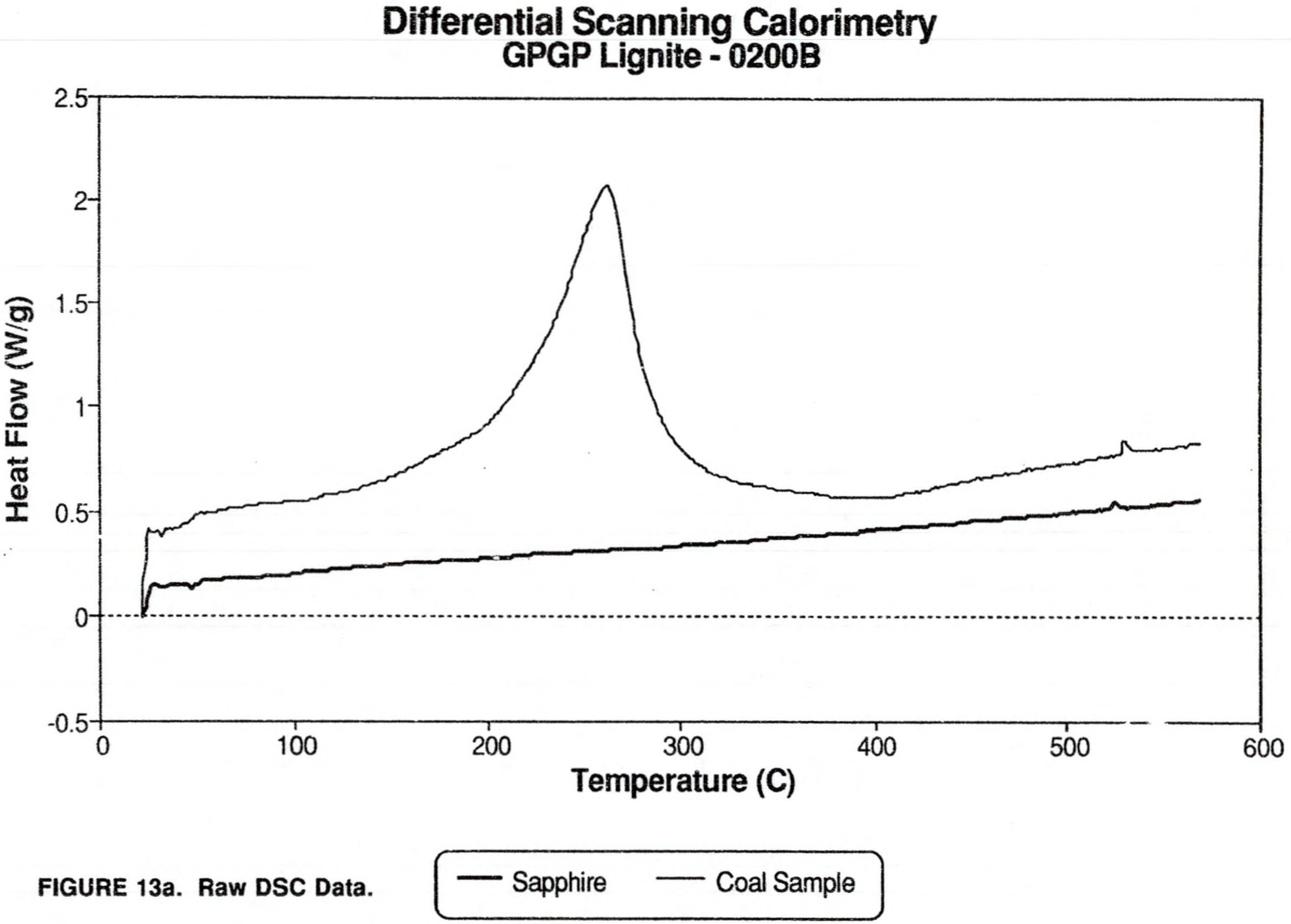


FIGURE 13a. Raw DSC Data.

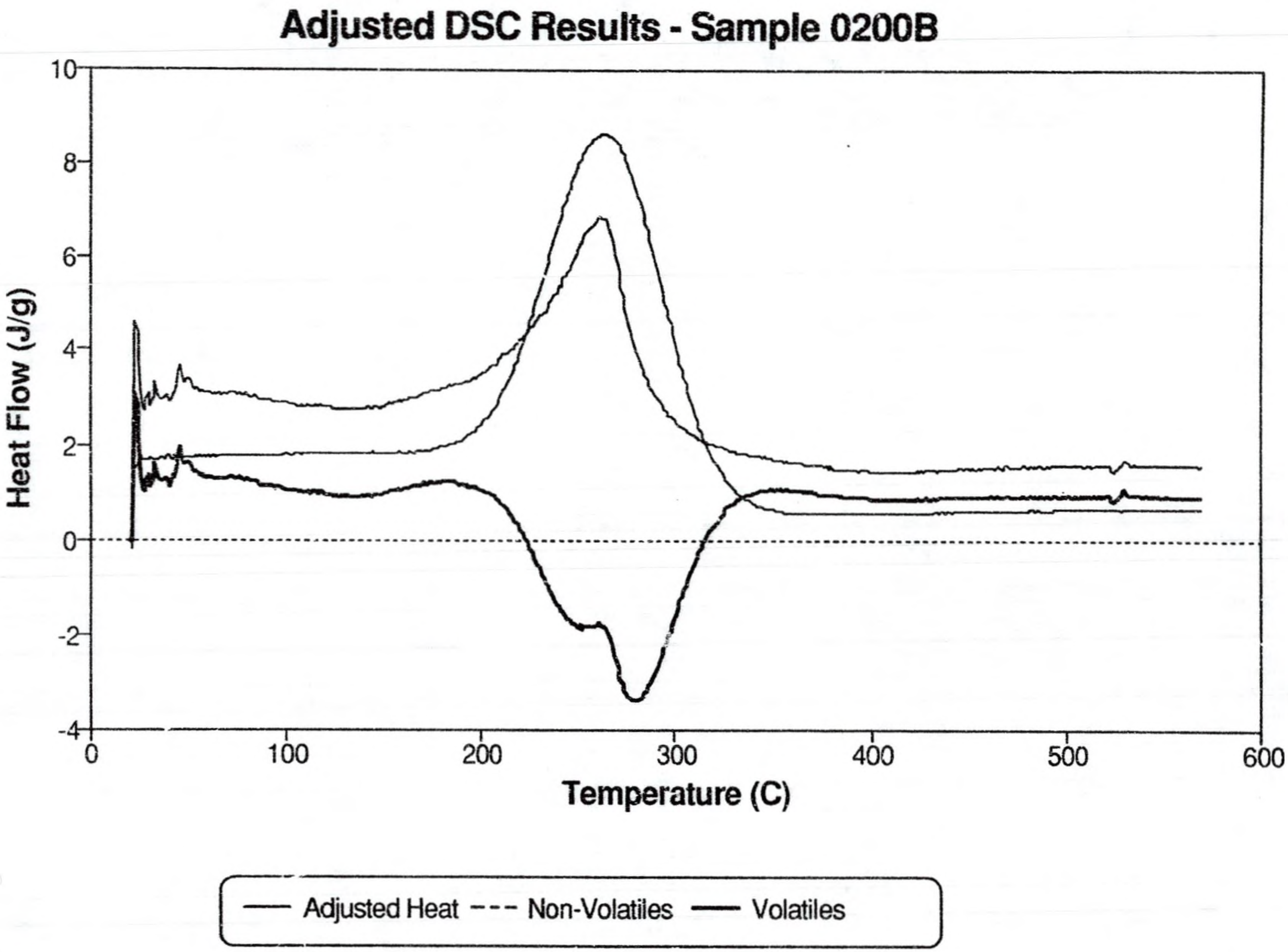
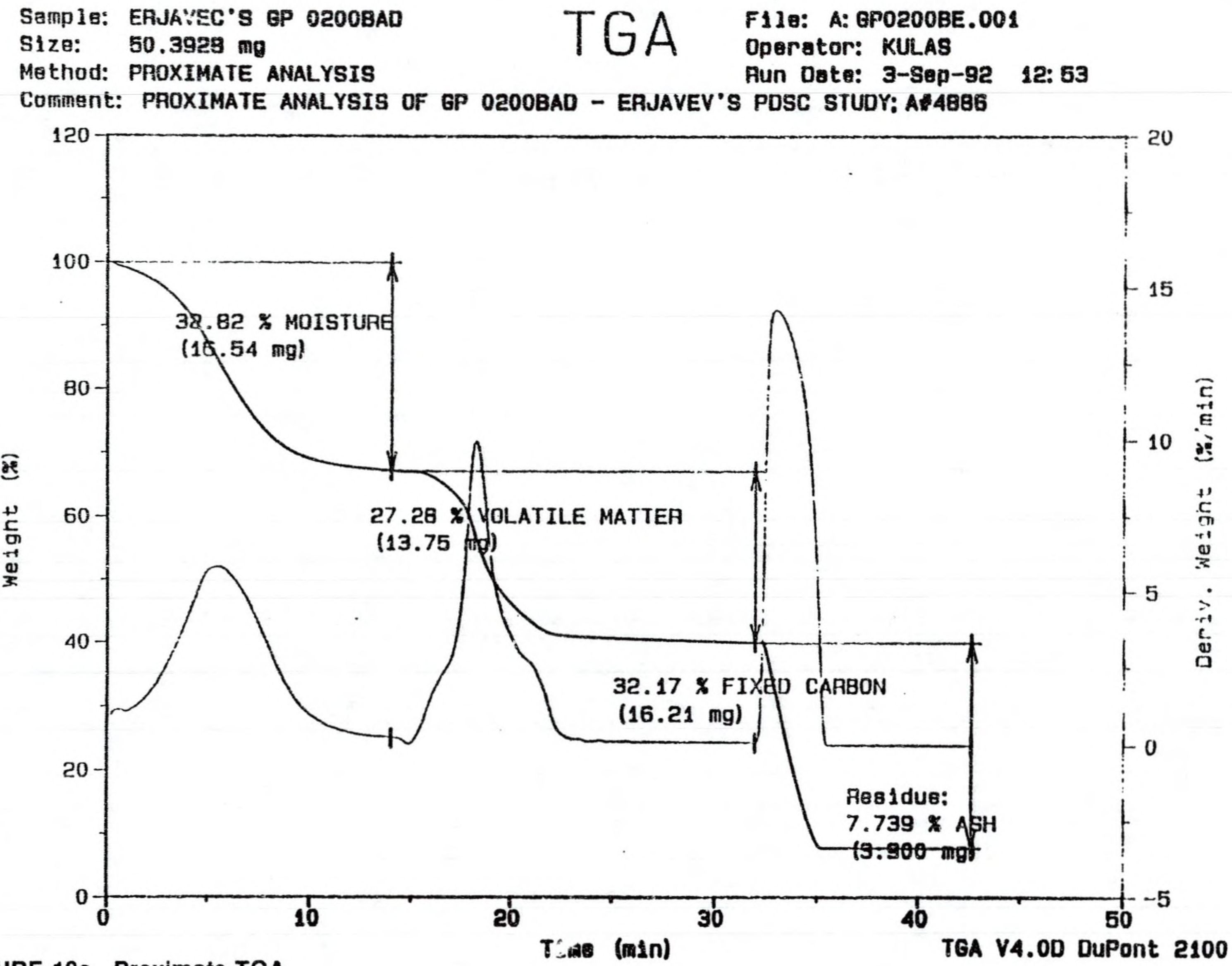


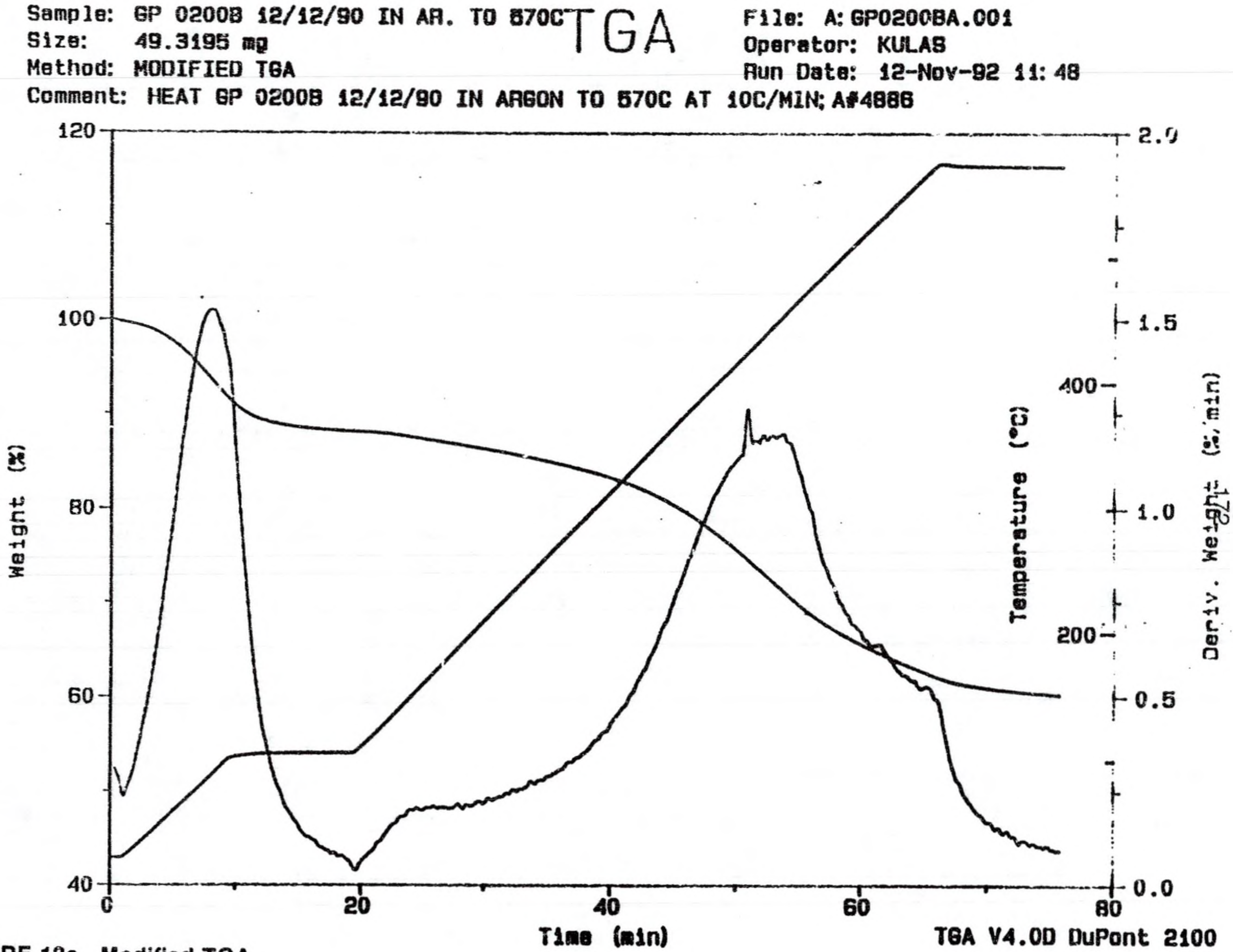
FIGURE 13b. Adjusted DSC Data.



Sample: ERJAVEC'S GP 0200BAD
Size: 50.3928 mg
Method: PROXIMATE ANALYSIS
Comment: PROXIMATE ANALYSIS OF GP 0200BAD - ERJAVEV'S PDSC STUDY; A#4886

File: A: GP0200BE.001
Operator: KULAS
Run Date: 3-Sep-92 12:53

FIGURE 13c. Proximate TGA.



Sample: GP 0200B 12/12/90 IN AR. TO 570C
Size: 49.3195 mg
Method: MODIFIED TGA
Comment: HEAT GP 0200B 12/12/90 IN ARGON TO 570C AT 10C/MIN; A#4886
File: A: GP0200BA.001
Operator: KULAS
Run Date: 12-Nov-92 11: 48

FIGURE 13c. Modified TGA.

```
DSC Standard                                       09/04/92 10:35:29  Page  1

File:  A:ERJAV.103        Run Date:  3-Sep-92   12:19
Program:  DSC V4.0B       Run Number:  100

DuPont 2100 Thermal Analysis -- DSC

Sample:       PDSC OF GP 1000N 9/3/92
Size:        11.5000 mg
Cell Constant:   1.2013
Operator:     KULAS
Method:       DSC
Comment:      PDSC OF GP 1000N FOR ERJAVEC'S PDSC STUDY; A#4686

Peak  Start   Onset    Max     Stop        Area
        °C      °C      °C      °C
      31.99   32.89  262.38  577.55    1043. J/g
      37.35  209.22  263.40  566.52    616.6 J/g
     110.72  211.70  263.40  330.80    560.4 J/g
```

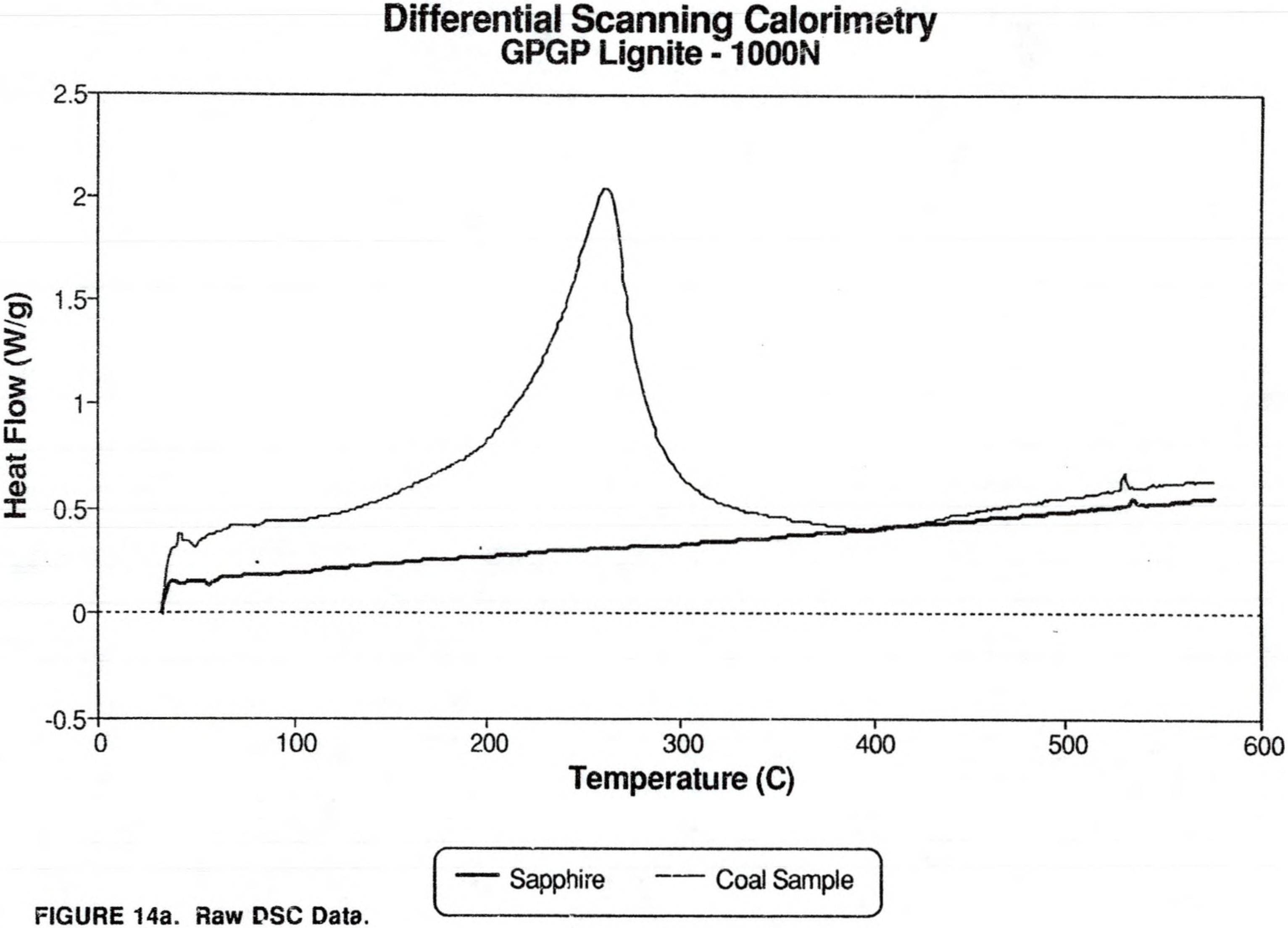


FIGURE 14a. Raw DSC Data.

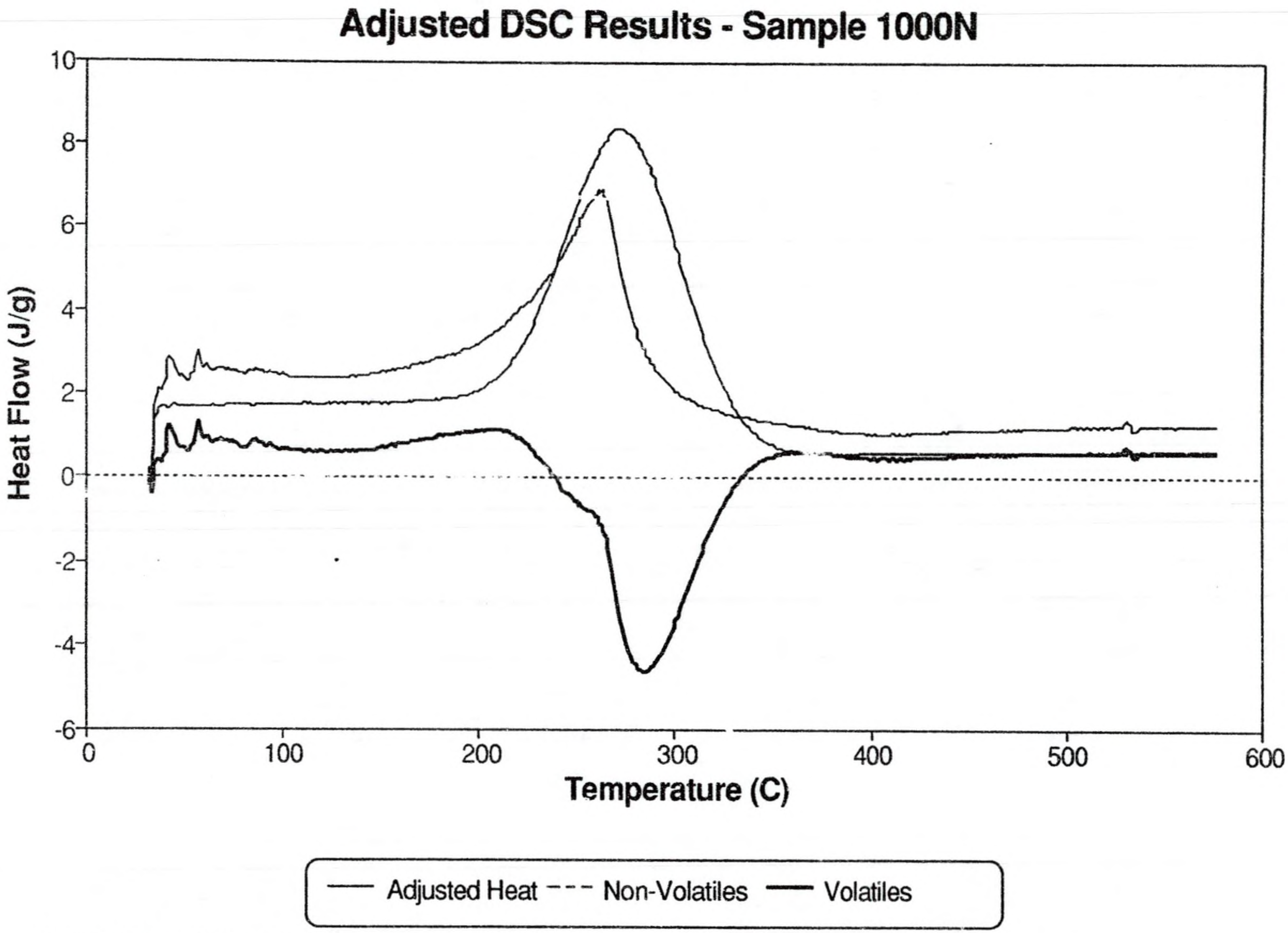
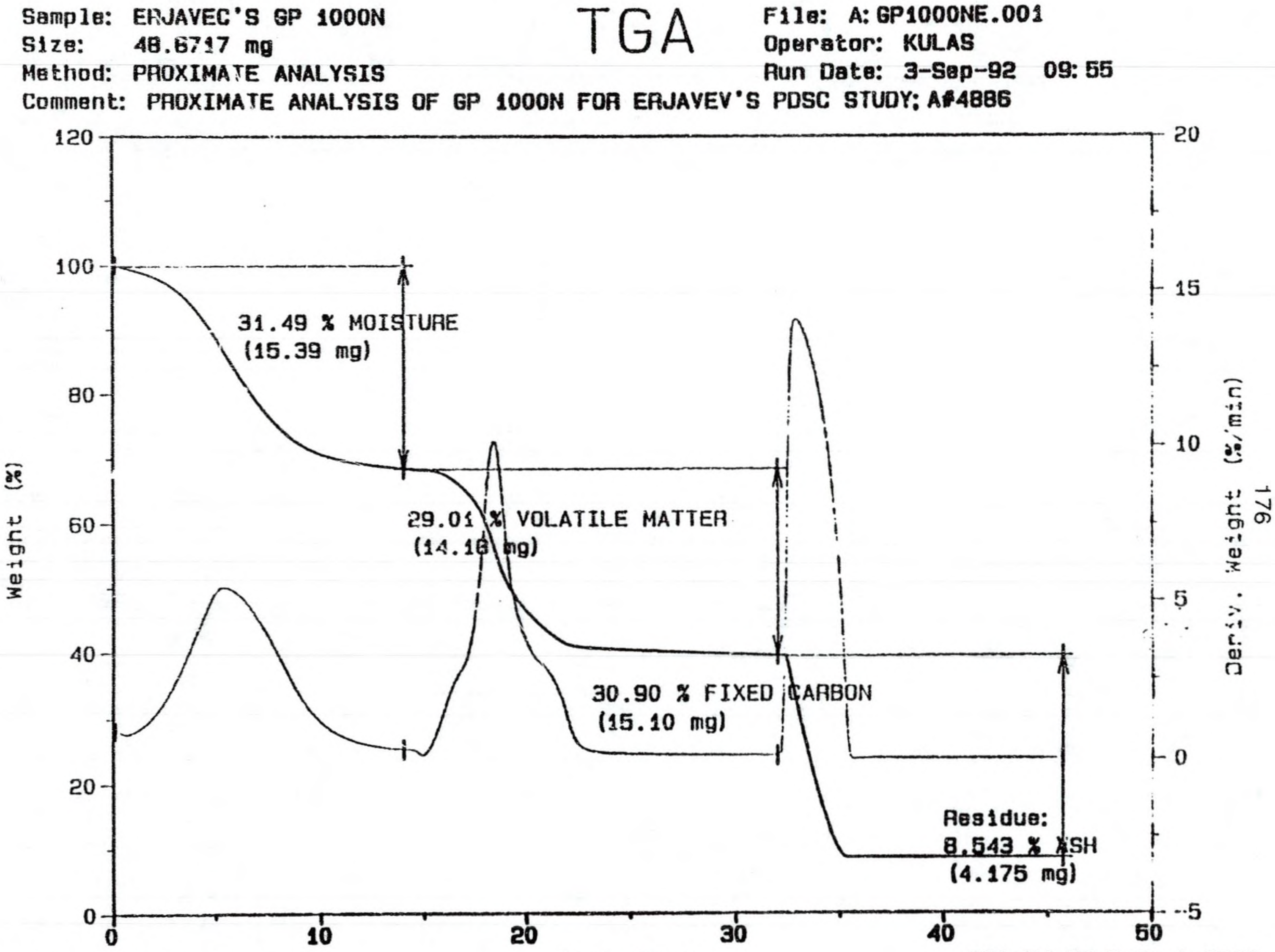


FIGURE 14 b Adjusted DSC Data.



Sample: ERJAVEC'S GP 1000N
Size: 48.6717 mg
Method: PROXIMATE ANALYSIS
Comment: PROXIMATE ANALYSIS OF GP 1000N FOR ERJAVEV'S PDSC STUDY; A#4886

File: A: GP1000NE.001
Operator: KULAS
Run Date: 3-Sep-92 09:55

FIGURE 14c. Proximate TGA.

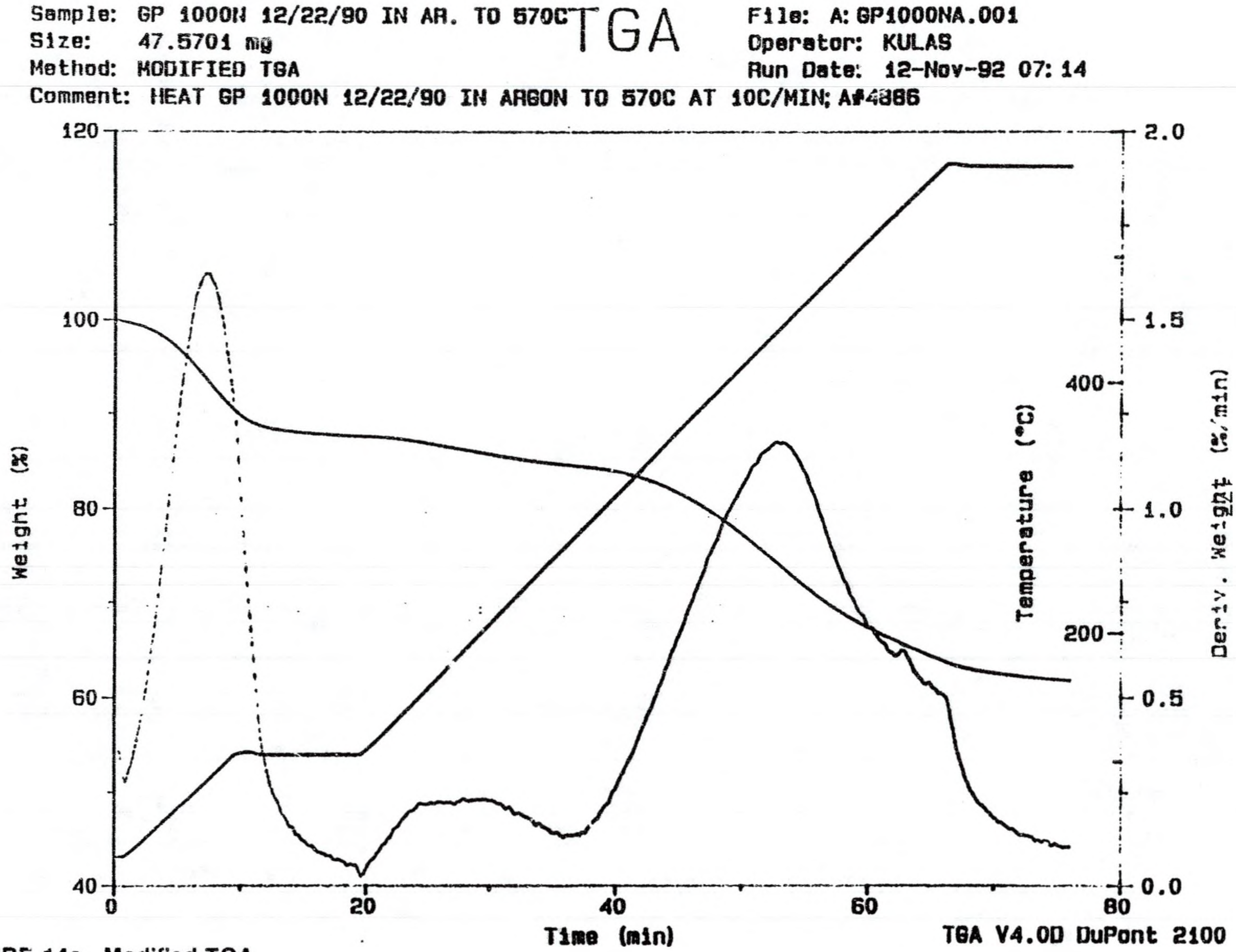


FIGURE 14c. Modified TGA.

```
DSC Standard                                          09/02/92 16:27:49  Page  1

File:  A:ERJAV.006          Run Date:  27-Aug-92 10:33
Program:  DSC V4.0B         Run Number:  96

DuPont 2100 Thermal Analysis -- DSC

Sample:      PDSC OF GP 1600N
Size:       10.4000 mg
Cell Constant:   1.2013
Operator:    KULAS
Method:      DSC
Comment:     PDSC OF GREAT PLAINS'1600N FOR ERJAVEC;  A#4886

Peak   Start    Onset     Max     Stop       Area
        °C       °C       °C       °C
       30.36    30.66   259.80   576.90    963.5 J/g
       37.06   207.26   259.80   566.52    486.1 J/g
      110.72   208.75   259.80   330.80    503.8 J/g
```

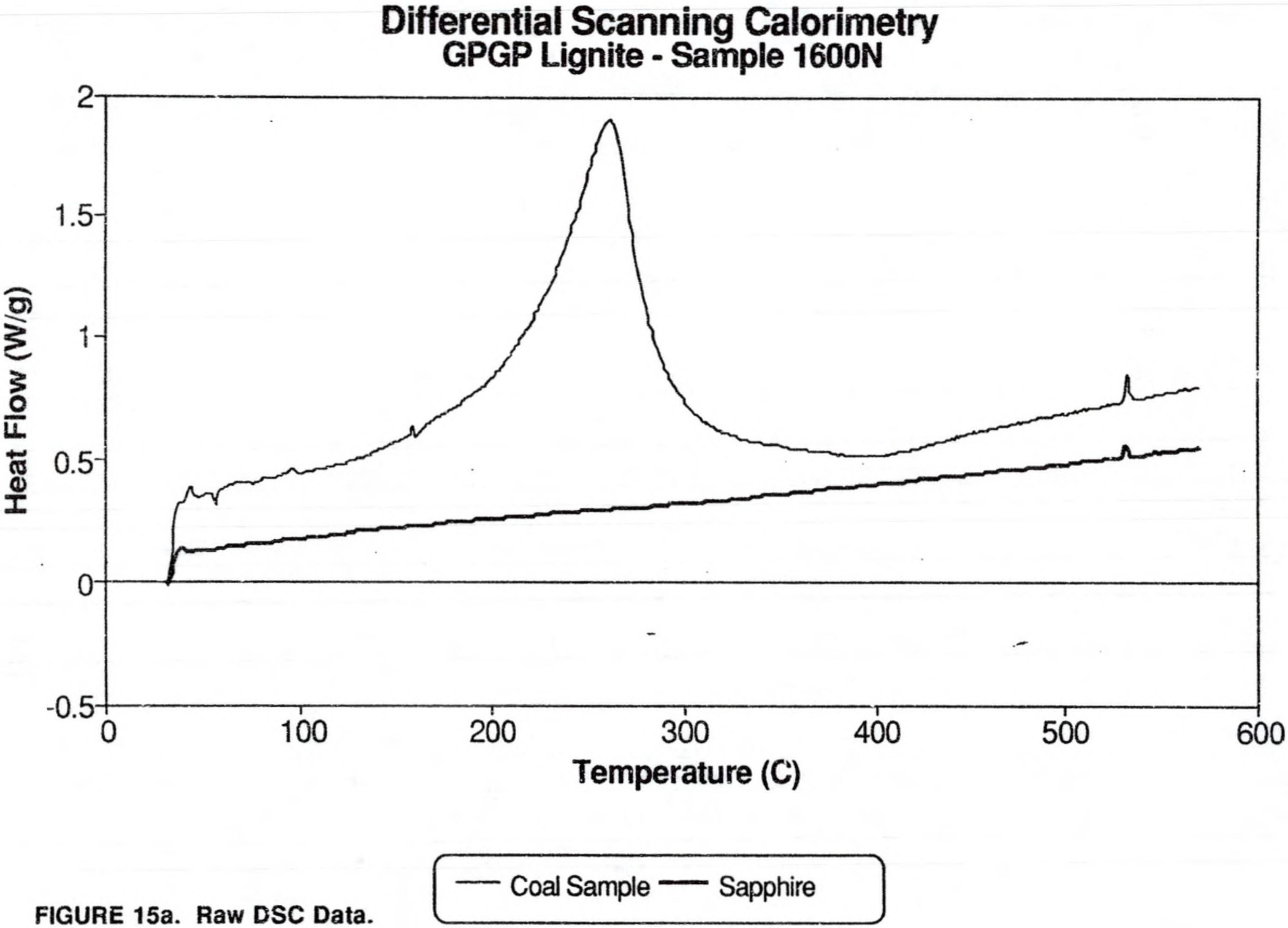


FIGURE 15a. Raw DSC Data.

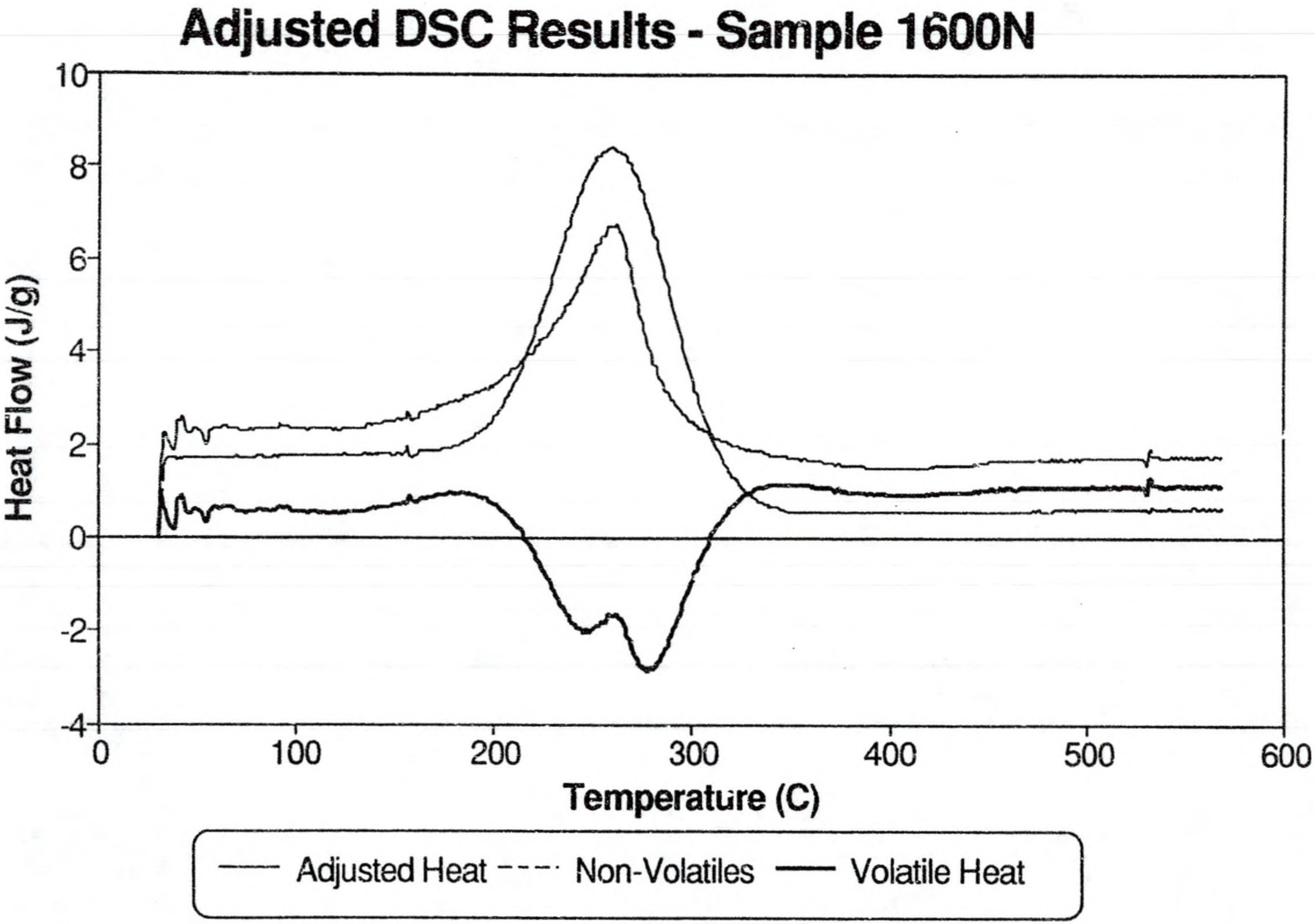


FIGURE 15b. Adjusted DSC Data.

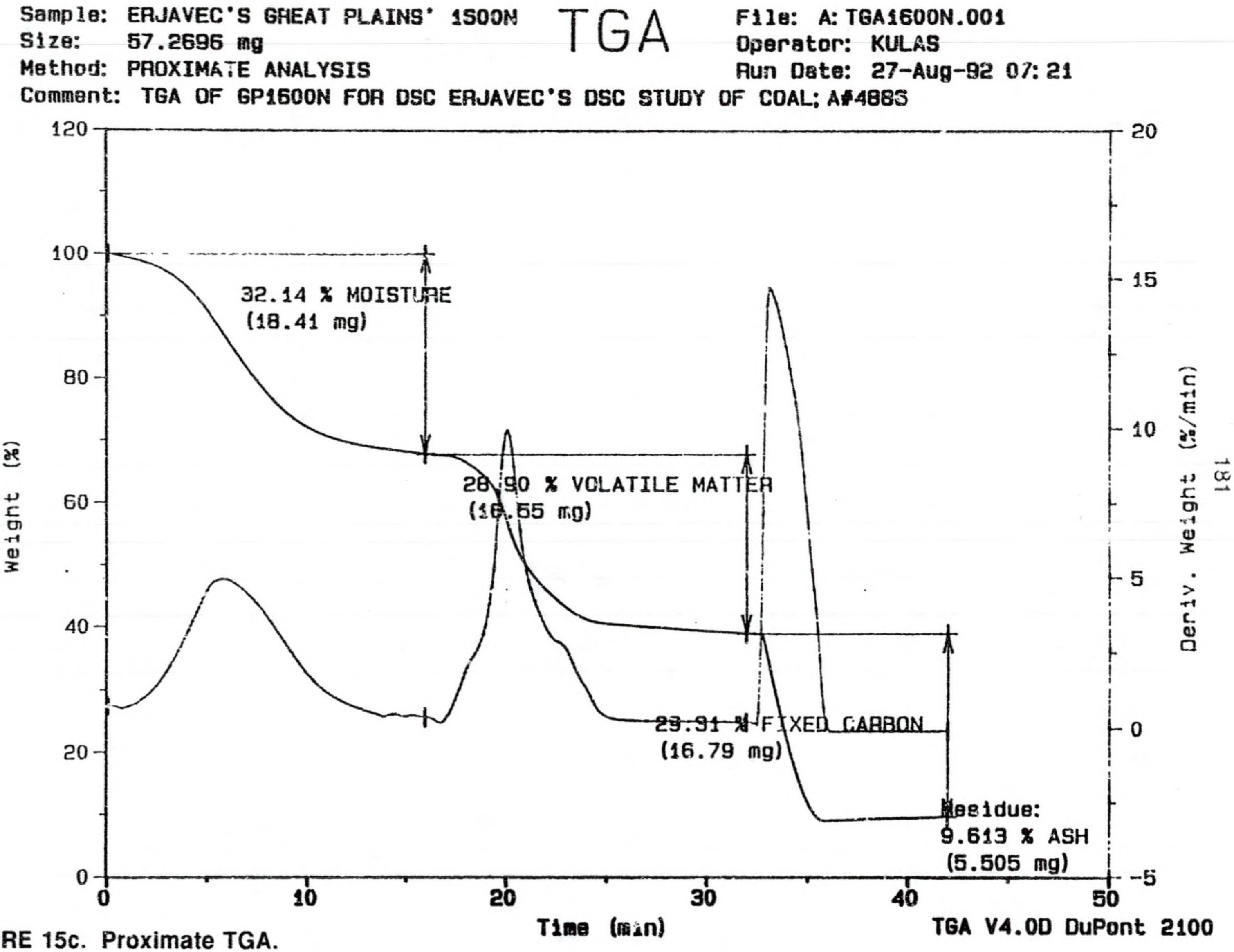
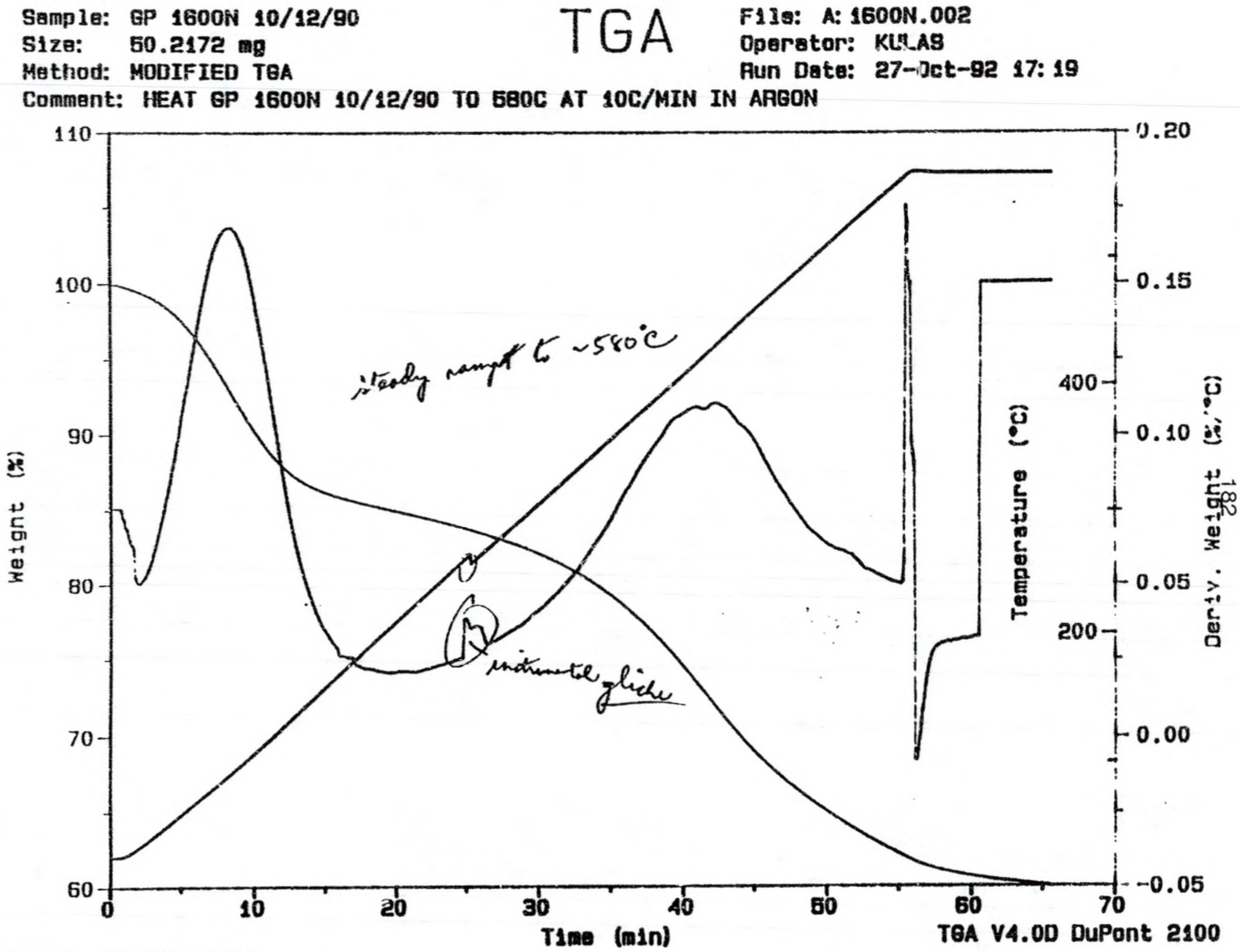


FIGURE 15c. Proximate TGA.



Sample: GP 1600N 10/12/90
Size: 50.2172 mg
Method: MODIFIED TGA
Comment: HEAT GP 1600N 10/12/90 TO 580C AT 10C/MIN IN ARGON

File: A:1600N.002
Operator: KULAS
Run Date: 27-Oct-92 17:19

steady ramp to ~580°C

instrumental glitch

FIGURE 15c. Modified TGA.

```
DSC Standard                                        09/04/92 10:49:09  Page  1

File:  A:ERJAV.104         Run Date:  3-Sep-92   13:43
Program:  DSC V4.0B        Run Number:  101

DuPont 2100 Thermal Analysis -- DSC

Sample:     PDSC OF GP 1400G 9/3/92
Size:     11.7000 mg
Cell Constant:   1.2013
Operator:   KULAS
Method:     DSC
Comment:    PDSC OF GP 1400G FOR ERJAVEC'S PDSC STUDY; A#4886

Peak   Start    Onset     Max     Stop        Area
         °C       °C       °C       °C
       31.48    32.28   263.64   578.80    964.8 J/g
       38.40   213.29   263.64   566.52    573.1 J/g
      110.72   215.59   263.64   330.80    524.7 J/g
```

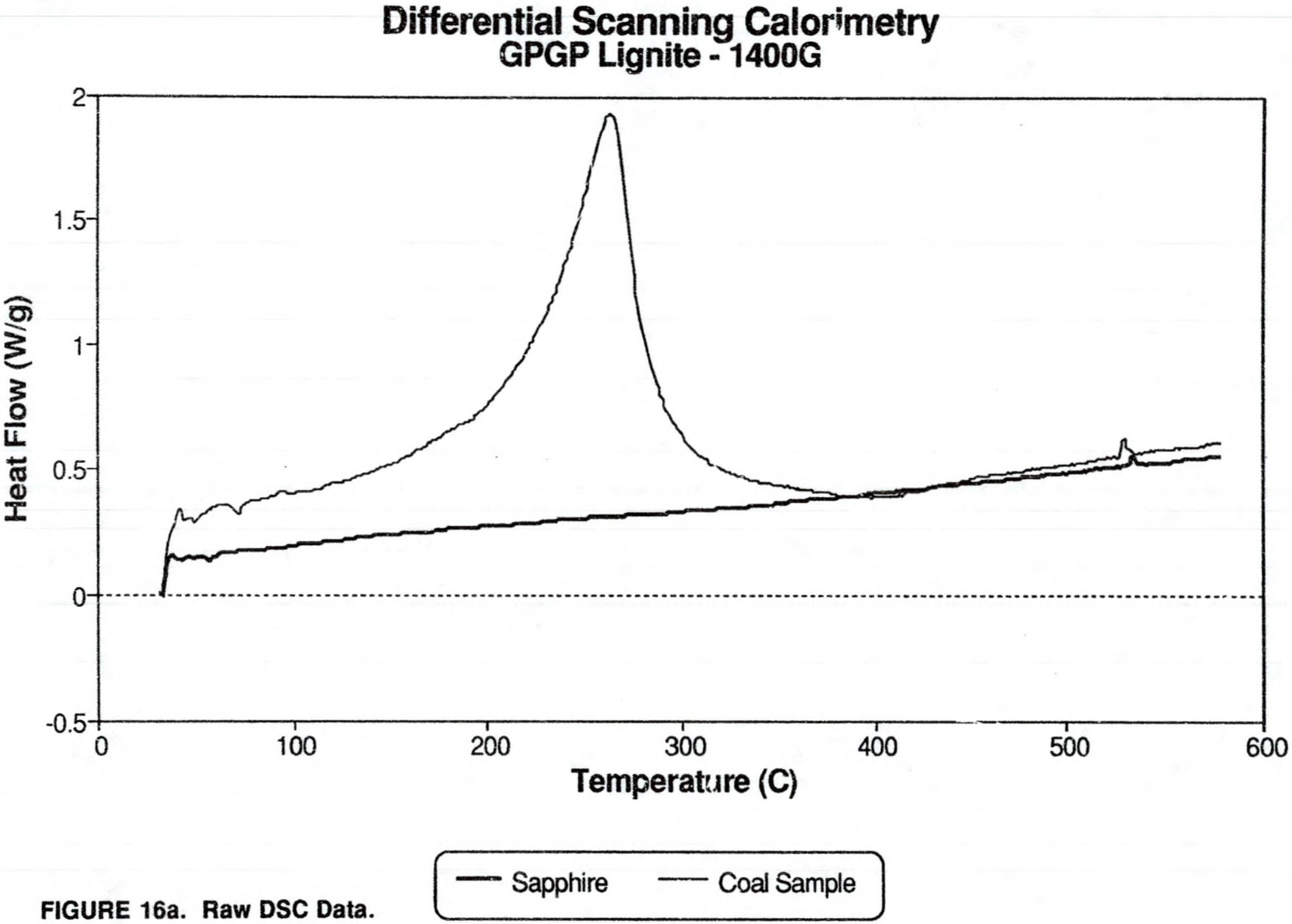


FIGURE 16a. Raw DSC Data.

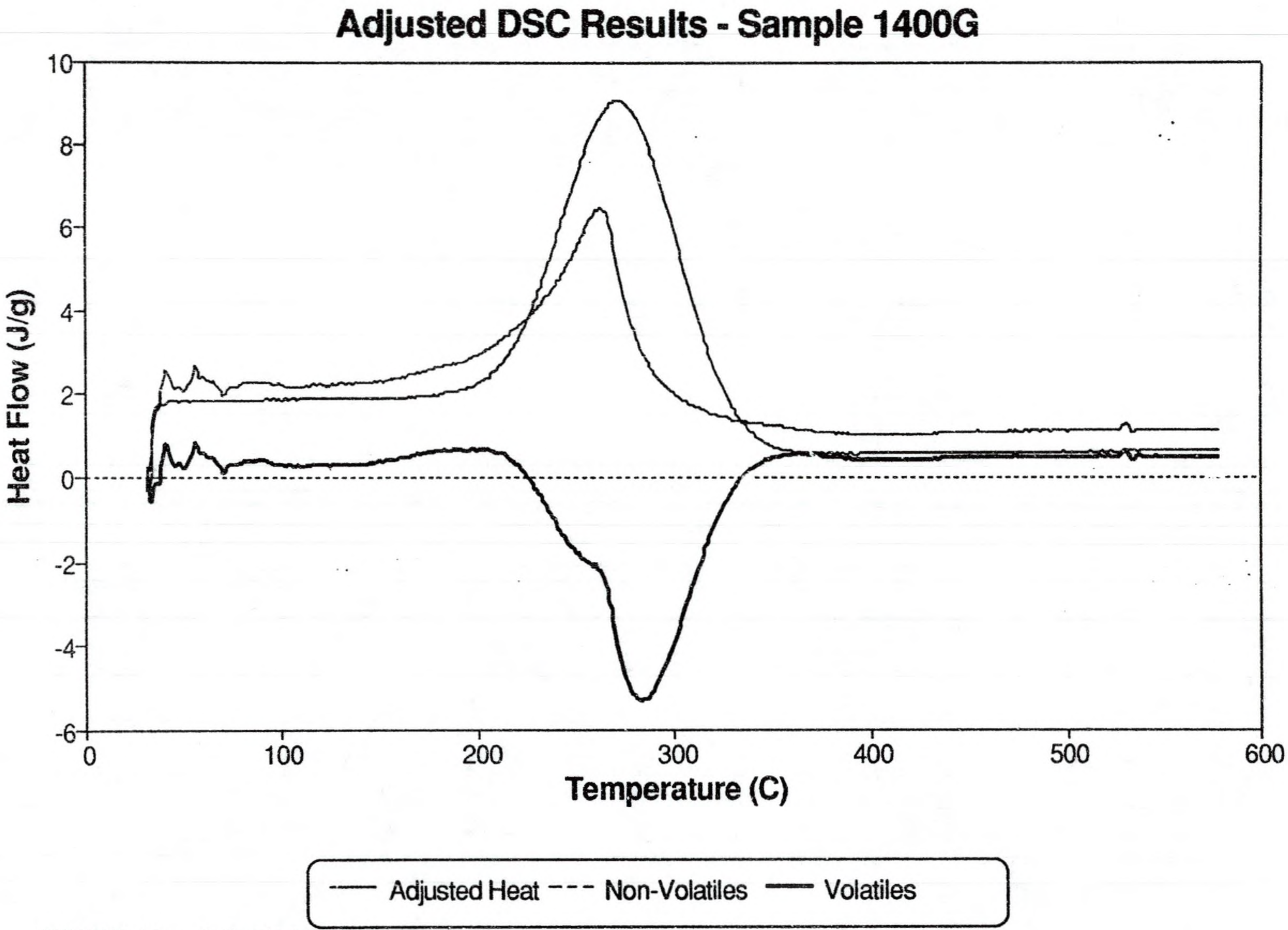
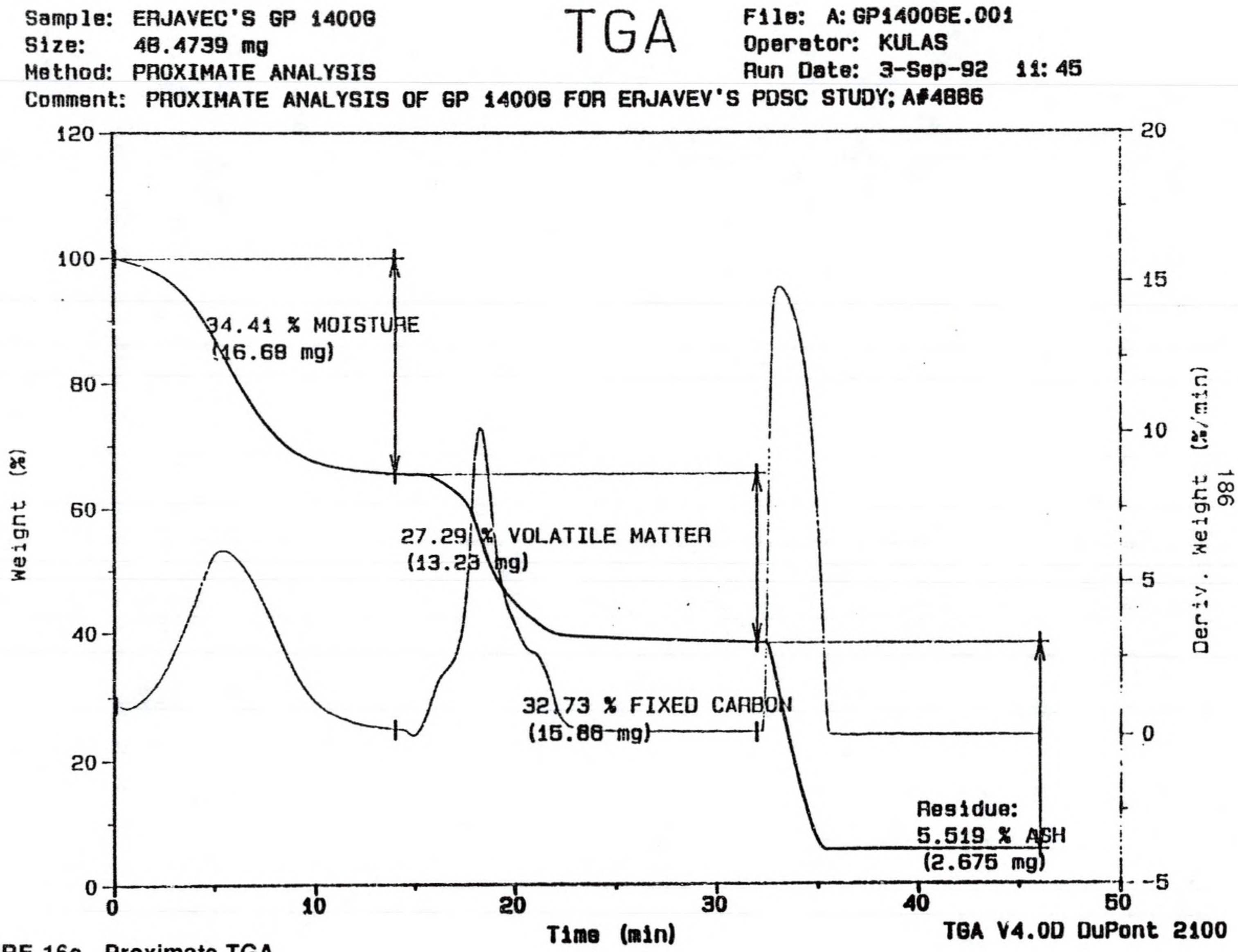


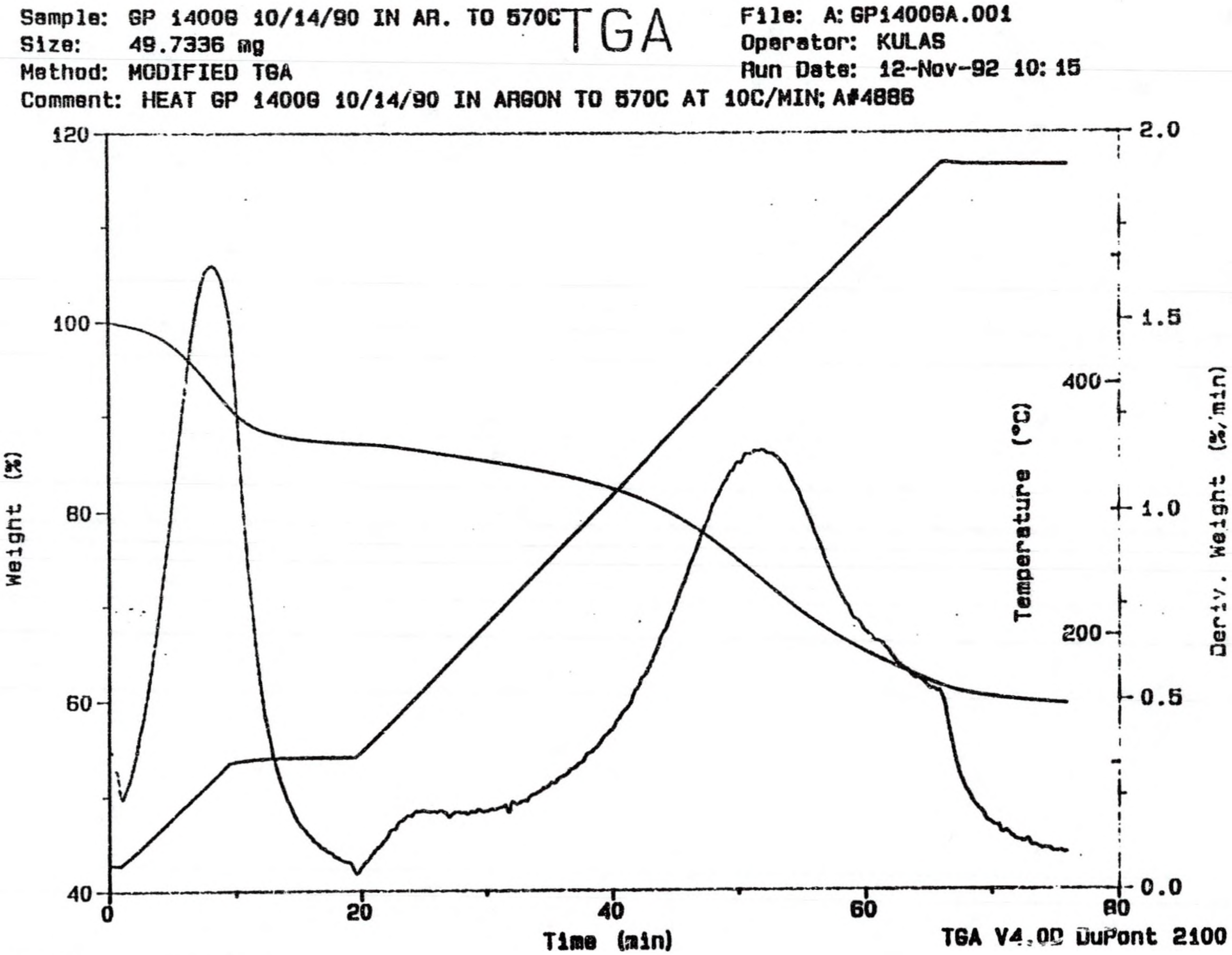
FIGURE 16b. Adjusted DSC Data.



Sample: ERJAVEC'S GP 1400G
Size: 48.4739 mg
Method: PROXIMATE ANALYSIS
Comment: PROXIMATE ANALYSIS OF GP 1400G FOR ERJAVEV'S PDSC STUDY; A#4886

File: A:GP1400GE.001
Operator: KULAS
Run Date: 3-Sep-92 11:45

FIGURE 16c. Proximate TGA.



Sample: GP 1400G 10/14/90 IN AR. TO 570C

Size: 49.7336 mg

Method: MODIFIED TGA

Comment: HEAT GP 1400G 10/14/90 IN ARGON TO 570C AT 10C/MIN; A#4886

File: A: GP1400GA.001

Operator: KULAS

Run Date: 12-Nov-92 10: 15

FIGURE 16c. Modified TGA.

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DSC Standard                                        09/04/92 10:44:48   Page  1

File:  A:ERJAV.102          Run Date:  3-Sep-92   10:43
Program:  DSC V4.0B         Run Number:  99

DuPont 2100 Thermal Analysis -- DSC

Sample:      PDSC OF GP 2200G 9/3/92
Size:       12.4000 mg
Cell Constant:   1.2013
Operator:    KULAS
Method:      DSC
Comment:     PDSC OF GP 2200G FOR ERJAVEC'S PDSC STUDY; A#4886

Peak  Start    Onset     Max     Stop       Area
        °C       °C       °C       °C
      32.42    32.59   268.38   579.74    1125. J/g
      37.06   232.44   268.38   566.52    599.4 J/g
     110.72   234.04   268.38   330.80    507.6 J/g
```

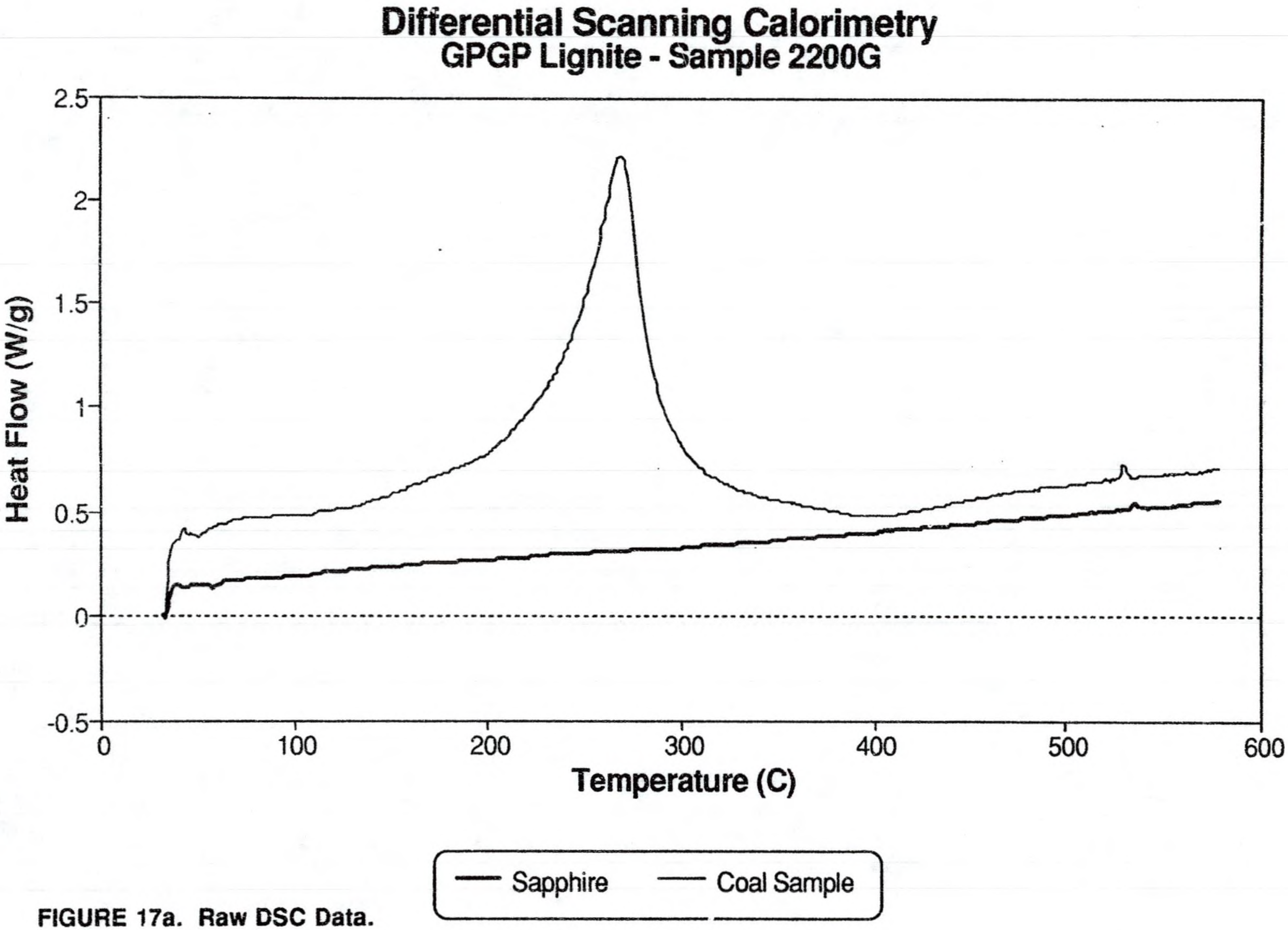
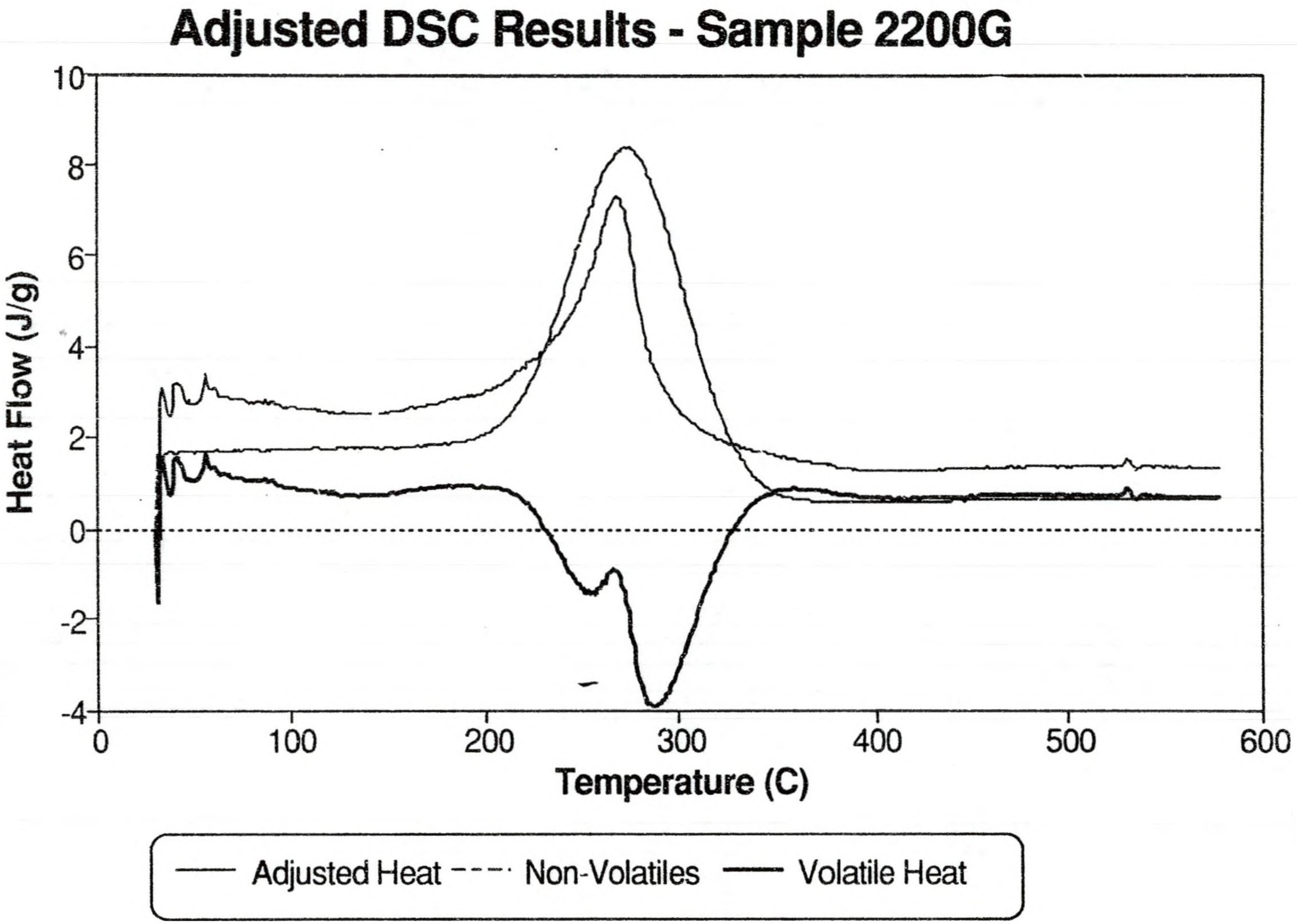


FIGURE 17a. Raw DSC Data.



Adjusted DSC Results - Sample 2200G

FIGURE 17b. Adjusted DSC Data.

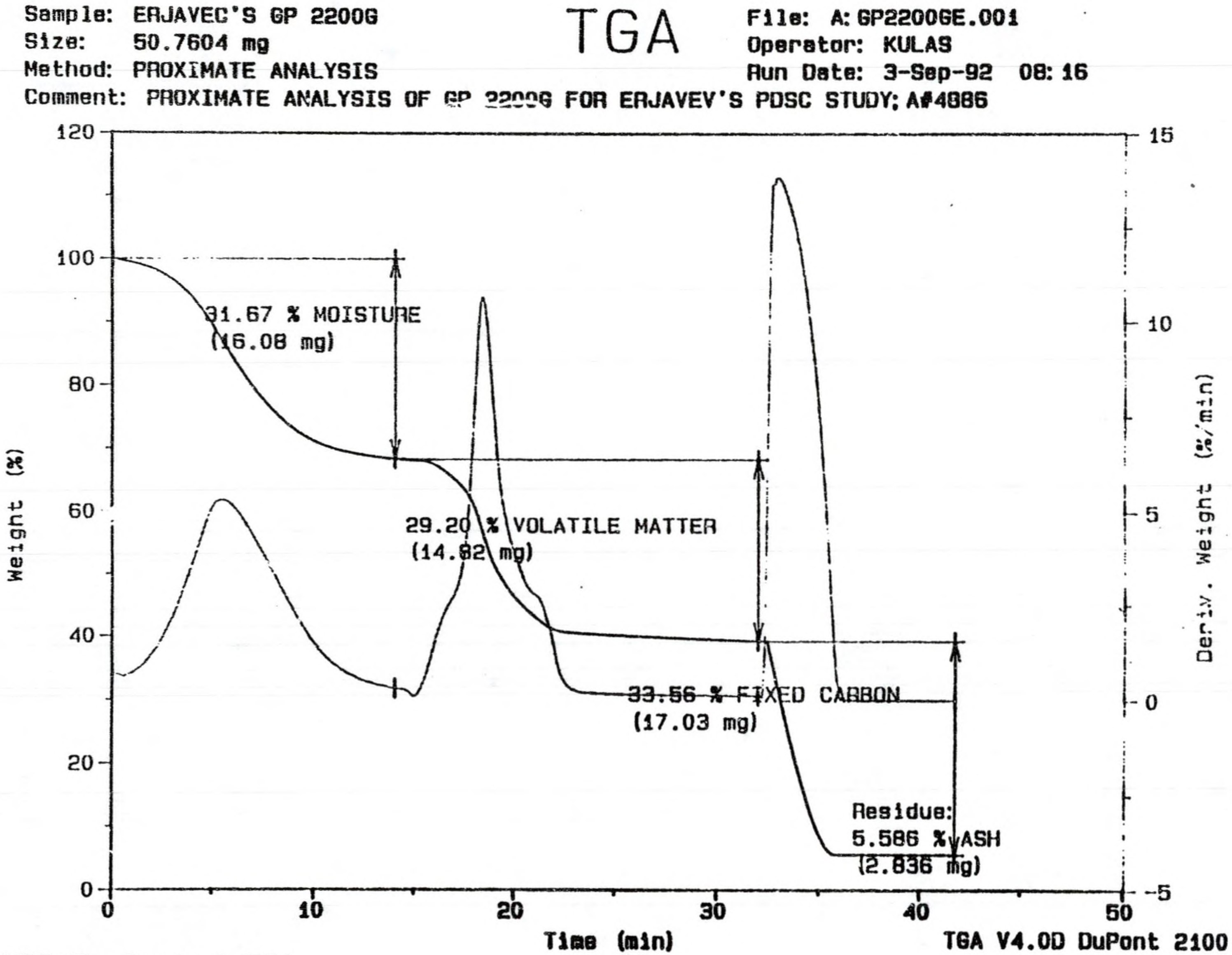
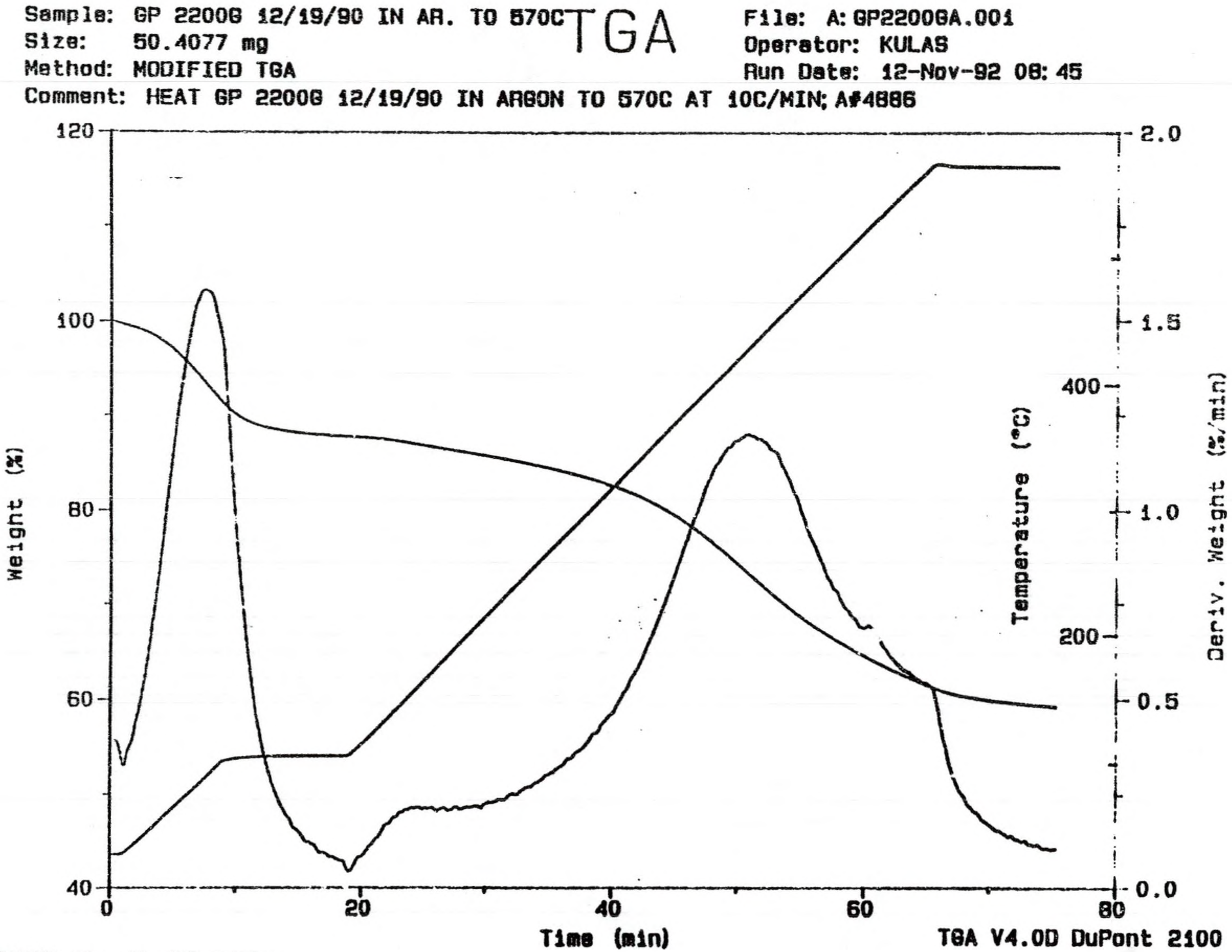


FIGURE 17c. Proximate TGA.



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