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Evaluation and Modification of ASPEN Fixed-Bed Gasifier Models for Inclusion in an Integrated Gasification Combined-Cycle Power Plant Simulation

Technical Note

By
J.M. Stefano

U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
P.O. Box 880
Morgantown, West Virginia 26507-0880

MASTER

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Summary

Several Advanced System for Process Engineering (ASPEN) fixed-bed gasifier models have been evaluated to determine which is the most suitable model for use in an integrated gasification combined-cycle (IGCC) power plant simulation. Four existing ASPEN models were considered: RGAS, a dry ash gasifier model developed by Halcon/Scientific Design Company; USRWEN, the WEN II dry ash gasifier model originally developed by C. Y. Wen at West Virginia University; the slagging gasifier model developed by Massachusetts Institute of Technology (MIT) and based on Continental Oil Company's (CONOCO) design study for the proposed Pipeline Demonstration Plant; and the ORNL dry ash gasifier model developed by Oak Ridge National Laboratory for the simulation of the Tri-States Indirect Liquefaction Process.

Because none of the models studied were suitable in their present form for inclusion in an IGCC power plant simulation, the SLAGGER model was developed by making significant modifications to the MIT model. The major problems with the existing ASPEN models were most often inaccurate material and energy balances, limitations of coal type, or long run times. The SLAGGER model includes simplifications and improvements over the MIT model, runs quickly (less than 30 seconds of computer time on a VAX-11/780), and gives more accurate mass and energy balances.

Introduction

ASPEN simulations of IGCC power plants have been previously developed at the Morgantown Energy Technology Center (METC). These simulations include one that is based on a fluidized-bed gasifier and another that uses an entrained-flow reactor. None has been developed, to date, that uses the most commercialized gasifier, the fixed-bed. The fixed-bed gasifier has several advantages over the other gasifier types that make it attractive for use in an IGCC. These advantages include a high cold gas efficiency and low oxidant requirements. The dry ash fixed-bed gasifier can also operate efficiently with air rather than oxygen, eliminating the need for a costly oxygen plant. In general, the disadvantages of the fixed-bed gasifier include the limited ability to handle fines and caking coals, and the production of tars and oils that can cause problems of downstream plugging. In the slagging mode, the fixed-bed gasifier offers the advantage of a lower steam consumption. Unfortunately, the slagging gasifier is generally thought to require oxygen or oxygen-enriched air for use as the oxidant stream.

The purpose of this evaluation is to determine which of the available ASPEN fixed-bed gasifier models is the most suitable for inclusion in a zero-order IGCC power plant simulation. A zero-order simulation performs basic mass and energy balances using a minimal number of ASPEN unit operation blocks, and tracks major environmental species such as SO_x and NO_x. A suitable gasifier model must be able to (1) perform basic mass and energy balances using a minimum number of ASPEN unit operation models, (2) run relatively quickly, and (3) handle changes in feed type and operating conditions with simple changes to the input file.

Several ASPEN fixed-bed gasifier models exist and were evaluated with respect to the above factors. These models are listed in Table 1.

TABLE 1. ASPEN FIXED-BED GASIFIER MODELS CONSIDERED FOR IGCC SIMULATION

Model Name	Developer	Dry Ash/Slagging	Unique Features
RGAS	Halcon/SD	Dry Ash	Countercurrent flow Kinetic model; two kinetic routines available
USRWEN	C. Y. Wen (WVU)	Dry Ash	Kinetic model
MIT	MIT	Slagging	Nonkinetic model Employs a limestone fluxing agent
ORNL	ORNL	Dry Ash	Nonkinetic model

Integrated Gasification Combined-Cycle (IGCC) Power Generation

In an IGCC configuration, a gasifier produces hot raw gas from coal, steam, and oxygen (or air). Following any required temperature reduction, this raw gas can be treated in either high or low temperature sulfur and particulate removal systems. The cleaned gas is sent to the combustion turbines and is burned to produce power. Hot exhaust gas from these turbines is cooled by generating, superheating, and reheating steam. The steam is then sent to steam turbines to generate additional power. The total power generated is a combination of that generated in the combustion turbines and that from the steam turbines. A general block diagram of an IGCC power plant using low-temperature gas cleanup is shown in Figure 1.

At the beginning of this evaluation, the coal type and mode of operation (dry ash or slagging) had not yet been established for the simulation of the fixed-bed IGCC plant. Therefore, the models were not examined in any order or tested with the data from a specific design study of an IGCC plant. The following sections outline the results of the evaluation of the ASPEN fixed-bed gasifier models in the order they were studied.

RGAS Gasifier Model

RGAS is a rigorous model of a countercurrent flow, dry ash gasifier. The model determines the material balance based on a kinetic subroutine. It was developed by Halcon/Scientific Design in a simulation of the Great Plains Gasification Plant (Benjamin 1985, Rinard and Benjamin 1985). The model, based on a Lurgi Mark IV gasifier, was developed from kinetic models and experimental data obtained from literature. The model was specifically tailored for the North Dakota lignite coal used at the Great Plains Plant.

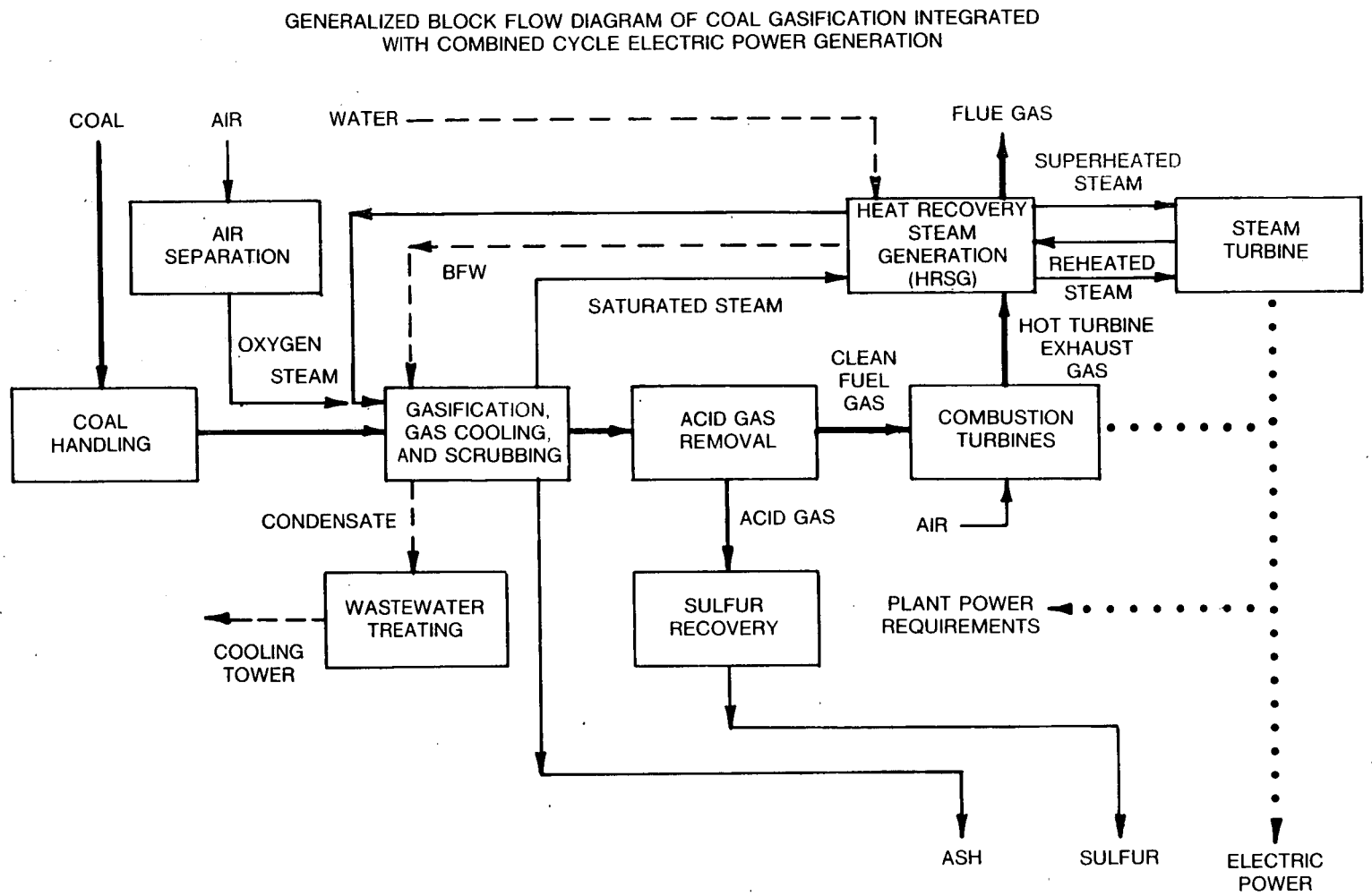

FIGURE 1. GENERALIZED BLOCK FLOW DIAGRAM OF COAL GASIFICATION INTEGRATED WITH COMBINED-CYCLE ELECTRIC POWER GENERATION

Reference: Simbeck, Dickenson, and Oliver 1983.

RGAS can be run with either of two gasification kinetic subroutines; one was taken from the WEN II model developed by C. Y. Wen of West Virginia University, and the other was taken from the DENN-1D model developed by Morton Denn of the University of Delaware. The choice of kinetic subroutines enhances the model's flexibility.

In RGAS, devolatilization kinetics are based on the ultimate yield-temperature curve of lignite coal. It is assumed that devolatilization occurs throughout an appreciable portion of the reactor. The presence of volatile species throughout the upper portion of the gasifier affects the chemical equilibrium of the system. Halcon reports that this simulation technique is more realistic than the more common method of handling devolatilization after convergence on fixed carbon. Heating and drying of the coal is assumed to take place instantaneously at the top of the gasifier.

The gasification reactions contained in this model are as follows:

$$C + 2H_2 \rightarrow CH_4$$

$$C + CO_2 \rightarrow 2CO$$

$$C + H_2O \rightarrow CO + H_2$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

The heat necessary to sustain these reactions is provided by the following combustion reactions:

$$C + \tfrac{1}{2}O_2 \rightarrow CO$$

$$C + O_2 \rightarrow CO_2$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O$$

Depending on which of the kinetic subroutines is chosen, some or all of the reactions above are used.

RGAS determines gasifier outlet gas composition, the amount of steam generated in the jacket, the temperature profile of the reactor, and the products of devolatilization in the product gas stream. The major system parameters, such as reactor size, feed rates, and process conditions, can be easily adjusted in the input file. A sample input file for RGAS utilizing the Denn kinetic subroutine is listed in Appendix A.

The limitation of this model is its dependence on lignite. Because the model is specifically designed to simulate the Great Plains Gasification Plant, the model is tailored to lignite. The gasification kinetics can be changed in the subroutine, and some data does exist in literature for bituminous and subbituminous coal gasification kinetic constants. The problem involves devolatilization kinetic data, which is given in the model as the yield-temperature curve for lignite. Yield-temperature curve data is not readily available for other coal types; this, therefore, decreases the flexibility of the model.

Because of this dependence on coal type, only a lignite case could be run to test the model's predictiveness. An Illinois No. 6 coal was tried, but the model had difficulty with it and never ran to completion. It was noted in this unsuccessful run that the error messages given by the model are vague and give the user little assistance in determining what needs to be done to correct the problem.

Additionally, RGAS was developed with a proximate analysis on a wet basis. This is contrary to ASPEN's convention, which requires that the proximate analysis be given on a dry basis (Massachusetts Institute of Technology 1982b). The model was tested with a proximate analysis on a dry basis, and the simulation would not run to completion. This inconsistency in RGAS with the proximate analysis has been corrected at Halcon/Scientific Design, and the modified files are currently being sent to METC. It appears that the modifications made to the original version of RGAS have not changed the results.

The original input files for RGAS delivered by Halcon were based on non-proprietary design data from the Great Plains Gasification Facility. These files run successfully, and the results are listed in Table 2.

No detailed operating data is available for the Great Plains Gasification Plant; therefore, there is no experimental reference case to compare to the simulated results. Instead, a literature case cited (Elliott 1981) was run in RGAS as a basis of comparison. The results for this literature case for lignite tested in a BGC/Lurgi dry-ash gasifier are compiled in Table 3. Both the Wen and Denn kinetic subroutines of RGAS have been tested with this literature data. Only the case utilizing Denn kinetics runs successfully. The case with RGAS using Wen kinetics incurs an error in the reactor block. The fix could not be determined partly because insufficient information was provided by the error message.

The results that are listed in Table 3 for RGAS tested with literature data show a close match with respect to outlet gas composition. The major difference appears to be an underprediction of the amount of hydrocarbons (CH_4 and CxHy) formed. The results of the literature case (in Table 3) are also similar to the results of the Great Plains simulation (in Table 2), suggesting that RGAS satisfactorily predicts the dry ash gasification of lignite, particularly if the Denn kinetic subroutine is used.

For comparison, USRWEN (which is discussed in more detail later in the report) was also tested with these same sets of lignite data. The results for the Great Plains Case are listed in Table 2. USRWEN would not run with the literature case due to a divide by zero error.

The length of time required to run RGAS is long (600 to 700 seconds). This is almost three times longer than the simulation time required for the entire entrained-flow gasifier IGCC simulation. This translates into a significant increase in the real time spent by the user to perform such a simulation. Because of the model's limitation to coal type and its relatively slow run time, RGAS was not chosen for inclusion in the proposed fixed-bed IGCC simulation.

TABLE 2. RGAS AND USRWEN RUN RESULTS WITH GREAT PLAINS LIGNITE DATA

Coal Proximate Analysis	Input Values
Volatile Matter (%, MF basis)	44.16
Fixed Carbon (%, MF basis)	46.34
Moisture (%, as received)	25.54
Ash (%, MF basis)	9.50
Gasifier Conditions	
Pressure (psia)	445
Steam/Coal (lb/lb)	.97
Oxygen/Coal (lb/lb)	.20

Raw Gas Composition (vol %)	RGAS		USRWEN
	Denn Kinetics	Wen Kinetics	
CO	16.08	16.08	10.83
H_2	40.26	40.64	42.51
CH_4	8.46	8.32	12.22
CxHy	0.93	0.93	N/C
H_2S	0.52	0.51	0.46
CO_2	33.57	33.33	33.42
N_2	0.18	0.19	0.58
Gas Heating Value (Btu/scf)	N/C	N/C	288
Offgas Temperature (°F)	617	613	1,408
Tars/Coal (lb/lb)	.05	.05	.05
Cold Gas Efficiency (%)	N/C	N/C	59.7
Carbon Conversion (%)	74.06	74.11	90.3
CPU Time for Simulation (sec)	796	735	418

N/C -- Not calculated by model.

TABLE 3. RGAS RUN RESULTS WITH NORTH DAKOTA LIGNITE LITERATURE CASE

Coal Proximate Analysis	Input Values	
Volatile Matter (%, MF basis)	44.3	
Fixed Carbon (%, MF basis)	46.3	
Moisture (%, as received)	34.3	
Ash (%, MF basis)	9.4	
Gasifier Conditions		
Pressure (psia)	440	
Steam/Coal (lb/lb)	1.07	
Oxygen/Coal (lb/lb)	0.20	
Raw Gas Composition (vol%)	**Reference**	**RGAS with Denn Kinetics**
CO	15.9	14.21
H_2	39.2	40.04
CH_4	10.8	8.06
CxHy	1.2	0.85
H_2S	0.4	0.51
CO_2	32.2	35.20
N_2	0.3	0.54
Gas Heating Value (Btu/scf)	306	N/C
Offgas Temperature (°F)	Not Given	525
Tars/Coal (lb/lb)	Not Given	.05
Carbon Conversion (%)	Not Given	82.19
CPU Time for Simulation (sec)	N/A	658

N/C -- Not calculated by model.

N/A -- Not applicable.

USRWEN Gasifier Model

Essentially, USRWEN is the WEN-II model converted into an ASPEN user model. A user model is a user-developed FORTRAN program describing a unit operation that is executed through ASPEN. (Massachusetts Institute of Technology 1982b). The WEN-II model is a dry ash gasifier model developed by C. Y. Wen at West Virginia University (Wen, Chen, and Onozaki 1982). This steady-state model takes into consideration the kinetics of the gasification reactions as well as the dimensions of the gasifier. The reactions considered in this model are listed below. The value of x is calculated by linear interpolation in the model and determines the primary composition of CO and CO_2

$$C + \frac{1}{x} O_2 \rightarrow (2 - \frac{2}{x}) CO + (\frac{2}{x} - 1) CO_2$$

$$C + H_2O \rightarrow CO + H_2$$

$$H_2O + CO \rightleftarrows H_2 + CO_2$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O$$

$$C + CO_2 \rightarrow 2CO$$

$$C + 2H_2 \rightarrow CH_4$$

The temperature and gas composition are assumed to be uniform along the radial direction; consequently, it is a one-dimensional model. The major assumptions of the model are the following: (1) devolatilization is assumed to occur separately from the other reactions at the top of the gasifier; (2) all gas-solid reactions are represented by volumetric reactions, and combustion occurs according to the shrinking core model. The shrinking core model accounts for the reduction in the size of the particle core as the reaction proceeds inward; (3) at every point in the gasifier, there is no difference between the gas and solid temperatures; (4) the temperature at the bottom of the gasifier is assumed to be equal to the inlet temperature of the oxidant and steam; (5) the amount of volatile matter produced is specified by the user and does not change with operating conditions; (6) the carbon/hydrogen/oxygen ratio in tar is the same as that in the original coal; (7) all nitrogen in the volatile gas appears as nitrogen gas, and all sulfur appears as H_2S; (8) devolatilization is assumed to be thermally neutral.

Three sets of kinetic data are available in the program. The data are for bituminous, subbituminous, and lignite coals. Caution is advised when using the default values for these constants since they are listed in a different order in the user manual than in the program itself. It is suggested that kinetic data be given by the user in the last line of the input file to ensure that the correct values are used. Also recommended is the use of the tuned kinetic data determined by Halcon/Scientific Design in their simulation of the Great Plains Gasification Plant if the feed is a lignite coal (Rinard and Benjamin 1985). In Appendix B, a sample input file for USRWEN is listed.

USRWEN has been run with the same sets of lignite data as was RGAS to compare the results. The results of the case using Great Plains data are listed on Table 2 along with the RGAS results. From this comparison, it is seen that USRWEN does not do as well as RGAS in predicting raw gas composition and temperature for the gasification of lignite. For the literature case, USRWEN would not run to completion. The program encounters a divide by zero error whenever the carbon flow rate out of the reactor is calculated to be zero (corresponding to 100 percent carbon conversion). Therefore, no results for the literature case are listed in Table 3 for USRWEN.

The USRWEN model was also run with a more commonly used coal, Illinois No. 6 (Woodall-Duckham 1974). The results in Table 4 show that USRWEN gives significantly better predictions for this bituminous coal than it does for lignite. The major discrepancies noted in the Illinois No. 6 simulation are the low prediction of methane and the overestimation of heat loss by an order of magnitude.

A third case was tried in the slagging mode with Illinois No. 6 coal (Scott 1981). The model did not run in this mode, most likely because of the marked difference in the steam requirement and the upper temperature limit on the kinetic equations.

USRWEN is more flexible than RGAS because it contains kinetic data for several coals. Unfortunately, it still takes about 400 seconds of computer time. Although the simulation time is about twice as fast as that of RGAS, it is still relatively too slow for the zero-order IGCC simulation.

Based on the evaluation of these two kinetic models, it was concluded that a faster, simpler model is needed for the IGCC simulation. The choice was between two nonkinetic models, the MIT model (Massachusetts Institute of Technology 1981) and the ORNL model (Barker and others 1983). At this point in the study, it was determined that a design study of an IGCC utilizing a BGC/Lurgi slagging gasifier would be the basis for the simulation (delaMora and others 1985). The decision was made to test the MIT model because it was designed to simulate a slagging gasifier. Additionally, previous METC experience with the ORNL model indicated that the energy and material balances in the devolatilization routine do not close, nor does the overall energy balance. Consequently, the ORNL model was never fully evaluated for the purpose of this study.

MIT Gasifier Model

The MIT gasifier model was developed by MIT to simulate the proposed Continental Oil Company's Pipeline Gas Demonstration Plant (Massachusetts Institute of Technology 1981). The gasifier model, which is based on the BGC/Lurgi slagging gasifier, comprises many relatively simple ASPEN unit operation blocks, unlike the more rigorous models previously examined which have a detailed code contained in one ASPEN unit operation block.

This model divides the gasifier into three sections. At the top of the gasifier, the moisture in the coal is evaporated by the heat of the rising hot gases. In the middle region, the coal devolatilizes according to a user routine called NYLD. The remaining gases, ungasified carbon, and the flux (represented by pure $CaCO_3$) go on to the bottom of the gasifier. There the carbon and

TABLE 4. USRWEN RUN RESULTS WITH ILLINOIS NO. 6 LITERATURE CASE

Coal Proximate Analysis	Input Values	
Volatile Matter (%, MF basis)	33.96	
Fixed Carbon (%, MF basis)	43.24	
Moisture (%, as received)	13.68	
Ash (%, MF basis)	9.12	
Gasifier Conditions		
Pressure (psia)	365	
Steam/Coal (lb/lb)	2.63	
Oxygen/Coal (lb/lb)	0.50	
Raw Gas Composition (vol %)	**Reference**	**USRWEN**
CO	16.3	17.3
H_2	39.8	46.6
CH_4	8.7	4.8
CxHy	0.6	N/C
H_2S	1.1	0.9
CO_2	32.1	28.9
N_2	1.4	1.6
Gas Heating Value (Btu/scf)	279	270
Offgas Temperature (°F)	1,158	1,122
Tars/Coal (lb/lb)	0.02	0.07
Heat Loss (Btu/hr)	2.62×10^6	5.01×10^7
Cold Gas Efficiency (%)	75.2	79.5
Carbon Conversion (%)	99.7	99.2
CPU Time for Simulation (sec)	N/A	411

N/C -- Not calculated by model.

N/A -- Not applicable.

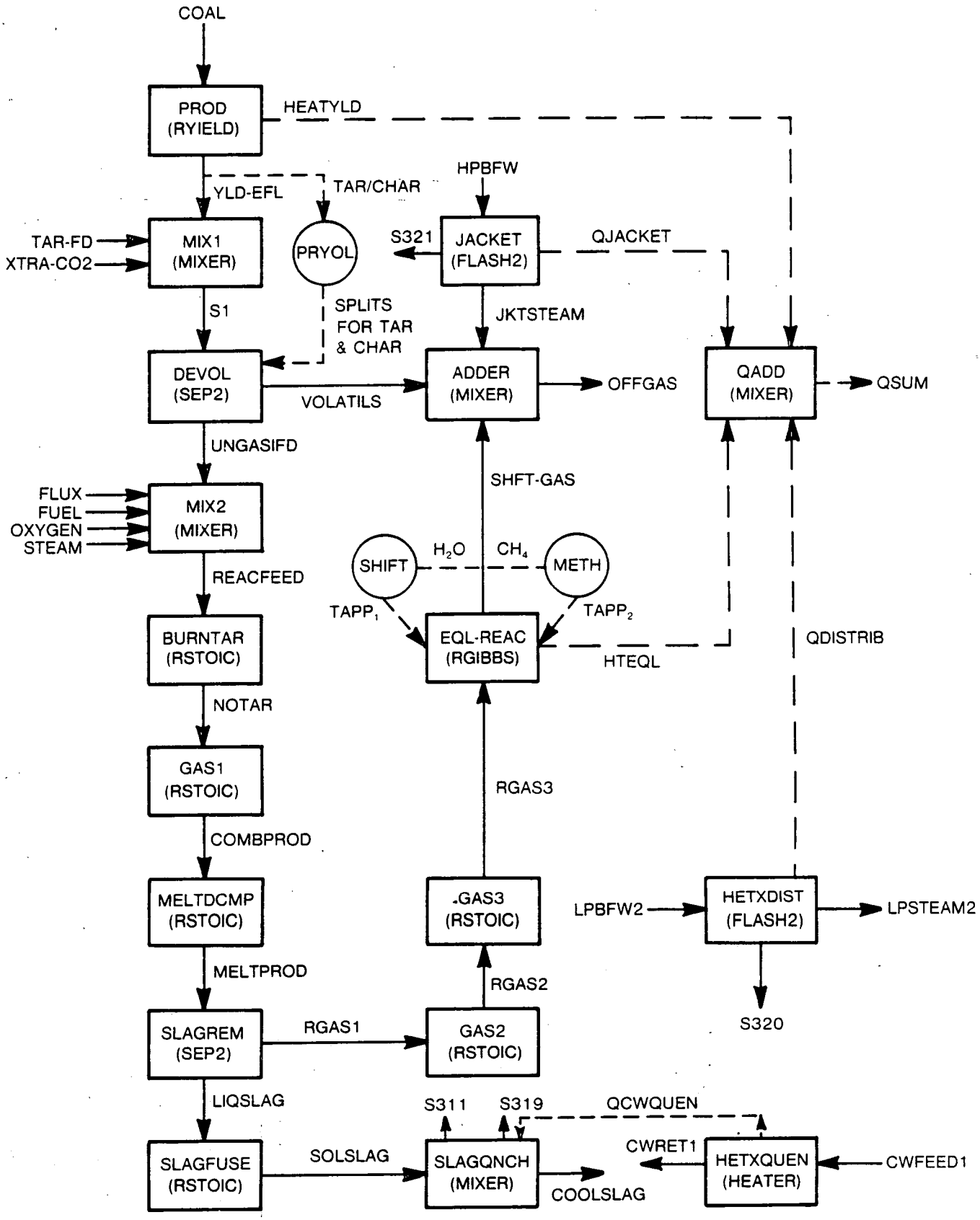

FIGURE 2. ASPEN BLOCK DIAGRAM OF THE MIT GASIFIER MODEL

Reference: Massachusetts Institute of Technology, 1981.

recycle tar react with oxygen and liberate enough heat to melt the flux and ash. The gasification products and devolatilization gases are mixed together to form the product gas. A block diagram of the MIT gasifier model is shown in Figure 2. To calculate properties such as volume, enthalpy, entropy, Gibbs free energy, and fugacity coefficients for each of the components, the MIT model utilizes the Redlich-Kwong-Soave equation of state. Additionally, the model allows for specification of ultimate analyses for the hydrocarbons. Therefore, the chemical formulas chosen to represent these components are used only for physical property determinations, and the user-supplied ultimate analyses are used to determine their compositional makeup.

The user devolatilization routine, NYLD, contains yield splits that match the Ohio No. 9 coal conversion product rates found in CONOCO's Pipeline Gas Demonstration Plant design study. The ultimate analyses of the coal, tar, phenols, naphtha, oil, and char are provided as inputs. The moisture in the coal, determined from the proximate analysis, is assumed to vaporize completely. The amounts of ash, carbon, hydrogen, nitrogen, sulfur, and oxygen formed from the coal is calculated from the ultimate analysis. Then the amount of hydrocarbons formed from these components is determined as a fraction of moisture- and ash-free (MAF) coal. Any remaining sulfur and nitrogen is distributed among the sulfur (H_2S, COS, CS_2, C_4H_4S) and nitrogen (NH_3, N_2) compounds according to those fractions given in CONOCO's design study.

Since the yields in the NYLD routine are set, the relative amounts of tar, phenol, naphtha, oil, char, C_2-C_4, H_2S, COS, CS_2, and C_4H_4S will always be the same, but the total amounts will be different depending on the ultimate analysis of the coal. Therefore, the model has a limited capability for predicting product gas composition when different coals are used; however, the splits given in the routine NYLD should be modified when using very different coals.

This nonkinetic model calculates the following from given feed rates and compositions of the oxidant, steam, and coal: offgas temperature, offgas composition, temperature at the bottom of the gasifier, temperature of the quenched slag, cooling duties, and overall heat and mass balances. Appendix C contains an input file for the MIT model.

Originally, the MIT gasifier model would not run. It encountered a problem in ASPEN's RGIBBS reactor model. The RGIBBS model is an equilibrium reactor that minimizes Gibbs free energy in determining phase and chemical equilibrium (Massachusetts Institute of Technology 1982a). When RGIBBS calculated the density of the exit gas, it was dividing by zero. The density is calculated by dividing the mass flow by the total volume, and in the initial pass through RGIBBS, the total volume was equal to zero. The reason for a zero volume was never determined. Since it was not critical that the density of the stream be calculated, a fix was added to the RGIBBS code which enabled it to bypass the density calculation whenever the total volume is zero.

Results of the MIT simulation, after the above fix was added, are listed in Table 5. The MIT input file contains data from the Pipeline Gas Demonstration Plant design study. The study lists the coal used as Illinois No. 6. However, the devolatilization routine, according to MIT's documentation, is based on an Ohio No. 9 coal. Since the most detailed slagging data set available for a BGC/Lurgi slagging gasifier is a case using Pittsburgh No. 8 coal (Scott 1981), the MIT model results initially have been compared to it.

TABLE 5. COMPARISON OF MIT MODEL AND SLAGGER*

	Reference	MIT	SLAGGER
Coal Proximate Analysis	Input Values		
Volatile Matter (%, MF basis)	38.05	35.9	38.05
Fixed Carbon (%, MF basis)	51.89	41.0	51.89
Moisture (%, as received)	4.88	2.5	4.88
Ash (%, MF basis)	10.06	23.1	10.06
Gasifier Conditions			
Pressure (psia)	349	450	350
Steam/Coal (lb/lb)	0.36	0.31	0.36
Oxygen/Coal (lb/lb)	0.53	0.43	0.51
Raw Gas Composition (vol %)	Results		
CO	56.50	58.08	55.84
H_2	27.14	27.43	27.63
CH_4	6.02	6.78	6.04
CxHy	0.64	0.37	0.61
H_2S	0.49	2.04	0.59
CO_2	4.03	4.59	4.25
N_2	4.79	0.60	4.66
NH_3	0.38	0.63	0.37
COS	0.03	0.11	0.03
Gas Heating Value (Btu/scf)	Not Given	N/C	N/C
Offgas Temperature (°F)	937	1,053	931
Tars/Coal (lb/lb)	0.09	0.14	0.07
Heat Loss (Btu/hr)	7.7×10^6	N/C	N/C
Cold Gas Efficiency (%)	89.2	N/C	N/C
Carbon Conversion (%)	99	100	96
CPU Time for Simulation (sec)	N/A	54.95	29.82

* SLAGGER was run without the quench section of the simulation.

N/C -- Not calculated by model.

N/A -- Not applicable.

The MIT gasifier model predicted the outlet gas composition fairly well except for the amount of hydrogen sulfide (H_2S) and nitrogen (N_2). The excess H_2S predicted could be partly due to the difference in the sulfur content of the coals. The coal listed in the CONOCO design study contains 4.88 percent sulfur, whereas the coal from Scott (1981) contains only 1.67 percent sulfur. The difference in the amount of N_2 may be due to differences in oxygen purity. Because the flow of heat streams in the MIT model flowsheet are ambiguous and difficult to follow, no comparison of heat loss is made.

The simulation time for this model is about 55 seconds, which is much shorter than that of the more rigorous kinetic models. Even though the run time for this model is favorable, it would be desirable if the results were more accurate. Additionally, certain awkward features of the model need to be changed before it can be recommended as the suitable model for the IGCC simulation.

Because the MIT model is the only available ASPEN model that handles slagging operation, and because it appears that modifications to it can produce a more flexible, accurate model, it was decided that a new version of the MIT model be developed. Therefore, the remainder of METC's effort has been devoted to enhancing the MIT model.

SLAGGER Gasifier Model

The modified version of the MIT model developed in this study is called SLAGGER. A block diagram of this model is given in Figures 3 and 4. By comparing it to the MIT model in Figure 2, it is obvious that the basic logic for the gasifier section of the flowsheet is the same. Some changes have been made to reflect more realistic gasifier operation and to allow the model to be more flexible.

The devolatilization routine, NYLD, has been left unchanged mainly because no better devolatilization routine exists that can be easily substituted. It is suggested, however, that the split fractions for the devolatilization products in the NYLD source code be modified when different coals are used. Some changes to these fractions have been made to give better results for a Pittsburgh No. 8 coal. These split fractions are listed in the comment section of the SLAGGER input file listed in Appendix D. Also remaining unchanged are the global physical property option set and the component list.

A modification to the method of recycling tar has been made. The MIT model requires the user to give the flow rate of recycle tar in the stream TAR-FD (see Figure 2). To provide for steady-state recycle, the recycled tar and char is sent to the stream VOLATILS, encounters no further reaction, and exits with the raw gas. The FORTRAN block, PYROL, is responsible for setting the flow rate of tar and char to be burned equal to the amount of tar and char produced during coal pyrolysis. A FORTRAN block allows the user to insert FORTRAN statements into the flowsheet computations (Massachusetts Institute of Technology 1982b). Subsequently, the only tar and char burned is that produced during devolatilization.

In SLAGGER, the stream TAR-FD is deleted and the user specifies in a separator block called DEVOL the fraction of tar and oil that will end up in the raw

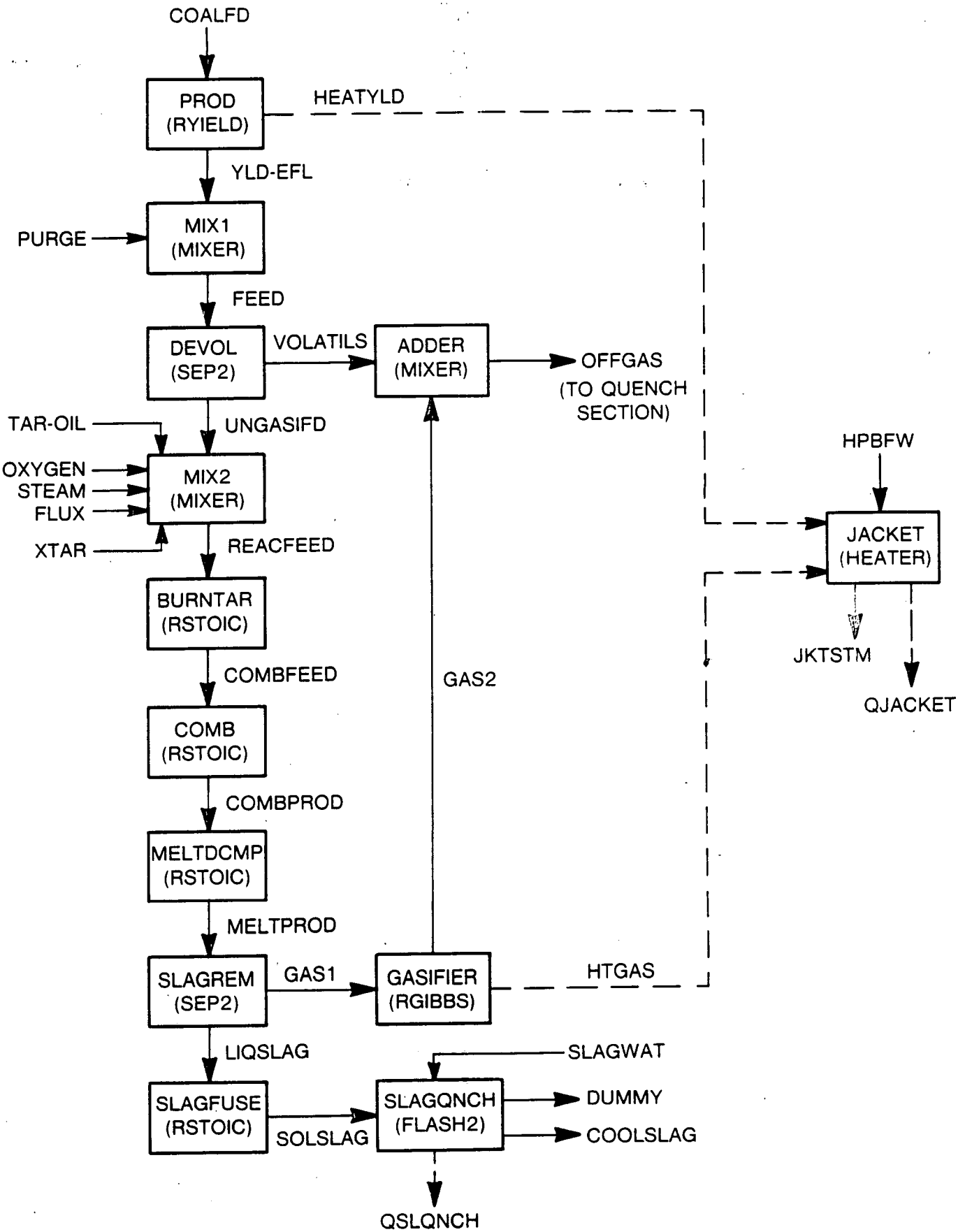

FIGURE 3. ASPEN BLOCK DIAGRAM OF THE GASIFIER SECTION OF SLAGGER

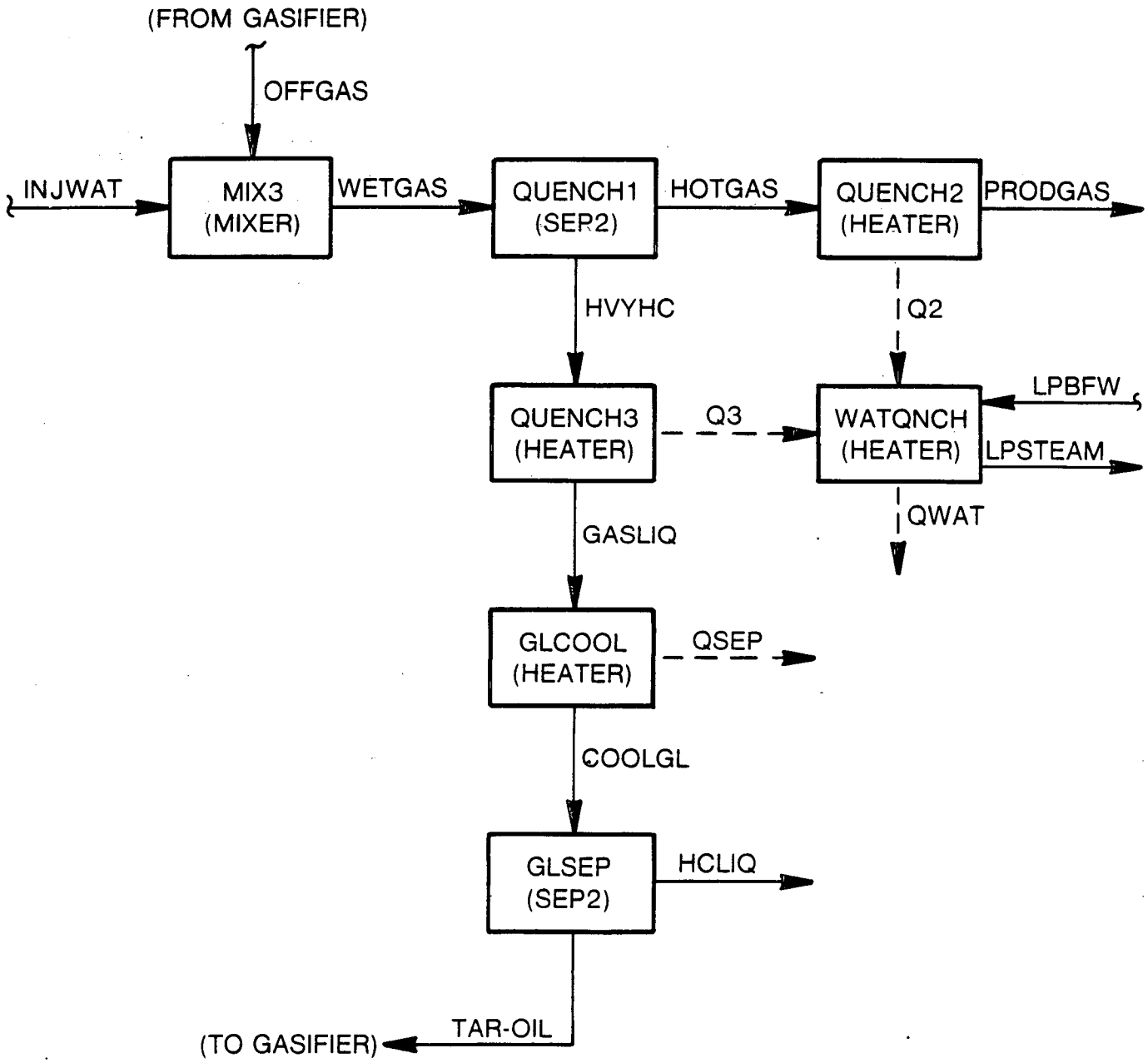

FIGURE 4. ASPEN BLOCK DIAGRAM OF THE QUENCH SECTION OF SLAGGER

gas. This tar and oil then proceeds to the quench section and can be recycled back to the gasifier. Instead of the char being split and some sent directly to the products, it flows through to the combustion and gasification sections and is completely reacted. Because of these changes, the PYROL block is no longer necessary.

The stream XTAR has been added to the MIX2 block. This stream, which contains a very small amount of tar and oil, is necessary to satisfy the block RGIBBS in the case where there is no tar recycle. RGIBBS will not run successfully if any of the specified reactants are not present in the feed. Therefore, the XTAR stream will always give RGIBBS some small amount of tar and oil to react even when there is no recycle. The effect on the material balance by adding this small amount of tar and oil is negligible.

Another change is that the stream XTRA-CO2 is renamed PURGE in the SLAGGER flowsheet. This stream is actually the gas used to pressurize the lockhopper. In the conceptual design of the Pipeline Gas Demonstration Plant, the gas used is carbon dioxide (CO_2), which comes from the Benfield CO_2 removal unit. However, it is likely that other inert gases such as N_2 would be used for this purpose in an IGCC power plant. Therefore, a more generic name for this stream is more suitable.

Another stream is deleted in block MIX2. The FUEL stream in the MIT input file consists of methane gas. This gas comes from the methanation unit of the Pipeline Gas Demonstration Process. This stream does not exist in an IGCC system and, therefore, is deleted.

Other stream and block changes are made to the slag quenching vessel (SLAGQNCH). In SLAGQNCH, the Stream Nos. S311 and S319 of the MIT model are process water streams from other sections of the plant. In SLAGGER, these are combined into one stream called SLAGWAT. The DUMMY stream in block SLAGQNCH in SLAGGER is added because the FLASH2 unit operation block requires an outlet vapor stream even if no vapor exists. The reason for changing the MIXER to a FLASH2 is to set the outlet pressure and temperature so that the amount of heat released at those conditions can be calculated. This is necessary since the literature case used as a basis for this simulation (Scott 1981) does not provide the amount of water used to quench the slag. Therefore, a design specification (DES-SPEC) block is used to vary the amount of water needed to quench the slag to a specified temperature and pressure. A DES-SPEC is used to specify that a flowsheet variable or a function of a flowsheet variable attains a desired value (Massachusetts Institute of Technology 1982b). If the amount of water used in the quenching of the slag is known, a MIXER block can be used, and the DES-SPEC will no longer be needed. The heat exchangers in the MIT model, HETXQUEN and HETXDIST, are not necessary for a simulation of only the gasifier section, and so they are deleted.

A major change in the block JACKET is also noted in SLAGGER. In the Pipeline Gas Demonstration Plant design, steam from the jacket is mixed with the product gas. In SLAGGER the steam produced from the jacket is not mixed with the product gas, but instead is available for use somewhere else in the combined-cycle plant.

Major changes in the gasifier blocks have also been made. The MIT model simulates the combustion and gasification zones with the following blocks:

BURNTAR, GAS1, GAS2, GAS3, and EQL-REAC. In GAS1, all the oxygen is consumed in the incomplete combustion of carbon to form CO and CO_2. In GAS2, the following reactions occur so that 90 percent of the CO_2 is reacted, and 50 percent of the water is reacted:

$$C + CO_2 \rightarrow 2CO$$

$$C + H_2O \rightarrow CO + H_2.$$

The methanation reaction listed below proceeds in GAS3 until all of the unreacted carbon is converted. This ensures that the model achieves 100 percent carbon conversion.

$$C + 2H_2 \rightarrow CH_4.$$

In the last reactor block, two reversible reactions occur, and their extents are determined by DES-SPECS SHIFT and METH. These reactions are

$$CO_2 + H_2 \leftrightarrow CO + H_2O, \text{ and}$$

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O.$$

The original MIT file includes a FORTRAN block that calculates the coefficients for the tar and char combustion reactions based on their ultimate analyses. Modifications have been made to this routine to include calculations for oil burning reaction coefficients. Several errors were noted with this routine but they have been corrected.

In SLAGGER, fewer reactor blocks and reactions are considered for the gasification and combustion zones. The blocks are BURNTAR, COMB, and GASIFIER. BURNTAR is the same as the block BURNTAR in the MIT model; however, the corrected version of the FORTRAN block COEFFS is used to determine the coefficients for the tar, char, and oil burning reactions. In block COMB, all of the feed oxygen is reacted in the incomplete combustion of carbon. The GASIFIER block contains the following reactions:

$$C + CO_2 \leftrightarrow 2CO$$

$$C + H_2O \leftrightarrow CO + H_2$$

$$C + 2H_2 \leftrightarrow CH_4$$

$$CO + H_2O \leftrightarrow CO_2 + H_2.$$

This block is an equilibrium reactor that is based on a temperature approach to equilibrium. Therefore, it can respond to various coal types and gasifier conditions if the user adjusts the temperature approach. Note that the reaction $CO + 3H_2 \leftrightarrow CH_4 + H_2O$, is neglected. This reaction is not cited as a major gasification reaction (Elliott 1981), nor is it cited in any other literature examined for this study. Therefore, its effect is assumed to be insignificant. The temperatures for each of the reactions in block GASIFIER for a Pittsburgh No. 8 coal have been determined and are listed in the comment section of the SLAGGER input file listed in Appendix D.

Other changes in SLAGGER include reworking the heat streams (denoted by dashed lines in Figures 2 and 3). SLAGGER takes the heat released (or absorbed) from each of the gasifier sections and sends them to block JACKET. Once again, the report (Scott 1981) does not list the amount of high-pressure boiler feedwater (HPBFW) used in the jacket, so a DES-SPEC, like the one used around the slag quenching vessel, is used to calculate the feedwater needed to produce steam at specified conditions. This DES-SPEC can be removed if the flow of HPBFW is known.

The gasifier section of SLAGGER was run alone utilizing a Pittsburgh No. 8 coal and a limestone flux (Scott 1981). The results are listed in Table 5. Note that the outlet gas compositions predicted by SLAGGER more closely match the experimental data than do the results of the CONOCO model. This portion of SLAGGER runs in less than 30 seconds of computer time.

To more closely resemble an actual slagging gasifier, a quench and gas-liquor separator section was developed and added to SLAGGER to allow the recycle of tar and oil. This portion of the SLAGGER model is shown in the flowsheet in Figure 4. The hot raw gas (OFFGAS) is initially quenched with injected quench water. Then the wet gas proceeds to the gas cooling section represented by blocks QUENCH1 and QUENCH2. The heavy hydrocarbons that are separated in block QUENCH1 are cooled in block QUENCH3. The heat streams from the gas cooling and hydrocarbon cooling blocks are sent to a HEATER block called WATQNCH. Here, low-pressure boiler feed water absorbs the heat, producing low-pressure steam. A DES-SPEC is used to calculate the amount of low-pressure boiler feed water needed since this flow rate was not given in the study used to validate this section of the simulation (Simbeck 1983). If this flow rate is known, this DES-SPEC can be deleted.

Blocks GLCOOL and GLSEP cool and separate the light hydrocarbons (naphtha and phenol) and the tar and oil. The stream containing the tar and oil (TAR-OIL) is recycled back to the gasifier, specifically to block MIX2. The heat stream, QSEP, from the gas-liquor separator is included so that the energy needed for cooling can be accounted for when the model is integrated into other flowsheets.

Note that a SEP block, which not only separates an inlet stream into two or more outlet streams but also allows for an outlet heat stream, could have been used in some instances instead of the coupled SEP2 and HEATER blocks. Unfortunately, when a SEP block was used in this simulation, it did not correctly perform the specified separations. The use of a FLASH2 block would have been better. FLASH2 determines the composition and conditions of two outlet streams (one vapor and one liquid) when feed streams are mixed and flashed at specified conditions (Massachusetts Institute of Technology 1982b). This would have been a more predictive unit operation block, but it did not predict a liquid phase at the conditions specified in SLAGGER. Therefore, the combination SEP2 and HEATER blocks, although less predictive, proved to be the most successful.

Other problems occurred during the development of the quench section. The flash calculations were not converging in some of the quench section blocks. Originally, it was thought that the heavy hydrocarbon chosen to represent the tar ($C_{12}H_{42}$) had poor physical property data and was causing the flash problems. However, a lighter hydrocarbon ($C_{15}H_{30}$) was tried with no change in the flash

calculations. The next step was to relax the tolerance for the flash calculations and increase the maximum number of iterations for these calculations, but both of these steps had unsuccessful results. The physical property option set was changed from the Redlich-Kwong-Soave (RKS) equation of state to the ideal gas law, and the flash calculations converged. It is not understood why the ideal gas law allows the flash calculation to converge when the RKS equation of state does not. However, since this different option set allows the quench portion of SLAGGER to run successfully, the flowsheet is divided into two sections so that this property option set can be supplied to the quench section.

A literature case that recycles tar and oil was used to validate the SLAGGER model. This case, unlike the previous SLAGGER validation case, uses an Illinois No. 6 coal and does not use a fluxing agent (Simbeck 1983). The results of SLAGGER with recycle are compared to literature values in Table 6. The major decrepancies with regards to product composition occur for methane, carbon dioxide, and the light hydrocarbons. The predicted compositions of the devolatilization products, which include the light hydrocarbons could be improved if the split fractions in NYLD are modified to better represent an Illinois No. 6 coal. For this test case, these splits were left at the values determined for a Pittsburgh No. 8 coal. Likewise, the composition of methane and carbon dioxide can also be improved if the temperature approaches in the block RGIBBS are changed. Additionally, not using a limestone flux affects the values used for the temperature approach since the amount of CO_2 that enters the RGIBBS block will be less than when a limestone flux is used.

In summary, SLAGGER, which contains an actual recycle loop, gives accurate results for product gas composition and light hydrocarbon production, allows the user more flexibility with respect to recycling heavy hydrocarbons, more closely resembles the slagging gasifier in the IGCC design study, and runs in about one-minute of computer time on a VAX 11/780.

TABLE 6. RESULTS OF SLAGGER WITH QUENCH SECTION

Input Values			
Proximate Analysis		**Ultimate Analysis**	
Volatile Matter (MF Basis, %)	42.97	Carbon	69.5
Fixed Carbon (MF Basis, %)	46.00	Hydrogen	5.3
Moisture (As Received, %)	14.20	Oxygen	10.0
Ash (MF Basis, %)	11.03	Sulfur	3.9
		Nitrogen	1.3
		Ash	10.0
Gasifier Conditions			
Pressure (psia)	465		
Stean/Coal (lb/lb)	0.30		
Oxygen/Coal (lb/lb)	0.51		

Results

	Reference		SLAGGER	
Raw Gas Composition	(lb/hr)	(Vol %)	(lb/hr)	(Vol %)
CH_4	72	3.8	76	4.3
C_2H_4, C_2H_6	13	0.4	24	0.5
H_2	63	26.4	54	24.4
CO	1521	46.0	1434	46.3
CO_2	149	2.9	161	3.3
H_2S	39	1.0	42	1.1
COS	6	0.1	4	0.1
N_2	93	2.8	95	3.0
H_2O	348	16.3	332	16.7
NH_3	7	0.3	5	0.3
	2311	100.0	2227	100.0
Naphtha	13		16	
Phenols	6		2	
	19		18	
Raw Gas Temperature (°F)	280		302	
Carbon Conversion (%)	100		100	
CPU Time for Simulation (Sec)	N/A		60.6	

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APPENDIX A

RGAS Input File
(With Denn Kinetic Subroutine)

```
;-----------------------------------------------------------------------
;-----------------------------------------------------------------------
;
;                        HALCON SD GROUP, INC.
;
;                                TITLE
; GREAT PLAINS GASIFICATION PLANT - ASPEN SIMULATION OF A SINGLE GASIFIER
;
;                              DESCRIPTION
;       LURGI GASIFIER SIMULATION USING RGAS UNIT OPERATION BLOCK
;
; AUTHOR: B. W. BENJAMIN                              DATE: JUNE 13, 1984
;
;   USER SUBROUTINES REQUIRED: 1 - KINETICS SUBROUTINE
;                                  DELKIN FORTRAN
;
;
;-----------------------------------------------------------------------
;-----------------------------------------------------------------------
TITLE  'GASIFIER SIMULATION - PFTR/DRKGS VERSION USING DENN KINETICS'
;   --------------------- OK AS OF 07-16-84 ---------------------
DESCRIPTION "BEULAH LIGNITE IN LURGI MARK IV USING DENN KINETICS
             WITH MODIFIED KINETIC PARAMETERS"
;   --------------------- OK AS OF 07-16-84 ---------------------
IN-UNITS SI
OUT-UNITS SI
;   --------------------- OK AS OF 07-16-84 ---------------------
SIM-OPTIONS RESULTS-PASS=1 HMB-RESULTS=2
HISTORY MSG-LEVEL PROPERTIES=2 SIMULATION=2 STREAM=2
;   --------------------- OK AS OF 07-16-84 ---------------------
RUN-CONTROL MAX-TIME=850.
;   --------------------- OK AS OF 07-16-84 ---------------------
COMPONENTS  O2 OXYGEN                     / H2O WATER                    /
            H2 HYDROGEN                   / CO CARBON-MONOXIDE           /
            CO2 CARBON-DIOXIDE            / CH4 METHANE                  /
            N2 NITROGEN                   / AR ARGON                     /
            HCL HYDROGEN-CHLORIDE         / H2S HYDROGEN-SULFIDE         /
            H3N AMMONIA                   / COS CARBONYL-SULFIDE         /
            CS2 CARBON-DISULFIDE          / CHN HYDROGEN-CYANIDE         /
            C2H4 ETHYLENE                 / C2H4O2-1 ACETIC-ACID         /
            C2H6 ETHANE                   / C3H6-2 PROPYLENE             /
            C3H6O-1 ACETONE               / C3H8 PROPANE                 /
            C4H4S THIOPHENE               / C4H8-1 1-BUTENE              /
            C4H8-2 CIS-2-BUTENE           / C4H8-3 TRANS-2-BUTENE        /
            C4H8O-3 METHYL-ETHYL-KETONE   / C4H10-1 N-BUTANE             /
            C5H5N PYRIDINE                / C6H6 BENZENE                 /
            C6H6O PHENOL                  / C6H14-1 N-HEXANE             /
            C7H8 TOLUENE                  / C7H8O-3 O-CRESOL             /
            C10H8 NAPHTHALENE             / C10H22-1 N-DECANE            /
            COOL WATER                    / COAL
;   --------------------- OK AS OF 07-16-84 ---------------------
```

```
FORMULA O2 O2 / H2O H2O / H2 H2 / CO CO / CO2 CO2 / CH4 CH4 / N2 N2
;   --------------------- OK AS OF 07-16-84 ---------------------
ATTR-COMPS    COAL   PROXANAL  ULTANAL  SULFANAL
;   --------------------- OK AS OF 07-16-84 ---------------------
NC-PROPS    COAL    ENTHALPY HCOALGEN 3 1 1 1 / DENSITY DCHARIGT
;
;GRUMMEL AND DAVIS CORRELATION FOR COAL ENTHALPY USED
;
;   --------------------- OK AS OF 07-16-84 ---------------------
PROP-DATA   ;   HEAT CAPACITY DATA
     PROP-LIST CP1C
     PVAL COAL 1. 0. 0. 0. & ; MOISTURE
               .223 .000218 0. 0. & ; FIXED CARBON (WEN)
               .43862 1.5414D-04 0. 0. & ; PRIMARY VOLATILES (NEUTRAL)
               .43862 1.5414D-04 0. 0. & ; SECONDARY VOLATILES (NEUTRAL)
               .18 .00014 0. 0. ; ASH
;   --------------------- OK AS OF 07-16-84 ---------------------
PROPERTIES  SYSOPO GLOBAL
;   --------------------- OK AS OF 07-16-84 ---------------------
FLOWSHEET
     GSMX IN = STM-FD O2-FD              OUT = STM-O2
;
;STEAM AND OXYGEN MIXED FEED
;
     RCTR IN = STM-O2 COAL-FD COOL-IN    OUT = PROD-GS CHAR COOL-OUT
;
;GASIFIER
;INLET STREAM ORDER - GAS FEED, COAL FEED, COOLANT FEED
;OUTLET STREAM ORDER - PRODUCT GAS , CHAR-ASH EFFLUENT, COOLANT + STEAM
;
;   --------------------- OK AS OF 07-16-84 ---------------------
DEF-STREAMS MIXNC ALL
;   --------------------- OK AS OF 07-16-84 ---------------------
STREAM  COOL-IN
        SUBSTREAM MIXED PRES=3.892468D+06 V-FRAC=0.0 MASS-FLOW=11.94375
        MOLE-FRAC COOL 1.
;   --------------------- OK AS OF 07-16-84 ---------------------
STREAM  STM-FD
        SUBSTREAM MIXED TEMP=672.0488889 PRES=3.892468D+06 V-FRAC=1 &
                  FLASH-OPTION=1-PHASE
        MASS-FLOW H2O 11.94375
        SUBSTREAM NC TEMP=672.0488889 PRES=3.892468D+06
;   --------------------- OK AS OF 07-16-84 ---------------------
STREAM  O2-FD
        SUBSTREAM MIXED TEMP=416.4933334 PRES=3.720142D+06 V-FRAC=1 &
                  FLASH-OPTION=1-PHASE
        MASS-FLOW O2 2.49375 / AR 0.000315
        SUBSTREAM NC TEMP=416.4933334 PRES=3.720142D+06
```

```
;   ---------------------- OK AS OF 07-16-84 ---------------------
STREAM  COAL-FD
        SUBSTREAM MIXED TEMP=298.16 PRES=3.065304D+06 V-FRAC=1 &
                  FLASH-OPTION=1-PHASE
        SUBSTREAM NC TEMP=298.16 PRES=3.065304D+06
        MASS-FLOW  COAL 12.2766
        COMP-ATTR COAL PROXANAL (25.53983619 34.50483991 &
                                 32.88160834 7.073715562 )/
                       ULTANAL (9.50 65.97 4.16 1.27 0.02 1.18 17.92)/
                       SULFANAL (0. 0. 0.)
;
;COAL DATA FROM DOW USING ONLY CHAR-ASH RATIO
;
;   ---------------------- OK AS OF 07-16-84 ---------------------
BLOCK   GSMX   MIXER
        PARAM PRES=3.065304D+06 NPK=1 KPH=1
;   ---------------------- OK AS OF 07-16-84 ---------------------
BLOCK   RCTR   RGAS
        SUBROUTINE KINET=DELKIN
;*********************************************************************
;********** DO NOT CHANGE THE VALUES OF CODE, NOUT, OR STATE **********
;*********************************************************************
        PARAM  CODE=6 NOUT=10 STATE=1 &
               LENGTH=3.000D+00 DIAM=4.000D+00 &
               PRES=3.065304D+06 PRESDP=0.0 UCP=1.70D+02 &
               ESP=3.000D-02 TEST1=0.10D-02
;              USE ESP FOR MAXIMUM INCREMENT (PRMT(3))
;                  SET ESP TO ABOUT 1% OF TOTAL LENGTH
;              USE TEST1 FOR ERROR CRITERIA (PRMT(4))
        COOLANT CPRES=3.892468D+06 NPK=2 TINIT=672.0488889
        UVEC NINTK=1 NREALK=75 NIWK=3 NWK=42 NREALP=53 NWP=4 NREALQ=12
;            NCC    = NUMBER OF CONVENTIONAL COMPONENTS (INCLUDE COOL)
;            NNCC   = NUMBER OF NON-CONVENTIONAL COMPONENTS = 1 (COAL)
;            NINTK  = ITERATIONS FOR CARBON CONVERGENCE (15 SUGGESTED)
;            NREALK = REAL VECTOR OF DIMENSION (NCC + 40)
;            NIWK   = SUBSTREAMS INDICATOR
;            NWK    = REAL WORK VECTOR OF DIMENSION (NCC + NNCC + NR)
;            NREALP = REAL VECTOR OF DIMENSION (NCC + 18)
;            NWP    = REAL WORK VECTOR OF DIMENSION 4 FOR CONVERGENCE
;            NREALQ = REAL VECTOR OF DIMENSION (12)
        INTK 10
        REALK .00000D-00 3.8612D-03 7.9434D-04 8.0075D-03 6.0537D-03   &
;             O2         H2O        H2         CO         CO2
              1.1116D-02 2.7054D-04 0.0000D-00 1.2771D-05 7.2865D-04   &
;             CH4        N2         AR         HCL        H2S
              1.4993D-03 3.1213D-05 3.1213D-05 4.9421D-07 1.0925D-04   &
;             H3N        COS        CS2        CHN        C2H4
              9.6761D-05 7.8085D-04 1.0925D-04 1.4514D-05 1.2485D-04   &
;             C2H4O2-1   C2H6       C3H6-2     C3H6O-1    C3H8
              1.1081D-05 1.0925D-04 0.0000D-00 0.0000D-00 1.6049D-04   &
```

```
;            C4H4S       C4H8-1      C4H8-2      C4H8-3      C4H8O-3
             6.2427D-05  1.2381D-05  7.8033D-05  1.5399D-04  5.1242D-05   &
;            C4H10-1     C5H5N       C6H6        C6H6O       C6H14-1
             1.6049D-04  4.0811D-04  1.1393D-04  7.9334D-05  0.0000D-00   &
;            C7H8        C7H8O-3     C10H8       C10H22-1    COOL
;
;      REACTION ORDER (UNIVERSITY OF DELAWARE MODEL)
;     REACTION 1:      Q  * C   + 1.0 * O2 --- 2 * ( Q - 1.0 ) * CO
;                                               + ( 2.0 - Q ) * CO2
;     REACTION 2:     1.0 * H2O + 1.0 * C  === 1.0 * CO  + 1.0 * H2
;     REACTION 3:     1.0 * CO2 + 1.0 * C  === 2.0 * CO
;     REACTION 4:     2.0 * H2  + 1.0 * C  === 1.0 * CH4
;     REACTION 5:     1.0 * H2O + 1.0 * CO === 1.0 * CO2 + 1.0 * H2
;
;            1.79D+06    27000.      613.        42000.      367.8        &
             1.79D+05    27000.      61.3        42000.      36.78        &
;            ADJ/RC 1    AE 1        RC 2        AE 2        EFF/RC 3
;            42000.      8.356D-06   16046.      3.D+06      14400.       &
             42000.      8.356D-05   16046.      3.D+07      14400.       &
;            AE 3        ADJ/RC 4    AE 4        RC 5        AE 5
             0.          0.          0.          0.          0.           &
;          SPACE FOR MISCELLANEOUS KINETIC CONSTANTS
             0.          0.          0.          0.          0.           &
;          SPACE FOR MISCELLANEOUS KINETIC CONSTANTS
             0.4         0.6         2.367       0.          1.3          &
;            VOID BED    VOID COAL   DIAM COAL   COAL DEN    CHAR DEN
             0.5         1.333333    0.6         0.01408     0.01408      &
;            ASH DEN     C/O2        SCHMIDT     O2 DIFF     H2O DIFF
             1.          0.          0.          0.          0.           &
;            MODEL
             1.0         950.00000   1255.3822   0.001       0.500
;            VMD         TVOLLO      TVOLHI      ITER 1      ITER 2
;          REALK  OPERATING DATA VECTOR FOR PROGRAM
;          REALK       1 = KGMOLES OF VOLATILE O2  MADE/KG VOLATILE MATTER
;          REALK       2 = KGMOLES OF VOLATILE H2O MADE/KG VOLATILE MATTER
;          REALK       3 = KGMOLES OF VOLATILE H2  MADE/KG VOLATILE MATTER
;          REALK       4 = KGMOLES OF VOLATILE CO  MADE/KG VOLATILE MATTER
;          REALK       5 = KGMOLES OF VOLATILE CO2 MADE/KG VOLATILE MATTER
;          REALK       6 = KGMOLES OF VOLATILE CH4 MADE/KG VOLATILE MATTER
;          REALK       7 = KGMOLES OF VOLATILE N2  MADE/KG VOLATILE MATTER
;          REALK       8 = KGMOLES OF VOLATILE ??? MADE/KG VOLATILE MATTER
;          ...
;          REALK  NCC-1 = KGMOLES OF VOLATILE ??? MADE/KG VOLATILE MATTER
;          REALK     NCC = 0. (DUMMY SPACE FOR COOLANT)
; (UWV)    REALK NCC+ 1 = REACTION 1 RATE ADJUSTMENT
; (UDEL)   REALK NCC+ 1 = RATE CONSTANT OF REACTION 1
; (UDEL)   REALK NCC+ 2 = ACTIVATION ENERGY OF REACTION 1
;          REALK NCC+ 3 = RATE CONSTANT OF REACTION 2
;          REALK NCC+ 4 = ACTIVATION ENERGY OF REACTION 2
; (UWV)    REALK NCC+ 5 = EFFECTIVENESS FACTOR FOR ASH ON REACTION 3
```

```
; (UDEL)   REALK NCC+ 5 = RATE CONSTANT OF REACTION 3
; (UDEL)   REALK NCC+ 6 = ACTIVATION ENERGY OF REACTION 3
; (UWV)    REALK NCC+ 7 = REACTION 4 RATE ADJUSTMENT
; (UDEL)   REALK NCC+ 7 = RATE CONSTANT OF REACTION 4
; (UDEL)   REALK NCC+ 8 = ACTIVATION ENERGY OF REACTION 4
;          REALK NCC+ 9 = RATE CONSTANT OF REACTION 5
;          REALK NCC+10 = ACTIVATION ENERGY OF REACTION 5
;          REALK NCC+21 = BED VOID FRACTION
; (UDEL)   REALK NCC+22 = COAL VOID FRACTION
;          REALK NCC+23 = INITIAL PARTICLE DIAMETER (CM)
; (UWV)    REALK NCC+24 = INITIAL DENSITY OF CHAR/ASH FEED (GM/CU.CM.)
; (UDEL)   REALK NCC+25 = INITIAL DENSITY OF CHAR FEED (GM/CU.CM.)
; (UDEL)   REALK NCC+26 = INITIAL DENSITY OF ASH FEED (GM/CU.CM.)
; (UWV)    REALK NCC+27 = RATIO OF CO TO CO2 IN REACTION 1
; (UDEL)   REALK NCC+27 = RATIO OF C  TO O2  IN REACTION 4
; (UDEL)   REALK NCC+28 = SCHMIDT NUMBER
; (UDEL)   REALK NCC+29 = DIFFUSION CONSTANT FOR OXYGEN (SQ.CM./SEC)
; (UDEL)   REALK NCC+30 = DIFFUSION CONSTANT FOR WATER (SQ.CM./SEC)
; (UDEL)   REALK NCC+31 = MODEL TYPE: 1 = ASH SEGREGATION
;                                     2 = SHELL PROGRESSIVE
;                                     3 = HOMOGENEOUS
;          REALK NCC+32 = MISCELLANEOUS
;          REALK NCC+33 = MISCELLANEOUS
;          REALK NCC+34 = MISCELLANEOUS
;          REALK NCC+35 = MISCELLANEOUS
;        REALK NREALK-4 = FRACTION VOLATILE MATTER RELEASED BY PYROLYSIS
;        REALK NREALK-3 = FINAL TEMPERATURE FOR VOLATILE MATTER RELEASE
;        REALK NREALK-2 = INITIAL TEMPERATURE FOR VOLATILE MATTER RELEASE
;        REALK NREALK-1 = FRACTION UNCONVERTED FIXED CARBON 1ST ITERATION
;        REALK NREALK = FRACTION UNCONVERTED FIXED CARBON 2ND ITERATION
       REALP .025 .025 .025 .025 .025 .025 .0   .0   .0   .0   &
             .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   &
             .0   .0   .0   .0   .0   .0   .0   .0   .0   .0   &
             .0   .0   .0   .0   .0   .010 .0   .010 .005 .005 &
             .005 .005 .0   .0   .0   .0   .0   .0   .0   .0   &
             .010 .8   .0
;            REALP  ERROR CRITERIA VECTOR FOR INTEGRATION
;*****************************************************************
;**************** SUM OF REALP COMPONENTS MUST BE ONE ****************
;*****************************************************************
;            REALP        1 = OXYGEN MOLE FRACTION
;            REALP        2 = WATER MOLE FRACTION
;            REALP        3 = HYDROGEN MOLE FRACTION
;            REALP        4 = CARBON MONOXIDE MOLE FRACTION
;            REALP        5 = CARBON DIOXIDE MOLE FRACTION
;            REALP        6 = METHANE MOLE FRACTION
;            REALP        7 = NITROGEN MOLE FRACTION
;            REALP        8 = 0.0 = ?? MOLE FRACTION
;            ...
;            REALP NCC -  1 = 0.0 = ?? MOLE FRACTION
```

```
;            REALP NCC      = COOL (H2O) MOLE FRACTION
;            REALP NCC +  1 = TOTAL GAS FLOW
;            REALP NCC +  2 = WEIGHT FRACTION MOISTURE (PROXANAL)
;            REALP NCC +  3 = WEIGHT FRACTION FIXED CARBON (PROXANAL)
;            REALP NCC +  4 = WEIGHT FRACTION VOLATILE MATTER (PROXANAL)
;            REALP NCC +  5 = WEIGHT FRACTION ASH (PROXANAL)
;            REALP NCC +  6 = WEIGHT FRACTION ASH (ULTANAL)
;            REALP NCC +  7 = WEIGHT FRACTION CARBON (ULTANAL)
;            REALP NCC +  8 = WEIGHT FRACTION HYDROGEN (ULTANAL)
;            REALP NCC +  9 = WEIGHT FRACTION NITROGEN (ULTANAL)
;            REALP NCC + 10 = WEIGHT FRACTION CHLORINE (ULTANAL)
;            REALP NCC + 11 = WEIGHT FRACTION SULFUR (ULTANAL)
;            REALP NCC + 12 = WEIGHT FRACTION OXYGEN (ULTANAL)
;            REALP NCC + 13 = WEIGHT FRACTION PYRITIC (SULFANAL)
;            REALP NCC + 14 = WEIGHT FRACTION SULFATE (SULFANAL)
;            REALP NCC + 15 = WEIGHT FRACTION ORGANIC (SULFANAL)
;            REALP NCC + 16 = TOTAL SOLID FLOW
;            REALP NCC + 17 = PROCESS TEMPERATURE
;            REALP NCC + 18 = HEAT LOSS TO COOLANT
        REALQ 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
        STOI REAC=1 SSID=NC      COMP=COAL COEF=-4.
        STOI REAC=1 SSID=MIXED   COMP=O2   COEF=-3.
        STOI REAC=1 SSID=MIXED   COMP=CO   COEF= 2.0
        STOI REAC=1 SSID=MIXED   COMP=CO2  COEF= 2.0
        STOI REAC=2 SSID=NC      COMP=COAL COEF=-1.
        STOI REAC=2 SSID=MIXED   COMP=H2O  COEF=-1.
        STOI REAC=2 SSID=MIXED   COMP=CO   COEF= 1.
        STOI REAC=2 SSID=MIXED   COMP=H2   COEF= 1.
        STOI REAC=3 SSID=NC      COMP=COAL COEF=-1.
        STOI REAC=3 SSID=MIXED   COMP=CO2  COEF=-1.
        STOI REAC=3 SSID=MIXED   COMP=CO   COEF= 2.
        STOI REAC=4 SSID=NC      COMP=COAL COEF=-1.
        STOI REAC=4 SSID=MIXED   COMP=H2   COEF=-2.
        STOI REAC=4 SSID=MIXED   COMP=CH4  COEF= 1.
        STOI REAC=5 SSID=MIXED   COMP=CO   COEF=-1.
        STOI REAC=5 SSID=MIXED   COMP=H2O  COEF=-1.
        STOI REAC=5 SSID=MIXED   COMP=CO2  COEF= 1.
        STOI REAC=5 SSID=MIXED   COMP=H2   COEF= 1.
;*********************************************************************
;************** TEMPERATURE PROFILE STORAGE (N + 2 POINTS)*************
;******* (1 ZERO POINT +  N INTERMEDIATE POINTS + 1 FOR MAXIMUM) ******
;*********************************************************************
        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.
;   -------------------- OK AS OF 07-16-84 --------------------
REPORT STREAMS BLOCKS FLOWSHEET
;STREAM-REPORT SUPPLEMENTAL OPTIONS=MOLE-FRAC
;   -------------------- OK AS OF 07-16-84 --------------------
```

APPENDIX B

USRWEN Input File

```
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;*                                                                            *
;* AUTHOR       :  B. SCOTT BREWSTER          DATE :  5/15/84                *
;*                                                                            *
;* SHORT TITLE :  METC PILOT PLANT SIMULATION
;*                                                                            *
;* DESCRIPTION :  THIS IS A SIMULATION OF THE METC FIXED-BED COAL GASIFIER
;*                SYSTEM.  THE C.Y. WEN MODEL IS USED TO SIMULATE THE
;*                GASIFIER; AND ADDITIONAL BLOCKS ARE INCLUDED TO ACCOUNT
;*                FOR PARTICULATE LOADINGS
;*                                                                            *
;* NUMBER OF PDF RECORDS REQUIRED:  100
;*                                                                            *
;* USER DATA FILES:                                                           *
;*           FILENAME:           FILETYPE (USRPP1A,ETC)      DISK PATHNAME:   *
;*           NONE                                                             *
;*                                                                            *
;* USER INSERT FILES:                                                         *
;*           FILENAME:           FILETYPE (INSERT)           DISK PATHNAME:   *
;*           NONE                                                             *
;*                                                                            *
;* USER SUBROUTINES REQUIRED:                                                 *
;*           FILENAME:    DESCRIPTION:                   DISK PATHNAME:      *
;*           USRWEN.FOR   WEN CODE                       DBB0:[DRF.ASPEN]
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;
TITLE           'METC PILOT PLANT'
;
DESCRIPTION    "THIS IS A SIMULATION OF THE METC FIXED-BED COAL GASIFIER
                SYSTEM.  THE C.Y. WEN MODEL IS USED TO SIMULATE THE
                GASIFIER; AND ADDITIONAL BLOCKS ARE INCLUDED TO ACCOUNT
                FOR PARTICULATE LOADINGS"
;
PROPERTIES  SYSOP3 GLOBAL
;
HISTORY         PROPERTIES= 2 SIMULATION= 4 STREAM= 6
;
IN-UNITS SI
OUT-UNITS SI
;
COMPONENTS CO CO/H2 H2/CO2 CO2/N2 N2/H2O H2O/O2 O2/CH4 CH4/
           H2S H2S/TARVAPOR C12H26/
           COAL-ASH/SOLIDTAR/AR AR
;
NC-PROPS COAL-ASH   DENSITY DCOALIGT/ENTHALPY HCJ1BOIE
NC-PROPS SOLIDTAR   DENSITY DCHARIGT/ENTHALPY HCJ1BOIE
;
ATTR-COMPS  COAL-ASH PROXANAL ULTANAL           SULFANAL/
            TARVAPOR          ULTANAL CLASS=CV          /
            SOLIDTAR PROXANAL ULTANAL           SULFANAL
;
```

```
FLOWSHEET   GASIFIER
    WEN         IN= COAL AIR STEAM      OUT= WENGAS  WENASH QWEN
    FLYMIX      IN= WENGAS HOTFLY       OUT= OFFGAS
    SPLITASH    IN= WENASH              OUT= COLDFLY ASHOUT
    FLYHETR     IN= COLDFLY             OUT= HOTFLY QFLYASH
    QMIX        IN= QWEN QFLYASH        OUT= QGASIF
;
DEF-STREAMS  MIXNC ALL/
             HEAT  QWEN QFLYASH QGASIF
;
STREAM  COAL
   SUBSTREAM  NC TEMP=298.16  PRES=3.065304D+06
      MASS-FLOW  COAL-ASH 12.2766
;
                              ;        ASH    C       H    N
      COMP-ATTR COAL-ASH      ULTANAL (9.50  65.97  4.16 1.27 &
                              ;         CL   S    O
                              0.02 1.18 17.92)/
;
                              ;            H2O            FC
                              PROXANAL (25.53983619     46.34 &
                              ;            VM             ASH
                                        44.16            9.5)/
;
                              ;        PYRITIC SULFATE ORGANIC
                              SULFANAL( 0.0      0.0     0.0)
STREAM   STEAM
   SUBSTREAM MIXED TEMP=672.0488889 PRES=3.892468D+06 V-FRAC=1 &
                   FLASH-OPTION=1-PHASE
      MASS-FLOW  H2O   11.94375
;
STREAM   AIR
   SUBSTREAM MIXED TEMP=416.4933334 PRES=3.720142D+06 V-FRAC=1 &
                   FLASH-OPTION=1-PHASE
      MASS-FLOW O2 2.49375 /N2 0.000315
;
BLOCK WEN USER
      DESCRIPTION  'WEN FIXED-BED GASIFIER MODEL'
      BLOCK-OPTIONS HMB-RESULTS=2 SIM-LEVEL=4
      SUBROUTINE  USRWEN1 USRWEN1
      PARAM  NINT=15 NREAL=244
      FLASH-SPECS  WENGAS  0/WENASH  0
;                  (OUTLET STREAMS ARE FLASHED INTERNALLY IN THE BLOCK)
      INT  2 &;(1=DESIGN MODE, 2=SIMULATION MODE)
           3 &;(1=BITUMINOUS COAL, 2=SUBBITUMINOUS COAL, 3=LIGNITE)
           0  ;(GAS COMP AND TEMP PROFILE PLOTS, 0=NO, 1=YES)
      REAL 9995.36  &; HEATING VALUE, BTU/LB WET COAL
           459.7    &; PRESSURE, PSIG
           13.12    &; BED DIAMETER, FT
           0.79     &; COAL PARTICLE SIZE, INCHES
```

```
            1.        &; FRACTION VOLATILE MATTER RELEASED DURING PYROLYSIS
            9.84      &; CARBON CONVERSION RATIO (DESIGN MODE) OR
                       ; BED HEIGHT (SIMULATION MODE), FT
            0.4       &; BED VOIDAGE
            29.8      &; OVERALL WALL HEAT TRANSFER COEFFICIENT, BTU/HR-FT**2-F
            700.0     &; WALL TEMPERATURE, F
            1.1       &; RATE COEFF OF CHAR-STEAM RXN, MOL/MOL C-ATM-S
            30000.    &; ACT ENERGY OF CHAR-STEAM RXN, CAL/MOL
            0.5       &; EFFECT FACTOR OF WATER-GAS-SHIFT RXN
            1.1       &; RATE COEFF OF CHAR-CO2 RXN, MOL/MOL C-ATM-S
            30000.     ; ACT ENERGY OF CHAR-CO2 RXN, CAL/MOL
;
BLOCK FLYMIX MIXER
  PARAM NPK=1
;
BLOCK SPLITASH FSPLIT
  FRAC COLDFLY 0.15/ASHOUT 0.85
;
TRANSFER FLYTEMP
  SET       BLOCK-VAR  BLOCK=FLYHETR VARIABLE=TEMP
  EQUAL-TO STREAM-VAR STREAM=WENGAS VARIABLE=TEMP
  EXECUTE BEFORE FLYHETR
;
BLOCK FLYHETR HEATER
  PARAM NPK=1
;
BLOCK QMIX MIXER
  PARAM NPK=1
;
```

APPENDIX C

MIT Input File

```
;
TITLE 'GASIFIER SIMULATION - NON KINETICS MODEL'
;
DESCRIPTION "ASPEN SIMULATION OF THE BRITISH GAS/LURGI GASIFIER FOR METC"
;
;
IN-UNITS ENG
;
HISTORY  MSG-LEVEL PROPERTIES=2 STREAMS=8 SIMULATION=8
;
RUN-CONTROL MAX-TIME = 200.
;
;
COMPONENTS  O2 OXYGEN/ N2 NITROGEN/ H2O WATER/ H2 HYDROGEN/CO CARBON-MONOXIDE/
            CO2  CARBON-DIOXIDE/CH4  METHANE/H2S  HYDROGEN-SULFIDE/
            NH3  AMMONIA/TAR  C21H42/ COAL/ CACO3-S/ CACO3-L/ ASH /CARBON/
            OIL C11H10-2/PHENOL  C6H6O/ NAPHTHA  C6H6/ C2-TO-C4 C3H8/
            COS COS/ CS2 CS2/ C4H4S C4H4S/ CAO/ CHAR
;
FORMULA H2O H2O      ;  NEEDED FOR SYSOP12
;
;
PROPERTIES  SYSOP3  GLOBAL /  ;  RKS EQN. OF STATE  FOR PROCESS STREAMS
            SYSOP12;  ASME STEAM TABLE CORRELATIONS FOR STEAM AND COOLING WATER
;
FLOWSHEET
;
     PROD       IN= COALFD                          OUT= YLD-EFL  HEATYLD
     MIX1       IN= YLD-EFL TAR-FD XTRA-CO2       OUT= S1
     DEVOL      IN= S1                            OUT= VOLATILS  UNGASIFD
     MIX2       IN= UNGASIFD FLUX FUEL OXYGEN STEAM  OUT= REACFEED
     BURNTAR    IN= REACFEED                      OUT= NOTAR
     GAS1       IN= NOTAR                         OUT= COMBPROD
     MELTDCMP   IN= COMBPROD                      OUT= MELTPROD
     SLAGREM    IN= MELTPROD                      OUT= RGAS1 LIQSLAG
     SLAGFUSE   IN= LIQSLAG                       OUT= SOLSLAG
     SLAGQNCH   IN= SOLSLAG S319 S311 QCWQUEN     OUT= COOLSLAG
     GAS2       IN= RGAS1                         OUT= RGAS2
     GAS3       IN= RGAS2                         OUT= RGAS3
     EQL-REAC   IN= RGAS3                         OUT= SHFT-GAS  HTEQL
     JACKET     IN= HPBFW                         OUT= JKTSTEAM S321  QJACKET
     HETXQUEN   IN= CWFEED1                       OUT= CWRET1  QCWQUEN
     HETXDIST   IN= LPBFW2                        OUT= LPSTEAM2 S320 QDISTRIB
     ADDER      IN= VOLATILS SHFT-GAS JKTSTEAM    OUT= OFFGAS
     QADD       IN= HEATYLD QJACKET HTEQL QDISTRIB   OUT= QSUM
;    IN THE MIT FILE THE STREAM HEATYLD WAS CALLED QYLD.  THE MIT
;    REPORT ON THIS PROJECT SHOWED IT COMING FROM BLOCK PROD AND
;    THUS THE STREAM WAS RENAMED HEATYLD BY RAB 12/14/81
;
;
```

```
ATTR-COMPS     COAL      PROXANAL  ULTANAL  SULFANAL  COALMISC  /
               CHAR      PROXANAL  ULTANAL  SULFANAL  COALMISC  /
               ASH       AOXANAL   GENANAL                      /
;
               TAR       ULTANAL   CLASS = CV                    /
               PHENOL    ULTANAL   CLASS = CV                    /
               NAPHTHA   ULTANAL   CLASS = CV                    /
               OIL       ULTANAL   CLASS = CV
;
NC-PROPS    COAL        ENTHALPY  HCOALGEN * 2 * * / DENSITY  DCOALIGT
NC-PROPS    ASH         ENTHALPY  ENTHLUSR         / DENSITY  DNSTYGEN
NC-PROPS    CHAR        ENTHALPY  HCOALGEN * 2 * * / DENSITY  DCHARIGT
;
INSERT * RKSKIJ  H2  CH4  CO  CO2  H2O  H2S  NAPHTHA
;  FURTHER RKSKIJ'S
PROP-DATA  COMP-LIST       H2S  CO2   CO   CH4   C2-TO-C4   NAPHTHA
     BCVAL RKSKIJ 1 1 N2  .14 -.022 .046 .0319   .0807    .2131
PROP-DATA  COMP-LIST        CH4  C2-TO-C4  NAPHTHA  PHENOL  OIL  TAR
     BCVAL RKSKIJ 1 1 H2O  .085    .16      .2       .2     .3   .5
     BCVAL RKSKIJ 1 1 H2S  .085    .16      .2       .2     .3   .5
;
PROP-DATA
;
     COMP-LIST   ASH
        CVAL  DENGEN 1 1 2.0D3
;
     PROP-LIST              MW    /   DHSFRM    /   DGSFRM
       PVAL   CARBON       12.01 /   0.0       /     0.0
       PVAL   CACO3-S     100.09 / -1.207473D9 / -1.127830D9
       PVAL   CACO3-L     100.09 / -1.154260D9 / -1.127830D9
       PVAL   CAO          56.08 / -0.634719D9 / -0.603569D9
;
     PROP-LIST           CPSPO1
       PVAL  CARBON     1.7154E+04  4.268  0.0  0.0  -2.786E+08  298  2300
       PVAL  CACO3-S      1.045863D5  2.193883D1 0D0 0D0 -2.595816D9 298 1200
       PVAL  CACO3-L      1.045863D5  2.193883D1 0D0 0D0 -2.595816D9 298 1200
       PVAL  CAO        0.496554D5  0.452174D1 0D0 0D0 -0.695009D9 298 2888
;
     PROP-LIST            VSPOLY
       PVAL  CARBON      5.54E-03  0.0  0.0  0.0  0.0  0.0  2.0E+03
       PVAL  CACO3-S       3.694D-2  0D0 0D0 0D0 0D0 0D0 2D3
       PVAL  CACO3-L       3.694D-2  0D0 0D0 0D0 0D0 0D0 2D3
       PVAL  CAO         1.676D-2  0D0 0D0 0D0 0D0 0D0 2D3
;
;
DEF-STREAM-CLASS  SLAG  SUBS= MIXED  CISOLID  NC
;
DEFS SLAG ALL / &
  CONVEN  XTRA-CO2 HPBFW JKTSTEAM S311 S319 STEAM OXYGEN FUEL &
          S320 CWFEED1 CWRET1 LPBFW2 LPSTEAM2 S321 / &
  HEAT    HTEQL HEATYLD QJACKET QCWQUEN QDISTRIB QSUM
;
```

```
STREAM  LPBFW2  TEMP = 250.  PRES = 150.
      MASS-FLOW  H2O  10320.3
;
;
STREAM  S311  TEMP = 143.  PRES = 102.4
      MASS-FLOW  H2O  38625.
;
STREAM  S319  TEMP = 85.  PRES = 49.4
      MASS-FLOW  H2O  5000.
;
STREAM  COALFD ;NAME CHANGED FROM COAL TO COALFD BY RAB 12/11/81
     SUBSTREAM MIXED TEMP=77. PRES=14.4 MASS-FLOW=1.D-10
          MASS-FRAC CO2 1.  ;ADDED BY LEG 12/8/81
          COMP-ATTR TAR     ULTANAL (0.   95.00 5.00 0.   0.   0.    0.  )
          COMP-ATTR PHENOL  ULTANAL (0.   76.58 6.42 0.   0.   0.   17.00)
          COMP-ATTR NAPHTHA ULTANAL (0.   85.07 9.32 0.39 0.   1.56  3.66)
          COMP-ATTR OIL     ULTANAL (0.   85.65 8.36 0.59 0.   1.40  4.00)
;
     SUBSTREAM NC  TEMP=77.  PRES=14.4
          MASS-FLOW  COAL   104720.
          COMP-ATTR  COAL   PROXANAL (2.5 41.0 35.9 23.1)                /
                            ULTANAL (23.1 60.0 4.35  1.0 0.04  4.8  6.7) /
                            SULFANAL (0.16 0.06 0.47)                   /
                            COALMISC ( *  *  *  0.5  * )
;
          COMP-ATTR  CHAR   PROXANAL (0.0  84. 7. 9.)                   /
                            ULTANAL  (9.  84. 7. 0. 0. 0. 0.)           /
                            SULFANAL (.16 .06 .47)                      /
                            COALMISC ( *  *  *  0.8  * )
;
          COMP-ATTR  ASH    GENANAL (100. 0. 0. 0. 0. 0. 0. 0. 0. 0.)
;
;
STREAM     FLUX
       SUBSTREAM  CISOLID  TEMP=77  PRES=14.4
          MASS-FLOW  CACO3-S  10472
;
STREAM  TAR-FD
    SUBSTREAM MIXED  TEMP= 158. PRES= 514.4
     MASS-FLOW  TAR  9704.
    SUBSTREAM  NC  TEMP = 158.  PRES = 514.4
     MASS-FLOW  CHAR  1571.
          COMP-ATTR  CHAR   PROXANAL (0.0  84. 7. 9.)                   /
                            ULTANAL  (9.  84. 7. 0. 0. 0. 0.)           /
                            SULFANAL (.16 .06 .47)                      /
                            COALMISC ( *  *  *  0.8  * )
;
;
STREAM  OXYGEN  TEMP=275  PRES=544.4
    MASS-FLOW  O2  44574 / N2  794
```

```
;
STREAM  STEAM  TEMP=750  PRES=564.4
    MASS-FLOW  H2O  32074
;
STREAM  XTRA-CO2  TEMP=460.  PRES=450.
     MASS-FLOW  CO2  3386.
;
STREAM  FUEL  PRES = 534.4  TEMP = 100.
     MOLE-FLOW  CH4  6.5/ H2  .3/ CO2  .1/ N2  .2/
;
STREAM  HPBFW TEMP=250.  PRES=804.4
     MASS-FLOW  H2O  11830.
;
STREAM  CWFEED1  TEMP=85.  PRES=74.4
     MOLE-FLOW  H2O   84178.2
;
;
;                UNIT OPERATION BLOCKS' SPECIFICATIONS
;
;
BLOCK   MIX1     MIXER
      PARAM  450.  1
;
BLOCK   PROD    RYIELD
   PARAM  PRES=450.  TEMP=1000. NPK=1  KPH=1
     SUBROUTINE  USER = NYLD
     USER-VECS 1 1 1 1
;
BLOCK  MIX2  MIXER
    PARAM  450. 1
;
BLOCK  DEVOL  SEP2
    FLASH-SPECS  STRM= VOLATILS  PRES= 450.  NPK=1  KPH=1
    FRAC  SUBS=MIXED  STRM=VOLATILS &
     COMP= N2 CO H2S NH3 OIL PHENOL NAPHTHA C2-TO-C4   &
           O2 H2O H2 CO2 CH4 COS CS2 C4H4S &
     FRAC= 1.  1. 1.  1.  1.   1.      1.     1.  &
           0. 1  .31  .3   0  1   1    1
     MOLES  SUBS=MIXED  STRM=UNGASIFD  COMP=TAR  FLOW=11.1
     MASS   SUBS=NC     STRM=UNGASIFD  COMP=CHAR FLOW=111.
;
    SUBS-FRAC  SUBS=CISOLID  STRM= UNGASIFD  FRAC = 1.0
;
     FRAC  SUBS=NC  STRM=UNGASIFD  COMP= ASH  FRAC=1.0
;
;
BLOCK  BURNTAR  RSTOIC
     PARAM Q=0 PRES=450
     STOICH  1  MIXED O2 -.88065/ TAR -0.03267 / CO2 .761299/ H2O .238701
     CONV    1  MIXED  TAR  1.0
    STOICH  2  NC CHAR -9.554/ MIXED O2 -.83415/ CO2  .6683/ H2O  .3317
    CONV    2  NC    CHAR  1.0
;
```

```
BLOCK   GAS1   RSTOIC
    PARAM   Q=0    PRES= 450
    STOICH  1  CISOLID CARBON -1.013/ MIXED O2 -1/ CO .026/ CO2 .987
    CONV    1  MIXED O2  1.0
;
BLOCK  MELTDCMP  RSTOIC
;
;  THIS  BLOCK MELTS THE FLUX AND THEN DECOMPOSES IT TO GAS AND SOLID.
;
    STOICH  1  CISOLID  CACO3-S -1/ CACO3-L .1073/ CAO .8927/MIXED CO2 .8927
    CONV    1  CISOLID  CACO3-S  1.0
;
BLOCK  GAS2  RSTOIC
    PARAM  Q=0   PRES= 450
    STOICH 1 CISOLID  CARBON -1 / MIXED CO2 -1/ CO 2
    CONV   1 MIXED    CO2  .90
    STOICH  2  CISOLID CARBON -1/ MIXED H2O -1/ CO 1/ H2 1
    CONV    2  MIXED  H2O  .50
;
BLOCK  GAS3  RSTOIC
;
;  THIS TAKES ALL REMAINING CARBON INTO GAS
;
    PARAM  Q=0  PRES=450
    STOICH 1 CISOLID  CARBON -1/ MIXED H2 -2 / CH4 1
    CONV   1 CISOLID  CARBON  1.0
;
BLOCK  SLAGREM  SEP2
   SUBS-FRAC  SUBS=MIXED  STRM=RGAS1  FRAC=1.0
   SUBS-FRAC  SUBS=NC  STRM=LIQSLAG  FRAC=1.0
   FRAC  SUBS=CISOLID  STRM=RGAS1  &
       COMP=  CARBON  CACO3-S  CACO3-L  CAO  &
       FRAC=    1.0     0.0      0.0    0.0
;
BLOCK  SLAGFUSE  RSTOIC
     PARAM   Q=0   PRES=40.
     STOICH  1  CISOLID CACO3-L  -1/ CACO3-S 1
     CONV 1 CISOLID  CACO3-L  1.0
;
BLOCK  SLAGQNCH  MIXER
    PARAM  PRES = 27.
;
;
BLOCK  EQL-REAC  RGIBBS
       PARAM  TEMP= 1200.  PRES= 450.   NAT=4  NPHS=1 NPX=1 NR=2  IDEL=1
       PROD  H2 1/ CO 1/ CO2 1/ H2O 1/ CH4 1/ N2 1
       ATOM  H2 2 2/CO 1 1/ CO 3 1/CO2 1 1/CO2 3 2/H2O 2 2/
             H2O 3 1/CH4 1 1/CH4 2 4/ N2 4 2
       STOI  1  CO -1/H2O -1/CO2 1/H2 1
       STOI  2  CO -1/H2 -3/CH4 1/H2O 1
       DELT  1  2620./ 2  399.
;
```

```
BLOCK  ADDER  MIXER
    BOPT SMLV=6 STLV=6
;
BLOCK  HETXQUEN   HEATER
    PROPERTIES  SYSOP12
    PARAM  TEMP = 105.  PRES = -25.
;
BLOCK  JACKET  FLASH2
     PROPERTIES  SYSOP12
     PARAM  PRES = 470.4  V=.97  TEST=457.
;
BLOCK  HETXDIST  FLASH2
     PROPERTIES  SYSOP12
      PARAM  V = .97089   PRES = 64.4
;
BLOCK  QADD MIXER
;
DES-SPEC METH
     DEFINE FCH4 MOLE-FLOW SHFT-GAS MIXED CH4
     SPEC FCH4 TO 471.4
     TOL-SPEC 5.
     VARY BLOCK-VAR BLOCK=EQL-REAC SENTENCE=DELT VARIABLE=TAPP ID1=2
     LIMITS -300. 2000.
DES-SPEC SHIFT
     DEFINE FH2O MOLE-FLOW SHFT-GAS MIXED H2O
     SPEC FH2O TO 622.7
     TOL-SPEC 6.
     VARY BLOCK-VAR BLOCK=EQL-REAC SENTENCE=DELT VARIABLE=TAPP ID1=1
     LIMITS 0.0 3700.
;
FORTRAN  PYROL
     DEFINE TARFL2 BVAR DEVOL MOLES FLOW 1 MIXED UNGASIFD
     DEFINE CHRFL2 BVAR DEVOL MASS FLOW 1 NC UNGASIFD
     DEFINE TARFL1 MOLE-FLOW YLD-EFL MIXED TAR
     DEFINE CHRFL1 MASS-FLOW YLD-EFL NC CHAR
F     TARFL2 = TARFL1
F     CHRFL2 = CHRFL1
     EXECUTE BEFORE DEVOL
;
;SEQ A HFS GAS1 MELTDCMP SLAGREM SLAGFUSE SLAGQNCH (RETURN HFS)
;SEQUENCE ORDER1  HETXDIST HETXQUEN JACKET PROD MIX1 PYROL DEVOL MIX2 BURNTAR &
;   GAS1 MELTDCMP SLAGREM SLAGFUSE SLAGQNCH  GAS2 GAS3 EQL-REAC &
;                 QADD ADDER
;
;  THE END
```

APPENDIX D

SLAGGER Input File

```
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;*                                                                            *
;* AUTHOR      :  JULIANNE M. STEFANO        DATE :  MAY 1985                *
;*                                                                            *
;* SHORT TITLE :  ASPEN SIMULATION OF A SLAGGING FIXED-BED GASIFIER           *
;*                                                                            *
;* DESCRIPTION :  THIS IS A NON-KINETIC SIMULATION OF A SLAGGING FIXED-BED    *
;*                GASIFIER.  THE DEVOLATILIZATION ROUTINE IS BASED ON THE     *
;*                USER MODEL, NYLD, DEVELOPED BY MIT IN THE SIMULATION OF     *
;*                THE PIPELINE GAS DEMONSTRATION PLANT.  THE COEFFICIENTS     *
;*                FOR THE COMBUSTION OF TAR, CHAR, AND OIL ARE DETERMINED BY  *
;*                THE FORTRAN BLOCK, COEFFS.  THE GASIFICATION REACTIONS USED *
;*                TO MODEL THE GASIFICATION ZONE ARE:                         *
;*                     C + H2O ---> CO + H2                                   *
;*                     C + CO2 ---> 2CO                                       *
;*                     C + 2H2 ---> CH4                                       *
;*                     CO + H2O ---> CO2 + H2                                 *
;*                NO KINETICS ARE CONSIDERED.  INSTEAD THE TEMPERATURE        *
;*                APPROACH TO EQUILIBRIUM IS USED IN AN RGIBBS BLOCK. A       *
;*                LIMESTONE FLUX IS ADDED TO FORM A SLAG WITH THE ASH.        *
;*                THE FORTRAN BLOCK, CHKMELT, CHECKS TO SEE THAT THE          *
;*                TEMPERATURE AT THE BOTTOM OF THE BED IS HIGH ENOUGH TO      *
;*                MELT THE SLAG AND ASH.  THE OFFGAS IS COOLED AND THE HEAVY  *
;*                HYDROCARBONS CONDENSE.  THE TAR AND OIL ARE RECYCLED TO THE *
;*                GASIFIER FOR FURTHER REACTION.                              *
;*                                                                            *
;* NUMBER OF PDF RECORDS REQUIRED: 100                                        *
;*                                                                            *
;* USER DATA FILES REQUIRED:  NONE                                            *
;*                                                                            *
;* USER INSERT FILES REQUIRED:  NONE                                          *
;*                                                                            *
;* USER SUBROUTINES REQUIRED:  ASH11, CIDIDX, ENTHLU, NYLD, SAVMWU            *
;*                                                                            *
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;
;                          USING THIS INPUT FILE
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;
;
;  COMPONENTS
;
;  The compounds used to model the hydrocarbons formed during devolatilization
;  are:
;                        Tar          C21H42
;                        Naphtha      C6H6
;                        Phenol       C6H6O
;                        Oil          C11H10-2
;
;  These formulas are used for physical property calculations.  The actual
;  compositional makeup of these compounds is determined by their ultimate
;  analyses.  When these components are reacted, the reaction coefficients are
;  determined by a FORTRAN block based on the ultimate analysis.  Presently, the
;  FORTRAN block does not consider chlorine and sulfur.  Therefore, these
;  components should be absent from the analyses or the FORTRAN block must be
;  modified.
```

```
;
; Limestone is modeled as pure CaCO3.
;
; Ash is considered a pure component with a distinct melting point and heat
; capacity as a function of temperature.
;
; The component names must remain the same as those in this input file or else
; the user routine NYLD will not recognize the components.
;
;
; PROPERTIES
;
; The heating value of coal is supplied in COALMISC.
;
; Physical property data for CARBON and CaCO3-L are not present in the ASPEN
; data bank.  Therefore, the data for these components are given in the PROP-
; DATA paragraph.
;
; Properties for ASH are also given in the PROP-DATA paragraph.
;
;
; SYSTEM PARAMETERS
;
; o  Devolatilization
;
; The devolatilization temperature is set in block PROD.  (A rough estimate for
; the temperature at which devolatilization occurs in a fixed-bed gasifier is
; about 1000 degrees F.)
;
; The subroutine, NYLD, sets the split of volatile matter.  These splits have
; been adjusted to the following values to give reasonable resluts for Pgh #8
; coal:
;       (as a function of moisture- and ash-free coal)
;                   Tar         .06648
;                   Phenol      .00246
;                   Naphtha     .01621
;                   Oil         .03442
;                   Char        .00205
;                   C3H8        .02459
;
; The distribution of sulfur compounds for any remaining sulfur (as a mass
; fraction of remaining sulfur) is:
;
;                   H2S         .9435
;                   COS         .05256
;                   CS2         .001314
;                   C4H4S       .002628
;
; The distribution of nitrogen compounds for any remaining nitrogen (as a
; mass fraction of remaining nitrogen) is:
;
;                   NH3         .2810
;                   N           .7190
;
; These fractions can be changed in the source code of NYLD.FOR to adjust
; for different coal types or gasifier conditions.
```

;
;
; o Tar recycle
;
; An actual recycle of tar and oil is simulated in this model. The user sets
; in block DEVOL a fraction of the original tar and oil that will be recycled.
; Presently, this fraction is set to 50 percent.
;
; (all other volatiles are sent to the product stream and encounter
; no further reaction)
;
;
; o Combustion
;
; The stoichiometric coefficients for the burning of tar, char, and oil are
; determined by the FORTRAN block COEFFS based on their ultimate analyses.
; If either the reactions or components are changed , appropriate changes
; must also be made to COEFFS. Presently, the FORTRAN block does not consider
; sulfur and chlorine.
;
;
; o Gasification
;
; A temperature approach to equilibrium is used to adjust the outlet gas
; composition. This is done by changing the values of DELT in the block
; GASIFIER for the appropriate reactions. The values of DELT are added to
; the reactor temperature to give the temperature at which the reaction is
; calculated. If different coals are used, the values for DELT may need to
; be adjusted. They will also need adjusted if the conditions of the reactor
; are changed.
;
; For a Pgh #8 coal type, the following temperatures were determined to be
; suitable at a pressure of 350 psia:
;
; $C + H_2 \rightarrow CO + H_2$ 1550 F
; $C + CO_2 \rightarrow 2CO$ 1525 F
; $C + 2H_2 \rightarrow CH_4$ 1100 F
; $H_2O + CO \rightarrow CO_2 + H_2$ 700 F
;
;
; O QUENCH, GAS COOLING, AND GAS-LIQUOR SEPARATION
;
; The offgas is first quenched with water to condense the hydrocarbons. The
; gas is further cooled while the hydrocarbons are separated into light
; hydrocarbons (naphtha and phenol) and heavy hydrocarbons (tar and oil).
; The blocks used in this section of the simulation are non-predictive. The
; amount of water that condenses out of the gas stream and is carrried down with
; the hydrocarbon liquids must be specified in the separator block QUENCH1.
; Also note that this section of the simulation utilizes SYSOPO (the ideal gas
; law) since this physical property option set allows the flash calculations in
; this section to converge. (The RKS eqn of state used in the gasifier portion
; of the simulation did not converge the flash calculations.) Also, a SEP block
; could be used in place of several SEP2 and HEATER block combinations. At the
; time that this simulation was developed, problems occured with the split
; specifications in the block so it was not used.
;

```
;  The amount of low pressure boiler feed water needed to cool the quenched gas
;  is calculated by the design specification WATQNCH.  A heat stream was included
;  for the gas-liquor cooling block, GLCOOL, so that the energy needed for this
;  cooling can be accounted for if this model is integrated into another simulation.
;
;
;  MODIFYING THE INPUT FILE
;
;  If the amounts of high pressure boiler feed water (HPBFW), low pressure boiler
;  feed water (LPBFW), and slag quenching water (SLAGWAT) are known, the design
;  specifications JACKET, SLAGQNCH, and WATQNCH should be deleted.  They are only
;  necessary if the flow of these streams is not known since they calculate the
;  flowrate based on the amount of heat released.
;
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;
;
TITLE 'SLAGGING FIXED-BED GASIFIER SIMULATION'
;
DESCRIPTION "NON-KINETIC ASPEN SIMULATION OF A SLAGGING FIXED-BED GASIFIER"
;
IN-UNITS ENG
OUT-UNITS ENG
;
HISTORY  MSG-LEVEL PROPERTIES=2  STREAM=4  SYSTEM=4 SIMULATION=4
;
;
;***************************************************************************
;
;                              COMPONENTS
;
;***************************************************************************
;
;
COMPONENTS  &
;
;                       *** MIXED COMPONENTS ***
;
   O2   OXYGEN        / N2   NITROGEN          / H2O   WATER/
   H2   HYDROGEN      / CO   CARBON-MONOXIDE   / CO2  CARBON-DIOXIDE/
   CH4  METHANE       / H2S  HYDROGEN-SULFIDE  / NH3  AMMONIA/
   TAR  C21H42        / OIL  C11H10-2          / PHENOL  C6H6O/
   NAPHTHA  C6H6      / C2-TO-C4  C3H8         / COS  COS/
   CS2  CS2           / C4H4S  C4H4S/  &
;
;
;                       *** CISOLID COMPONENTS ***
;
    CACO3-L  CACO3-L  /  CACO3-S  CACO3        /  CARBON  CARBON/
    CAO   CAO    /  &
;
;
;                          *** NC COMPONENTS ***
;
    COAL     /    ASH    /    CHAR
```

```
;
;
;*************************************************************************
;
;                              PROPERTIES
;
;*************************************************************************
;
PROPERTIES  SYSOP3  GLOBAL /  ;  RKS EQN. OF STATE  FOR GASIFIER SECTION
            SYSOP0 SEC2/  ; IDEAL GAS LAW USED FOR QUENCH SECTION
            SYSOP12 ;  ASME STEAM TABLE CORRELATIONS FOR STEAM AND COOLING WATER
;
FORMULA H2O H2O      ;  NEEDED FOR SYSOP12
;
;
ATTR-COMPS    COAL     PROXANAL  ULTANAL  SULFANAL  COALMISC  /
              CHAR     PROXANAL  ULTANAL  SULFANAL  COALMISC  /
              ASH      AOXANAL   GENANAL                     /
;
              TAR      ULTANAL   CLASS = CV                   /
              PHENOL   ULTANAL   CLASS = CV                   /
              NAPHTHA  ULTANAL   CLASS = CV                   /
              OIL      ULTANAL   CLASS = CV
;
NC-PROPS   COAL       ENTHALPY  HCOALGEN 6 2 * * / DENSITY  DCOALIGT
NC-PROPS   ASH        ENTHALPY  ENTHLUSR         / DENSITY  DNSTYGEN
NC-PROPS   CHAR       ENTHALPY  HCOALGEN * 2 * * / DENSITY  DCHARIGT
;
;
PROP-DATA
;
     COMP-LIST   ASH
        CVAL  DENGEN 1 1 2.0D3
;
     PROP-LIST              MW     /   DHSFRM    /   DGSFRM
       PVAL   CARBON       12.011 /   0.0       /     0.0
       PVAL   CACO3-L      100.09  / -1.154260D9 / -1.127830D9
;
     PROP-LIST           CPSPO1
       PVAL  CARBON     3.049D+04 1.276 -9.603D-04 -1.020D+7 1.046D+09 200. 1500.
       PVAL  CACO3-L      1.045863D5  2.193883D1 0D0 0D0 -2.595816D9 298 1200
;
     PROP-LIST           VSPOLY
       PVAL  CARBON      5.34E-03  0.0  0.0  0.0  0.0  0.0  2500
       PVAL  CACO3-L       3.694D-2  0D0 0D0 0D0 0D0 0D0 2D3
;
;
```

```
;*************************************************************************
;
;                              FLOWSHEET
;
;*************************************************************************
;
FLOWSHEET   SEC1
;
     PROD       IN= COALFD                              OUT= YLD-EFL  HEATYLD
     MIX1       IN= YLD-EFL PURGE                       OUT= FEED
     DEVOL      IN= FEED                                OUT= VOLATILS  UNGASIFD
     MIX2       IN= UNGASIFD FLUX OXYGEN STEAM XTAR TAR-OIL  OUT= REACFEED
     BURNTAR    IN= REACFEED                            OUT= COMBFEED
     COMB       IN= COMBFEED                            OUT= COMBPROD
     MELTDCMP   IN= COMBPROD                            OUT= MELTPROD
     SLAGREM    IN= MELTPROD                            OUT= GAS1 LIQSLAG
     SLAGFUSE   IN= LIQSLAG                             OUT= SOLSLAG
     SLAGQNCH   IN= SOLSLAG SLAGWAT                     OUT= DUMMY COOLSLAG QSLQNCH
     GASIFIER   IN= GAS1                                OUT= GAS2  HTGAS
     ADDER      IN= GAS2 VOLATILS                       OUT= OFFGAS
     JACKET     IN= HPBFW  HEATYLD  HTGAS               OUT= JKTSTEAM  QJACKET
;
FLOWSHEET  SEC2
;
     MIX3       IN= OFFGAS INJWAT                       OUT= WETGAS
     QUENCH1    IN= WETGAS                              OUT= HOTGAS HVYHC
     QUENCH2    IN= HOTGAS                              OUT= PRODGAS Q2
     QUENCH3    IN= HVYHC                               OUT= GASLIQ Q3
     WATQNCH    IN= LPBFW Q2 Q3                         OUT= LPSTEAM QWAT
     GLCOOL     IN= GASLIQ                              OUT= COOLGL QSEP
     GLSEP      IN= COOLGL                              OUT= HCLIQ TAR-OIL
;
;
;*************************************************************************
;
;                          STREAM SPECIFICATIONS
;
;*************************************************************************
;
DEF-STREAM-CLASS  MIXCINC  SUBS= MIXED  CISOLID  NC
;
DEFS MIXCINC ALL /
  CONVEN  PURGE STEAM OXYGEN HPBFW JKTSTEAM /
  HEAT    HTGAS HEATYLD QJACKET QSLQNCH Q2 Q3 QWAT QSEP
;
;
;=========================================================================
;  ILLINOIS #6 COAL FEED
;    COAL ANALYSIS TAKEN FROM EPRI AP-3109 AND ASPEN MANUAL
;    FLOWRATE OF COAL TAKEN FROM AP-3109
;     NAPHTHA AND OIL ULTANALS TAKEN FROM EPRI AP-1922,
;     TAR AND PHENOL FROM CONOCO PIPELINE GAS DEMONSTRATION PLANT STUDY
;  (the analysis for oil has been normalized because it originally contained
;   sulfur and chlorine.)
;=========================================================================
;
```

```
STREAM  COALFD
     SUBSTREAM MIXED TEMP=77. PRES=14.7
          COMP-ATTR TAR     ULTANAL (0.   95.00 5.00 0.   0.   0.    0.  )
          COMP-ATTR PHENOL  ULTANAL (0.   76.58 6.42 0.   0.   0.   17.00)
          COMP-ATTR NAPHTHA ULTANAL (0.06 91.46 7.51 0.11 0.04 0.19 0.63 )
          COMP-ATTR OIL     ULTANAL (0.07 88.01 7.53 0.8  0.0  0.0  3.59 )
;
;
     SUBSTREAM NC  TEMP=77.  PRES=14.7
          MASS-FLOW  COAL   1263.
;
;
;==========================================================================
;   COAL PROXANAL, ULTANAL, AND HEATING VALUE TAKEN FROM EPRI AP-3109
;==========================================================================
;
          COMP-ATTR  COAL   PROXANAL (14.2 46.00 42.97 11.03)/
                            ULTANAL (10.0 69.5 5.3 1.3 0.0 3.9 10.0)/
                            SULFANAL (1.84 .03 2.03)/
                            COALMISC ( 11235. *  *  0.5  * )
;
;
;=========================================================================
;   ALL CHAR ATTRIBUTES TAKEN FROM MIT SIMULATION, EXCEPT SULFANAL WHICH
;   WAS CHANGED TO MATCH THAT OF ILL #6 COAL
;=========================================================================
;
          COMP-ATTR  CHAR   PROXANAL (0.0  84. 7. 9.)                  /
                            ULTANAL  (9.  84. 7. 0. 0. 0. 0.)          /
                            SULFANAL (0.  0.  0.)/
                            COALMISC ( *  *  *  0.8  * )
;
;
          COMP-ATTR  ASH    GENANAL (100. 0. 0. 0. 0. 0. 0. 0. 0. 0.)
;
;
;=========================================================================
;  LIMESTONE IS ADDED TO MIX WITH MELTED ASH FORMING A EUTECTIC SOLUTION
;  CALLED SLAG -- THE FLUX:ASH RATIO WAS LISTED AS 1.2 IN EPRI AP-1922
;=========================================================================
;
STREAM   FLUX
       SUBSTREAM  CISOLID  TEMP=77.  PRES=14.7
           MASS-FLOW  CACO3-S  0.0
;
;
;=========================================================================
;  98% BY VOLUME OXYGEN FEED TO THE REACTOR
;  STREAM CONDITIONS TAKEN FROM THE CONOCO PIPELINE REPORT
;  FLOWRATE TAKEN FROM AP-3109
;=========================================================================
;
STREAM  OXYGEN  TEMP=275.  PRES=500.
    MASS-FLOW  O2  630. / N2  11.
;
;
```

```
;==========================================================================
;  SUPERHEATED HIGH-PRESSURE STEAM TO THE REACTOR
;     STREAM CONDITIONS AND FLOWRATE TAKEN FROM EPRI REPORT AP-3109
;==========================================================================
;
STREAM  STEAM  TEMP=620.  PRES=415.
     MASS-FLOW  H2O  379.
;
;
;==========================================================================
;  PURGE STREAM TO PRESSURIZE THE LOCKHOPPER
;     STREAM CONDITIONS TAKEN FROM THE CONOCO PIPELINE GAS REPORT
;     FLOWRATE TAKEN FROM AP-3109
;==========================================================================
;
STREAM  PURGE  TEMP=750.  PRES=550.
     MASS-FLOW  N2  74.
;
;
;==========================================================================
;  HIGH PRESSURE BOILER FEED WATER TO COOLING JACKET
;     STREAM CONDITIONS TAKEN FROM THE CONOCO PIPELINE GAS REPORT
;     FLOWRATE IS AN INITIAL GUESS AND IS VARIED BY DES-SPEC JACKET
;==========================================================================
;
STREAM  HPBFW TEMP=250.  PRES=780.4
     MASS-FLOW  H2O  2500.
;
;
;==========================================================================
;  COOLING WATER FOR SLAG QUENCH
;     NO AVAILABLE DATA FOR CONDITIONS OF SLAG QUENCH WATER, THEREFORE THE
;     CONDITIONS ARE AN EDUCATED GUESS.   FLOWRATE IS AN INITIAL GUESS AND
;     IS VARIED BY DES-SPEC SLAGQNCH
;==========================================================================
;
STREAM  SLAGWAT TEMP=100.  PRES=50.
     MASS-FLOW  H2O  10000.
;
;==========================================================================
;  A SMALL AMOUNT OF TAR AND OIL IS NECESSARY TO SATISFY THE UNIT OPERATION
;  BLOCK RGIBBS WHICH IS USED TO SIMULATE THE GASIFIER
;==========================================================================
;
STREAM  XTAR  TEMP=300.  PRES=350.
     MASS-FLOW  TAR  1.0D-5 / OIL  1.0D-5
;
;==========================================================================
;  THE CONDITIONS FOR THE WATER WHICH COOLS THE GASIFIER EXIT GAS ARE TAKEN
;  FROM EPRI REPORT NO. 3980 ON THE USE OF BGC/LURGI IN AN IGCC  --  THE FLOW
;  RATE IS VARIED BY DES-SPEC WATQNCH
;==========================================================================
;
STREAM  LPBFW TEMP=220.  PRES=75.
     MASS-FLOW  H2O  250.
```

```
;
;=========================================================================
;  THE CONDITIONS AND COMPOSITION OF THE QUENCH INJECTION WATER ARE UNKNOWN
;  THE CONDITIONS ARE TAKEN FROM EPRI REPORT 3980
;  THE COMPOSITION IS ASSUMED TO BE PURE WATER AND THE FLOWRATE IS TAKEN FROM
;     EPRI REPORT 3109
;=========================================================================
;
STREAM  INJWAT TEMP=158.  PRES=525.
     MASS-FLOW  H2O  84.
;
;
;
;*************************************************************************
;
;                 UNIT OPERATION BLOCK SPECIFICATIONS
;
;*************************************************************************
;
;
BLOCK   PROD    RYIELD  ; THE GENERAL TEMP FOR DEVOLATILIZATION IN A FIXED-BED
;                         GASIFIER IS  ~1000 F.   PRES= 465 TAKEN FROM AP-3109
   DESCRIPTION "THIS BLOCK PERFORMS COAL DEVOLATILIZATION AND PYROLYSIS
               ACCORDING TO THE USER SUBROUTINE NYLD DEVELOPED BY MIT"
   PARAM  PRES=465.  TEMP=1000. NPK=1  KPH=1
     SUBROUTINE  USER = NYLD
     USER-VECS 1 1 1 1
;
;
BLOCK   MIX1     MIXER
    DESCRIPTION "THIS BLOCK MIXES THE PRODUCTS OF COAL DEVOLATILIZATION
                 AND PYROLYSIS WITH THE PURGE GAS"
    PARAM  PRES=465.
;
;
BLOCK  DEVOL  SEP2
    DESCRIPTION "THIS BLOCK SEPARATES THE VOLATILE PRODUCTS FROM THE TAR, OIL,
                CHAR, AND ASH."
    FLASH-SPECS  STRM= VOLATILS  PRES= 465.  NPK=1  KPH=1
;
    FRAC  SUBS=MIXED  STRM=VOLATILS &
            COMP= N2 CO H2S NH3  PHENOL NAPHTHA C2-TO-C4   &
                     H2O H2 CO2 CH4 COS CS2 C4H4S TAR OIL &
            FRAC= 1.  1. 1.  1.   1.      1.     1.  &
                      1.  1.  1.  1.  1.  1.  1.   0.5  0.5/
;
                      STRM=UNGASIFD COMP= O2 TAR OIL  FRAC = 1. 0.5 0.5
;
    SUBS-FRAC  SUBS=CISOLID  STRM= UNGASIFD  FRAC = 1.0 /
               SUBS=NC  STRM=UNGASIFD  FRAC=1.0
;
;
BLOCK  MIX2  MIXER
    DESCRIPTION "THIS BLOCK MIXES THE TAR, OIL, CHAR, AND ASH WITH THE FLUX,
                 OXYGEN, STEAM, AND RECYCLE STREAM."
    PARAM  465.
```

```
;
;
BLOCK  BURNTAR  RSTOIC
    DESCRIPTION "THIS BLOCK PERFORMS COMPLETE COMBUSTION OF THE CHAR AND
                 PARTIAL COMBUSTION OF THE TAR AND OIL-- THE FORTRAN BLOCK
                 COEFFS DETERMINES THE STOICIOMETRIC COEFFICIENTS FOR
                 THESE REACTIONS"
    PARAM Q=0 PRES=465. NPK=1
    STOICH  1  MIXED TAR -100. / O2 -100. / CO2 100./ H2O 100.
    CONV    1  MIXED  TAR  0.5
    STOICH  2  NC CHAR -1.0/ASH 1.0/MIXED O2 -1.0/CO2  1.0/H2O  1.0
    CONV    2  NC    CHAR  1.0
    STOICH  3  MIXED OIL -100. / O2 -100. / CO2 100./ H2O 100.
    CONV    3  MIXED OIL  0.5
;
;
BLOCK   COMB   RSTOIC
    DESCRIPTION "THIS BLOCK REACTS ALL THE REMAINING OXYGEN BY PERFORMING
                INCOMPLETE COMBUSTION OF CARBON"
    PARAM   Q=0    PRES= 465
    STOICH  1  CISOLID CARBON -1.013/ MIXED O2 -1.0/ CO .026/ CO2 .987
    CONV    1  MIXED O2  1.0
;
;
BLOCK  MELTDCMP  RSTOIC
    DESCRIPTION "THIS BLOCK MELTS THE FLUX AND DECOMPOSES 89.2% OF IT INTO
                 GASEOUS CO2 AND SOLID CAO"
    PARAM  Q=0  PRES=465
    STOICH  1  CISOLID  CACO3-S -1/ CACO3-L .1073/ CAO .8927/ MIXED CO2 .8927
    CONV    1  CISOLID  CACO3-S  1.0
;
;
BLOCK  SLAGREM  SEP2
    DESCRIPTION "THIS BLOCK SEPARATES THE SLAG (ASH AND FLUX) FROM THE
                CARBON AND GASES"
    FLASH-SPECS  LIQSLAG  NPK = 1  KPH = 3
    SUBS-FRAC  SUBS=NC  STRM=LIQSLAG FRAC=1.0/
               SUBS=MIXED  STRM=GAS1  FRAC=1.0
    FRAC  SUBS=CISOLID  STRM=GAS1  &
       COMP=  CARBON  CACO3-S  CACO3-L  CAO  &
       FRAC=    1.0     0.0      0.0    0.0  /
;
;
BLOCK  SLAGFUSE  RSTOIC  ; PRES=40 IS AN EDUCATED GUESS
     DESCRIPTION "THIS BLOCK SOLIDIFIES THE MOLTEN CACO3"
     PARAM   Q=0   PRES=40.  NPK=1  KPH=3
     STOICH  1  CISOLID CACO3-L  -1/ CACO3-S 1
     CONV 1 CISOLID  CACO3-L  1.0
;
;
BLOCK  SLAGQNCH  FLASH2  ; CONDITIONS ARE TAKEN FROM CONOCO PIPELINE GAS REPORT
     DESCRIPTION "THIS BLOCK MIXES THE HOT SLAG WITH QUENCH WATER"
     PARAM  PRES = 12.  TEMP= 158.  KODE = 2
;
;
```

```
BLOCK  GASIFIER  RGIBBS
     DESCRIPTION "THIS BLOCK PERFORMS THE GASIFICATION REACTIONS AND THE
                  WATER-GAS SHIFT REACTION"
     PARAM  TEMP=800  PRES=465  NAT=6  NPHS=1  NR=6  IDEL=1
     PROD CARBON 0/ N2 1/ CO 1/ H2 1/ H2O 1/ CH4 1/ CO2 1/TAR 1/OIL 1
;                        C  /  H  /  O  /  N  / TAR/ OIL
     ATOM  CARBON  1    1  /  *  /  *  /  *  /  * /  * /
           N2      1    *  /  *  /  *  /  2  /  * /  * /
           H2O     1    *  /  2  /  1  /  *  /  * /  * /
           CO      1    1  /  *  /  1  /  *  /  * /  * /
           CO2     1    1  /  *  /  2  /  *  /  * /  * /
           H2      1    *  /  2  /  *  /  *  /  * /  * /
           CH4     1    1  /  4  /  *  /  *  /  * /  * /
           TAR     1    *  /  *  /  *  /  *  /  1 /  * /
           OIL     1    *  /  *  /  *  /  *  /  * /  1
;
     STOI  1  CARBON -1/ H2O -1/ CO 1/ H2 1
     STOI  2  CARBON -1/ CO2 -1/ CO 2
     STOI  3  CARBON -1/ H2 -2/ CH4 1
     STOI  4  H2O -1/ CO -1/ CO2 1/ H2 1
     STOI  5  TAR -1/ TAR 1
     STOI  6  OIL -1/ OIL 1
;
     DELT 1  +850
     DELT 2  +825
     DELT 3  +300
     DELT 4  -100
;
;
BLOCK  ADDER  MIXER
     DESCRIPTION "THIS BLOCK MIXES THE PRODUCTS OF GASIFICATION WITH
                  THE PRODUCTS OF DEVOLATILIZATION TO OBTAIN THE OFFGAS
                  FROM THE GASIFIER"
     PARAM  NPK=1  KPH=1
;
;
BLOCK  JACKET  HEATER  ; STEAM T & P TAKEN FROM CONOCO PIPELINE GAS REPORT
     DESCRIPTION "THIS BLOCK SIMULATES THE STEAM JACKET WHERE STEAM IS
                 PRODUCED FROM THE HEATING OF HIGH PRESSURE BOILER FEED
                 WATER"
     PROPERTIES SYSOP12
     PARAM  PRES = 428.  TEMP = 450.  KODE = 2
;
;
BLOCK  MIX3  MIXER
     DESCRIPTION "THIS BLOCK MIXES THE INJECTION WATER WITH THE EXIT GAS FROM
                 THE GASIFIER"
;
;
BLOCK  QUENCH1  SEP2
     DESCRIPTION "THIS BLOCK SEPARATES THE GAS FROM THE TAR, OIL, PHENOL,
                 NAPHTHA, INJECTION WATER, AND ANY UNREACTED CARBON"
     FRAC  SUBS=CISOLID STRM=HVYHC COMP=CARBON  FRAC=1/
           SUBS=MIXED  STRM=HVYHC COMP=TAR OIL PHENOL NAPHTHA &
                        FRAC=1  1  1  1/
```

```
                        STRM=HOTGAS &
                         COMP= N2 H2O H2 CO CO2 CH4 H2S NH3  &
                               C2-TO-C4 COS CS2 C4H4S &
                         FRAC=  1 .83  1  1  1   1   1  1  &
                                  1     1   1     1
;
;
BLOCK  QUENCH2  HEATER
     PARAM  TEMP= 302   PRES= 300.5
;
;
BLOCK  QUENCH3  HEATER
     PARAM  TEMP= 203   PRES= 250
;
;
BLOCK  WATQNCH  HEATER
     DESCRIPTION "THIS BLOCK CALCULATES THE AMOUNT OF LOW PRESSURE BOILER FEED
                 WATER NEEDED TO QUENCH THE GASIFIER OFFGAS"
     PROPERTIES SYSOP12
     PARAM TEMP=275 PRES=45
;
;
BLOCK  GLCOOL HEATER
     DESCRIPTION "THIS BLOCK COOLS THE GAS-LIQUOR TO SPECIFIED TEMP AND PRES
                 AND ACCOUNTS FOR THE COOLING DONE IN THE GAS-LIQUOR SEPARATOR"
     PARAM   TEMP=158. PRES=115.
;
;
BLOCK  GLSEP  SEP2
     DESCRIPTION "THIS BLOCK SEPARATES THE TAR, OIL, AND ANY UNREACTED CARBON
                 FROM THE REST OF THE STREAM.  THEY ARE RECYCLED TO THE
                 GASIFIER"
     FLASH-SPECS  TAR-OIL TEMP=158. PRES=115./
                  HCLIQ   TEMP=158. PRES=115.
     FRAC  SUBS=CISOLID  STRM=TAR-OIL COMP=CARBON  FRAC=1/
           SUBS=MIXED    STRM=TAR-OIL COMP=TAR OIL FRAC=1 1/
                         STRM=HCLIQ   COMP=NAPHTHA  PHENOL H2O &
                                      FRAC=  1       1      1
;
;
TEAR-STREAMS  TAR-OIL
;
;*************************************************************************
;
;                              DESIGN SPECIFICATIONS
;
;*************************************************************************
;
;
DES-SPEC JACKET
;    DESCRIPTION "THIS DESIGN SPECIFICATION VARIES THE FLOWRATE OF HIGH PRESSURE
;                BOILER FEED WATER TO PRODUCE STEAM AT A SPECIFIED TEMP AND PRES,
;                THEREFORE REMOVING THE HEAT FROM THE GASIFIER"
    DEFINE Q STRM-ATTR-VAR ATTR=HEAT VAR=Q STREAM=QJACKET
    SPEC Q TO 0.0
    TOL-SPEC 100.
    VARY STREAM-VAR STREAM=HPBFW VAR=MASS-FLOW
    LIMITS   100.  500000.
```

```
;
;
DES-SPEC SLAGQNCH
;    DESCRIPTION "THIS DESIGN SPECIFICATION VARIES THE FLOWRATE OF QUENCH WATER
;                 IN THE SLAG QUENCH VESSEL UNTIL THE SLAG IS COOLED TO ITS
;                 SPECIFIED TEMP AND PRES, THEREFORE REMOVING HEAT FROM THE SLAG."
     DEFINE Q STRM-ATTR-VAR ATTR=HEAT VAR=Q STREAM=QSLQNCH
     SPEC Q TO 0.0
     TOL-SPEC 100.
     VARY STREAM-VAR STREAM=SLAGWAT VAR=MASS-FLOW
     LIMITS  100.  100000.
;
DES-SPEC WATQNCH
;    DESCRIPTION "THIS DESIGN SPECIFICATION VARIES THE FLOWRATE OF BOILER FEED
;                WATER IN THE QUENCH SECTION UNTIL THE GAS AND GAS-LIQUOR ARE
;                COOLED TO THEIR SPECIFIED TEMP AND PRES."
     DEFINE Q STRM-ATTR-VAR ATTR=HEAT VAR=Q STREAM=QWAT
     SPEC Q TO 0.0
     TOL-SPEC 100.
     VARY STREAM-VAR STREAM=LPBFW VAR=MASS-FLOW
     LIMITS  100.  10000.
;
;*****************************************************************************
;
;                              FORTRAN BLOCKS
;
;*****************************************************************************
;
;
FORTRAN CHKMELT
     DESCRIPTION "THIS FORTRAN BLOCK DETERMINES WHETHER THE TEMPERATURE
                  AT THE BOTTOM OF THE GASIFIER IS HIGH ENOUGH TO MELT
                  THE FLUX AND CALCULATES THE CONVERSION OF SOLID
                  CACO3 TO LIQUID CACO3 TO BE USED IN THE FLUX
                  MELTING AND DECOMPOSITION BLOCK."
     DEFINE  TCACO3  SVAR  COMBPROD  CISOLID  TEMP
     DEFINE  RLIQID  BVAR  MELTDCMP  CONV  CONV  ID1=1
F     IF (TCACO3 .GT. 2340.) GOTO 88
F     WRITE (NHSTRY,222) TCACO3
F 222 FORMAT (' TEMPERATURE OF',F8.2,'  IS TOO LOW FOR FLUX TO MELT.'
F    1,' NO CO2 IS EVOLVED.')
F     RLIQID = 0.0
F     GOTO 99
F  88 WRITE (NHSTRY,223) TCACO3
F 223 FORMAT (' TEMPERATURE OF',F9.2,' IS HIGH ENOUGH FOR FLUX TO MELT.'
F    1,' CO2 IS EVOLVED.')
F     RLIQID = 1.0
F  99 CONTINUE
     EXECUTE BEFORE MELTDCMP
;
;
FORTRAN COEFFS
     DESCRIPTION "THIS BLOCK CALCULATES THE STOICHIOMETRIC COEFFICIENTS
                  FOR TAR, CHAR, AND OIL COMBUSTION BASED ON THE ULTIMATE
                  ANALYSES OF THE COMPONENTS.  CHAR CAN BE COMPOSED ONLY OF
                  ASH, CARBON, AND HYDROGEN.  TAR AND OIL CANNOT CONTAIN
                  SULFUR OR CHLORINE."
```

```
;
      DEFINE WTA1 CATV REACFEED MIXED TAR  ULTANAL 1
      DEFINE WTC1 CATV REACFEED MIXED TAR  ULTANAL 2
      DEFINE WTH1 CATV REACFEED MIXED TAR  ULTANAL 3
      DEFINE WTN1 CATV REACFEED MIXED TAR  ULTANAL 4
      DEFINE WTO1 CATV REACFEED MIXED TAR  ULTANAL 7
;
      DEFINE WTA2 CATV REACFEED NC    CHAR ULTANAL 1
      DEFINE WTC2 CATV REACFEED NC    CHAR ULTANAL 2
      DEFINE WTH2 CATV REACFEED NC    CHAR ULTANAL 3
;
      DEFINE WTA3 CATV REACFEED MIXED OIL  ULTANAL 1
      DEFINE WTC3 CATV REACFEED MIXED OIL  ULTANAL 2
      DEFINE WTH3 CATV REACFEED MIXED OIL  ULTANAL 3
      DEFINE WTN3 CATV REACFEED MIXED OIL  ULTANAL 4
      DEFINE WTO3 CATV REACFEED MIXED OIL  ULTANAL 7
;
      DEFINE TAR1   BVAR BURNTAR STOICH COEF ID1=1 MIXED TAR
      DEFINE CO21   BVAR BURNTAR STOICH COEF ID1=1 MIXED CO2
      DEFINE H2O1   BVAR BURNTAR STOICH COEF ID1=1 MIXED H2O
      DEFINE O21    BVAR BURNTAR STOICH COEF ID1=1 MIXED O2
      DEFINE ZN1    BVAR BURNTAR STOICH COEF ID1=1 MIXED N2
      DEFINE ASH1   BVAR BURNTAR STOICH COEF ID1=1 NC    ASH
;
      DEFINE CHAR2  BVAR BURNTAR STOICH COEF ID1=2 NC    CHAR
      DEFINE ASH2   BVAR BURNTAR STOICH COEF ID1=2 NC    ASH
      DEFINE O22    BVAR BURNTAR STOICH COEF ID1=2 MIXED O2
      DEFINE CO22   BVAR BURNTAR STOICH COEF ID1=2 MIXED CO2
      DEFINE H2O2   BVAR BURNTAR STOICH COEF ID1=2 MIXED H2O
;
      DEFINE OIL3   BVAR BURNTAR STOICH COEF ID1=3 MIXED OIL
      DEFINE CO23   BVAR BURNTAR STOICH COEF ID1=3 MIXED CO2
      DEFINE H2O3   BVAR BURNTAR STOICH COEF ID1=3 MIXED H2O
      DEFINE O23    BVAR BURNTAR STOICH COEF ID1=3 MIXED O2
      DEFINE ZN3    BVAR BURNTAR STOICH COEF ID1=3 MIXED N2
      DEFINE ASH3   BVAR BURNTAR STOICH COEF ID1=3 NC    ASH
;
C
C  STOICHIOMETRIC COEFFICIENTS FOR TAR COMBUSTION
C  BASIS IS 100 LB-MOL OF TAR
C  TAR MOLECULAR WEIGHT IS TAKEN AS C21H42
C
F      TARMW = 294.6D0
F      CMOLS = TARMW * WTC1 / 12.01D0
F      HMOLS = TARMW * WTH1 / 1.008D0
F      OMOLS = TARMW * WTO1 / 16.0D0
F      TAR1 = -1.D2
F      CO21 = CMOLS
F      H2O1 = HMOLS/2.D0
F      O21  = (-(2.D0 * CO21 + H2O1) / 2.D0) + OMOLS
F      ZN1  = TARMW * WTN1 / 14.01D0
F      ASH1 = TARMW * TAR1 * (WTA1/1.0D2)
F      WRITE (NHSTRY,10) WTA1,WTC1,WTH1,WTN1,WTO1,TAR1,
F     1                  CO21,H2O1,O21,ZN1,ASH1
```

```
F  10   FORMAT(1X,'ULTIMATE ANALYSIS FOR TAR',/,10X,
F    1  'PERCENT ASH      = ',F10.5,/,10X,'PERCENT CARBON = ',F10.5,
F    2  /,10X,'PERCENT HYDROGEN = ',F10.5,/,10X,'PERCENT NITROGEN  =',
F    3  F10.5,/,10X,'PERCENT OXYGEN = ',F10.5,/,1X,
F    4       'STOICHIOMETRIC COEFFICIENTS FOR TAR COMBUSTION',/,10X,
F    5       'TAR = ',F10.5,' LB',/,10X,
F    6       'CO2  = ',F10.5,' LB-MOL',/,10X,
F    7       'H2O  = ',F10.5,' LB-MOL',/,10X,
F    8       'O2   = ',F12.5,' LB-MOL',/,10X,
F    9       'N2   = ',F10.5,' LB-MOL',/,10X,
F    1       'ASH  = ',F10.5,' LB',/)
C
C  STOICHIOMETRIC COEFFICIENTS FOR OIL COMBUSTION
C  BASIS IS 100 LB-MOLE OF OIL
C  OIL MOLECULAR WEIGHT IS TAKEN TO BE C11H10
C
F     OILMW  = 142.
F     CMOLS3 = OILMW * WTC3 / 12.01D0
F     HMOLS3 = OILMW * WTH3 / 1.008D0
F     OMOLS3 = OILMW * WTO3 / 16.0D0
F     OIL3   = -1.D2
F     CO23   = CMOLS3
F     H2O3   = HMOLS3/2.D0
F     O23    = (-(2.D0 * CO23 + H2O3) / 2.D0) + OMOLS3
F     ZN3    = OILMW * WTN3 / 14.01D0
F     ASH3   = -OIL3 * OILMW * (WTA3/1.0D2)
F     WRITE (NHSTRY,20) WTA3,WTC3,WTH3,WTN3,WTO3,OIL3,
F    1                  CO23,H2O3,O23,ZN3,ASH3
F 20   FORMAT(1X,'ULTIMATE ANALYSIS FOR OIL',/,10X,
F    1   'PERCENT ASH = ',F10.5,/,10X,'PERCENT CARBON = ',F10.5,/,10X,
F    2   'PERCENT HYDROGEN = ',F10.5,/,10X,'PERCENT NITROGEN = ',F10.5,
F    3   /,10X,'PERCENT OXYGEN = ',F10.5,/,1X,
F    4       'STOICHIOMETRIC COEFFICIENTS FOR OIL COMBUSTION',/,10X,
F    5       'OIL = ',F10.5,' LB',/,10X,
F    6       'CO2 = ',F10.5,' LB-MOL',/,10X,
F    7       'H2O = ',F10.5,' LB-MOL',/,10X,
F    8       'O2  = ',F12.5,' LB-MOL',/,10X,
F    9       'N2  = ',F10.5,' LB-MOL',/,10X,
F    1       'ASH = ',F10.5,' LB',/)
C
C  STOICHIOMETRIC COEFFICIENTS FOR CHAR COMBUSTION
C  BASIS IS 1 LB OF CHAR
C
F     CHAR2 = -1.D0
F     ASH2  = -CHAR2*WTA2/1.D2
F     CO22  = -CHAR2*WTC2/1.D2/12.01
F     H2O2  = -CHAR2*WTH2/1.D2/1.008/2.D0
F     O22   = -(2.D0 * CO22 + H2O2) / 2.D0
F     WRITE (NHSTRY,30) WTA2,WTC2,WTH2,CHAR2,CO22,H2O2,O22,ASH2
F  30 FORMAT(1X,'ULTIMATE ANALYSIS FOR CHAR',/,10X,
F    1       'PERCENT ASH        = ',F10.5,/,10X,'PERCENT CARBON = ',
F    2       F10.5,/,10X,'PERCENT HYDROGEN = ',F10.5,/,1X,
F    3       'STOICHIOMETRIC COEFFICIENTS FOR CHAR COMBUSTION',/,10X,
F    4       'CHAR = ',F10.5,' LB',/,10X,
F    5       'CO2  = ',F10.5,' LB-MOL',/,10X,
F    6       'H2O  = ',F10.5,' LB-MOL',/,10X,
F    7       'O2   = ',F10.5,' LB-MOL',/,10X,
F    8       'ASH  = ',F10.5,' LB',/)
     EXECUTE BEFORE BURNTAR
```