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DOE/MC/26291--3029-Vol.2

DE92 001125

Development of Standardized Air-Blown Coal Gasifier/ Gas Turbine Concepts for Future Electric Power Systems
Volume II
Appendix A: Fixed Bed Gasifier and Sulfur Sorbent Regeneration Subsystem Computer Model Development

Final Report

E. Blough
W. Russell
J.W. Leach

August 1990

Work Performed Under Contract No.: DE-AC21-89MC26291

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
Morgantown, West Virginia

By
CRS Sirrine, Inc.
Power Division
Greenville, South Carolina

MASTER

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DOE/MC/26291-3029, Vol. 2
(DE92001125)

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Morgantown, West Virginia 26507-0880

By
CRS Sirrine, Inc.
Power Division
P.O. Box 5456
Greenville, South Carolina 29606-5456

August 1990

MODELING OF STANDARDIZED INTEGRATED COAL GASIFICATION COMBINED CYCLE POWER PLANTS

Technical Report

Submitted to

CRS Sirrine Incorporated

August 15, 1990

Prepared by

Eric Blough
William Russell
James W. Leach

Mechanical & Aerospace Engineering
North Carolina State University
Raleigh, NC 27695-7910

ABSTRACT

Computer models have been developed for evaluating conceptual designs of integrated coal gasification combined cycle power plants. An overall system model was developed for performing thermodynamic cycle analyses, and detailed models were developed for predicting performance characteristics of fixed bed coal gasifiers and hot gas clean up subsystem components. The overall system model performs mass and energy balances and does chemical equilibrium analyses to determine the effects of changes in operating conditions, or to evaluate proposed design changes. An existing plug flow model for fixed bed gasifiers known as the Wen II model was revised and updated. Also, a spread sheet model of a zinc ferrite sulfur sorbent regeneration subsystem was developed. Parametric analyses were performed to determine how performance depends on variables in the system design. The work was done to support CRS Sirrine Incorporated in their study of standardized air blown coal gasifier gas turbine concepts.

TABLE OF CONTENTS

Page

LIST OF FIGURES

LIST OF TABLES

1 INTRODUCTION

There is a need for cost effective and environmentally acceptable power generation systems that can utilize our nations vast coal resources. Thus, integrated coal gasification combined cycle (IGCC) power plants are now under intense study because of their potential for accomplishing clean and cheap conversion of energy in coal. IGCC systems that burn low BTU coal gas produced in air blown fixed bed gasifiers appear to have economic advantages. The hot pressurized coal gas from the gasifier is cleaned prior to combustion in a gas turbine. The volume of the coal gas that is cleaned is much less than the volume of the stack gases that must be cleaned in a conventional plant. Also, the sulfur in the coal gas is in the form of hydrogen sulfide which can be removed more efficiently than can sulfur dioxide in flue gases. The overall efficiency of the combined cycle plant is expected to be in excess of 40%. Thus, carbon dioxide emissions as well as sulfur dioxide omissions will be reduced.

Research and development on IGCC systems has been in progress for the last two decades, and several demonstration plants have been built. The demonstration plants in the United States have operated on medium BTU gas produced by oxygen blown entrained flow gasifiers. Plants are now being designed to burn cheaper low BTU gas from air blown fixed bed gasifiers, and a demonstration plant that will process about 1000 tons of coal per day will be built near Tallahassee Florida in the early 1990's.

The work documented in this report was done in support of a larger study conducted by CRS Sirrine Incorporated for the United States Department of Energy on low cost standardized IGCC systems designs. Our work is concerned with the development of computer models. We have developed an overall IGCC system model for performing thermodynamic cycle analysis, and have also worked towards the development of detailed computer models of two of the major components in the IGCC system.

The overall system model is useful for evaluating the effects of changes in operating conditions or of changes in subsystem designs on the net plant efficiency and power output. We have revised and updated an existing Fortran model of a fixed bed coal gasifier to gain a better understanding of the gasification process and to determine the effects of variations in coal properties such as moisture content and particle size on the plant performance. We have also developed a new spread sheet model for analyzing the regeneration and sulfur recovery process in a hot gas cleanup system that employs zinc ferrite to remove hydrogen sulfide from the coal gas.

Two computer models have been developed for analyzing the coal gasifier. One model simulates the detailed processes that occur within the gasifer. It contains chemical reaction rate equations, conservation equations, heat transfer correlations, a devolatilization model, and other information needed for analyzing the gasifier from basic principles. It is useful for predicting local temperatures within the gasifier, carbon conversion efficiency, product gas composition, and other detailed information about the gasification process. This model originated at West Virginia University. We have made extensive modifications in the present work. A second computer model of the coal gasifier was developed for evaluating IGCC system designs. This model performs mass and energy balances, and is capable of predicting the product gas composition based on chemical equilibrium assumptions. It can also accept experimentally determined gas compositions as input. It is useful for predicting how the gasifier operating conditions affect the overall system performance. For example, it could be used to determine how the overall power plant efficiency changes when the steam flow to the gasifier is reduced.

Hot gas cleanup will contribute to the success of the IGCC. Conventional processes for removing impurities from coal gas must operate at low temperatures, and the plant cycle efficiency would suffer if the gas had to be cooled for cleaning before it is burned in the combustor. The zinc ferrite sorbent hot gas cleanup system is a promising alternative to conventional scrubber technology. However, the zinc ferrite is expensive and must be regenerated when it becomes charged with sulfur. The sorbent regeneration process and sulfur recovery subsystem should be integrated into the overall plant design. We have developed a computer model to gain an understanding of how this should be done, and have done parametric analysis to determine how the required gas flows depend on variables in the subsystem design.

2. IGCC POWER PLANT SIMULATION

This section provides a detailed description of a computer model that was developed for evaluating the overall performance of integrated coal gasification combined cycle (IGCC) plants. The model is useful for evaluating the effects of changes in the system configuration (or of improvements in individual component performance) on the net cycle efficiency and power output. It performs thermodynamic analysis of the individual components of the system and accounts for mass and energy balances. Also, in the gasifier and combustor where chemical reactions occur, the model can perform chemical equilibrium calculations to determine the composition of the product gas streams. It does not account for reaction kinetics, but gives the user the option of inputting the product gas composition when chemical equilibrium calculations are not acceptable. Whether the product gas compositions are computed by the model or provided by the user, the model computes product gas flows and temperatures to insure that mass and energy are conserved.

The IGCC plant employs a fired heat recovery steam generator (HRSG) which provides low pressure steam for the coal gasification and high pressure steam for the Rankine cycle power plant. The computer model contains steam tables and source code for analyzing the HRSG and Rankine cycle plant.

2.1 IGCC Plant Description

An Integrated Gasification Combined Cycle Power Plant using a GE MS7001 EA gas turbine utility power plant computer model is illustrated in Figure 2.1. Air flows into the gas turbine compressor at a mass flow rate of about 600 lbm/sec. The air is pressurized in the compressor to a pressure of about 200 psi, and the temperature increases to around 800° F. This compressed air is divided into three streams. About 5 percent of the air by-passes the combustor and is used for cooling purposes in the turbine. About 9 percent of the air is sent to a booster compressor for use in the gasification process. The remaining air is sent to the combustor.

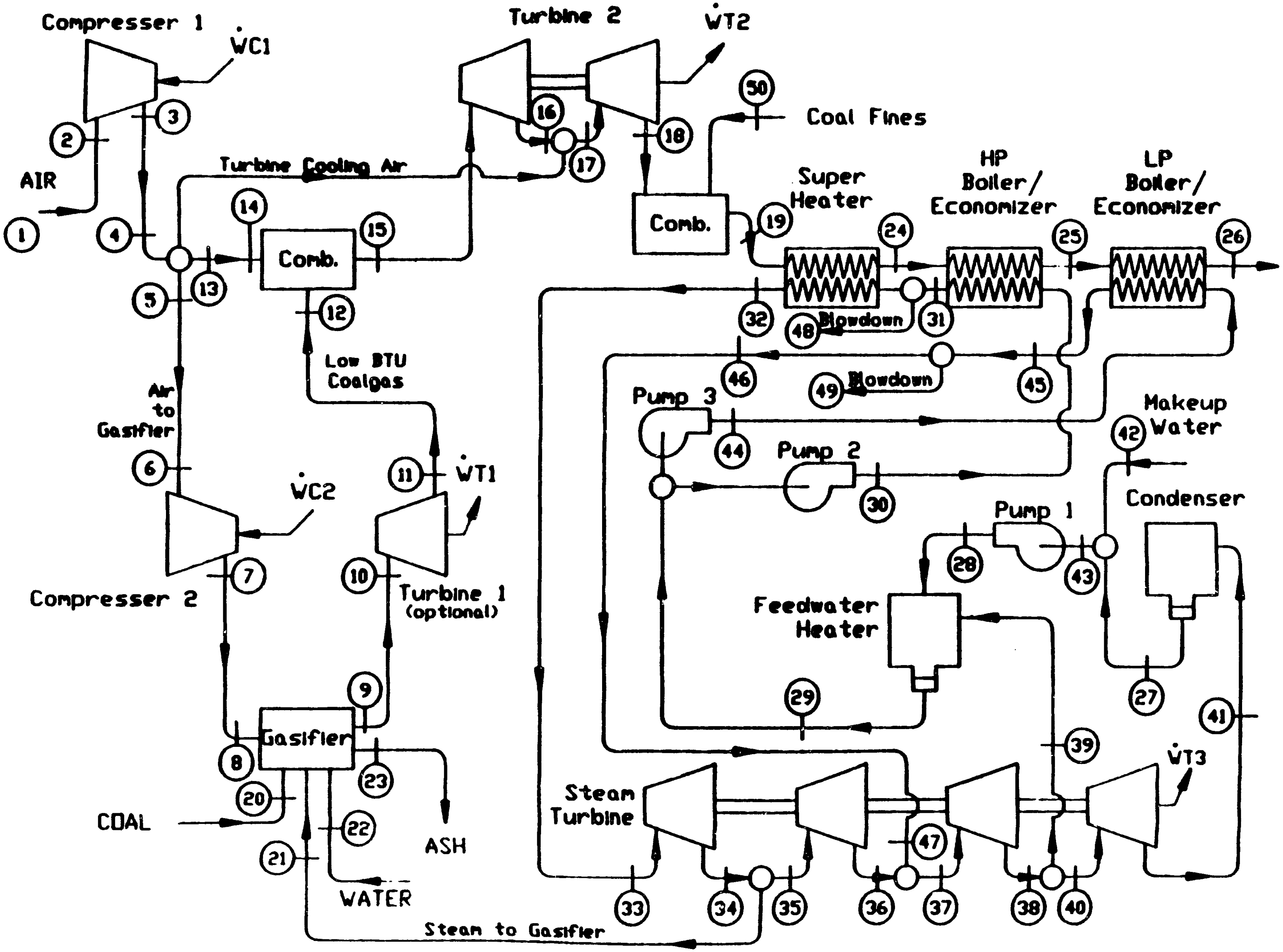


Figure 2.1 GE MS7001 EA Heavy-Duty Gas Turbine

The air that is sent to the gasifier is increased in pressure to 300 psi, and increased in temperature to 1070 °F. In the gasifier, coal, steam, water, and air are mixed and react to produce a low BTU gas that will be burned in the gas turbine combustor. This raw gas leaving the gasifier is purified in a hot gas cleanup unit before it is throttled to the pressure of the combustor. The hot gas cleanup unit is described in detail in Section 4. Our model contains an optional turbine that could derive power from the high pressure coal gas that flows from the gasifier. This turbine will not be employed in the actual IGCC system. It was included in the model so that we could make computations to determine how the overall system efficiency is affected by the throttling of the high pressure coal gas.

The low BTU gaseous fuel is mixed with air and burned in the gas turbine combustor. The mass flow rate exiting the combustor is about 600 lbm/sec and 2100 °F. The pressure at this location is close to 175 psi. These gases now expand through the turbine area creating power.

Our model contains equations for a fired heat recovery steam generator. Originally, this component was added to the model so that we could evaluate the effect of burning coal fines. It appears that this is undesirable because of the sulfur in the fines. However, it may prove to be advantageous to burn clean coal gas in the heat recovery steam generator. We have arbitrarily made example computations for the case when the exhaust gas is heated to 1250 F before it is used to raise steam. In this case the mass flow rate of the exhaust gas is almost 650 lbm/sec. This flow is sent to the heat recovery part of the Integrated Gasification Combined Cycle.

2.2 Combustor Model Using Equilibrium Constants

The computer model of the combustor determines the firing temperature and the combustor product gas composition for given fuel gas properties and fuel flow rates. It can make calculations based on complete combustion while accounting for combustor losses, or it can do chemical equilibrium calculations to determine the equilibrium fractions of carbon monoxide, hydroxyl, nitric oxide, and other radicals in the combustor product gases. One way of determining the combustion temperature is to use an energy balance of the products and reactants coupled with equilibrium equations that allow the extent of reaction to be determined as a function of temperature.

For example, Figure 2.1 shows that the reactants for the combustor are the products of the gasifier from stage 12 and the air from compressor 1 at stage 14. Consequently, a straight forward calculation can be performed. Below is the complete combustion equation for the reaction of N_2, O_2, CO_2, CO, H_2O, H_2, CH_4, C_2H_6, H_2S, and SO_2.

$$\begin{gathered}
n_{N2}N_2 + n_{CO2}CO_2 + n_{CO}CO + n_{H_2}H_2 + n_{H_2O}H_2O + \\
n_{CH_4}CH_4 + n_{SO_2}SO_2 + n_{C_2H_6}C_2H_6 + n_{H_2S}H_2S + \\
Z \times O_2 + Z \times 3.77 \times N_{AIR} \times N_2 \longrightarrow (n_{H_2S} + n_{SO_2})SO_2 + \\
(n_{CO_2} + n_{CO} + n_{CH_4} + 2n_{C_2H_6})CO_2 + (Z \times 3.77 \times N_{AIR} + n_{N_2} + \\
(Z - 1/2\, n_{CO} - 1/2\, n_{H_2} - 2\, n_{CH_4} - 7/2\, n_{C_2H_6} - 3/2\, n_{H_2S})O_2 + \\
(n_{H_2} + n_{H_2O} + 2n_{CH_4} + 3n_{C_2H_6} + n_{H_2S})H_2O
\end{gathered} \tag{2.1}$$

In the above equation "N_{AIR}" may be chosen to be either one or zero. If the user chooses one, the computer model simulates the combustion of the products with air. If the user chooses zero for this parameter the computer model simulates the combustion with pure oxygen.

The extent of the reaction that will occur for each of the products can be determined from chemical equilibrium analyses. Below are the equilibrium equations for the reactions in the combustor.

Balancing Constant	**Equation**	
x_1	$2CO_2 \Longleftrightarrow 2CO + O_2$	(2.2)
x_2	$2SO_2 + 2H_2O \Longleftrightarrow 2H_2S + 3O_2$	(2.3)
x_3	$2H_2O \Longleftrightarrow 2H_2 + O_2$	(2.4)

$$x_4 \qquad 2H_2O \Longleftrightarrow H_2 + 2OH \tag{2.5}$$

$$x_5 \qquad N_2 + O_2 \Longleftrightarrow 2NO \tag{2.6}$$

$$x_6 \qquad CO_2 + 2H_2O \Longleftrightarrow 2O_2 + CH_4 \tag{2.7}$$

$$x_7 \quad 2CO_2 + 3H_2O \Longleftrightarrow 7/2O_2 + C_2H_6 \tag{2.8}$$

where 'x_N' represents the extent of reaction that each of the above equations will experience at a given temperature. The reaction equation for incomplete combustion is:

$$\begin{gathered}
n_{N_2}N_2 + n_{CO_2}CO_2 + n_{CO}CO + n_{H_2}H_2 + n_{H_2O}H_2O + \\
n_{CH_4}CH_4 + n_{SO_2}SO_2 + n_{C_2}H_6C_2H_6 + n_{H_2S}H_2S + \\
Z \times O_2 + Z \times 3.77 \times N_{AIR} \times N_2 \longrightarrow (n_{H_2S} + n_{SO_2} - 2x_2)SO_2 + \\
(n_{CO_2} + n_{CO} + n_{CH_4} + 2n_{C_2H_6} - 2x_1 - x_6 - 2x_7)CO_2 + \\
(Z \times 3.77 \times N_{AIR} + n_{N_2} - x_5)N_2 + (2x_1)CO + (2x_2)H_2S + (2x_4)OH + \\
(n_{H_2} + n_{H_2O} + 2n_{CH_4} + 3n_{C_2H_6} + n_{H_2S} - 2x_2 - 2x_3 - 2x_4 - \\
2x_6 - 3x_7)H_2O + (Z - 1/2\, n_{CO} - 1/2\, n_{H_2} - 2\, n_{CH_4} - 7/2\, nC_2H_6 - \\
3/2\, n_{H_2S} + x_1 + 3x_2 + x_3 - x_5 + 2x_6 + 7/2\, x_7)O2 + (2x_5)NO + \\
(2x_3 + x_4)H_2 + (x_6)CH_4 + (x_7)C_2H_6
\end{gathered} \tag{2.9}$$

The extent of each reaction may be calculated at any temperature and pressure by solving equilibrium equations. In general, for the equation

$$v_A A + v_B B \Longleftrightarrow v_C C + v_D D \tag{2.10}$$

The equilibrium equation can be written as:

$$\ell n \frac{(Y_C P/P_o)^{vD}(Y_D P/P_o)^{vD}}{(Y_A P/P_o)^{vA}(Y_B P/P_o)^{vB}} = \frac{v_C G_C + v_D G_D - v_A G_A - v_B G_B}{RT} \tag{2.11}$$

By writing the equilibrium equations for our combustion problem, we obtain the following:

For equation $2CO_2 \Longleftrightarrow 2CO + O_2$:

$$\ell n \frac{(Y_{CO}P.100)^2(Y_{O_2}P/100)^1}{(Y_{CO_2}P/100)^2} = \frac{2G_{CO_2} - 2G_{CO} - G_{O_2}}{RT} \tag{2.12}$$

For equation $2SO_2 + 2H_2O \Longleftrightarrow 2H_2S + 3O_2$:

$$\ell n \frac{(Y_{H_2S}P/100)^2(Y_{O_2}P/100)^3}{(Y_{SO_2}P/100)^2(Y_{H_2O}P/100)^2} = \frac{2G_{SO_2} + 2G_{H_2O} - 2G_{H_2S} - 3G_{O_2}}{RT} \tag{2.13}$$

For equation $2H_2O \Longleftrightarrow 2H_2 + O_2$:

$$\ell n \frac{(Y_{H_2}P/100)^2(Y_{O_2}P/100)^1}{(Y_{H_2O}P/100)^2} = \frac{2G_{H_2O} - 2G_{H_2} - G_{O_2}}{RT} \tag{2.14}$$

For equation $2H_2O \Longleftrightarrow H_2 + 2OH$:

$$\ell n \frac{(Y_{H_2}P/100)^1(Y_{OH}P/100)^2}{(Y_{H_2O}P/100)^2} = \frac{2G_{H_2O} - 2G_{H_2} - 2G_{OH}}{RT} \tag{2.15}$$

For equation $N_2 + O_2 \Longleftrightarrow 2NO$:

$$\ell n \frac{(Y_{NO}P/100)^2}{(Y_{N_2}P/100)^1(Y_{O_2}P.100)^1} = \frac{G_{N_2} + G_{O_2} - 2G_{NO}}{RT} \tag{2.16}$$

For equation $CO_2 + 2H_2O \Longleftrightarrow 2O_2 + CH_4$:

$$\ell n \frac{(Y_{O_2}P/100)^2(Y_{CH_4}P/100)^1}{(Y_{CO_2}P/100)^1(Y_{H_2O}P/100)^2} = \frac{G_{CO_2} + 2G_{H_2O} - 2G_{O_2} - G_{CH_4}}{RT} \tag{2.17}$$

For equation $2CO_2 + 3H_2O \Longleftrightarrow 7/2O_2 + C_2H_6$:

$$\ell n \frac{(Y_{O_2}P/100)^{7/2}(Y_{C_2H_6}P/100)^1}{(Y_{CO_2}P/100)^2(Y_{H_2})P/100)^3} = \frac{2G_{CO_2} + 3G_{H_2O} - 7/2G_{O_2} - G_{C_2H_6}}{RT} \qquad (2.17)$$

An energy balance was used to determine the combustion temperature. This balance included the enthalpies of the reactants, enthalpies of the products, and a combustion efficiency parameter.

Because the combustion temperature is a function of the extent of reaction which is in turn a function of temperature, a Newton-Raphson iterative process is used. With the Newton-Raphson method accurate solutions can be obtained with as few as five iterations.

Although the above analysis is included in our model, and is useful for determining amounts of disassociation that may occur within a combustion process, it is not actually needed for determining the temperature of the reaction, the main objective of this part of the program. There is excess air in the gas turbine combustor, and the firing temperatures are low enough that little dissociation occur. Thus it is acceptable to assume that complete combustion occurs. For this reason later versions of this program only calculated the complete combustion temperature, which was found to be extremely close to temperatures calculated in the analyses using equilibrium equations.

It should be noted that the overall system model described here assumes that the combustor design is adequate for accomplishing complete combustion of low BTU coal gas. Separate computer models which account for turbulent mixing of the fuel and air, chemical kinetics, radiation heat transfer, and other details of reacting flows are needed to predict whether a combustor design is indeed adequate. Two computer models of gas turbine combustors were evaluated in a separate task of the IGCC system study.

2.3 Gasifier Model Using Equilibrium Constants

A detailed model of a fixed bed coal gasifier was developed separately, and is described in Section 3. It is useful for predicting allowable coal feed rates for given gasifier dimensions, local temperatures within the gasifier (which is needed to predict whether ash fusion is a potential problem), carbon conversion efficiency, and other specific information about the coal gasifier. A less detailed model is needed for the overall system analysis. The requirements in this case are that the model must conserve mass and energy, and must account for the chemical composition of the coal gas. Chemical equilibrium analysis are not as useful for predicting gas compositions in the gasifier as they are in the combustor because temperatures are lower in the gasifier. Chemical equilibrium may not be approached because the reaction rates are slow.

It was also found that equilibrium analysis tended to under predict the amount of heavier hydrocarbons in the coal gas. The result of this is that the model tended to underpredict the heating value of the coal gas and overpredicted the gas exit temperatures. The model predicted that too little of the energy originally in coal remained as stored chemical energy in the product gas and that too much was stored as sensible energy in the gas.

Nevertheless, the model predictions base on equilibrium analysis are adequate for the purpose of the study. For example, based on chemical equilibrium analyses, the model predicted that the lower heating value of the dry product gases is 163 BTU/scf. Based on experimental gas compositions, the heating value is 168 BTU/scf. To compensate for this error, the model predicted that the gas temperatures for the chemical equilibrium case is about 300 °F higher than for the case with experimental gas composition. The user has the option of inputting the experimental gas composition when it is known.

The first step in developing the equation for the chemical equilibrium analysis is to create a complete gasification equation from the known reactants. The equation is:

$$n_C C + n_{H_2}H_2 + n_{O_2}O_2 + n_{N_2}N_2 + n_S S + z_1 H_2O + z_2(O_2 + 3.77z_2N_2) \longrightarrow$$

$$(n_C - 2z_2 - 2n_{O_2})CO + (2z_2 + 2n_{O_2})CO_2 + (n_{H_2} + n_C - n_S)H_2 + (z_1 - n_C)H_2O +$$

$$(3.77z_2 + n_{N_2})N_2 + n_S H_2S \tag{2.19}$$

The next step is to write the important equilibrium equations needed to determine the amounts of O_2, N_2, CO, CO_2, H_2, H_2, CH_2, C_2H_6, H_2O, SO_2, and H_2S as a function of temperature and pressure. The reactions that are considered are:

$$x_1 \qquad H_2 + CO_2 \Longleftrightarrow H_2O + CO \tag{2.20}$$

$$x_2 \qquad CO + 3H_2 \Longleftrightarrow CH_4 + H_2O \tag{2.21}$$

$$x_3 \quad 2CO + 5H_2 \Longleftrightarrow C_2H_6 + 2H_2O \tag{2.22}$$

$$x_4 \quad H_2S + 2H_2O \Longleftrightarrow SO_2 + 3H_2 \tag{2.23}$$

where x_1, x_2, x_3, and x_4 signify the extent of the reaction of each of the above equations. These equations can now be combined with equation 19 to give:

$$\begin{gathered} n_C C + n_{H_2}H_2 + n_{O_2} + n_{N_2} + n_S S + z_1 H_2O + z_2(O_2 + 3.77z_2N_2) \longrightarrow \\ (n_C - 2z_2 - 2n_{O_2} + x_1 - x_2 - 2x_3)CO + (2z_2 + 2n_{O_2} - x_1)CO_2 + \\ (n_{H_2} + n_C - n_S - x_1 - 3x_2 - 5x_3 + 3x_4)H_2 + (z_1 - n_C + x_1 + x_2 + 2x_3 - 2x_4)H_2O + \\ (3.77z_2 + n_{N_2})N_2 + (n_S - x_4)h_2S + x_2CH_4 + x_3C_2H_6 + x_4SO_2 \end{gathered} \tag{2.24}$$

Equation 24 is simply a balanced reaction equation in which all of the components that are of significance in the coal gas appear as products. The values of x_1 through x_4, which specify the amount of each component, are obtained by minimizing the Gibbs energy of the product gas mixture. The following equations establish the conditions for which the Gibbs energy is a minimum:

$$\frac{dG}{dx_1} = \frac{DG}{dx_2} = \frac{dG}{dx_3} = \frac{dG}{dx_4} = 0 \tag{2.25}$$

By writing an equation for the Gibbs energy of the mixture of produced gases in Equation 2.24 and differentiating with respect to x_1 through x_4 we obtain the following:

$$\ell n \frac{(Y_{H_2O}P/P^0)^1(Y_{CO}P/P^0)^1}{(Y_{H_2}P/P^0)^1(Y_{CO_2}P/P^0)^1} = \frac{G_{H_2} + G_{CO_2} - G_{H_2O} - G_{CO}}{RT} \tag{2.26}$$

$$\ell n \frac{(Y_{CH_4}P/P^0)^1(Y_{H_2O}P/P^0)^1}{(Y_{CO}P/P^0)^1(Y_{H_2}P/P^0)^3} = \frac{G_{CO} + 3G_{H_2} - G_{CH_4} - G_{H_2O}}{RT} \tag{2.27}$$

$$\ell n \frac{(Y_{C_2H_6}P/P^0)^1(Y_{H_2O}P/P^0)^2}{(Y_{CO}P/P^0)^2(Y_{H_2}P/P^0)^5} = \frac{2G_{CO} + 5G_{H_2} - G_{C_2H_6} - 2G_{H_2O}}{RT} \tag{2.28}$$

$$\ell n \frac{(Y_{SO_2}P/P^0)^1(Y_{H_2}P/P^0)^3}{(Y_{H_2S}P/P^0)^1(Y_{H_2O}P/P^0)^2} = \frac{G_{H_2S} + 2G_{H_2O} - G_{SO_2} - 3G_{H_2}}{RT} \tag{2.29}$$

The mole fractions of the product gases may be expressed in terms of x_1 through x_4 using Equation 2.24. A Newton Raphson search procedure is then employed to solve Equation 2.26 through Equation 2.29 for x_1 through x_4. However a fifth variable (temperature) must be considered because the Gibbs energies in Equation 2.26 through Equation 2.29 are temperature dependent.

The product gas temperature may be determined from the energy equation which is written below in terms of the enthalpies of the gaseous components, heat losses, change of energies of the ash, and the heat of formation of the coal.

$$n_{air}h_{air} + n_{liq\ water}h_{liq\ water} + n_{stream}h_{stream} + m_{coal}h_{f\ coal} =$$

$$g_{loss} + \sum n_{prod}h_{prof} + m_{ash}(E_{ash\ @2} - E_{ash\ @1}) \qquad (2.30)$$

Once again, a Newton-Raphson method was used to solve the five non-linear equations. However, the solution to the equations for the gasifier is not as straight forward as the solution to the equation for the gas turbine combustor. The gasification process is at a lower temperature with much smaller amounts of oxygen. Convergence was much more difficult. In particular, determining the values of x_1 through x_4 was very tedious. Because the gasification reactions are done in an oxygen poor environment, the amount of oxygen in the product gas is extremely low. Consequently, while iterating towards the solution, the amount of oxygen might be temporarily calculated to be less than zero. However, before another iteration could compensate for this error, the program would crash. For the above reason, initial guesses in the Newton Raphson search could not be totally random.

2.4 Compressor and Turbine Model

Standard equations for the compressor and the turbine are used in the computer model. The work needed for the compressors or the work produced by the turbines are calculated using the following equations:

$$Compressor\ Work = \dot{m}_{air} * Cp_{air} * Delta\ Temp \qquad (2.31)$$

$$Turbine\ Work = \dot{m}_{products} * Cp_{products} * Delta\ Temp \qquad (2.32)$$

The following are the compressor and turbine equations used to determine exiting temperatures given a prescribed pressure ratio.

For the Turbine:

$$T_{out} = T_{in} * \left(\frac{P_{out}}{P_{in}}\right)^{\left[\frac{turbine\ eff * (k_{prod} - 1)}{k_{prod}}\right]} \tag{2.33}$$

For the Compressor:

$$T_{out} = T_{in} * \left(\frac{P_{out}}{P_{in}}\right)^{\left[\frac{(k_{air} - 1)}{compressor\ eff\ *\ k_{air}}\right]} \tag{2.34}$$

2.5 Computer Model of Heat Recovery Cycle

The gas turbine exhaust is at a low pressure (approximately atmospheric) but at a high temperature (approximately 1000 °F). By using heat exchangers to cool the exhaust gas while heating water to make steam, waste energy in the low pressure exhaust gas can be rendered into useful energy in high pressure steam.

For the heat recovery steam generator (HRSG) and bottoming cycle, the pressures at every point in the cycle are set to optimize the cost and efficiency of the overall plant. Other knowns include the temperature of the exhaust gas entering the HRSG, the mass flowrate of the exhaust gas, the heat exchanger sizes, and the turbine and pump efficiencies. The temperature of the steam leaving the superheater is set by the temperature of the exhaust gas. From all the given information, the properties and mass flow rates at each point on the cycle can be determined.

In our bottoming cycle model, the starting and ending point for the calculations is at the condenser. First, the properties of water leaving the condenser are determined at saturated conditions. Equations for the pumps are then solved to determine the properties of the feedwater entering the boiler. An iterative process is used to determine both the properties of the gas and steam on either side of the superheater and the high pressure boiler/economizer. Finally, the properties of the steam returning to the condenser are determined by solving equations for the turbines. The calculations for each separate component of the system are described in detail below.

2.5.1 Pumps

The knowns for the pump calculations are the pump efficiency, the pressures on both sides of the pump, and the properties of the water entering the pump. Assuming incompressible flow, the following formula is used to determine the amount of work done by the pump per kilogram of feedwater.

$$W_{pump} = \frac{v \cdot (P_{exit} - P_{enter})}{\eta_p} \tag{2.35}$$

Also, the enthalpy of the exiting water is determined using the following formulas.

$$h_{exit} = W_{pump} + h_{enter} \tag{2.36}$$

The above procedure is repeated for each of the three pumps.

2.5.2 Boilers/Economizers and Superheaters

The knowns for the models of the boilers/economizers are the inlet exhaust gas temperature, the size of the boilers, and the inlet and exit properties of the steam.

In our model, the overall UA for the boiler is divided into two regions, the preheat region and the boiling region. Since the steam leaving the boilers is saturated at the design pressure, the properties for steam are known for both the entrance and the exit of the boiler. Also since the exhaust gas exit temperature is not known, the overall UA is written in terms of steam temperatures, and mass flow rates only. An energy balance is performed for each of these regions yeilding the following energy equations.

$$q_1 = (\dot{m}c_p)_{gas}(T_{GI} - T_{G2}) = (UA)_1 \Delta T_{M1} \tag{2.37}$$

$$q_2 = (\dot{m}c_p)_{gas}(T_{G1} - T_{GI}) = (UA)_2 \Delta T_{M2} \tag{2.38}$$

where ΔT_M is the logarithmic mean temperature for the region. Equations 2.37 and 2.38 are solved for their respective UA values, and are added together to give one equation for the overall UA value for the boiler/economizer.

$$UA = (\dot{m}c_p)_{gas} \left[\frac{1}{1 - \frac{T_{S2} - T_{S1}}{T_{GI} - T_{G1}}} \ln \left(\frac{T_{GI} - T_{S2}}{T_{G1} - T_{S1}} \right) + \ln \left(\frac{T_{G1} - T_{S2}}{T_{GI} - T_{S2}} \right) \right] \tag{2.39}$$

where:

T_{G1} ≡ Exhaust gas inlet temperature (known)
T_{GI} ≡ Exhaust gas temperature at interface of regions (unknown)
T_{G2} ≡ Exhaust gas outlet temperature (unknown)
T_{S1} ≡ Water inlet temperature (known)
T_{S2} ≡ Steam outlet temperaure (known)

The overall steady state energy equation for both regions is solved for the exhaust gas exit temperature, T_{G2}.

$$T_{G2} = T_{G1} - \frac{(\dot{m}c_p)_{water}}{(\dot{m}c_p)_{gas}} \left(T_{S2} - T_{S1} + \frac{h_{fg}}{c_{p,water}} \right) \tag{2.40}$$

where h_{fg} is the heat of vaporization for water. Also, an energy balance for the preheat region when solved for the exhaust gas boiling interface temperature provide the following equation.

$$T_{GI} = T_{G2} + \frac{T_{S2} - T_{S1}}{R} \tag{2.41}$$

where:

$$R \equiv \frac{(\dot{m}c_p)_{gas}}{(\dot{m}c_p)_{water}} \tag{2.42}$$

Equations 2.40 and 2/41 may be solved for the exhaust gas boiling interface temperature, T_{GI}.

$$T_{GI} = T_{G1} + \frac{1}{R} \frac{h_{fg}}{c_{p,water}} \tag{2.43}$$

Equations 2.39, 2.49, and 2.43 are combined to give a single equation for the overall UA.

$$\frac{UA}{(\dot{m}c_p)_{gas}} = \frac{1}{1-R} \ln \left(\frac{T_{G1} - T_{S2} + \frac{1}{R}\frac{h_{fg}}{c_{p,water}}}{T_{G1} - T_{S1} - \frac{1}{R}\left(\frac{h_{fg}}{c_{p,water}} + T_{S2} - T_{S1} \right)} \right)$$

$$+\ln\left(\frac{T_{G1}-T_{S2}}{T_{G1}-T_{S2}+\frac{1}{R}\frac{h_{fg}}{c_{p,water}}}\right) \tag{2.44}$$

In Eqn. 2.44 the only unknown is R, given by Eqn. 2.42. R is determined using the Newton-Raphson method, which means two trial values for R are required. To find these two trial values, the critical values for Eqn. 2.44 are determined. These critical values of R are defined as the values that make the denominators of either of logrithmic terms equate to zero. By equating these denominators to zero, the following expressions for R are determined.

$$R_{CRIT,1} = \frac{T_{S2}-T_{S1}+\frac{h_{fg}}{c_{p,water}}}{T_{G1}-T_{S1}} \tag{2.45}$$

$$R_{CRIT,2} = \frac{\frac{h_{fg}}{c_{p,water}}}{T_{G1}-T_{S2}} \tag{2.46}$$

The trial values of R must be larger than either of the critical values. R^* is defined as the larger of the two R_{CRIT} values. R^* is used in the following equations to determine the trial values for R.

$$R_1 = \frac{R^*}{1-\exp\left(\frac{-UA}{(\dot{m}c_p)_{gas}}\right)} \tag{2.47}$$

$$R_2 = R_1 + \left[\frac{UA}{(\dot{m}c_p)_{gas}}\right][R_1 - R^*] \tag{2.48}$$

Once Eqn. 2.44 is solved for R, the flowrate of feedwater is determined from Eqn. 2.42. The feedwater flowrate is needed to compute the power produced by the Rankine cycle.

2.5.3 Turbines

The knowns for the turbine calculations are the turbine efficiency, the properties of steam entering the turbine, and the pressure drop across the turbine. The properties of steam are calculated at the outlet pressure and the inlet entropy. The work for the turbine is then calculated using the following formula.

$$W_t = \eta_t\left(h_{enter} - h_{exit,isentropic}\right) \tag{2.49}$$

The actual exit enthalpy is then calculated using the following formula.

$$h_{exit,actual} = h_{enter} - W_{TURBINE} \tag{2.50}$$

The properties of the exhaust steam are re-calculated using the exit pressure and the above enthalpy.

2.5.4 Steam Tables

The steam table subroutine calculates the properties of steam from saturated liquid to superheated steam. The method used here is the one described in Reynolds [1] and Keenan [2]. A listing of the subroutines that make up the steam tables is included in the appendices.

2.6 Simulation Results

Five initial test cases were run to predict the overall system performance for the computer model. The Rankine bottoming cycle and heat recovery steam generator, which are described in Reference 1, were added to the model after the initial test cases were run. Separate cases were run to determine the performance of the combined cycle plant. The results of the initial test cases are summarized in Table 2.1 through Table 2.5.

As a first case the gas turbine was operated with methane fuel. A second run was made with a coal gas fuel when composition was determined experimentally. Table 2.1 shows that the cycle thermodynamic efficiency dropped from 32.14 % for methane fuel to 30.00 % for the coal gas fuel. Much of the loss in efficiency is due to the throttling of the high pressure coal gas as it flows from the gasifier to the combustor. This may be seen from the results of Table 2.3 in which a turbine was added to the system to replace the throttle valve. The efficiency improved to 31.45 % with the optional turbine. Two additional cases were run to establish the errors introduced by having the model compute the composition of the coal gas from equilibrium analysis. The results show that there is a negligible effect on the predicted overall system performance.

The overall system model is written such that it runs in an interactive mode. It prompts the user for needed information (such as the ultimate analysis of the coal), and provides a printout of the input data and the computed results. Table 2.6 shows the results of a typical run. It may be seen from the results in Table 2.6 that the fired HRSG and bottoming cycle increases the net shaft power by about 65 % and increases the thermodynamic efficiency (based on the lower heating value of the coal fed to the gasifier) to more than 41 %.

Table 2.1

```
                    **********************
                    **   COMMAND MENU   **
                    **********************

   Please type the number or letter of the variable
  you wish to change and PRESS ENTER.
      --------------------------------------------
                        (TOGGLE VALUES)
 1)               Fuel used in power system
                           METHANE
      --------------------------------------------
                        (INPUT VALUES)
 3)  Temperature of air at inlet (Location 1)......  298.15 K
 4)  Pressure of air at inlet (Location 1).........  101.32 KPA
 5)  Mass flow rate of air at inlet (Location 1)...  287.13 KG/SEC
 6)  Fraction of air used to cool blades...........   .050
 7)  Efficiancy of air compressors.................   .860
 8)  Efficiency of gas turbines....................   .920
 9)  Efficiency of combustor.......................   .950
 A)  Efficiency of pipes...........................   .950
 B)  Efficiency of generator and drive.............   .960
 I)                         STATISTICS
          (Amounts in moles - DRY & Sulfur FREE)
                   CO2....     .00000
                   CO.....     .00000
                   H2.....     .00000
                   CH4....    1.00000
                   CnHm...     .00000
                   N2.....     .00000
```

```
                    ENGLISH UNITS
location      degrees F       psi          lbm/sec
   1            76.67        14.69         633.00
   2            76.58        14.68         633.00
   3           719.52       171.80         633.00
   4           719.52       163.21         633.00
  11            80.00        21.75          11.01
  12           300.20       155.05          11.01
  13           719.52       163.21         601.35
  14           719.52       155.05         601.35
  15          2023.24       155.05         612.36
  16          1614.37        70.84         612.36
  17          1570.39        70.84         644.01
  18           956.83        14.79         644.01

                    METRIC UNITS
location      degrees K       KPA          kg/sec
   1           298.15       101.32         287.13
   2           298.10       101.27         287.13
   3           655.29      1184.81         287.13
   4           655.29      1125.57         287.13
  11           300.00       150.00           4.99
  12           422.33      1069.29           4.99
  13           655.29      1125.57         272.77
  14           655.29      1069.29         272.77
  15          1379.58      1069.29         277.77
  16          1152.43       488.57         277.77
  17          1128.00       488.57         292.12
  18           787.13       102.00         292.12
```

```
                 WORK INPUT/OUTPUT (KW)
   Work of FIRST COMPRESSOR --------->  106878.3
   Work of SECOND COMPRESSOR -------->    2019.9
   Work of FIRST TURBINE ------------>        .0
   Work of SECOND TURBINE ----------->  190480.8
TOTAL OUTPUT (including generator losses) -->   80258.4

         (BASED ON LOWER HEATING VALUE)
            Efficiency ---> 0.321420931316001370
            Heat Rate ---->  10618.4746152843030
```

Table 2.2

```
                  **********************
                  **   COMMAND MENU   **
                  **********************

  Please type the number or letter of the variable
 you wish to change and PRESS ENTER.
     ---------------------------------------------
                     (TOGGLE VALUES)
1)               Fuel used in power system
                          COALGAS
2)       Method of finding products leaving gasifier
                        EXPERIMENTAL
     ---------------------------------------------
                      (INPUT VALUES)
3)  Temperature of air at inlet (Location 1)......  298.15 K
4)  Pressure of air at inlet (Location 1).........  101.32 KPA
5)  Mass flow rate of air at inlet (Location 1)...  287.13 KG/SEC
6)  Fraction of air used to cool blades...........   .050
7)  Efficiency of air compressors.................   .860
8)  Efficiency of gas turbines....................   .920
9)  Efficiency of combustor.......................   .950
A)  Efficiency of pipes...........................   .950
B)  Efficiency of generator and drive.............   .960
C)  Efficiency of gasifier........................   .960
D)  Pressure in gasifier..........................  2068.43 KPA
E)  Fraction of air sent to gasifier..............   .085
F)                  COAL STATISTICS
               (Amounts in MASS FRACTIONS)
                  Carbon....   81.300
                 Hydrogen...    5.300
                  Oxygen....    9.800
                 Nitrogen...    1.700
                  Sulfur....    1.900
            Heating value of coal...  33725.0
        Percent WATER in coal as received...   .100
         Percent ASH in coal as received...   .100
G)  Amount of water added per mole of dry coal....   .500
I)                 PRODUCT STATISTICS
          (Amounts in moles - DRY & Sulfur FREE)
                 CO2....     .10300
                 CO.....     .21200
                 H2.....     .20100
                 CH4....     .04600
                 CnHm...     .00300
                 N2.....     .43500

J)             AUXILIARY TURBINE STATUS
                  ---> THROTTLE <---
```

ENGLISH UNITS

location	degrees F	psi	lbm/sec
1	76.67	14.69	633.00
2	76.58	14.68	633.00
3	719.52	171.80	633.00
4	719.52	163.21	633.00
5	719.52	163.21	53.80
6	719.52	155.05	53.80
7	1008.05	315.71	53.80
8	1008.05	299.92	53.80
9	1089.33	299.92	91.01
10	1089.33	284.93	91.01
11	1089.33	163.21	91.01
12	1089.33	155.05	91.01
13	719.52	163.21	547.54
14	719.52	155.05	547.54
15	2017.80	155.05	638.56
16	1616.27	70.84	638.56
17	1573.92	70.84	670.21
18	968.13	14.79	670.21
20	76.67	299.92	23.15
21	571.67	299.92	10.48
22	76.67	299.92	5.89
23	1340.00	299.92	2.31

METRIC UNITS

location	degrees K	KPA	kg/sec
1	298.15	101.32	287.13
2	298.10	101.27	287.13
3	655.29	1184.81	287.13
4	655.29	1125.57	287.13
5	655.29	1125.57	24.41
6	655.29	1069.29	24.41
7	815.58	2177.29	24.41
8	815.58	2068.43	24.41
9	860.74	2068.43	41.28
10	860.74	1965.01	41.28
11	860.74	1125.57	41.28
12	860.74	1069.29	41.28
13	655.29	1125.57	248.37
14	655.29	1069.29	248.37
15	1376.56	1069.29	289.65
16	1153.48	488.57	289.65
17	1129.56	488.57	304.01
18	793.41	102.00	304.01
20	298.15	2068.43	10.50
21	573.15	2068.43	4.75
22	298.15	2068.43	2.67
23	1000.00	2068.43	1.05

```
                   WORK INPUT/OUTPUT (KW)
        Work of FIRST COMPRESSOR ---------->  106878.3
        Work of SECOND COMPRESSOR --------->    4242.5
        Work of FIRST TURBINE ------------->        .0
        Work of SECOND TURBINE ------------>  196625.5
   TOTAL OUTPUT (including generator losses) -->   82084.6

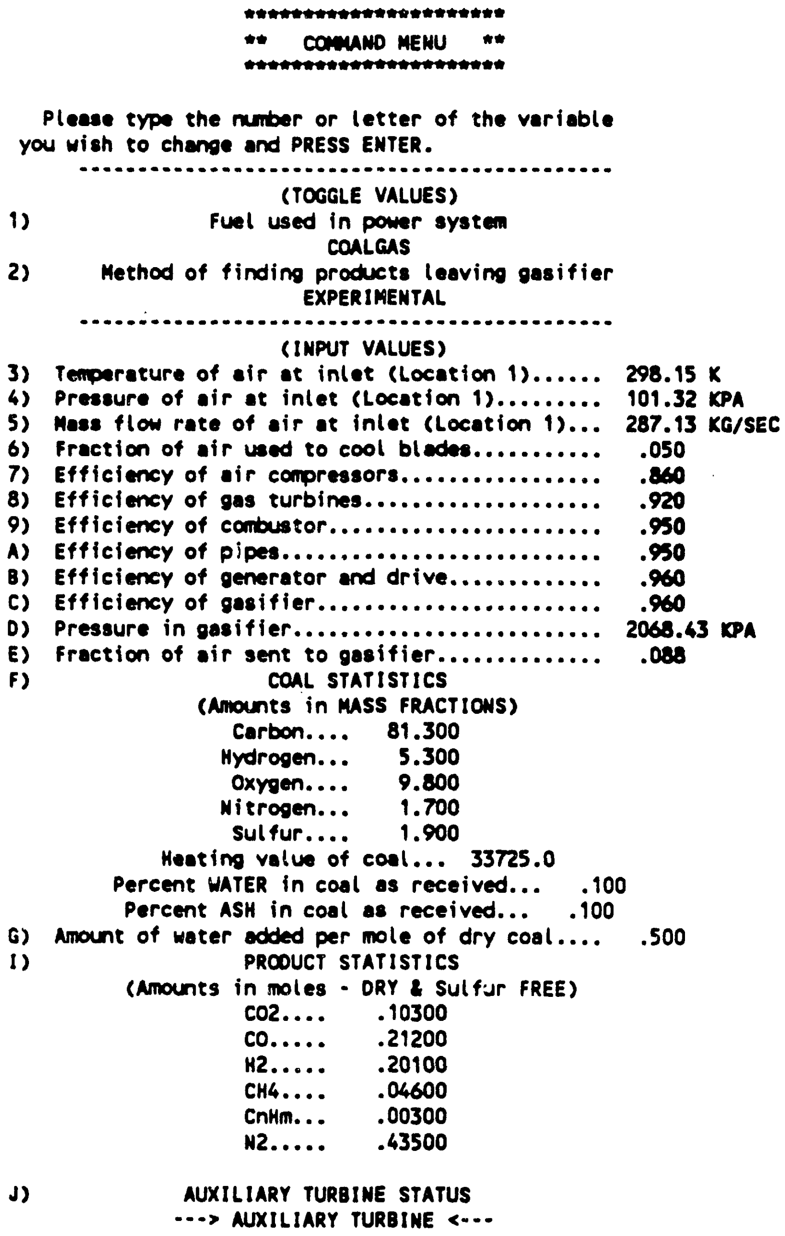
                   HIGHER HEATING VALUES
                     KJ/KG           BTU/SCF
     DRY BASIS      7129.39          189.78
     WET BASIS      6445.80          166.35

                   LOWER HEATING VALUES
                     KJ/KG           BTU/SCF
     DRY BASIS      6310.69          167.99
     WET BASIS      5705.60          147.25

                 HEAT RATES & EFFICIENCIES
                  (HIGHER HEATING VALUES)
     COAL EFFICIENCY ----------> .2897
     COAL HEAT RATE -----------> 11779.5
     GAS EFFICIENCY -----------> .3085
     GAS HEAT RATE ------------> 11064.3
                  (LOWER HEATING VALUES)
     COAL EFFICIENCY ----------> .3000
     COAL HEAT RATE -----------> 11375.4
     GAS EFFICIENCY -----------> .3485
     GAS HEAT RATE ------------>  9793.8

                      RELATIVE FLOWS
      LBM STEAM / LBM COAL ---->    .4527
    LBM STEAM&WATER / LBM COAL >    .7073
        LMB AIR / LBM COAL  --->   2.3243
    66.1660   STD FT^3 GAS OUT / LBM COAL
     .01221   LBM H2O / STD FT^3 GAS OUT
     .47499   STD FT^3 AIR / STD FT^3 GAS
```

Table 2.3



```
                    ***********************
                    **   COMMAND MENU   **
                    ***********************

  Please type the number or letter of the variable
 you wish to change and PRESS ENTER.
      -----------------------------------------------
                        (TOGGLE VALUES)
1)                Fuel used in power system
                            COALGAS
2)        Method of finding products leaving gasifier
                          EXPERIMENTAL
      -----------------------------------------------
                         (INPUT VALUES)
3)  Temperature of air at inlet (Location 1)......  298.15 K
4)  Pressure of air at inlet (Location 1).........  101.32 KPA
5)  Mass flow rate of air at inlet (Location 1)...  287.13 KG/SEC
6)  Fraction of air used to cool blades...........   .050
7)  Efficiency of air compressors.................   .860
8)  Efficiency of gas turbines....................   .920
9)  Efficiency of combustor.......................   .950
A)  Efficiency of pipes...........................   .950
B)  Efficiency of generator and drive.............   .960
C)  Efficiency of gasifier........................   .960
D)  Pressure in gasifier..........................  2068.43 KPA
E)  Fraction of air sent to gasifier..............   .088
F)                    COAL STATISTICS
               (Amounts in MASS FRACTIONS)
                   Carbon....   81.300
                  Hydrogen...    5.300
                   Oxygen....    9.800
                  Nitrogen...    1.700
                   Sulfur....    1.900
             Heating value of coal...  33725.0
         Percent WATER in coal as received...   .100
          Percent ASH in coal as received...   .100
G)  Amount of water added per mole of dry coal....   .500
I)                  PRODUCT STATISTICS
          (Amounts in moles - DRY & Sulfur FREE)
                    CO2....    .10300
                    CO.....    .21200
                    H2.....    .20100
                    CH4....    .04600
                    CnHm...    .00300
                    N2.....    .43500

J)              AUXILIARY TURBINE STATUS
               ---> AUXILIARY TURBINE <---
```

ENGLISH UNITS

location	degrees F	psi	lbm/sec
1	76.67	14.69	633.00
2	76.58	14.68	633.00
3	719.52	171.80	633.00
4	719.52	163.21	633.00
5	719.52	163.21	55.70
6	719.52	155.05	55.70
7	1008.05	315.71	55.70
8	1008.05	299.92	55.70
9	1089.33	299.92	94.22
10	1089.33	284.93	94.22
11	914.88	163.21	94.22
12	914.88	155.05	94.22
13	719.52	163.21	545.65
14	719.52	155.05	545.65
15	2024.98	155.05	639.87
16	1622.86	70.84	639.87
17	1580.28	70.84	671.52
18	973.39	14.79	671.52
20	76.67	299.92	23.97
21	571.67	299.92	10.85
22	76.67	299.92	6.10
23	1340.00	299.92	2.40

METRIC UNITS

location	degrees K	KPA	kg/sec
1	298.15	101.32	287.13
2	298.10	101.27	287.13
3	655.29	1184.81	287.13
4	655.29	1125.57	287.13
5	655.29	1125.57	25.27
6	655.29	1069.29	25.27
7	815.58	2177.29	25.27
8	815.58	2068.43	25.27
9	860.74	2068.43	42.74
10	860.74	1965.01	42.74
11	763.82	1125.57	42.74
12	763.82	1069.29	42.74
13	655.29	1125.57	247.51
14	655.29	1069.29	247.51
15	1380.54	1069.29	290.25
16	1157.14	488.57	290.25
17	1133.49	488.57	304.60
18	796.33	102.00	304.60
20	298.15	2068.43	10.87
21	573.15	2068.43	4.92
22	298.15	2068.43	2.77
23	1000.00	2068.43	1.09

```
                  WORK INPUT/OUTPUT (KW)
        Work of FIRST COMPRESSOR ---------> 106878.3
        Work of SECOND COMPRESSOR -------->   4392.2
        Work of FIRST TURBINE ------------>   6372.2
        Work of SECOND TURBINE -----------> 197676.5
TOTAL OUTPUT (including generator losses) -->   89067.1

                  HIGHER HEATING VALUES
                   KJ/KG            BTU/SCF
 DRY BASIS       7129.39             189.78
 WET BASIS       6445.80             166.35

                  LOWER HEATING VALUES
                   KJ/KG            BTU/SCF
 DRY BASIS       6310.69             167.99
 WET BASIS       5705.60             147.25

                HEAT RATES & EFFICIENCIES
                 (HIGHER HEATING VALUES)
 COAL EFFICIENCY ----------> .3037
 COAL HEAT RATE -----------> ~~14239.2~~
 GAS EFFICIENCY -----------> 3233
 GAS HEAT RATE ------------> ~~10556.8~~
                 (LOWER HEATING VALUES)
 COAL EFFICIENCY ----------> .3145
 COAL HEAT RATE -----------> ~~10853.6~~
 GAS EFFICIENCY -----------> .3652
 GAS HEAT RATE ------------> ~~9344.5~~

                     RELATIVE FLOWS
  LBM STEAM / LBM COAL ---->   .4527
LBM STEAM&WATER / LBM COAL >   .7073
    LMB AIR / LBM COAL  --->  2.3243
66.1660   STD FT^3 GAS OUT / LBM COAL
 .01221   LBM H2O / STD FT^3 GAS OUT
 .47499   STD FT^3 AIR / STD FT^3 GAS
```

Table 2.4

```
                    **********************
                    **   COMMAND MENU   **
                    **********************

   Please type the number or letter of the variable
  you wish to change and PRESS ENTER.
      --------------------------------------------
                        (TOGGLE VALUES)
 1)                Fuel used in power system
                            COALGAS
 2)          Method of finding products leaving gasifier
                   THEORETICAL -> (EQUILIBRIUM)
      --------------------------------------------
                         (INPUT VALUES)
 3)  Temperature of air at inlet (Location 1)......  298.15 K
 4)  Pressure of air at inlet (Location 1).........  101.32 KPA
 5)  Mass flow rate of air at inlet (Location 1)...  287.13 KG/SEC
 6)  Fraction of air used to cool blades...........   .050
 7)  Efficiency of air compressors.................   .860
 8)  Efficiency of gas turbines....................   .920
 9)  Efficiency of combustor.......................   .950
 A)  Efficiency of pipes...........................   .950
 B)  Efficiency of generator and drive.............   .960
 C)  Efficiency of gasifier........................   .960
 D)  Pressure in gasifier..........................  2068.43 KPA
 E)  Fraction of air sent to gasifier..............   .085
 F)                     COAL STATISTICS
                   (Amounts in MASS FRACTIONS)
                      Carbon....   81.300
                     Hydrogen...    5.300
                      Oxygen....    9.300
                     Nitrogen...    1.700
                      Sulfur....    1.900
                Heating value of coal...  33725.0
            Percent WATER in coal as received...   .100
             Percent ASH in coal as received...   .100
 G)  Amount of water added per mole of dry coal....   .500
```

```
         GASIFIER PRODUCTS
     CO2 ----------->   .2659543
     CO ------------>   .2940301
     H2 ------------>   .3370807
     CH4 ----------->   .1290224
     C2H6 ---------->   .0000098
     N2 ------------>   .8167270
     H2O ----------->   .2370947
     H2S ----------->   .0060322
```

```
                         ENGLISH UNITS
location     degrees F         psi          lbm/sec
    1           76.67         14.69          633.00
    2           76.58         14.68          633.00
    3          719.52        171.80          633.00
    4          719.52        163.21          633.00
    5          719.52        163.21           53.80
    6          719.52        155.05           53.80
    7         1008.05        315.71           53.80
    8         1008.05        299.92           53.80
    9         1391.71        299.92           91.01
   10         1391.71        284.93           91.01
   11         1391.71        163.21           91.01
   12         1391.71        155.05           91.01
   13          719.52        163.21          547.54
   14          719.52        155.05          547.54
   15         2013.36        155.05          638.56
   16         1612.49         70.84          638.56
   17         1570.32         70.84          670.21
   18          965.52         14.79          670.21
   20           76.67        299.92           23.15
   21          571.67        299.92           10.48
   22           76.67        299.92            5.89
   23         1340.00        299.92            2.31

                         METRIC UNITS
location     degrees K         KPA           kg/sec
    1          298.15        101.32          287.13
    2          298.10        101.27          287.13
    3          655.29       1184.81          287.13
    4          655.29       1125.57          287.13
    5          655.29       1125.57           24.41
    6          655.29       1069.29           24.41
    7          815.58       2177.29           24.41
    8          815.58       2068.43           24.41
    9         1028.73       2068.43           41.28
   10         1028.73       1965.01           41.28
   11         1028.73       1125.57           41.28
   12         1028.73       1069.29           41.28
   13          655.29       1125.57          248.37
   14          655.29       1069.29          248.37
   15         1374.09       1069.29          289.65
   16         1151.38        488.57          289.65
   17         1127.96        488.57          304.01
   18          791.96        102.00          304.01
   20          298.15       2068.43           10.50
   21          573.15       2068.43            4.75
   22          298.15       2068.43            2.67
   23         1000.00       2068.43            1.05
```

```
                   WORK INPUT/OUTPUT (KW)
         Work of FIRST COMPRESSOR --------->  106878.3
         Work of SECOND COMPRESSOR -------->    4242.5
         Work of FIRST TURBINE ------------>        .0
         Work of SECOND TURBINE ----------->  196258.1
TOTAL OUTPUT (including generator losses) -->   81731.8

                   HIGHER HEATING VALUES
                    KJ/KG           BTU/SCF
  DRY BASIS        6734.40           185.53
  WET BASIS        6159.65           164.44

                   LOWER HEATING VALUES
                    KJ/KG           BTU/SCF
  DRY BASIS        5928.52           163.33
  WET BASIS        5422.55           144.76

                 HEAT RATES & EFFICIENCIES
                   (HIGHER HEATING VALUES)
  COAL EFFICIENCY ----------> .2885
  COAL HEAT RATE -----------> 11829.9
  GAS EFFICIENCY -----------> .3214
  GAS HEAT RATE ------------> 10618.7
                   (LOWER HEATING VALUES)
  COAL EFFICIENCY ----------> .2988
  COAL HEAT RATE -----------> 11424.0
  GAS EFFICIENCY -----------> .3651
  GAS HEAT RATE ------------>  9348.0

                      RELATIVE FLOWS
   LBM STEAM / LBM COAL ---->   .4527
LBM STEAM&WATER / LBM COAL >   .7073
     LMB AIR / LBM COAL  --->  2.3244
64.2324   STD FT^3 GAS OUT / LBM COAL
 .01258   LBM H2O / STD FT^3 GAS OUT
 .48931   STD FT^3 AIR / STD FT^3 GAS
```

Table 2.5

```
                 **********************
                 **   COMMAND MENU   **
                 **********************

  Please type the number or letter of the variable
 you wish to change and PRESS ENTER.
     ---------------------------------------------
                    (TOGGLE VALUES)
1)               Fuel used in power system
                         COALGAS
2)       Method of finding products leaving gasifier
                THEORETICAL -> (EQUILIBRIUM)
     ---------------------------------------------
                     (INPUT VALUES)
3)  Temperature of air at inlet (Location 1)......  298.15 K
4)  Pressure of air at inlet (Location 1).........  101.32 KPA
5)  Mass flow rate of air at inlet (Location 1)...  287.13 KG/SEC
6)  Fraction of air used to cool blades...........   .050
7)  Efficiency of air compressors.................   .860
8)  Efficiency of gas turbines....................   .920
9)  Efficiency of combustor.......................   .950
A)  Efficiency of pipes...........................   .950
B)  Efficiency of generator and drive.............   .960
C)  Efficiency of gasifier........................   .960
D)  Pressure in gasifier..........................  2068.43 KPA
E)  Fraction of air sent to gasifier..............   .088
F)                  COAL STATISTICS
              (Amounts in MASS FRACTIONS)
                  Carbon....   81.300
                 Hydrogen...    5.300
                  Oxygen....    9.800
                 Nitrogen...    1.700
                  Sulfur....    1.900
            Heating value of coal...  33725.0
        Percent WATER in coal as received...   .100
         Percent ASH in coal as received...   .100
G)  Amount of water added per mole of dry coal....   .500
```

```
                    GASIFIER PRODUCTS
                CO2 ----------->   .2659543
                CO ------------>   .2940301
                H2 ------------>   .3370807
                CH4 ----------->   .1290224
                C2H6 ---------->   .0000098
                N2 ------------>   .8167270
                H2O ----------->   .2370947
                H2S ----------->   .0060322



                      ENGLISH UNITS
location     degrees F        psi          lbm/sec
     1          76.67        14.69         633.00
     2          76.58        14.68         633.00
     3         719.52       171.80         633.00
     4         719.52       163.21         633.00
     5         719.52       163.21          55.70
     6         719.52       155.05          55.70
     7        1008.05       315.71          55.70
     8        1008.05       299.92          55.70
     9        1391.71       299.92          94.22
    10        1391.71       284.93          94.22
    11        1190.21       163.21          94.22
    12        1190.21       155.05          94.22
    13         719.52       163.21         545.65
    14         719.52       155.05         545.65
    15        2014.61       155.05         639.87
    16        1614.10        70.84         639.87
    17        1571.94        70.84         671.52
    18         967.44        14.79         671.52
    20          76.67       299.92          23.97
    21         571.67       299.92          10.85
    22          76.67       299.92           6.10
    23        1340.00       299.92           2.40

                      METRIC UNITS
location     degrees K        KPA          kg/sec
     1         298.15       101.32         287.13
     2         298.10       101.27         287.13
     3         655.29      1184.81         287.13
     4         655.29      1125.57         287.13
     5         655.29      1125.57          25.27
     6         655.29      1069.29          25.27
     7         815.58      2177.29          25.27
     8         815.58      2068.43          25.27
     9        1028.73      2068.43          42.74
    10        1028.73      1965.01          42.74
    11         916.78      1125.57          42.74
    12         916.78      1069.29          42.74
    13         655.29      1125.57         247.51
    14         655.29      1069.29         247.51
    15        1374.78      1069.29         290.24
    16        1152.28       488.57         290.24
    17        1128.85       488.57         304.60
    18         793.02       102.00         304.60
    20         298.15      2068.43          10.87
    21         573.15      2068.43           4.92
    22         298.15      2068.43           2.77
    23        1000.00      2068.43           1.09
```

```
                WORK INPUT/OUTPUT (KW)
      Work of FIRST COMPRESSOR ---------->  106878.3
      Work of SECOND COMPRESSOR --------->    4392.2
      Work of FIRST TURBINE ------------->    7377.8
      Work of SECOND TURBINE ------------>  196842.9
TOTAL OUTPUT (including generator losses) -->   89232.2

                HIGHER HEATING VALUES
                 KJ/KG            BTU/SCF
  DRY BASIS     6734.40            185.53
  WET BASIS     6159.65            164.44

                LOWER HEATING VALUES
                 KJ/KG            BTU/SCF
  DRY BASIS     5928.52            163.33
  WET BASIS     5422.55            144.76

               HEAT RATES & EFFICIENCIES
                (HIGHER HEATING VALUES)
  COAL EFFICIENCY ----------> .3042
  COAL HEAT RATE -----------> 11217.9
  GAS EFFICIENCY -----------> .3389
  GAS HEAT RATE ------------> 10069.4
                (LOWER HEATING VALUES)
  COAL EFFICIENCY ----------> .3151
  COAL HEAT RATE -----------> 10833.1
  GAS EFFICIENCY -----------> .3850
  GAS HEAT RATE ------------>  8864.4

                    RELATIVE FLOWS
   LBM STEAM / LBM COAL ---->    .4527
  LBM STEAM&WATER / LBM COAL >   .7073
     LMB AIR / LBM COAL  --->  2.3244
  64.2324   STD FT^3 GAS OUT / LBM COAL
   .01258   LBM H2O / STD FT^3 GAS OUT
   .48931   STD FT^3 AIR / STD FT^3 GAS
```

Table 2.6 IGCC System Computer Model Sample Run

```
                    **********************
                    **   COMMAND MENU   **
                    **********************

   Please type the number or letter of the variable
 you wish to change and PRESS ENTER.
      ---------------------------------------------
                       (TOGGLE VALUES)
1)               Fuel used in power system
                           COALGAS
2)      Method of finding products leaving gasifier
                 THEORETICAL -> (EQUILIBRIUM)
      ---------------------------------------------
                       (INPUT VALUES)
3)  Temperature of air at inlet (Location 1)......  298.15 K
4)  Pressure of air at inlet (Location 1).........  101.32 KPA
5)  Mass flow rate of air at inlet (Location 1)...  287.13 KG/SEC
6)  Fraction of air used to cool blades...........   .050
7)  Efficiency of air compressors.................   .860
8)  Efficiency of gas turbines....................   .920
9)  Efficiency of combustor.......................   .950
A)  Efficiency of pipes...........................   .950
B)  Efficiency of generator and drive.............   .960
C)  Efficiency of gasifier........................   .960
D)  Pressure in gasifier.......................... 2068.43 KPA
E)  Fraction of air sent to gasifier..............   .085
F)                    COAL STATISTICS
                (Amounts in MASS FRACTIONS)
                   Carbon....   81.300
                  Hydrogen...    5.300
                   Oxygen....    9.800
                  Nitrogen...    1.700
                   Sulfur....    1.900
             Heating value of coal...  33725.0
         Percent WATER in coal as received...   .100
          Percent ASH in coal as received...   .100
G)  Amount of water added per mole of dry coal....   .500
H)  Amount of air added per mole of dry coal......   .215

J)             AUXILIARY TURBINE STATUS
              ---> AUXILIARY TURBINE <---

             ----->  INPUT SELECTION  <-----
```

```
              (ENTER -> 0 <- TO CONTINUE ONWARD)

             GASIFIER PRODUCTS
         CO2 ----------->   .3129231
         CO ------------>   .2153383
         H2 ------------>   .2888830
         CH4 ----------->   .1607398
         C2H6 ---------->   .0000127
         N2 ------------>   .8167270
         H2O ----------->   .1511596
         H2S ----------->   .0060322

              ENGLISH UNITS                    METRIC
UNITS

 POINT  DEGREES F     PSI       LBM/SEC  |  DEGREES K       KPA KG/SEC
   1      76.67      14.69      607.04   |    298.15 101.32     275.35
   2      76.58      14.68      607.04   |    298.10 101.27     275.35
   3     812.16     192.41      607.04   |    706.76 1326.98    275.35
   4     812.16     182.79      607.04   |    706.76 1260.63    275.35
   5     812.16     182.79       51.60   |    706.76 1260.63     23.41
   6     812.16     173.65       51.60   |    706.76 1197.60     23.41
   7    1067.99     315.71       51.60   |    848.88 2177.29     23.41
   8    1067.99     299.92       51.60   |    848.88 2068.43     23.41
   9    1311.50     299.92       87.28   |    984.17 2068.43     39.59
  10    1311.50     284.93       87.28   |    984.17 1965.01     39.59
  11    1160.88     182.79       87.28   |    900.49 1260.63     39.59
  12    1160.88     173.65       87.28   |    900.49 1197.60     39.59
  13     812.16     182.79      525.09   |    706.76 1260.63    238.18
  14     812.16     173.65      525.09   |    706.76 1197.60    238.18
  15    2037.61     173.65      612.37   |   1387.56 1197.60    277.77
  16    1615.06      76.40      612.37   |   1152.81 526.92     277.77
  17    1577.14      76.40      642.72   |   1131.75 526.92     291.54
  18     946.16      14.79      642.72   |    781.20 102.00     291.54
  19    1249.64      14.79      646.32   |    949.80 102.00     293.17
  20      76.67     299.92       22.20   |    298.15 2068.43     10.07
  21     571.67     299.92       10.05   |    573.15 2068.43      4.56
  22      76.67     299.92        5.65   |    298.15 2068.43      2.56
  23    1340.00     299.92        2.22   |   1000.00 2068.43      1.01
  24    1043.10      14.79      642.72   |    835.06 102.00     291.54
  25     423.05      14.79      642.72   |    490.58 102.00     291.54
  26     370.77      14.79      642.72   |    461.54 102.00     291.54
  27     114.13       1.45       98.67   |    318.96 10.00       44.76
  28     114.22      20.30      107.95   |    319.01 140.00      48.97
  29     228.43      20.30      120.85   |    382.46 140.00      54.82
```

```
30    233.08    910.02    111.50  |  385.04 6276.00    50.58
31    533.13    910.02    111.50  |  551.74 6276.00    50.58
32   1049.66    910.02    108.15  |  838.70 6276.00    49.06
33   1044.26    864.52    108.15  |  835.70 5962.20    49.06
34    810.61    314.94    108.15  |  705.90 2172.00    49.06
35    810.61    314.94     98.10  |  705.90 2172.00    44.50
36    678.89    166.26     98.10  |  632.72 1146.65    44.50
37    652.07    166.26    107.17  |  617.82 1146.65    48.61
38    231.18     21.37    107.17  |  383.99 147.37     48.61
39    228.43     20.30     12.90  |  382.46 140.00      5.85
40    231.18     21.37     94.27  |  383.99 147.37     42.76
41    114.13      1.45     94.27  |  318.96 10.00      42.76
42    114.13      1.45      9.28  |  318.96 10.00       4.21
43    114.13      1.45    107.95  |  318.96 10.00      48.97
44    229.24    175.01      9.35  |  382.91 1207.00     4.24
45    370.52    175.01      9.35  |  461.40 1207.00     4.24
46    370.52    175.01      9.07  |  461.40 1207.00     4.11
47    366.37    166.26      9.07  |  459.09 1146.65     4.11
48    533.13    910.02      3.34  |  551.74 6276.00     1.52
49    370.52    175.01       .28  |  461.40 1207.00      .13
50     76.67     14.69      4.12  |  298.15 101.32      1.87
51   1249.64     14.79       .51  |  949.80 102.00       .23

                 TURBINE PRODUCTS
          N2    --------->  8.85554941
          O2    --------->  1.54963079
          CO2   --------->   .68902643
          CO    --------->   .00000000
          H2O   --------->   .76759235
          H2    --------->   .00000000
          CH4   --------->   .00000000
          C2H6  --------->   .00000000
          SO2   --------->   .00603224
          H2S   --------->   .00000000
          OH    --------->   .00000000
          NO    --------->   .00000000

               WORK INPUT/OUTPUT (KW)

WORK FROM MAIN GAS TURBINE (GE MS7001 HEAVY DUTY)
  Work of FIRST COMPRESSOR ---------> -117956.9
  Work of SECOND COMPRESSOR -------->   -3621.5
  Work of FIRST TURBINE ------------>    5065.8
  Work of SECOND TURBINE (optional)->  196727.5
```

```
 TOTAL OUTPUT OF GAS TURBINE (GE MS7001)-->   77006.3
Net Work of RECOVERY TURBINES ------->   49874.5
  ******* TOTAL OUTPUT OF SYSTEM ******* ->  126880.8

              HIGHER HEATING VALUES
                KJ/KG           BTU/SCF
DRY BASIS     6442.68            183.34
WET BASIS     6082.97            169.14

              LOWER HEATING VALUES
                KJ/KG           BTU/SCF
DRY BASIS     5709.15            162.46
WET BASIS     5390.40            149.88

             HEAT RATES & EFFICIENCIES

             GAS TURBINE EFFICIENCIES
              (HIGHER HEATING VALUES)
COAL EFFICIENCY ----------> .2835
COAL HEAT RATE -----------> 12040.9
GAS EFFICIENCY -----------> .3198
GAS HEAT RATE ------------> 10673.5
               (LOWER HEATING VALUES)
COAL EFFICIENCY ----------> .2935
COAL HEAT RATE -----------> 11627.8
GAS EFFICIENCY -----------> .3608
GAS HEAT RATE ------------>  9458.3


             COMBINED CYCLE EFFICIENCY
              (HIGHER HEATING VALUES)
COAL EFFICIENCY ----------> .3978
COAL HEAT RATE ----------->  8578.7
               (LOWER HEATING VALUES)
COAL EFFICIENCY ----------> .4120
COAL HEAT RATE ----------->  8284.4

                  RELATIVE FLOWS
  LBM STEAM / LBM COAL ---->   .4527
LBM STEAM&WATER / LBM COAL >   .7073
    LMB AIR / LBM COAL  ---> 2.3244
60.1027   STD FT^3 GAS OUT / LBM COAL
 .01178   LBM H2O / STD FT^3 GAS OUT
 .52293   STD FT^3 AIR / STD FT^3 GAS
```

2.7 Parametric Analysis

There are several parameters in the model (such as the compressor and turbine small stage efficiencies) for which exact numerical values are unavailable. Also, some parameters such as the percent moisture in the coal change on a day to day basis. Therefore, parametric analysis were performed to determine the effects of changes in several of the design variables on the overall system performance. Gas turbine stage efficiency, booster compressor stage efficiency, gasifier pressure, percent moisture in coal, and percent ash in coal were varied over a reasonable range. The results of the parametric analyses are discussed below with the following coal as input:

Table 2.7

```
          COAL STATISTICS
     (Amounts in MASS FRACTIONS)
        Carbon....   81.300
       Hydrogen...    5.300
        Oxygen....    9.800
       Nitrogen...    1.700
        Sulfur....    1.900
  Heating value of coal...  33725.0
```

2.7.1 Turbine Isentropic Efficiency

The small stage efficiency of the gas turbine was found to have a considerable effect on the exhaust temperatures and the turbine output power. Although this parameter is somewhat given for an existing turbine, it is easy to see how a high efficiency turbine is of the utmost importance. Figure 2.2 illustrates how the temperatures at locations 16, 17, and 18 are changed over a range of turbine efficiency. As the efficiency of the gas turbine increases, all three of these temperatures decrease. This is due to the fact that more energy is converted into usable work. Figure 2.3 shows how the turbine output sharply increases as the turbine efficiency increases. Although a certain amount of work can be regained at later steam turbine sections of the IGCC plant, the net affect of a decrease in turbine efficiency is still a loss in the overall power plant efficiency.

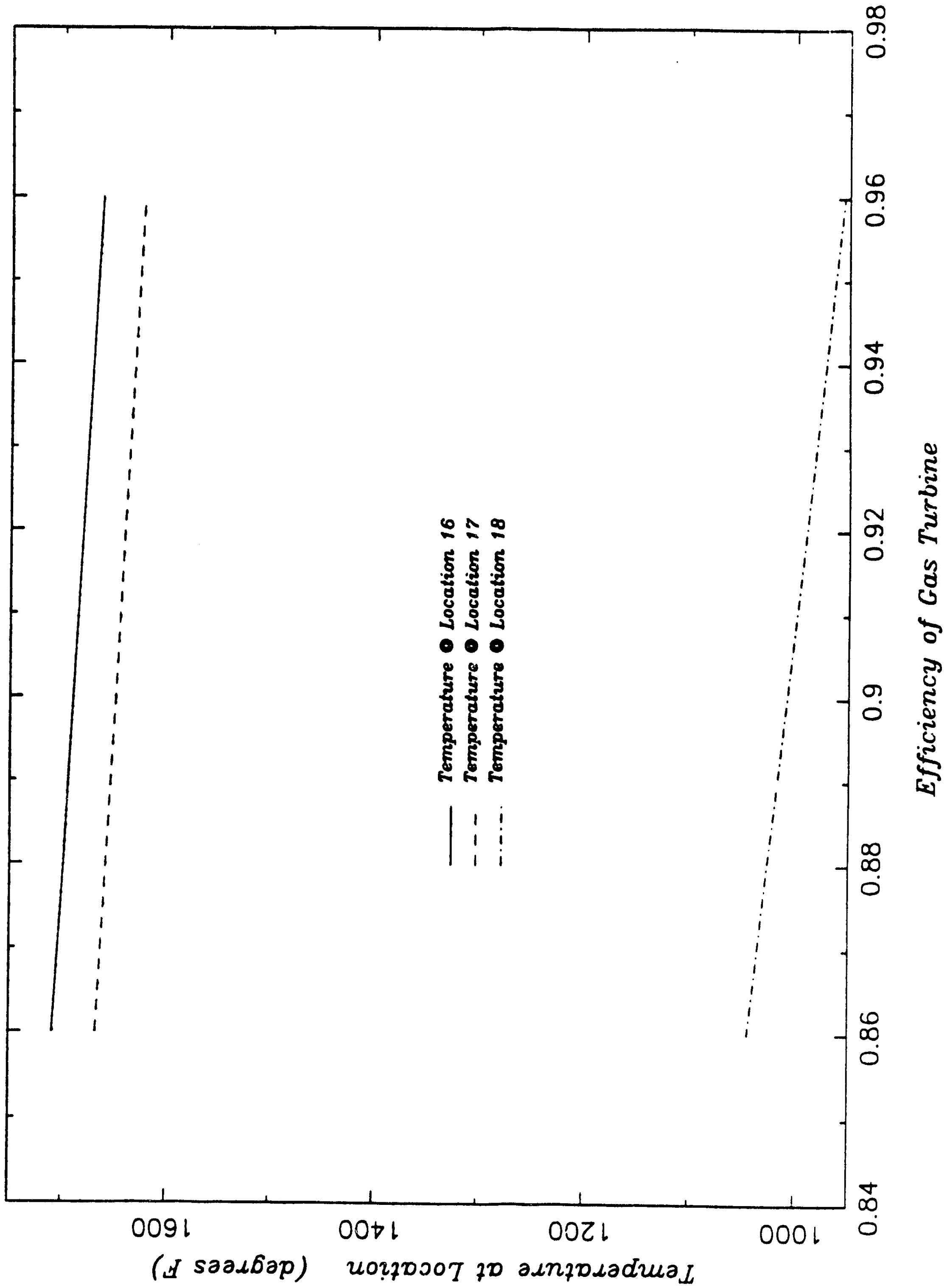


Figure 2.2 Temperature verses Efficiency of Gas Turbine

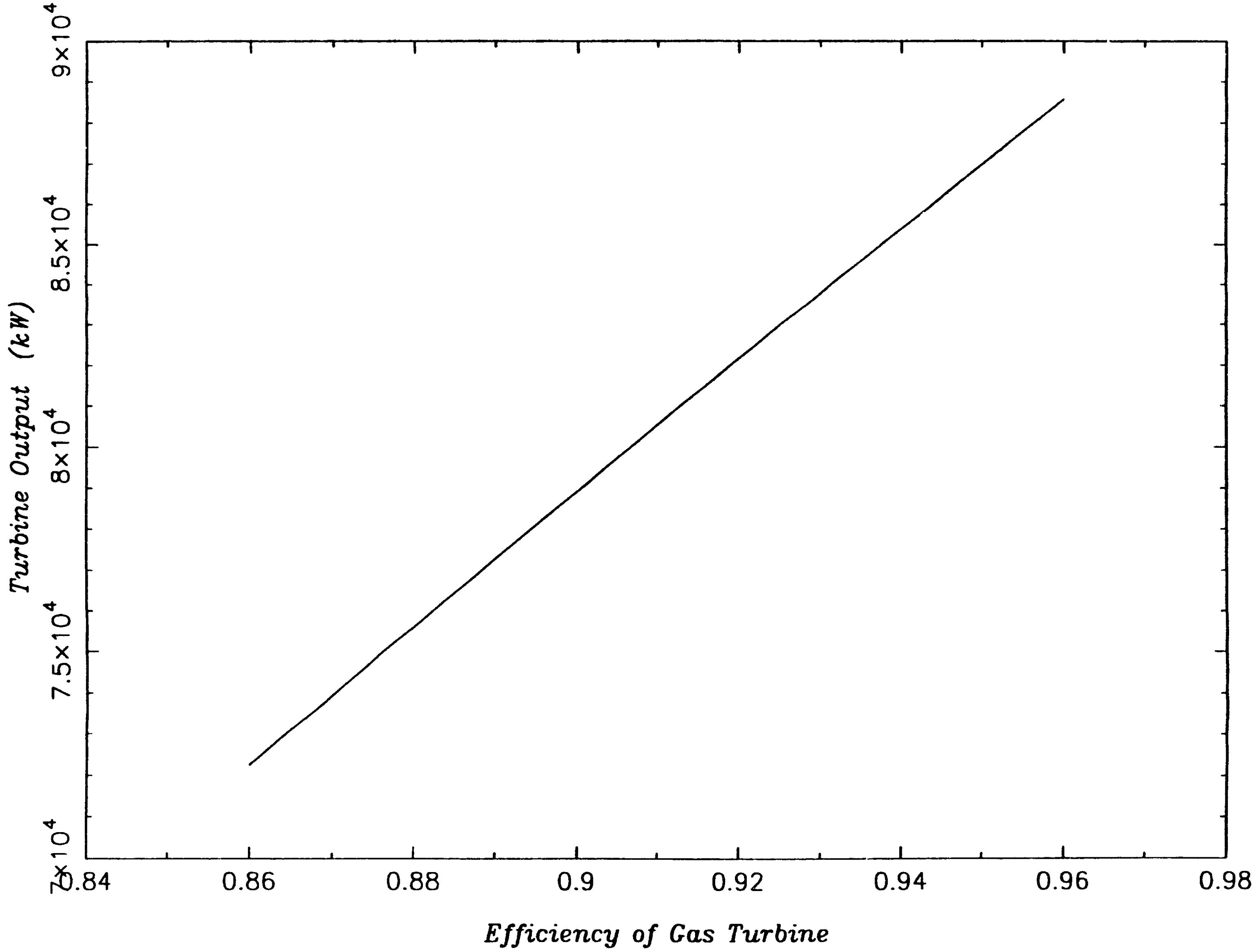


Figure 2.3 Turbine Output verses Efficiency of Gas Turbine

2.7.2 Booster Compressor Isentropic Efficiency

A change in the efficiency of the booster compressor altered the temperature after the compressor, which also changed the gasifier outlet temperature. Figure 2.4 illustrates the effect of these two temperatures as the efficiency of the compressor increases. However, Figure 2.5 shows that the turbine output is only slightly changed over a wide range of booster compressor efficiency.

2.7.3 Pressure in Gasifier

The pressure within the gasifier was found to greatly influence the temperatures before and after the gasifier as well as turbine output. Figure 2.6 illustrates the temperature changes around the gasifier. The temperature before the gasifier becomes higher at higher gasifier pressures as a result of the work input at the booster compressor. Consequently, the product gas temperature also increases in as the pressure in the gasifier is increased. Figure 2.7 shows that the turbine output slightly increases as the gasifier pressure increases.

2.7.4 Percent Water in Inlet Coal

The percent water in the inlet coal greatly affected gasifier temperatures, needed inlet coal mass flow rates, and of course turbine output work. Figure 2.8 shows how the gasifier exit temperature drops with an increase in percent water in the coal. In fact, Figure 2.9 shows that the temperature had even dropped although the coal mass flow rate had increased. Figure 2.10 illustrates how the turbine output decreases with an increase in the amount of moisture in the coal.

2.7.5 Percent Ash in Inlet Coal

The percent ash in the coal was found to have effects similar to the percent water in the coal. Figure 2.11 illustrates how the gasifier exit temperature slightly decreases as the

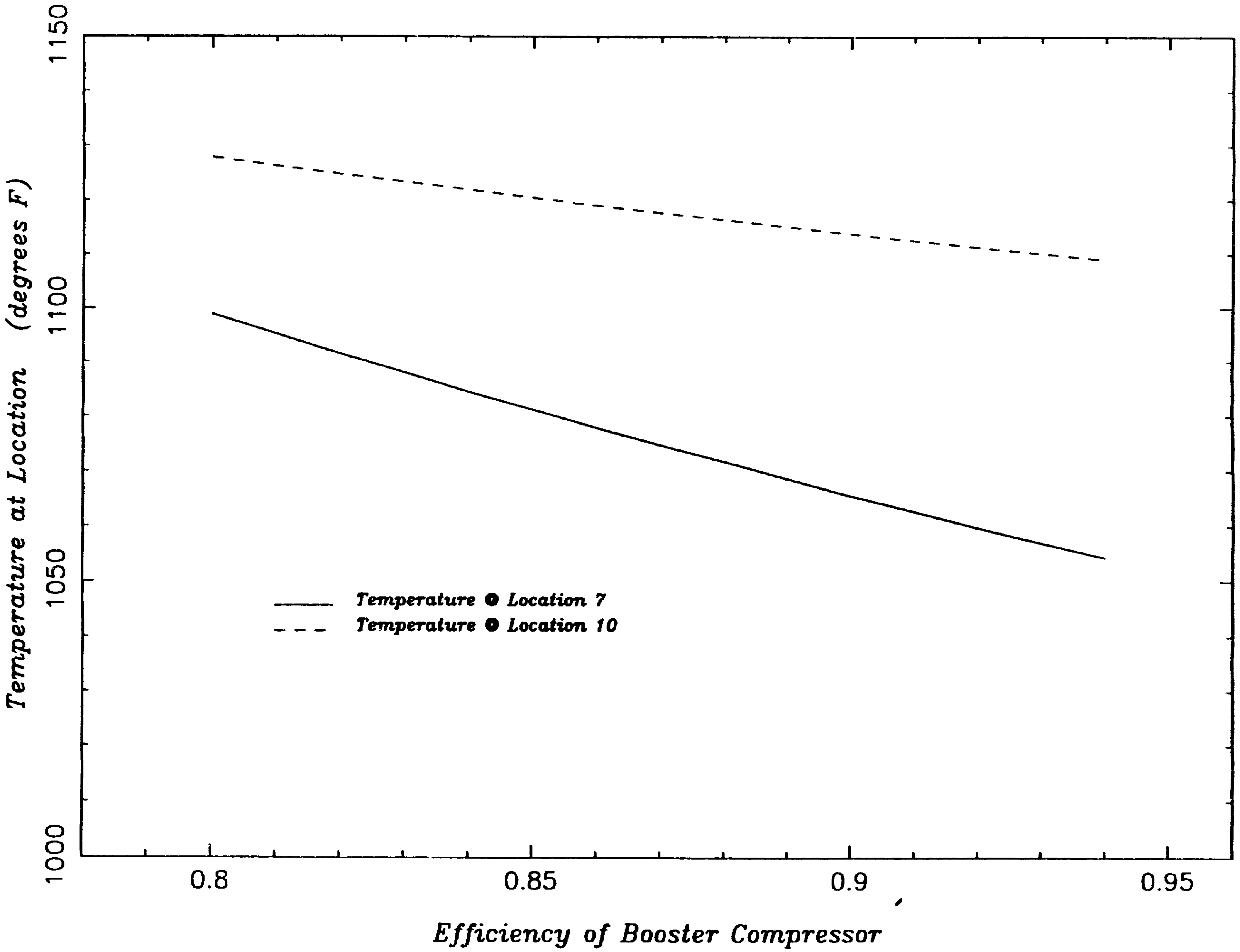


Figure 2.4 Temperature verses Efficiency of Booster Compressor

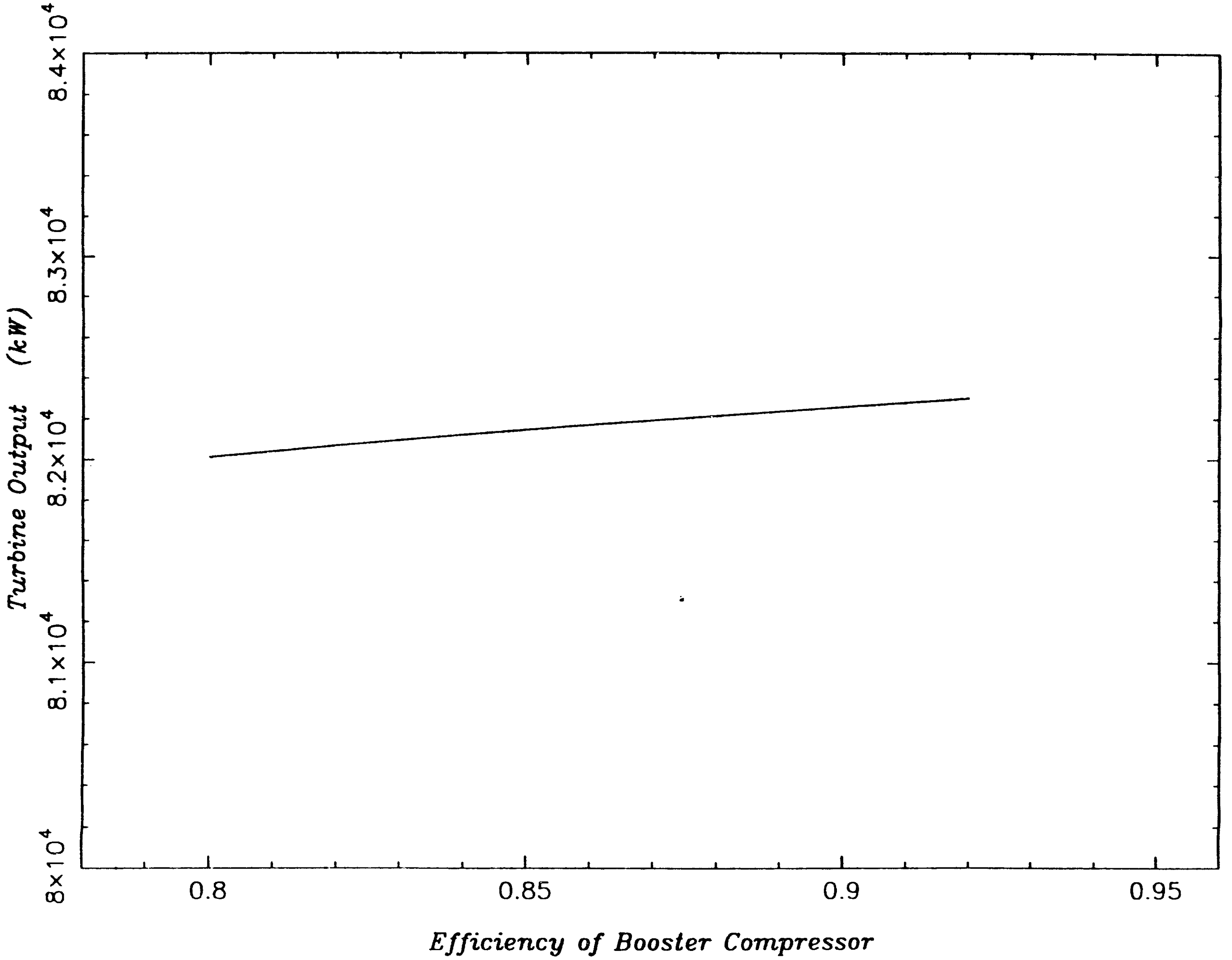


Figure 2.5 Turbine Output verses Efficiency of Booster Compressor

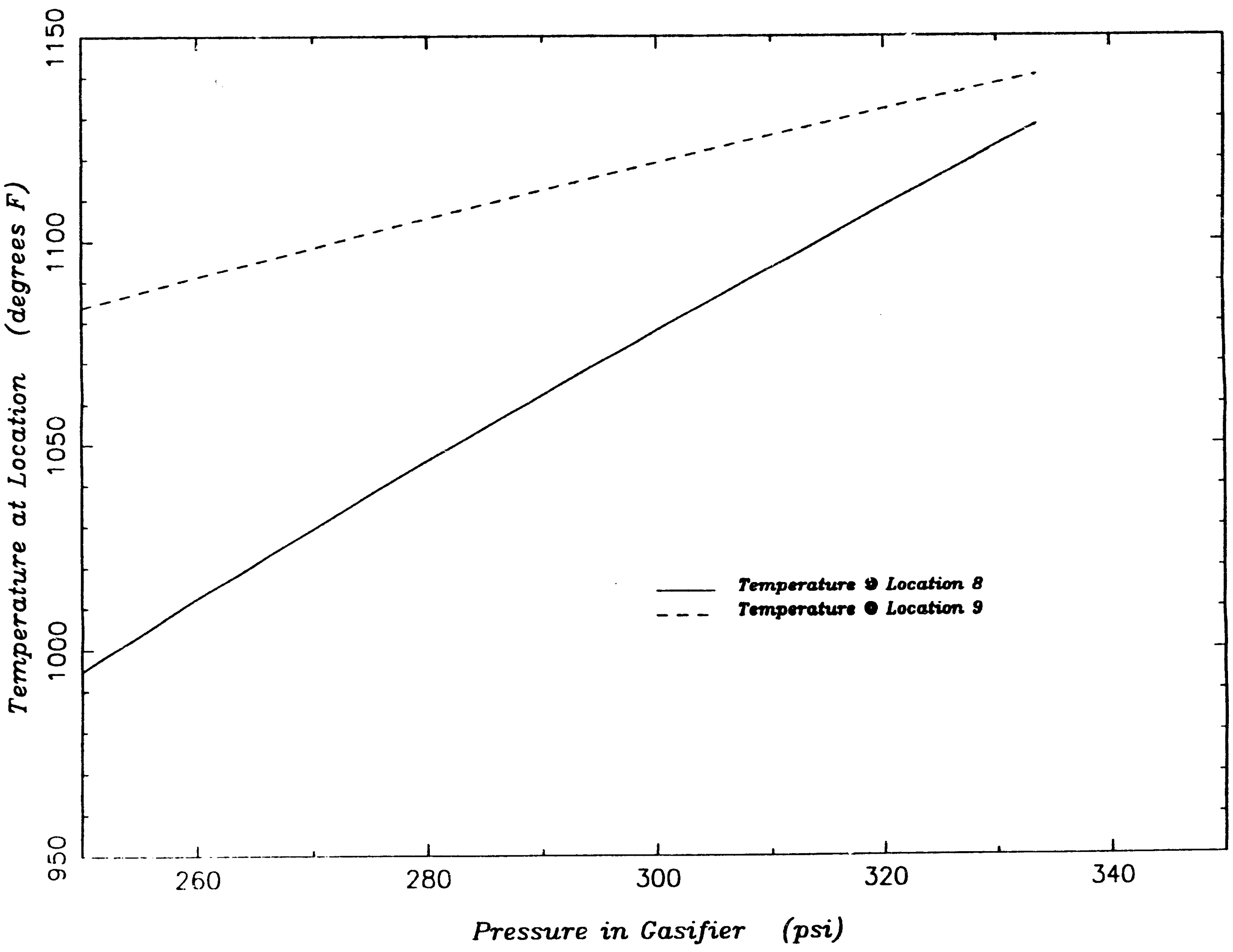


Figure 2.6 Temperature verses Pressure in Gasifier

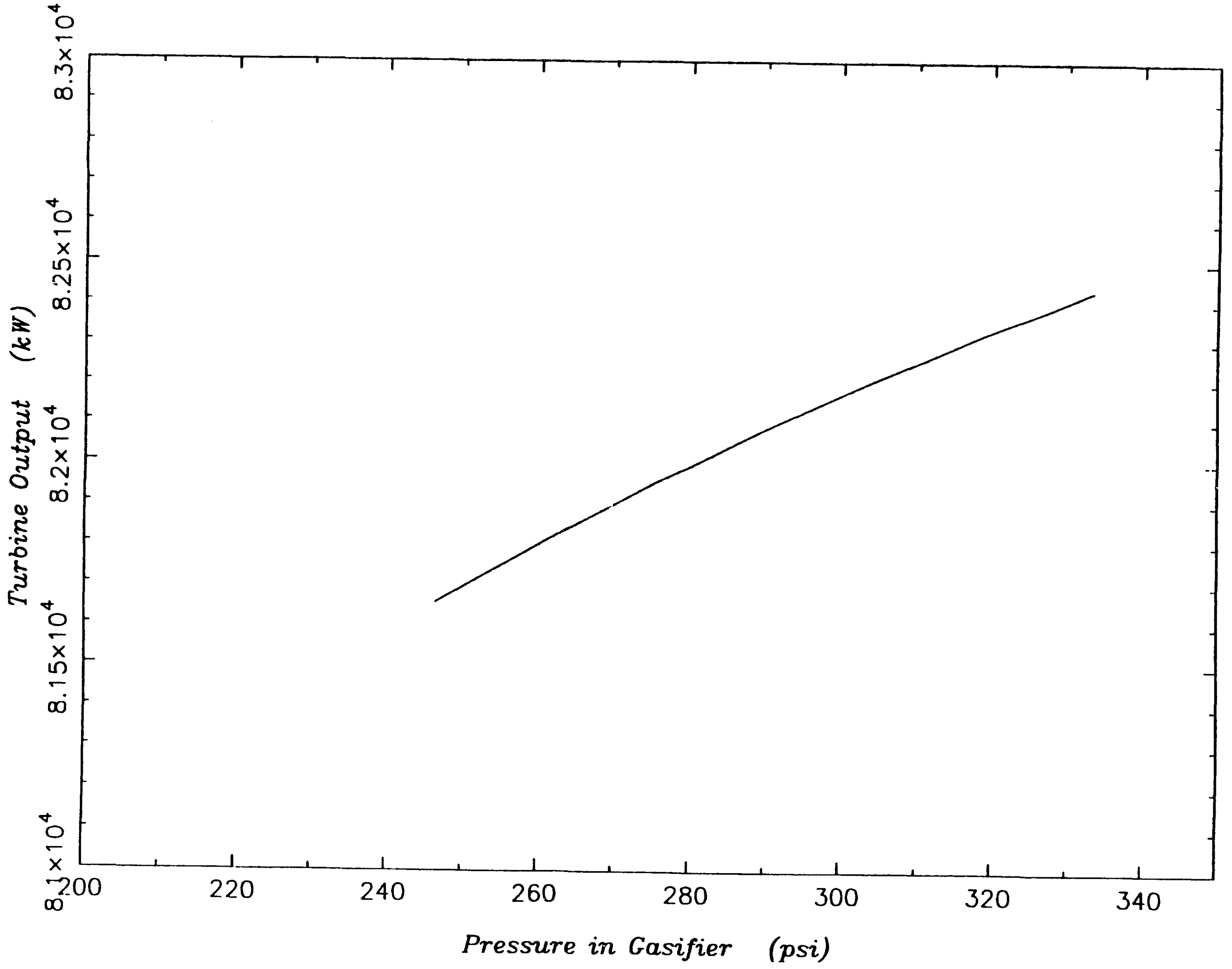


Figure 2.7 Turbine Output verses Pressure in Gasifier

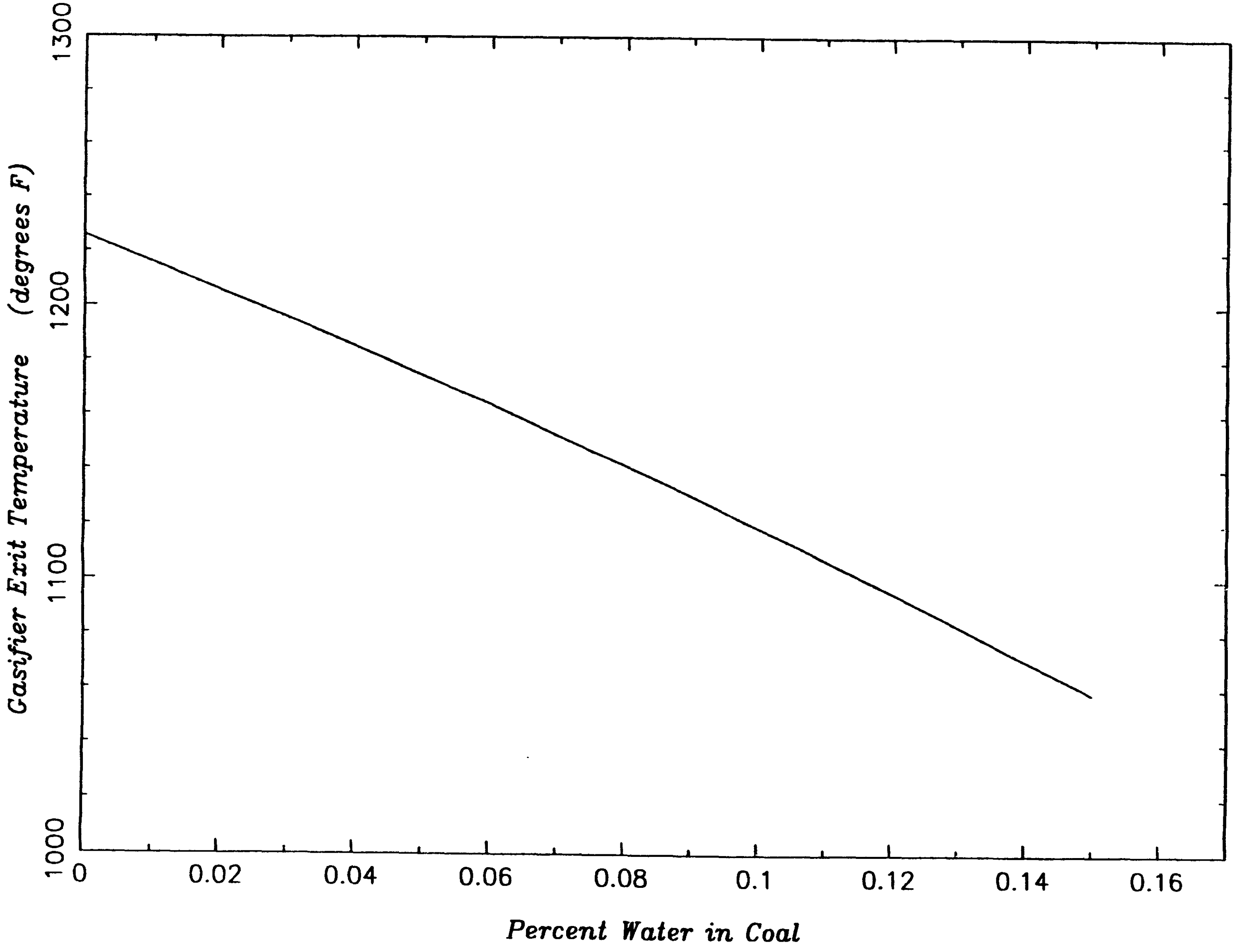


Figure 2.8 Gasifier Exit Temperature verses Percent Water in Coal

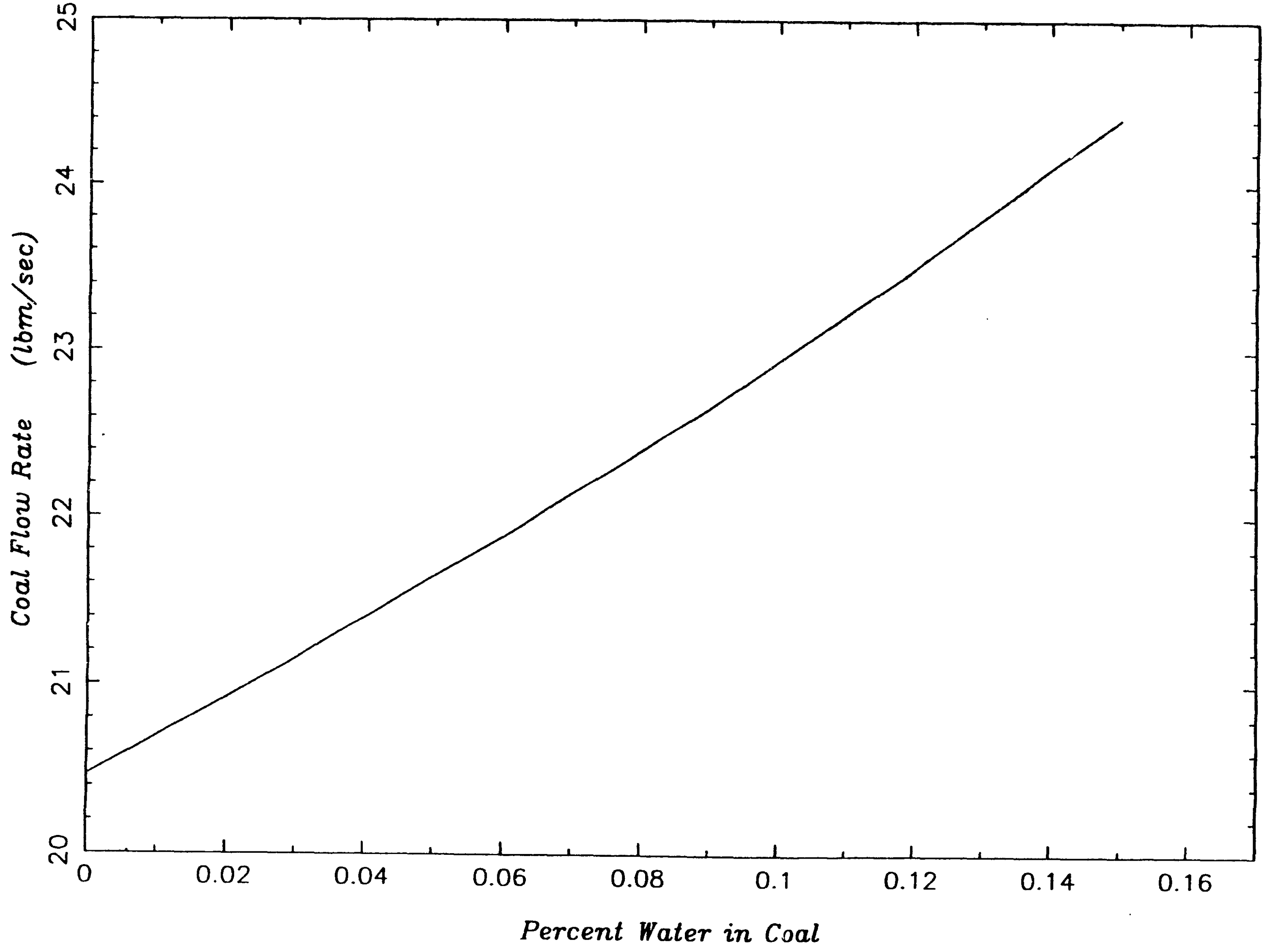


Figure 2.9 Coal Flow Rate verses Percent Water in Coal

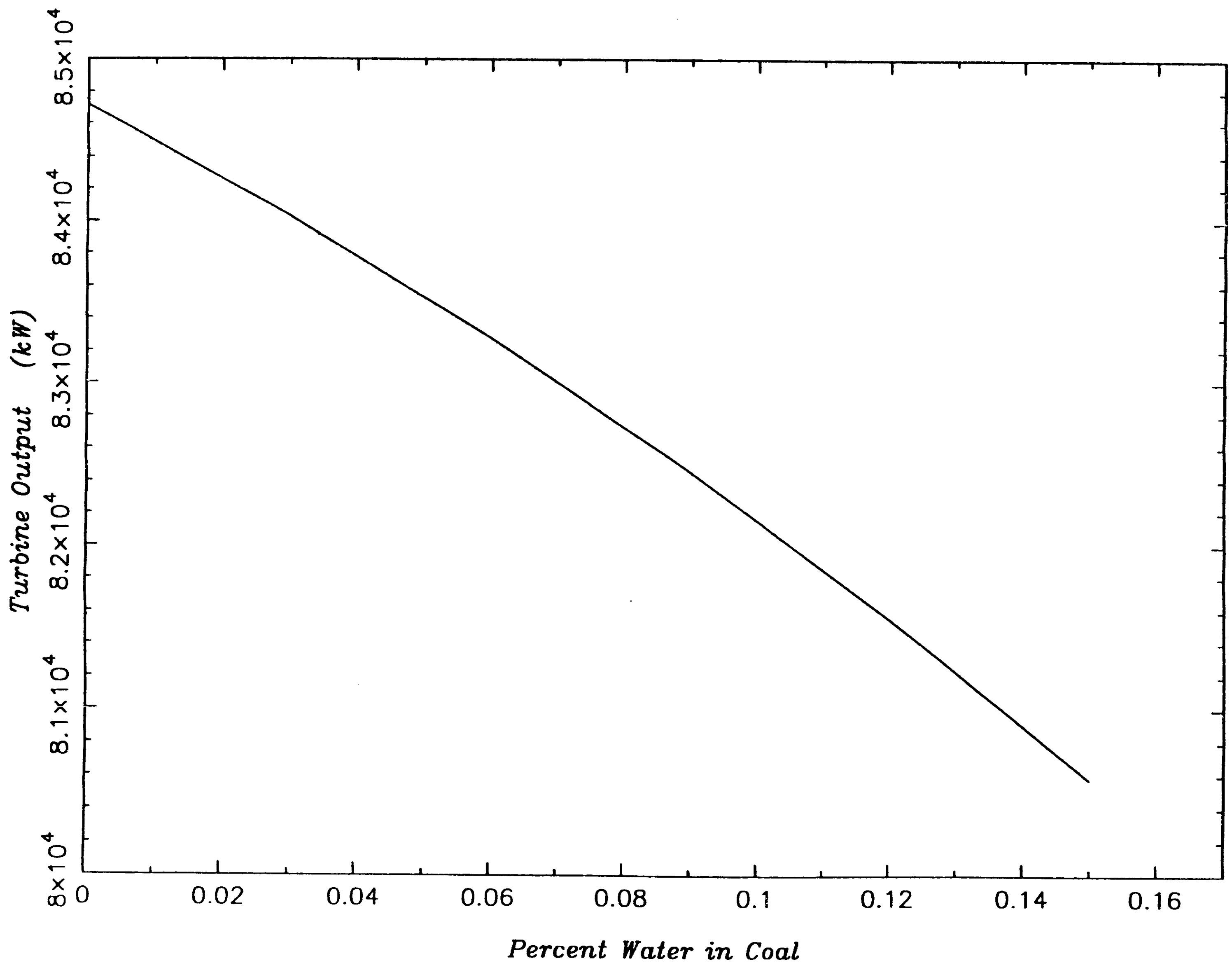


Figure 2.10 Turbine Output verses Percent Water in Coal

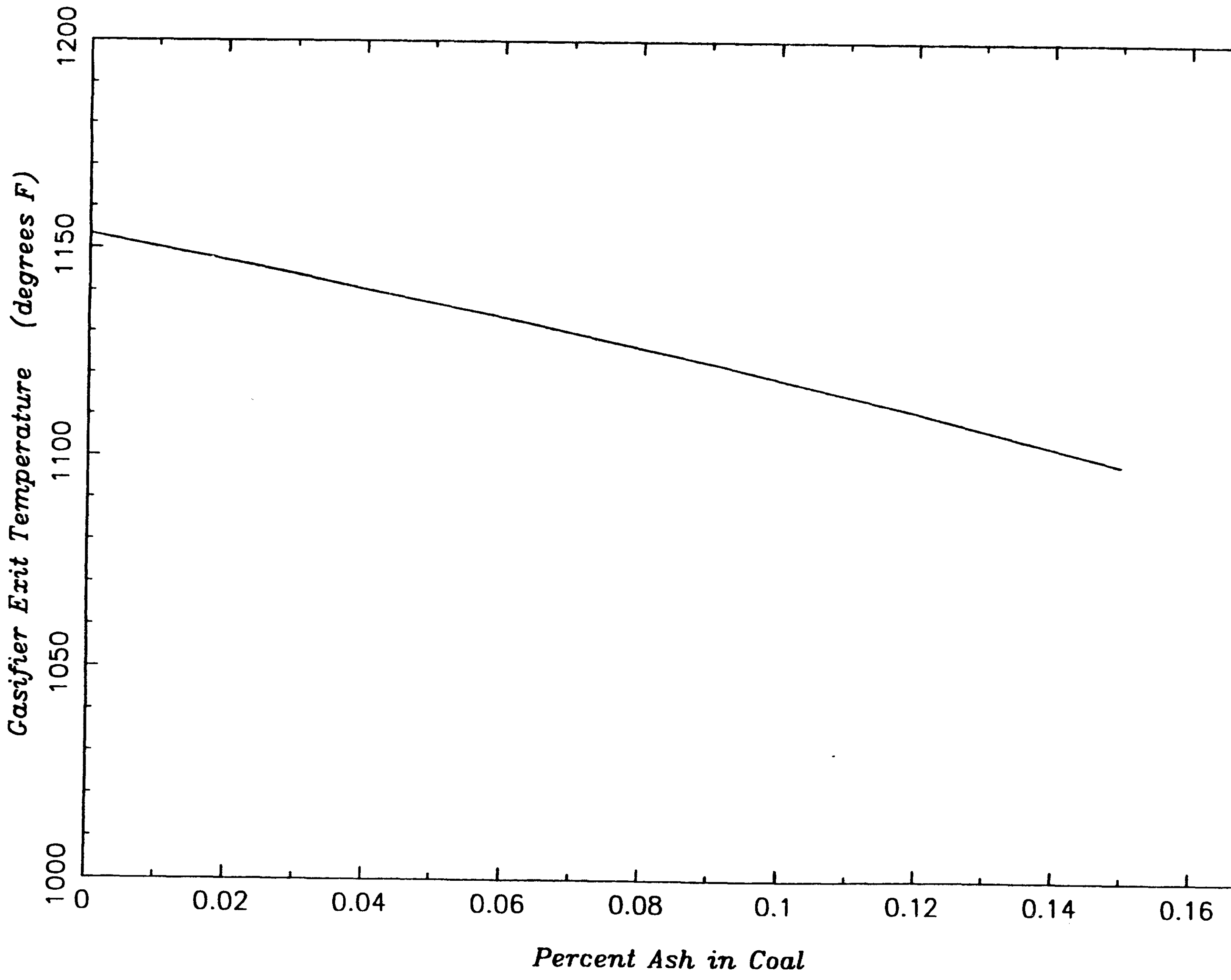


Figure 2.11 Gasifier Exit Temperature verses Percent Ash in Inlet Coal

percent ash is increased. Energy was lost in this system when the hot ash left without contributing in a positive way. Figure 2.12 illustrates the increase in the feed of the coal. Because the computer model was designed to work with a certain prescribed turbine output, more coal was needed when there were large losses due to the percent water or percent ash in the coal. Figure 2.13 shows how the ash flow rate increases as the percent ash in the coal becomes larger. It should not be a surprise to find that this relation is almost linear. Even though more coal was added to the system when the percent ash increased, there still existed turbine output losses. Figure 2.14 illustrates how the turbine output decreases as the percent ash in the coal increases.

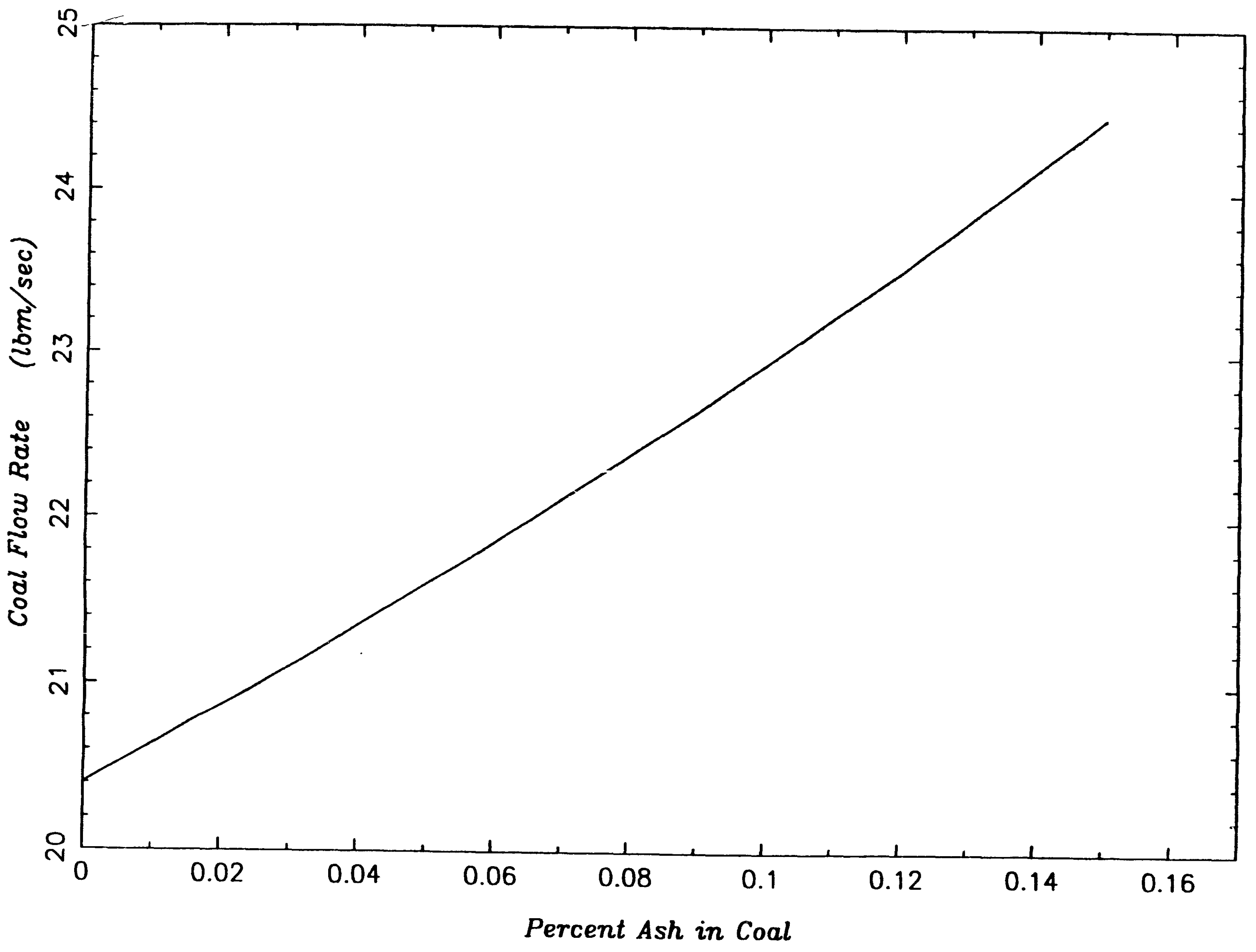


Figure 2.12 Coal Flow Rate verses Percent Ash in Coal

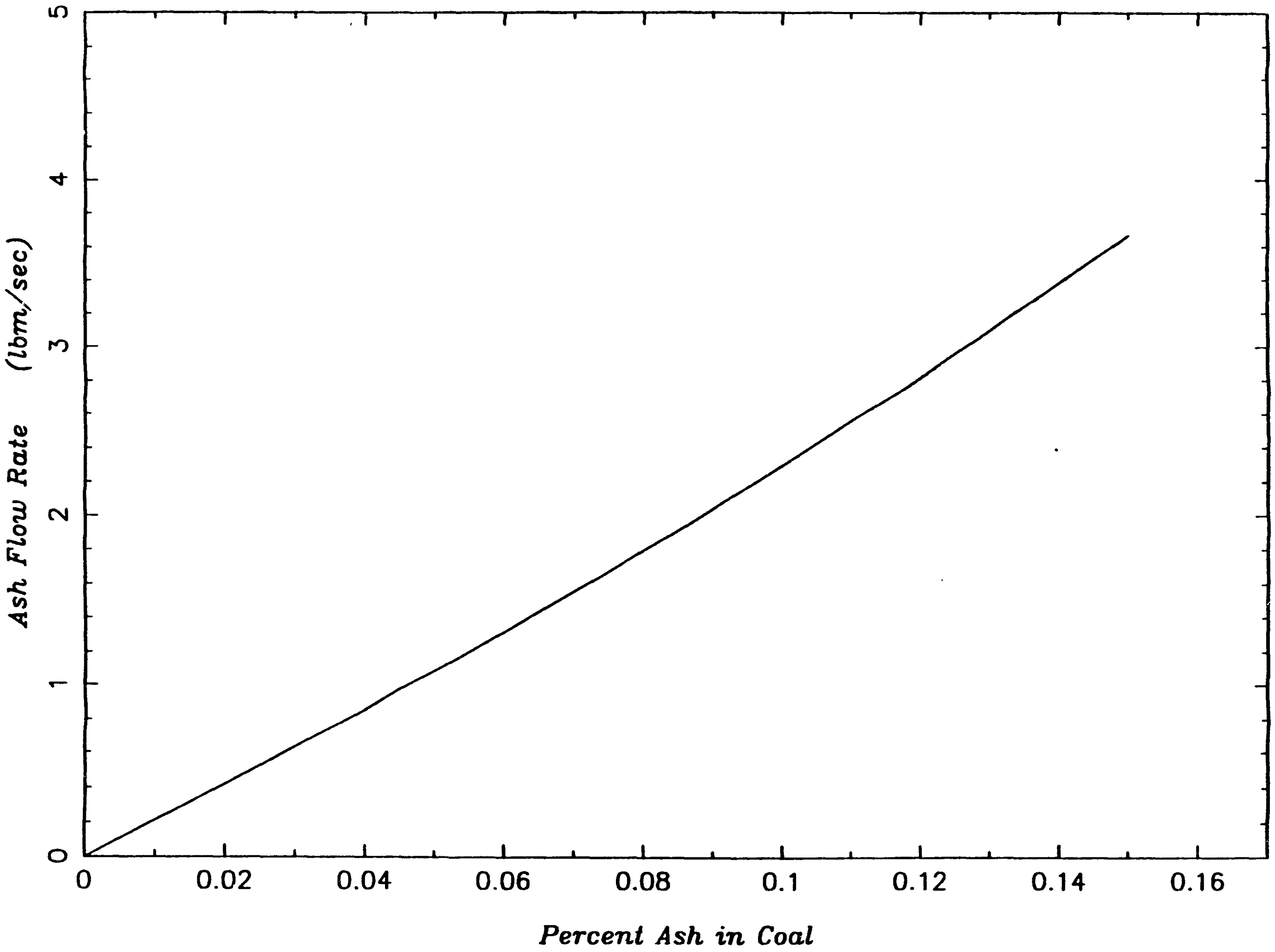


Figure 2.13 Ash Flow Rate verses Percent Ash in Coal

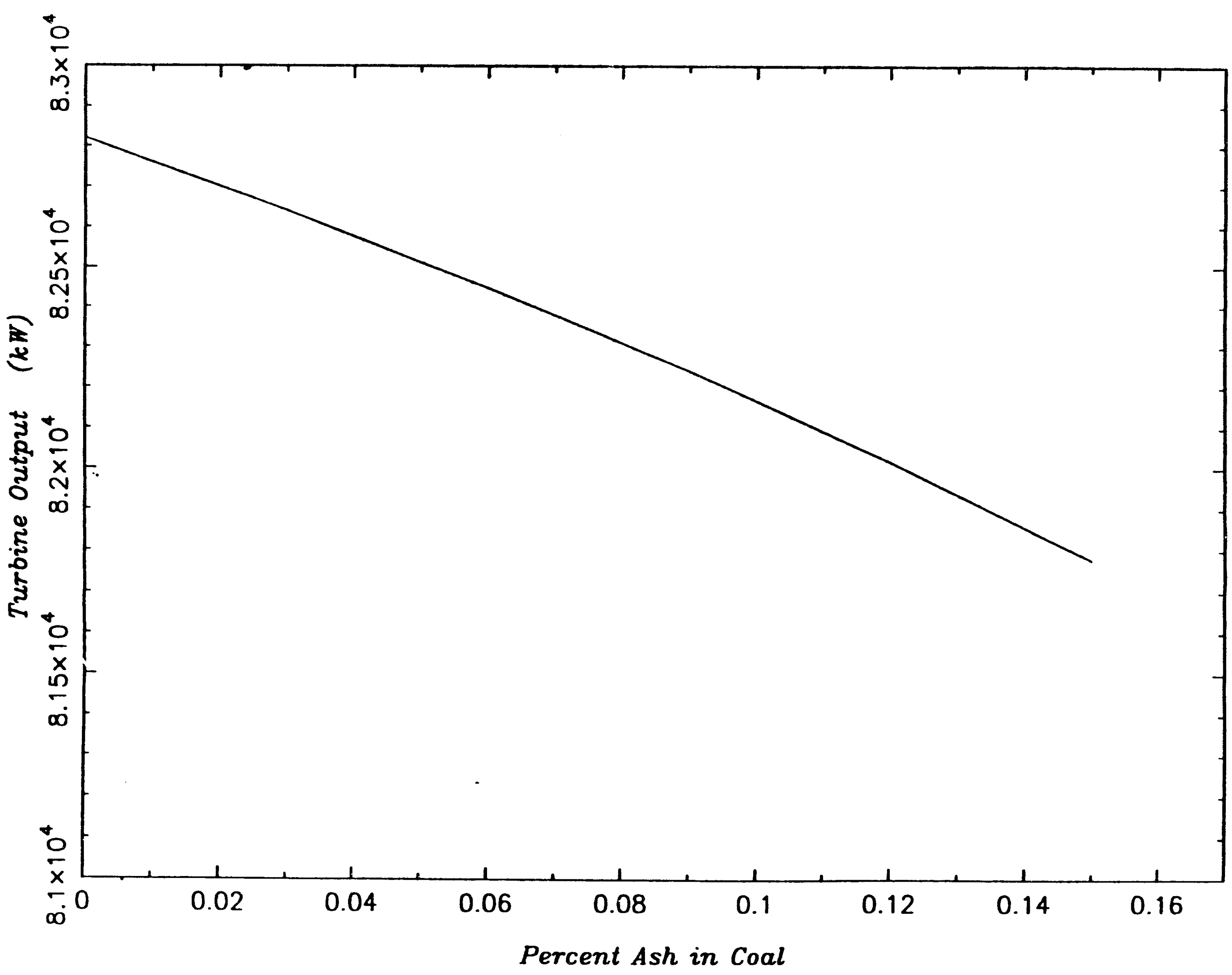


Figure 2.14 Turbine Output verses Percent Ash in Coal

3. FIXED BED COAL GASIFIER COMPUTER MODEL

A computer code, known as the Wen II model developed by Wen, Chen, and Onozaki [3] has been modified and applied to predict the performance of fixed bed gasifiers for the Standardized Air Blown Coal Gasifier/Gas Turbine Concept study. A copy of the source code was provided by the Morgantown Energy Technology Center (METC). Engineers at METC cautioned that the code employs several approximations that affect accuracy. A METC report [4] documents work done to evaluate the limitations of the model, and improved computer models of fixed bed gasifiers are now being developed under METC sponsorship. However, METC believes that the Wen II model is probably the best that is currently available.

Following a briefing at METC on limitations of the Wen II model, we studied the source code in detail, and ran several test cases to determine how model predictions compare to measurements. A decision was made to modify the Wen II code as described below before we made additional computer runs to predict gasifier performance.

1) The program would be modified to correct unrealistic calculations of quantities of tar and gas produced in the devolatilization of coal. The Wen II model contains equations for pulverized coal with particle diameters less than 0.01 centimeters. It predicts unrealistic results (such as negative mass flux) when applied at conditions needed for the present work. A decision was make to remove approximations in the model made to simplify mathematics, and to include effects such as temperature gradients within the solid that become important when the particle diameter is greater than 0.01 centimeters. The program would also be modified to account for energy needed to dry moisture from the coal prior to devolatilization.

2) The Wen II program would be modified so that it computes separate temperatures for the solid and gaseous phases. The model assumes that the solid and gas are at the same temperature. This permits a considerable simplification in mathematics. However, several investigations have expressed concern that this assumption may lead to serious errors in calculations for fixed bed gasifiers. Although it is expected that the temperatures of the solid and gas will be nearly the same at most locations in the gasifier, small difference may be important because reaction rates are very sensitive to temperature. The temperature differences may be significant in fixed bed gasifiers because the coal particles are relatively large. The consequences of the assumption have not been previously investigated. Therefore a decision was made to program separate energy equations for the solid and gaseous phases into the Wen II model so that differences in the temperatures of the two phases could be taken into account.

The modifications to the Wen II program were made so as to minimize the effects on the program structure. This was done so that a person who is familiar with the program would be able to recognize immediately where changes have been made, and could easily check to see whether the changes have been programmed correctly. When programming new equations, we used the same nomenclature that is in the original program, and tried to introduce as few new terms as possible. When describing the program modifications below we shall begin by describing the way that calculations were made in the original program, and shall then describe how the program has been modified. We discovered a few errors in the original program which we shall also discuss below when describing the program modifications.

3.1 GAS AND SOLID PHASE TEMPERATURE CALCULATIONS

3.1.1 Method Before Modifications

The Wen II program assumes that the gas and solid are at the same temperature. This common temperature is calculated by solving the following steady state energy equation:

$$\left[(\dot{m}c_p)_{gas} + (\dot{m}c_p)_{solid}\right] \frac{dT}{dz} = A\sum_{i=1}^{6} H_i R_i + h\pi D(T_w - T) \qquad (3.1)$$

The equation states that the increase in sensible energy in the gas and solid comes from energy released in chemical reactions and heat gain from the walls of the gasifier. H_i is the heat of reaction "i" in (cal/mole), R_i is the rate of the reaction per unit volume (moles/sec/cm^3), A is the cross sectional area of the gasifier (cm^2), and D is the diameter of the gasifier (cm).

We believe, however, that there is an error in the way that Eqn. 3.1 was programmed in the Wen II model. The error involves the sign of $(\dot{m}c_p)_{solid}$. The sign should be positive as it is in Eqn. 3.1 when the flow of the solid and gas is parallel. In this case (dT/dz) would be zero when there are no chemical reactions and no heat transfer from the wall. However, the sign of $(\dot{m}c_p)_{solid}$ should be negative when the solid and gas are in counterflow as they are in a fixed bed gasifier.

$$\left[(\dot{m}c_p)_{gas} - (\dot{m}c_p)_{solid}\right] \frac{dT}{dz} = A\sum_{i=1}^{6} H_i R_i + h\pi D(T_w - T) \tag{3.2}$$

With counterflow, (dT/dz) does not have to be zero when the right hand side of the equation vanishes. The gas and solid can change temperatures by transferring heat to each other. Also, the heat of reaction causes the gas temperatures to increase as the gas flows upwards, and the solid temperature to increase as the solid flow downwards. This sign error has probably not been detected earlier because $(\dot{m}c_p)_{solid}$ is small in comparison to $(\dot{m}c_p)_{gas}$. However, the term is not negligible. The sign error would affect the gas exit temperature and other calculated performance parameters, such as carbon conversion, which depend on temperature.

3.1.2 METHOD AFTER MODIFICATIONS

This section will address the modifications to the program concerning gas and solid phase temperature calculations. In addition, a small change was made to incorporate the devolatilization time of the coal. Wen II assumes that the devolatilization time is negligible in comparison to the gasification time. This assumption is true for very small coal particles (.01 cm), but for larger particles (2 to 5 cm), the devolatilization time is not negligible.

We have deleted the single energy equation and now solve two energy equations to determine the individual temperatures of the solid and gas. The energy equations that are solved in the modified version of the Wen II program are:

$$
\begin{aligned}
(\dot{m}c_p)_{gas}\frac{dT_g}{dz} &= f \cdot A\left(\sum R_iH_i + R_{coal}c_{p,s}(T_s - T_g)\right) \\
&+h\pi D(T_w - T_g) + h_cA\frac{6}{D_p}(1-\epsilon)(T_s - T_g)
\end{aligned}
\tag{3.3}
$$

$$
\begin{aligned}
&(\dot{m}c_p)_{solid}\frac{dT_s}{dz} = \\
&-(1-f)A\left(\sum R_iH_i + R_{coal}c_{p,s}(T_s - T_g)\right) + h_cA\frac{6}{D_p}(1-\epsilon)(T_s - T_g)
\end{aligned}
\tag{3.4}
$$

where f is the fraction of the energy released in chemical reactions that goes directly into the gas phase, $(6 \div D_p)(1-\epsilon)$ is the surface area of the solid phase per unit volume, and hc is the heat transfer coefficient between the gas and solid. The heat transfer coefficient should account for the thermal resistance of the ash layer that separates the gas and the reacting solid.

The actual value of f is unknown. It is probable that f is nearly unity since most of the reactions occur at the surface of the solid or in the gas phase. However, the effects of the ash layer, and of reactions that occur within the pores of the solid will cause f to be less than one. Parametric analysis indicate that the computed temperatures are not strongly dependent on the value of f.

In the revised program, rates for all reactions that invloved the char are computed at the average temperature of the solid and gas. Gas phase reactions rates are computed at the gas temperatures.

An iterative procedure is used to solve Eqn.'s 3.3 and 3.4. The iterative solution is necessary because the gas inlet temperatures is prescribed at the bottom of the gasifier while the solid temperatures is prescribed at the top. Equation 3.3 is solved first to obtain preliminary gas temperatures by integrating upwards though the gasifier and assuming that the solid temperature is the same as the gas temperature. Equation 3.4 is then solved to obtain preliminary solid temperatures by integrating downwards from the top of the gasifier. Equation 3.3 is then solved a second time to obtain corrected gas temperatures. In the second solution of Eqn. 3.3, heat transfer between the gas and solid is computed based on the corrected gas temperature and the preliminary solid temperature. The solid temperature is then corrected by solving Eqn. 3.4. The procedure is repeated until the updated temperatures agree with the temperature from the previous iteration.

Our experience indicates that convergence always occurs within a few iterations. We initially tried an iteration procedure that was very unstable. The unstable solution technique was one in which we attempted to guess the solid outlet temperature so that Eqn.'s 3.3 and 3.4 could be solved simultaneously. We anticipated that we could correct the assumed value of the solid outlet temperature until the computed solid temperature at the top of the gasifier matched the known solid inlet temperature. However the solution proved to be extremely sensitive to the assumed value of the solid outlet temperature. Underflows and overflows of exponents occurred for very reasonable trial values.

The heat transfer coefficient is computed using a correlation from the literature [8] for flow in packed beds.

$$h_c = 2.06 \cdot \frac{k}{D_p} Re^{.425} Pr^{.333} \tag{3.5}$$

This correlation does not account for the thermal resistance of the ash layer. By using a shape factor for conduction through a spherical shell [9], the heat transfer coefficient can be modified to compensate for the ash layer. The conduction heat transfer coefficent for the ash layer is given by:

$$h_{ash} = \frac{2 \cdot k_{ash}}{D_p} \left(\frac{\frac{r_i}{r_o}}{1 - \frac{r_i}{r_o}} \right) \tag{3.6}$$

where:

k_{ash} ≡ Conduction Heat transfer coefficient for the ash layer.
D_p ≡ Diameter of the coal particle.
r_i ≡ Radius of the coal particle.
r_o ≡ Radius of the coal particle plus the ash layer

The overall heat transfer coefficient is given by:

$$h_{overall} = \frac{1}{\frac{1}{h_c} + \frac{1}{h_{ash}}} \tag{3.7}$$

Since the surface area of the solid is very large, the calculated values of the solid and gas temperatures are nearly equal throughout most of the gasifier. Near the top, the gas temperature is greater than the solid temperature. Near the bottom of the gasifier, the solid temperature is greater that the gas temperature.

3.1.3 Programming the Changes

The solution to the energy equation for the gas phase is obtained by employing a numerical non-linear differential equation solver as in the original Wen II model. However, a semi analytical method was used to solve the solid phase energy equation. The numerical differential equation solver would have required small step sizes for this equation because $(\dot{m}c_p)_{solid}$ is small. The solids energy equation, Eqn. 3.4, is rewritten in the following form.

$$\frac{dT_s}{dx} + \frac{h_c A}{(\dot{m}c_p)_s} T_s = \frac{h_c A}{(\dot{m}c_p)_s} T_g + \frac{1-f}{(\dot{m}c_p)_s} A \sum_i H_{R,i} \tag{3.8}$$

The solution to this non homogeneous differential equation contains two parts, the complementary solution and the particular solution. The solution to the homogeneous equation is:

$$T_{s,comp} = C \exp\left(-\frac{h_c A}{(\dot{m}c_p)_s} x\right) \tag{3.9}$$

To obtain a particular solution, we assumed that the gas temperature could be represented by a linear function of x over small distances. The particular solution is:

$$T_{s,p} = A + \frac{T_{g,j} - T_{g,j-1}}{x_j - x_{j-1}} x \tag{3.10}$$

where A is a constant. Differentiating, we get:

$$\frac{dT_{s,p}}{dx} = \frac{T_{g,j} - T_{g,j-1}}{x_j - x_{j-1}} \tag{3.11}$$

Substituting Eqn.'s 3.10 and 3.11 into Eqn. 3.8, we get:

$$T_{p,s} = T_g + \frac{(1-f)\sum H_R}{h_c A} - \frac{(\dot{m}c_p)_s}{h_c A}\left[\frac{T_{g,j} - T_{g,j-1}}{x_j - x_{j-1}}\right] \tag{3.12}$$

Adding the complementary and the particular solution, Eqn.'s 3.9 and 3.12 and solving for the integration constant, we get:

$$\frac{T_{s,j-1} - T_{g,j-1} + \left(\frac{T_{g,j-1} - T_{g,j}}{x_{j-1} - x_j}\right)\frac{(\dot{m}c_p)_s}{h_c A} - \frac{(1-f)\sum H_R}{h_c A}}{T_{s,j} - T_{g,j} + \left(\frac{T_{g,j-1} - T_{g,j}}{x_{j-1} - x_j}\right)\frac{(\dot{m}c_p)_s}{h_c A} - \frac{(1-f)\sum H_R}{h_c A}} = \exp\left[-\frac{h_c A}{(\dot{m}c_p)_s}(x_{j-1} - x_j)\right] \tag{3.13}$$

This equation may be used to determine the solid temperature $T_{s,j-1}$ given $T_{s,j}$ and T_g. The solid temperature at the top of the gasifier, which is needed to initialize the solution of Eqn. 3.13, is obtained from an energy balance of the devolatilization zone. The heat transfer from the gas in the devolatilization zone is given by:

$$\begin{aligned}\dot{Q} \;=\; & D_{TAR} \cdot \left[h_{f,tarv} - h_{f,tarl} + c_{p,tar}(T_E - T_O)\right] \\ & + D_{GAS} \cdot \left[h_{f,gasv} - h_{f,tarl} + c_{p,gas}(T_E - T_O)\right] \\ & + D_{MOIST} \cdot \left[h_{fg} + c_{p,moist}(T_E - T_O)\right] \\ & + (COAL - D_{TAR} - D_{GAS} - D_{MOIST}) \cdot c_{p,solid}(T_C - T_O)\end{aligned} \tag{3.14}$$

also,

$$\dot{Q} = GAS \cdot c_{p,gas}(T_F - T_E) \tag{3.15}$$

where:

T_O ≡ Temperature of the coal entering the gasifier
T_C ≡ Temperature of the char leaving the devolatilization zone
T_F ≡ Temperature of the coalgas entering the devolatilization zone
T_E ≡ Temperature of the coalgas leaving the gasifier
h_{fg} ≡ Heat of vaporization for water
GAS ≡ The gas flowrate into devolatilization zone
D_{TAR} ≡ The amount of tar generated during devolatilization
D_{GAS} ≡ The amount of gas generated during devolatilization
D_{MOIST} ≡ The amount of moisture generated during devolatilization

A third equation is needed since there are three unknowns, $\dot{Q}, T_E,$ andT_C in Eqn.'s 3.14 and 3.15. The additional equation describes the way that heat transfer depends on the difference between the solid and gas temperatures. Here it is convenient to employ the concept of heat exchanger effectiveness.

$$T_C = T_O + \epsilon\,(T_F - T_O) \tag{3.16}$$

In counterflow heat transfer the effectiveness, ϵ, is given by

$$\epsilon = \frac{1-\Gamma}{1 - C\cdot\Gamma} \tag{3.17}$$

where:

$$\begin{aligned}
\Gamma &= \exp\left((C-1)\cdot N\right) && (3.18)\\
C &= \frac{(\dot{m}c_p)_{solid}}{(\dot{m}c_p)_{gas}} && (3.19)\\
N &= \frac{hA}{(\dot{m}c_p)_{solid}} && (3.20)
\end{aligned}$$

and where hA is the overall conductance in the devolatilization zone. Equations 3.14 through 3.16 were solved simultaneously to obtain a single expression for the gas exit temperature, T_E. After some algebraic manipulation the equation for the gas exit temperature, T_E, can be written in the following form.

$$T_E = \frac{(\dot{m}c_p)_{gas}T_F - A1 + C1\cdot T_C}{B1 + (\dot{m}c_p)_{gas}} \tag{3.21}$$

where:

$$\begin{aligned}
A1 &= D_{TAR}\cdot\left(h_{f,tar,v} - h_{f,tar,l} - c_{p,tar}T_O\right)\\
&\quad + D_{GAS}\cdot\left(h_{f,gas} - h_{f,tar,l} - c_{p,gas}T_O\right)\\
&\quad + D_{MOIST}\cdot\left(h_{f,g} - c_{p,steam}T_O\right)\\
&\quad + \left(D_{TAR} + D_{GAS} + D_{MOIST} - COAL\right)c_{p,solid}T_O && (3.22)\\
B1 &= D_{TAR}\cdot c_{p,tar} + D_{GAS}\cdot c_{p,gas} + D_{MOIST}\cdot c_{p,steam} && (3.23)\\
C1 &= \left(COAL - D_{TAR} - D_{GAS} - D_{MOIST}\right)c_{p,solid} && (3.24)
\end{aligned}$$

and $COAL$ is the coal feed rate into the top of the gasifier.

The overall conductance (hA) depends on the height of the devolatilization zone. Also, the height of the devolatilization zone must be subtracted from the gasifier height to obtain the effective column height for conversion of char to gas. The height of the devolatilization zone depends on the devolatilization time and the coal feed rate. An iterative procedure is employed in the revised program to calculate the devolatilization time. Initially the devolatilization time and the height of the gasifier column required for devolatilization are neglected. Preliminary gas temperatures and compositions at the top of the column are then computed assuming that the entire column height is available for conversion of char to gas. These preliminary gas temperatures and compositions are then used to estimate the devolatilization time. The effective height of the gasifier column is then recalulated accounting for the column height needed for devolatilization, and all of the calculations are repeated.

3.2 DEVOLATILIZATION CALCULATIONS

The subroutines of the Wen II program that compute quantities of tar and gas formed during the devolatilization of coal were rewritten to remove approximations in mathematics and to account for effects such as temperature gradients within the solid which become important as the particle diameter increases. These changes were necessary because the original model predicted unrealistic results for conditions needed in the present work.

Devolatilization has been studied in great depth in recent years, and new theories and models have been developed. References [5] and [6] discuss recent studies. The Wen II program should eventually be revised to incorporate the new knowledge. However, new devolatilization theory has not been added to the model in the present work. We have only refined the mathematics in Wen's original model.

In the Wen II model coal devolatilizes to form tar and char:

$$\text{Coal} \longrightarrow X_1 \text{tar} + (1 - X_1)\text{char} \tag{3.25}$$

where X_1 is the mass fraction of the coal that forms tar. The model accounts for subsequent cracking of the tar, and also accounts for the fact that some of the tar reverts back to char in a process called deposition. Thus the amount of tar produced during the devolatilization of coal is less than X_1 and the amount of char remaining after devolatilization is greater than $(1 - X_1)$. The net amount of tar produced depends on differences in the rates of devolatilization, cracking, and deposition. Thus it changes with temperature, particle diameter, and other properties of coal. However, in the Wen II model, the net amount of char remaining after devolitalization is not a variable. It is a constant that is specified by the user, depending on the type of coal being fed into the gasifier. For example, when the coal is Illinois #6, the user should specify that 91.6% of the volatile matter is released during devolatilization. The net amount of char remaining after devolatilization is then determined from the proximate analysis of the coal.

$$\text{char} = 100 - 0.916 \times \text{VM} - \text{MOISTURE} - \text{ASH} \tag{3.26}$$

In this way the program permits experimental data to be incorporated into the devolitalization model. However, the user is also required to provide the value of the parameter X_1 in Eqn. 3.25. Default values of X_1 are included in the model for various coal types. One problem with the model is that the user specified or default value of X_1 may not be consistent with the user specified value of char remaining after devolatilization. The Wen II program corrects for this problem as follows:

1) The amount of char remaining after devolatilization is calculated as the sum of $(1 - X_1)$ and the amount of char depositied within the pores of the coal particle during the devolatilization process. The quantity of deposited char depends on the rate of deposition and the time required for devolatilization.
2) If the calculated amount of char remaining after devolatilization is less than the user specified value, the program assumes that its devolatilization calculations were incorrect. It reduces the amounts of tar and gas formed so that more of the devolatilization mass appears in the form of char.
3) If the calculated amount of char remaining after devolatilization is greater than the user specified amount, the excess char is assumed to react with hydrogen gas to form methane.

$$C + 2H_2 \longrightarrow CH_4 \tag{3.27}$$

This correction sometimes leads to unrealistic results. The amount of hydrogen needed for the reaction may exceed the amount that is available is the gas stream. In this case the program predicts negative mass fractions of hydrogen and excessive mass fractions of methane in the product gas stream.

In the revised program, the value of X_1 is calculated internally. It is not specified by the user. The program adjusts X_1 until the calculated amount of carbon remaining after devolatilization agrees with the user specified amount. In this case corrections to the devolatilization calculations are not required.

3.3 TAR CALCULATIONS

The Wen II program calculates the quantity of tar produced by integrating rate equations. The net amount of tar produced is calculated as the amount devolatilized from the coal minus the amount lost through cracking and deposition. Thus, since the rate equations for devolatilization, cracking, and deposition depend on temperature, the quantity of tar produced from a given coal changes with the operating conditions. The model predicts that less tar will be produced when the coal particle diameter increases because the devolatilization process takes longer, and more time is thus available for cracking and deposition of tar. However, mathematical approximations are made in the model which limit the accuracy of the predictions.

Some boundary conditions were not satisfied when solving differential equations to calculate the mass of tar and gas evolved during devolatilization. Because of this, the calculated amount of tar flowing from the surface of the coal particle is not the same as the net amount generated within the particle after accounting for cracking and deposition. The discrepancy is signigicant as shown in Figure 3.1. The program has now been modified so that boundary conditions are satisfied and consistent results are obtained. This required extensive revision of the devolatilization subroutines. These revisions are described in detail below.

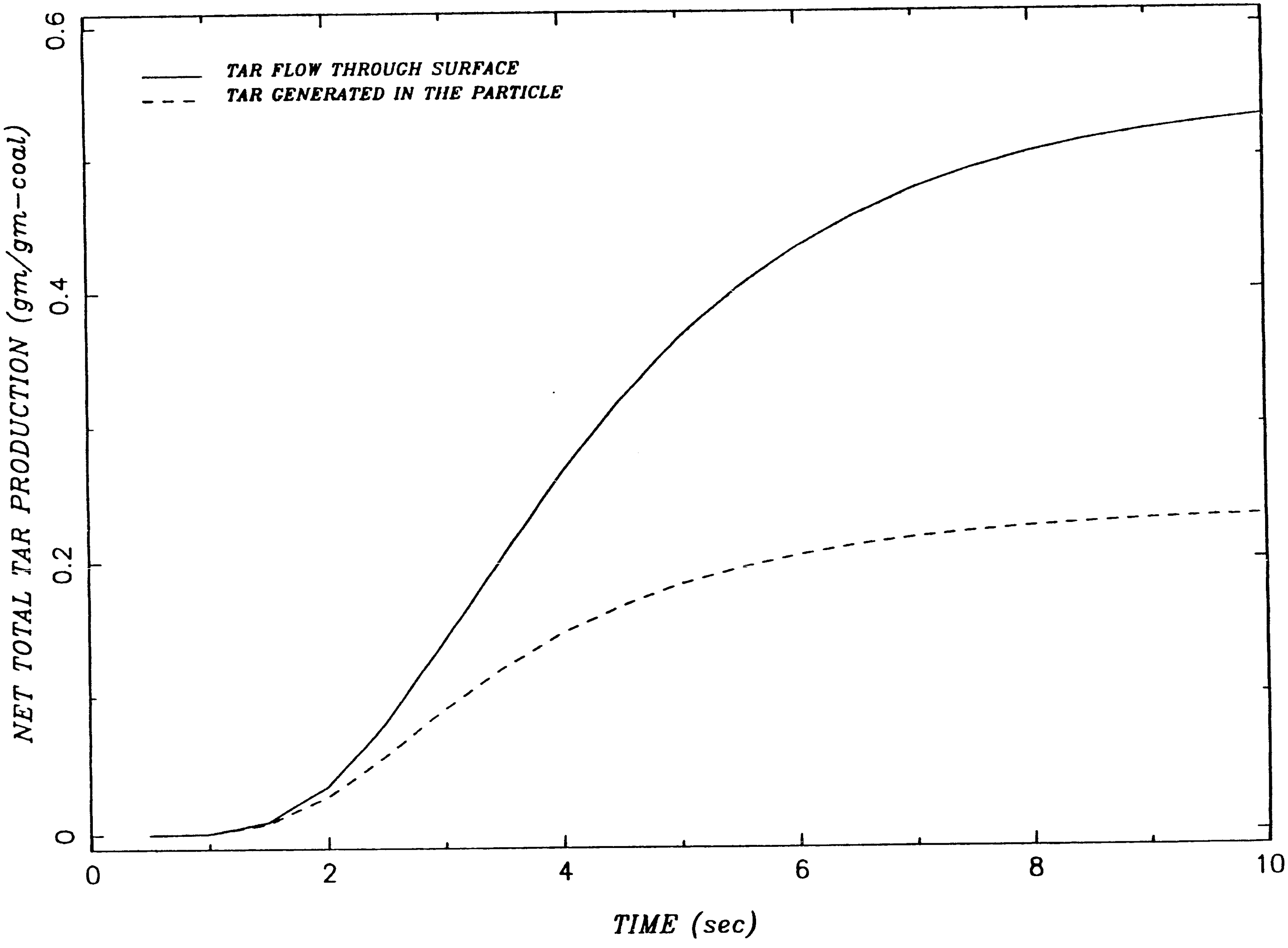


Figure 3.1: Comparison of Total Net Tar Generation for Flow Through the Particle Surface Versus Generation Inside the Particle.

We have also revised the subroutines to account for temperature gradients within the solid. Experiments indicate that devolatilization occurs in a relatively thin layer. The layer forms at the outside surface, which is heated first, and moves inwards as the temperature within the particle increases. The Wen II model, which was developed for pulverized coal assumes that the temperature within the particle is uniform. Thus, devolatilization occurs at the same time throughout the particle. No film develops. We have modified the program to account for temperature gradients within the particle. Figures 3.2 and 3.3 show some typical transients temperature profiles computed by the revised program. The energy equation solved to obtain these profiles accounts for heat needed to vaporize tars and gases. The program changes are documented below.

Initial results from the revised program indicated that very little tar was being formed in coal particles having diameters greater than 0.25 inches. The time required for devolatilization of these particles is sufficiently long that the program calculated that all of the tar cracked. We believe that the rate constant for cracking is too high. This constant was determined from experimental data for pulverized coal. Very high rates are required if cracking is to have any effect at all in this case. We have substituted rate constants from other sources [7], and the results are much more reasonable.

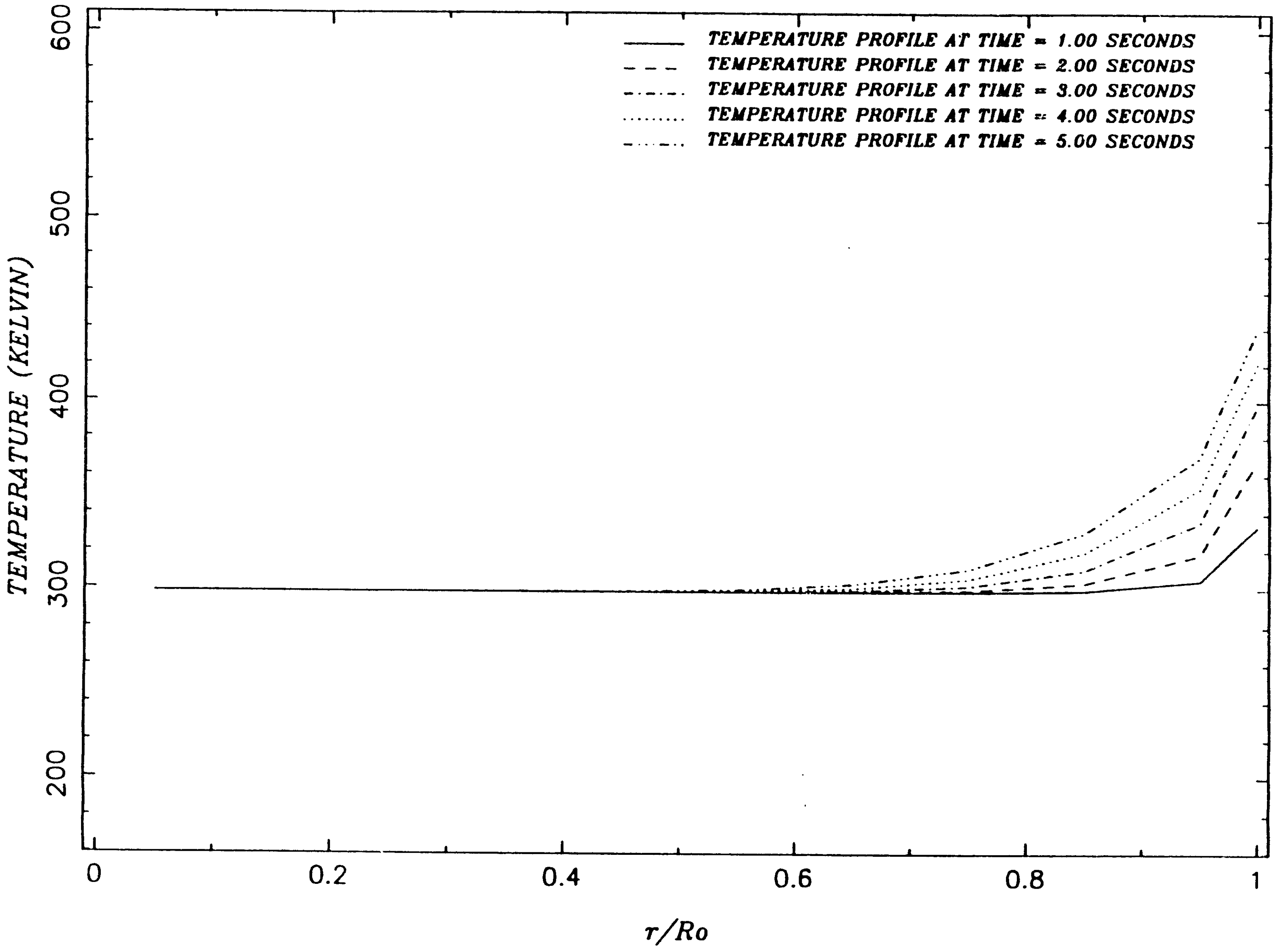


Figure 3.2: Comparison of Temperature Profiles at Various Times with a Particle Diameter of 0.5 inches.

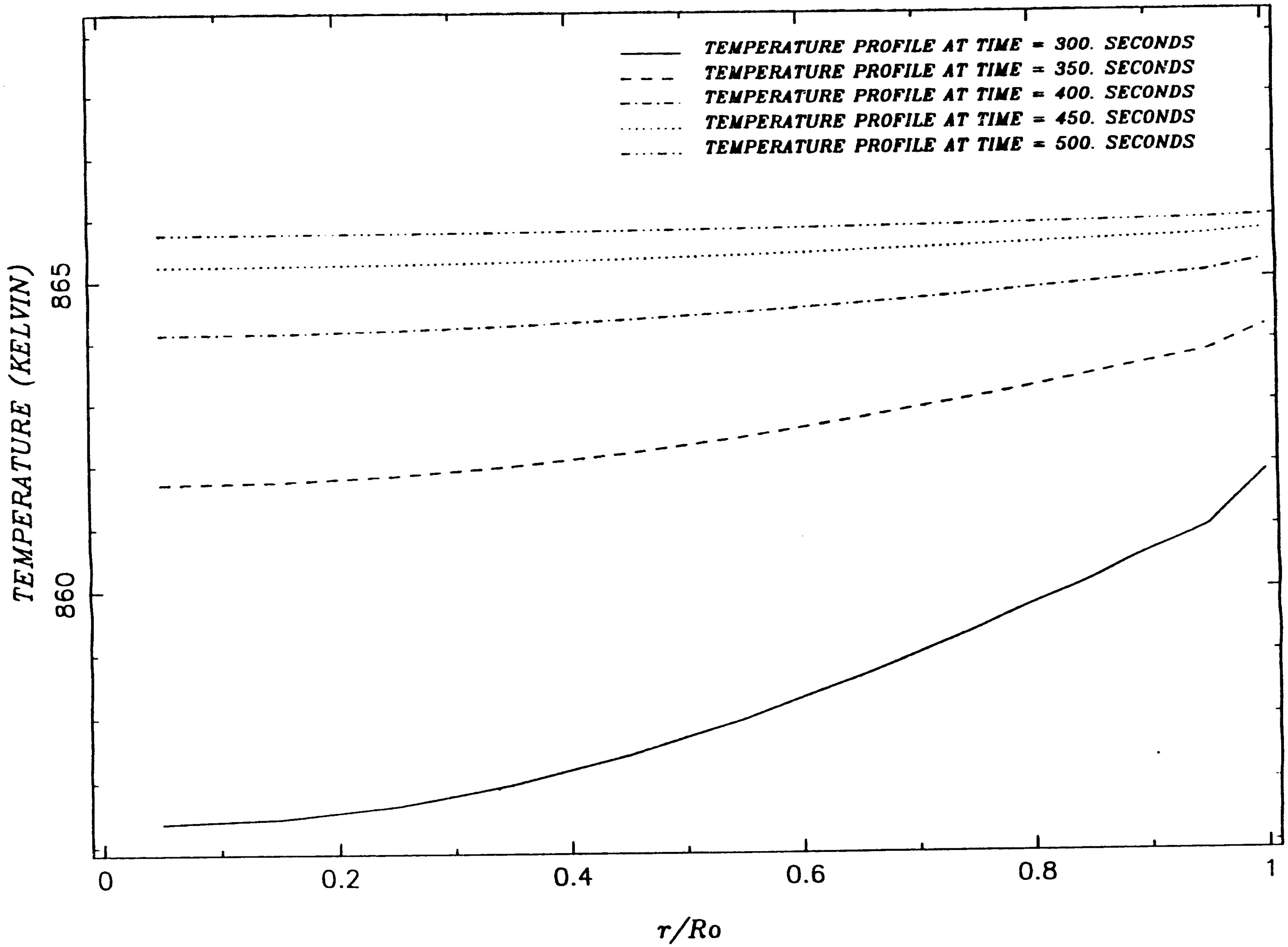


Figure 3.3: Comparison of Temperature Profiles at Various Times with a Particle Diameter of 0.5 inches.

3.3.1 METHOD BEFORE MODIFICATIONS

This section provides details of the way that the Wen II model accounted for the pyrolysis of coal. This will provide a starting point for discussing the program modifications. The Wen II model assumed that the three key reactions are: coal converted to tar and char, tar converted to product gas, and tar converted to char. These reactions were modeled using first order rate equations to give the reaction rates at various temperatures. Using conservation of species equations, both mass flux and species concentrations were calculated using a non- linear differential equation solver. These mass fluxes and concentrations were used in an overall energy equation and in coal particle weight loss calculation for each time interval.

The model bases the devolatilization of the coal particle on three reactions which occur simultaneously within the coal particle. The three reactions are devolatilization, cracking, and depostion.

*Devolatilization:

$$\text{Coal} \xrightarrow{k_1} X_1 \cdot \text{tar} + (1 - X_1) \cdot \text{char} \tag{3.28}$$

$$\text{Rate} = k_{10} \cdot exp\left(\frac{-E_{10}}{R_g T}\right) \cdot C_{\text{coal}} \tag{3.29}$$

*Cracking:

$$\text{Tar} \xrightarrow{k_2} \text{product gas} \tag{3.30}$$

$$\text{Rate} = k_{20} \cdot exp\left(\frac{-E_{20}}{R_g T}\right) \cdot C_{\text{tar}} \tag{3.31}$$

*Deposition:

$$\text{Tar} \xrightarrow{k_3} \text{char} \tag{3.32}$$

$$\text{Rate} = k_{30} \cdot exp\left(\frac{-E_{20}}{R_g T}\right) \cdot C_{\text{tar}} \tag{3.33}$$

The products of pyrolysis are tar, char, and product gas. Char is the undistillable material which remains in solid form; tar is material with a molecular weight greater than C_6, and appears in the vapor form; gas is material with a molecular weight ligher than C_6, i.e. CO, CH_4, CO_2, H_2O, etc., and appears in the vapor form. The rates of formation for tar, product gas, and the inert gas can be expressed in the following equations:

$$\mathrm{R_{tar}} = X_1 \cdot \mathrm{k_1} \cdot \mathrm{C_{coal}} - (k_2 + k_3) \cdot \mathrm{C_{tar}} \tag{3.34}$$

$$\mathrm{R_{gas}} = k_2 \cdot \mathrm{C_{tar}} \tag{3.35}$$

$$\mathrm{R_{inert\ gas}} = 0 \tag{3.36}$$

The coal particle is considered to be a porous sphere which retains its integrity during pyrolysis. The conservation equation that is solved for the gaseous species, is:

$$\frac{1}{\mathrm{r}^2} \cdot \frac{\partial}{\partial \mathrm{r}} \left(\mathrm{r}^2 \cdot \mathrm{N_i} \right) = \mathrm{R_i} \tag{3.37}$$

where $\mathrm{R_i}$ is the rate of generation of the species i due to chemical reactions.

$\mathrm{N_i}$ is the molecular flux of the species and can be expressed as the sum of the rate of diffusion in the radial direction plus bulk flow through the pores.

$$\mathrm{N_i} = -\mathrm{D_{eff,i}} \cdot \frac{\partial \mathrm{C_i}}{\partial \mathrm{r}} + \mathrm{W_i} \cdot \sum_j \mathrm{N_j} \tag{3.38}$$

$\mathrm{W_i}$, which is the weight fraction of species i, can be expressed in the following equation:

$$\mathrm{W_i} = \frac{\mathrm{C_i}}{\sum_j C_j} \tag{3.39}$$

The following equation is solved to determine the solid concentration.

$$\frac{\mathrm{dC_1}}{\mathrm{dt}} = \mathrm{R_1} \tag{3.40}$$

Finally, the flow of the gaseous species i across the gas film is given by:

$$N_i = k_{gi} \cdot \left[C_{i,s} - C_{i,b}\right] \tag{3.41}$$

where:

$C_{i,s}$ ≡ concentration of the gas species i at the surface.
$C_{i,b}$ ≡ concentration of the gas species i at the bulk gas stream.
k_{gi} ≡ is the mass-transfer coefficient across the gas film which can be estimated from an apropriate mass-transfer correlation.

Equations 3.37 and 3.38 are coupled first order differential equaitons. One of the required boundary conditions is provided by Eqn. 3.41. The second boundary condition is $N_i = 0$ at $r = 0$. In the Wen II program, the second boundary condition is not enforced. The coupled differential equations are solved by integrating numerically from the outside of the particle inwardly to $r = 0$. Thus, both boundary conditions are needed at the outside radius. The Wen II model estimates the unknown boundary condition for N_i at the surface, so that the integration can be performed, but does not correct the trial value so that $N_i = 0$ at $r = 0$. As a result, the program predicts inconsistent and erronous values for the mass flux. The net amount of tar produced inside the particle accounting for cracking and deposition is not the same as the amount of tar flowing through the surface of the particle. Figure 3.4 which graphs the tar mass flux predicted by the Wen II model, shows that the mass flux does not approach zero at the center of the particle.

3.3.2 METHOD AFTER MODIFICATIONS

The first item that was changed was the conservation equation for the gaseous species, i. The previous conservation equation neglected the amount of mass stored inside the particle. By neglecting the storage term, the conservation equation became an ordinary differential equation (ODE) which could be solved with a standard ODE solver. Including the storage

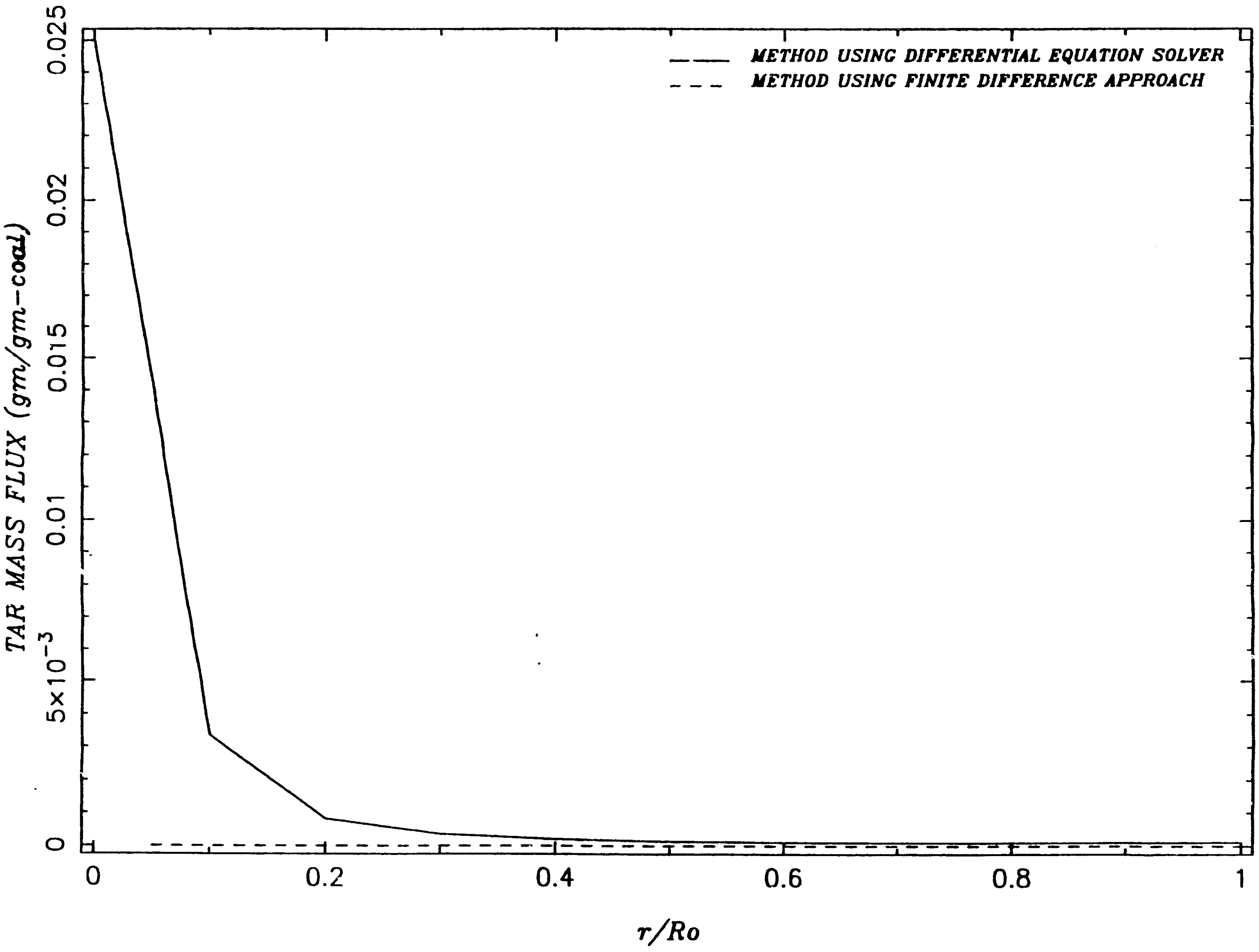


Figure 3.4: Comparison of Tar Mass Flux.

term in the gaseous species conservation equation results in the following partial differential equation:

$$\frac{1}{\mathrm{r}^2} \cdot \frac{\partial}{\partial \mathrm{r}} \left(\mathrm{r}^2 \cdot \mathrm{N_i} \right) + \frac{\partial \mathrm{C_i}}{\partial \mathrm{t}} = \mathrm{R_i} \tag{3.42}$$

A finite difference approach was employed to solve the partial differential equation. After the coal particle was divided into shells, appropriate equations for species conservation and mass flux were derived for each shell. The concentration of species, i, is calculated at the midpoint of the shell and the mass flux of the species is calculated at the shell boundary.

Equations are programmed for three types of nodes. The node equations are for the center shell, the middle shells, and the outer shell. Starting with a mass balance, the rate of storage equations were devired; and then using Fick's law, the subsequent mass-flux equations were derived. The following equations were developed in this manner.

For Node # 1:

$$N_1' \cdot 4\pi r_1^2 = \left(R_1 - \frac{dC_i}{dt} \right) \cdot \frac{4}{3}\pi r_1^3 \tag{3.43}$$

$$\frac{C_1' - C_i}{\Delta t} = R_1 - \frac{3N_1'}{r_1} \tag{3.44}$$

$$N_1' = -D_{eff} \left(\frac{C_2' - C_1'}{\Delta r} \right) + (C_1' + C_2') \cdot \frac{\sum N_1}{\sum C_1 + \sum C_2} \tag{3.45}$$

For Node # i for $1 < i < N$:

$$\left(N_i' \cdot 4\pi r_i^2 - N_{i-1}' \cdot 4\pi r_{i-1}^2 \right) = \left[R_i' - \frac{dC_i}{dt} \right] \left[\frac{4}{3}\pi \right] \left[r_i^3 - r_i^3 \right] \tag{3.46}$$

$$\frac{C_i' - C_i}{\Delta t} = R_i' - 3 \left(\frac{N_i' r_i^2 - N_{i-1}' r_{i-1}^2}{r_i^3 - r_{i-1}^3} \right) \tag{3.47}$$

$$N_i' = -D_{eff} \left(\frac{C_{i+1}' - C_i'}{\Delta r} \right) + (C_i' + C_{i+1}') \cdot \frac{\sum N_i}{\sum C_i + \sum C_{i+1}} \tag{3.48}$$

For Node # N:

$$\left(N'_N \cdot 4\pi r_N^2 - N'_{N-1} \cdot 4\pi r_{N-1}^2\right) = \left[R'_N - \frac{dC_N}{dt}\right]\left[\frac{4}{3}\pi\right]\left[r_N^3 - r_{N-1}^3\right] \tag{3.49}$$

$$\frac{C'_N - C_N}{\Delta t} = R'_N - 3\left(\frac{N'_N r_N^2 - N'_{N-1} r_{N-1}^2}{r_N^3 - r_{N-1}^3}\right) \tag{3.50}$$

$$N'_N = kg \cdot [C'_N - C'_B] + C'_N \frac{\sum N_N}{\sum C_N} \tag{3.51}$$

These equations are the governing mass-flux and concentration equations used to determine the amount of tar and gas generated during devolatilitization. They were solved implicitly using a tridiagonal matrix solver as described below. It should be noted that Eqn. 3.51, which prescribes the molecular flux at the boundary, is different from Eqn. 3.41, which is the corresponding equation in the Wen II model. The Wen II model neglects the bulk flow out of the particle surface.

The energy equation solved to determine the temperatures inside the particle accounts for energy transfer due to conduction, convection, and heats of reaction. A finite difference energy equation was generated for a sperical control volume. The general equation is:

$$\begin{aligned}
c_p \cdot \left(\frac{T'_i - T_i}{\Delta t}\right)\left(\frac{4\pi\left(r_i^3 - r_{i-1}^3\right)}{3}\right) = \\
-k_{coal}\left(\frac{T'_i - T'_{i-1}}{\Delta r}\right) 4\pi r_{i-1}^2 + k_{coal}\left(\frac{T'_{i+1} - T'_i}{\Delta r}\right) 4\pi r_i^2 \\
+M_{j,i-1} \cdot \left(H_{f,j} + c_{p,j}\left(\frac{T'_{i-1} + T'_i}{2}\right)\right) 4\pi r_{i-1}^2 \\
-M_{j,i} \cdot \left(H_{f,j} + c_{p,j}\left(\frac{T'_i + T'_{i+1}}{2}\right)\right) 4\pi r_i^2 \\
+\left(R_{tar} + R_{gas}\right) \cdot \left(H_{f,tar,l} + c_{p,tar} T'_i\right) \cdot \left(\frac{4\pi\left(r_i^3 - r_{i-1}^3\right)}{3}\right)
\end{aligned} \tag{3.52}$$

where:

$i \equiv$ The shell of the particle number
$j \equiv$ Species type; tar, gas, or inerts
$M \equiv$ Species mass flux
$R \equiv$ Species rate of generation
$H_f \equiv$ Enthalpy of formation

The above equation applies to all of the shells except for the last one which is in contact with the ambient gas. The only change to the above equation for the final shell is the deletion of the positive (+) conduction term and the addition of the following convection term:

$$+\,h \cdot (T_\infty - T_i')\, 4\pi r_N^2 \qquad (3.53)$$

Equation 3.52 with Eqn. 3.53 as a boundary condition determines the temperature profile across the particle. This equation was solved using the same tridiagonal matrix solver used for solving the species concentration equations.

The convective heat transfer coefficient in Eqn. 5.53 is computed from a correlation in the heat transfer literature [8] for flow in packed beds which is the same correlation that appears as Eqn. 3.5. The correlation requires average thermal properties for the gas mixture. A new subroutine (CONV) was written to calculate the heat transfer coefficient based on the average properties of the gas, the temperature, and the diameter of the particle.

3.1 PROGRAMMING THE CHANGES

This section converts the equations listed above into FORTRAN programming lines. It also discusses the changes to the affected subroutines called by the devolatilization subroutine. During the modification process, new subroutines were written to replace the devolatilization subroutine. The new subroutines are included in the appendices of this report.

The mass-flux and rate of storage equations were combined to get an overall conservaton equation in terms of the old and new concentrations. Each shell had its own conservation equation in terms of C_{i-1}, C_i, and C_{i+1}. This series of equations was then supplied to the tridiginal matrix solver (TRIDI) which produces the new values for concentrations. The species mass-fluxes are then determined given these new concentrations. The next three equations are the general species conservation equations for nodes 1, i, and N.

$$\frac{C_1' - C_1}{\Delta t} = R_1 - \frac{3}{r_1}\left[-D_{eff}\left(\frac{C_2' - C_1'}{\Delta r}\right) + (C_1' + C_2')\cdot\left(\frac{\sum_j N_1}{\sum_j C_1 + \sum_j C_2}\right)\right] \tag{3.54}$$

$$\begin{aligned}\frac{C_i' - C_i}{\Delta t} &= R_i \\ &-\frac{3r_i^2}{r_i^3 - r_{i-1}^3}\cdot\left[-D_{eff}\left(\frac{C_{i+1}' - C_i'}{\Delta r}\right) + \left(C_i' + C_{i+1}'\right)\cdot\left(\frac{\sum_j N_i}{\sum_j C_i + \sum_j C_{i+1}}\right)\right] \\ &+\frac{3r_{i-1}^2}{r_i^3 - r_{i-1}^3}\cdot\left[-D_{eff}\left(\frac{C_i' - C_{i-1}'}{\Delta r}\right) + \left(C_i' + C_{i-1}'\right)\cdot\left(\frac{\sum_j N_{i-1}}{\sum_j C_i + \sum_j C_{i-1}}\right)\right]\end{aligned} \tag{3.55}$$

$$\begin{aligned}\frac{C_N' - C_N}{\Delta t} &= R_N - \frac{3r_N^2}{r_N^3 - r_{N-1}^3}\cdot\left[kg\cdot(C_N' - C_B') + C_N'\frac{\sum_j N_N}{\sum_j C_N}\right] \\ &+\frac{3r_{N-1}^2}{r_N^3 - r_{N-1}^3}\left[-D_{eff}\left(\frac{C_N' - C_{N-1}'}{\Delta r}\right) + \left(C_N' + C_{N-1}'\right)\left(\frac{\sum_j N_{N-1}}{\sum_j C_N + \sum_j C_{N-1}}\right)\right]\end{aligned} \tag{3.56}$$

These equations were then used to calculated the species concentrations for tar, gas, and inerts and subsequently the mass fluxes for each.

TRIDI solves a matrix in the following form:

$$\begin{bmatrix} b_1 & c_1 & 0 & \cdots & & & \\ a_2 & b_2 & c_2 & 0 & \cdots & & \\ 0 & a_3 & b_3 & c_3 & 0 & \cdots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & \vdots & 0 & a_{N-2} & b_{N-2} & c_{N-2} & 0 \\ & & \vdots & 0 & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & \vdots & 0 & a_N & b_N \end{bmatrix} \times \begin{bmatrix} C_1' \\ C_2' \\ \vdots \\ \\ \\ C_{N-1}' \\ C_N' \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ \\ \\ d_{N-1} \\ d_N \end{bmatrix} \tag{3.57}$$

In the above matrix equation, the a's are the coefficents of the terms containing C_{i-1}; the b's are the C_i terms; c's are the C_{i+1}; and the d's contain everything else. For the particle energy equation the C's are changed to T's.

Since certain expressions appeared thoughout the equations for a, b, c, and d, the following constants were defined for the ease of programming (assume $r_o = 0$):

$$K1_i = \frac{3 \cdot \Delta t}{r_i^3 - r_{i-1}^3} \tag{3.58}$$

$$K2_i = r_i^2 \tag{3.59}$$

$$K3_i = \frac{Y1_i + Y2_i + Y3_i}{Y4_i + Y5_i + Y6_i + Y4_{i+1} + Y5_{i+1} + Y6_{i+1}} \tag{3.60}$$

$$K4_i = \frac{Y1_{i-1} + Y2_{i-1} + Y3_{i-1}}{Y4_i + Y5_i + Y6_i + Y4_{i-1} + Y5_{i-1} + Y6_{i-1}} \tag{3.61}$$

$$K5_i = \frac{\left(r_i^3 - r_{i-1}^3\right) \cdot \Delta t}{3} \tag{3.62}$$

$$K6_i = \left(\frac{Y1_i \cdot c_{p,tar}}{2} + \frac{Y2_i \cdot c_{p,gas}}{2} + \frac{Y3_i \cdot c_{p,inerts}}{2}\right) K2_i \Delta t \tag{3.63}$$

$$K7_i = (RATE_{tar} + RATE_{gas}) \cdot c_{p,tar} \cdot K5_i \tag{3.64}$$

$$K8_i = (Y1_i \cdot H_{f,tar,v} + Y2_i \cdot H_{f,gas} + Y3_i \cdot H_{f,inerts}) K2_i \Delta t \tag{3.65}$$

$$K9_i = (RATE_{tar} + RATE_{gas}) \cdot H_{f,tar,l} \cdot K5_i \tag{3.66}$$

$$K10_i = \frac{k_{coal} \cdot \Delta t \cdot K5_i}{\Delta r} \tag{3.67}$$

The following equations define the a's, b's, c's, and d's which were sent to TRIDI to find the new concentrations and temperatures. The equations will be grouped in 4's, the first set were applied to tar concentrations, the second were applied to gas concentrations, the third were applied to inerts concentrations, the forth and final set were applied to the temperatures.

$$a_{tar} = -K1_i K2_{i-1} \cdot \left(\frac{D_{eff}}{\Delta r} + K4_i\right) \tag{3.68}$$

$$b_{tar} = 1 + K1_i K2_i \left(\frac{D_{eff}}{\Delta r} + K4_i\right) - K1_i K2_{i-1} \left(\frac{-D_{eff}}{\Delta r} + k4_i\right)$$

$$+(CK2_i + CK3_i)\cdot\Delta t \tag{3.69}$$

$$c_{tar} = K1_i K2_i \left(\frac{-D_{eff}}{\Delta r} + K3_i\right) \tag{3.70}$$

$$d_{tar} = X1 \cdot CK1_i \cdot CCOAL_i \Delta t + Y4_i \tag{3.71}$$

$$a_{gas} = -K1_i K2_{i-1} \cdot \left(\frac{D_{eff}}{\Delta r} + K4_i\right) \tag{3.72}$$

$$b_{gas} = 1 + K1_i K2_i \left(\frac{D_{eff}}{\Delta r} + K4_i\right) - K1_i K2_{i-1} \left(\frac{-D_{eff}}{\Delta r} + K4_i\right) \tag{3.73}$$

$$c_{gas} = K1_i K2_i \left(\frac{-D_{eff}}{\Delta r} + K3_i\right) \tag{3.74}$$

$$d_{gas} = CK2_i \cdot Y4_i \Delta t + Y5_i \tag{3.75}$$

$$a_{inerts} = -K1_i K2_{i-1} \cdot \left(\frac{D_{eff}}{\Delta r} + K4_i\right) \tag{3.76}$$

$$b_{inerts} = 1 + K1_i K2_i \left(\frac{D_{eff}}{\Delta r} + K4_i\right) - K1_i K2_{i-1} \left(\frac{-D_{eff}}{\Delta r} + K4_i\right) \tag{3.77}$$

$$c_{inerts} = K1_i K2_i \left(\frac{-D_{eff}}{\Delta r} + K3_i\right) \tag{3.78}$$

$$d_{inerts} = Y6_i \tag{3.79}$$

$$a_{temp} = -K6_{i-1} - K10_{i-1} \tag{3.80}$$

$$b_{temp} = \frac{c_{p,coal} \cdot K5_i}{\Delta t} + K6_i - K6_{i-1} - K7_i + K10i + K10i - 1 \tag{3.81}$$

$$c_{temp} = K6_i - K10_i \tag{3.82}$$

$$d_{temp} = \frac{c_{p,coal} \cdot K5_i \cdot Y7}{\Delta t} - K8_i + K8_{i-1} + K9_i \tag{3.83}$$

where:

$CK1, CK2 \equiv$ Rate constants for devolatilization, cracking
$Y1, Y2, Y3 \equiv$ Mass flux of tar , gas, inerts

$Y4, Y5, Y6 \equiv$ Concentration of tar, gas, inerts
$Y7 \equiv$ Temperature of particle

The above equations apply for nodes greater than one and less than N. The equations for nodes i and N, which are listed in the source code in Appendix A, were obtained by only a slight variation of these equations.

In order to calculate an appropriate heat transfer coefficient, values for Prandtl Number, conductivity, specific heat, and viscosity were needed. These values were determined for each individual gas, $CO_2, H_2, \ldots$, and then averaged to obtain one value for each constant at the specified temperature. The Wen II program contained a subroutine to calulate the specific heats at a given temperature. In the new subroutine, CONV, Prandtl Numbers for each individual gas were averaged to obtain the Prandtl Number for the collective gas mixture. The conductivities for each gas were determined by using the following formula:

$$k_i = A + B \cdot T \tag{3.84}$$

The A's and B's were obtained by a curve fit to experimental data. The conductivities of individual gases were then averaged to obtain an effective conductivity of the gas mixture. The following equations were used to determine the heat transfer coefficient:

$$\mu_{avg} = \frac{\mathrm{Pr}_{avg} \cdot k_{avg}}{c_{p,avg}} \tag{3.85}$$

$$\mathrm{Re} = \frac{\sum_{i=1}^{7} \dot{m}_i \cdot D_p}{A \cdot \mu} \tag{3.86}$$

$$\mathrm{Nu} = \frac{2.06\mathrm{Re}^{.425}\mathrm{Pr}^{.333}}{\text{bed voidage}} \tag{3.87}$$

$$h = \frac{\mathrm{Nu} \cdot k_{avg}}{D_p} \tag{3.88}$$

where:

$D_p \equiv$ The diameter of the particle

$A \equiv$ The cross-sectional area of the gasifier

In test cases, we observed that the particle was still heating up when the tar production approached zero. Since the convergence criteria in the Wen II model was based on the tar and gas generation during devolatilization, the subroutine would stop prematurely. We now base the convergence criteria on temperature only, such that the subroutine will stop when the temperature at the center of the coal particle is within 1 °C of the gas temperature entering the devolatilization zone.

3.4 Comparisons of Results

Below we discuss the results of several test cases that were run to assess the accuracy of the computer model predictions, and to determine how the gasifier performance depends on input parameters such as coal particle size and gasifier bed height. We also ran several test cases to determine the effects of injecting water into the inlet air stream. Water injection would cool the air and reduce the amount of steam needed in the gasification process. The first two cases were run to compare the results of the orignial Wen II code and the modified code. The last ten cases were run to determine how the gasifier performance depends on input parameters and to determine the effects of water injection into the air stream.

3.4.1 Computer Model Predictions

In cases 1 and 2, experimental data from Ref. [7] are compared to the model predictions. The original model was run using the input data prescribed in Ref. [7], and the results were compared to results from the modified model and to the experimental data. Table 3.1 lists the input parameters for the two cases, with Table 3.2 listing the results.

As seen in Table 3.2, a discrepancy exists between calculated values of methane, hydrogen, tar production, and gas exit temperature. In the Wen II model most of the methane is produced during the devolatilization process, by hydrogasification according to Eqn. 3.27. The value of X_1 in Eqn. 3.25 can be adjusted to make the model predictions agree with measurements.In the modified program the value of X_1 is computed internally so that no hydrogasification occurs during the devolatilization process. The value of X_1 could easily be set by the model so that any prescribed amount of methane is formed by hydrogasification.

Table 3.1 Input Data for Cases 1 and 2

Coal Feed Rate, lbs/hr	8058.00

Proximate Analysis of Pittsburgh #8 Coal, Wt %

Moisture	4.58	Volatile matter	37.37
Ash	7.74	Fixed Carbon	50.31

Ultimate Analysis of Pittsburgh #8 Coal, Wt %

C	74.2	H_2	5.0	O_2	4.5
N_2	1.4	S	2.5	H_2O	4.58
Ash	7.74				

Heating Value of Coal, Btu/lb-wet coal	13441.80
Steam Feed Rate, lbs/hr	26145.00
Oxygen Feed Rate, lbs/hr	5005.00
Oxygen Content, mole ratio	0.94
Temperature of Coal, °F	77.00
Temperature of Steam, °F	700.00
Temperature of Oxygen, °F	700.00
Temperature of Wall, °F	700.00
Pressure, psig	350.00
Bed Diameter, ft	10.00
Bed Height, ft	10.00
Initial Coal Particle Size, in	0.79
Heat Transfer Coefficient, Btu/($ft^2 \cdot hr \cdot {}^\circ R$)	30.00
Bed Voidage	0.40

However, it is expected that most of the hydrogasificaton will occur following devolatilization. Other process are probably responsible for methane formation during devolatilization. Alternative methods for methane formation in the devolatilization will need to be addressed in future model developement.

The differences in the tar production are due to the tar cracking rate constants. The rate constant could be adjusted to make the model predictions agree with the experimental data. It should be noted that the Wen II model changes the coal particle diameter from 0.79 inch to 0.01 centimeter to obtain the results in Table 3.2. The Wen II model predicts zero tar production when the particle diameter is 0.79 inch. The modified code does not arbitrary change the particle diameter.

The gas outlet temperature depends on the heat transfer coefficient at the water cooled walls of the gasifier. The heat transfer coefficient specified for Table 3.2is h = 30 Btu/(hr ft^2 °F). This value appears to be too high because the heat loss to the walls is greater than is typical of fixed bed gasifiers. In additional test cases discribed below for a Lurgi Mark IV gasifier, we found that a heat transfer coefficient of h_c = 17 Btu/(hr ft^2 °F) resulted in the correct heat loss to the water jackets. This value would raise the gas outlet temperature in Table 3.2. However we have not attempted to fine tune the model to match experimental results in Cases 1 and 2. We only wish to show the effects of the program modifications.

Table 3.2 Comparison of Results to Experimental Data for Cases 1 and 2

	Experimental Results	Original Code Results	Modified Code Results
Total Gas Output, lbs mole/hr	771.0	859.56	690.39
Product Gas Composition, mole %			
CO	16.8	15.54	16.83
CO_2	31.3	30.01	30.34
H_2	39.2	44.52	49.82
CH_4	10.3	7.63	0.40
N_2	1.6	1.57	1.95
H_2S	0.7	0.73	0.91
Exit Steam Rate, lbs moles/hr	1189.0	1140.8	1250.9
Amount of Tar, lbs/hr	425.0	453.1	227.2
Temperature of Exit Gas, °F	1196.0	1208.5	1069.0
Maximum Temperature, °F	-	1942.0	1978.0
Carbon Conversion, %	98.9	98.5	99.1
Heating Value of Dry Gas, Btu/SCF	285.0	264.8	220.8
Heat Loss, 10^6 Btu	-	74.2	70.8

Figures 3.5 through 3.11 are a direct comparison of temperature and methane, carbon monoxide, carbon dioxide, hydrogen, water/steam, and oxygen molecular fluxes respectively. The original and modified versions produced very simular results. The gasification maximum temperature was slightly higher and the gas exit temperature was slightly lower than that of the original version.

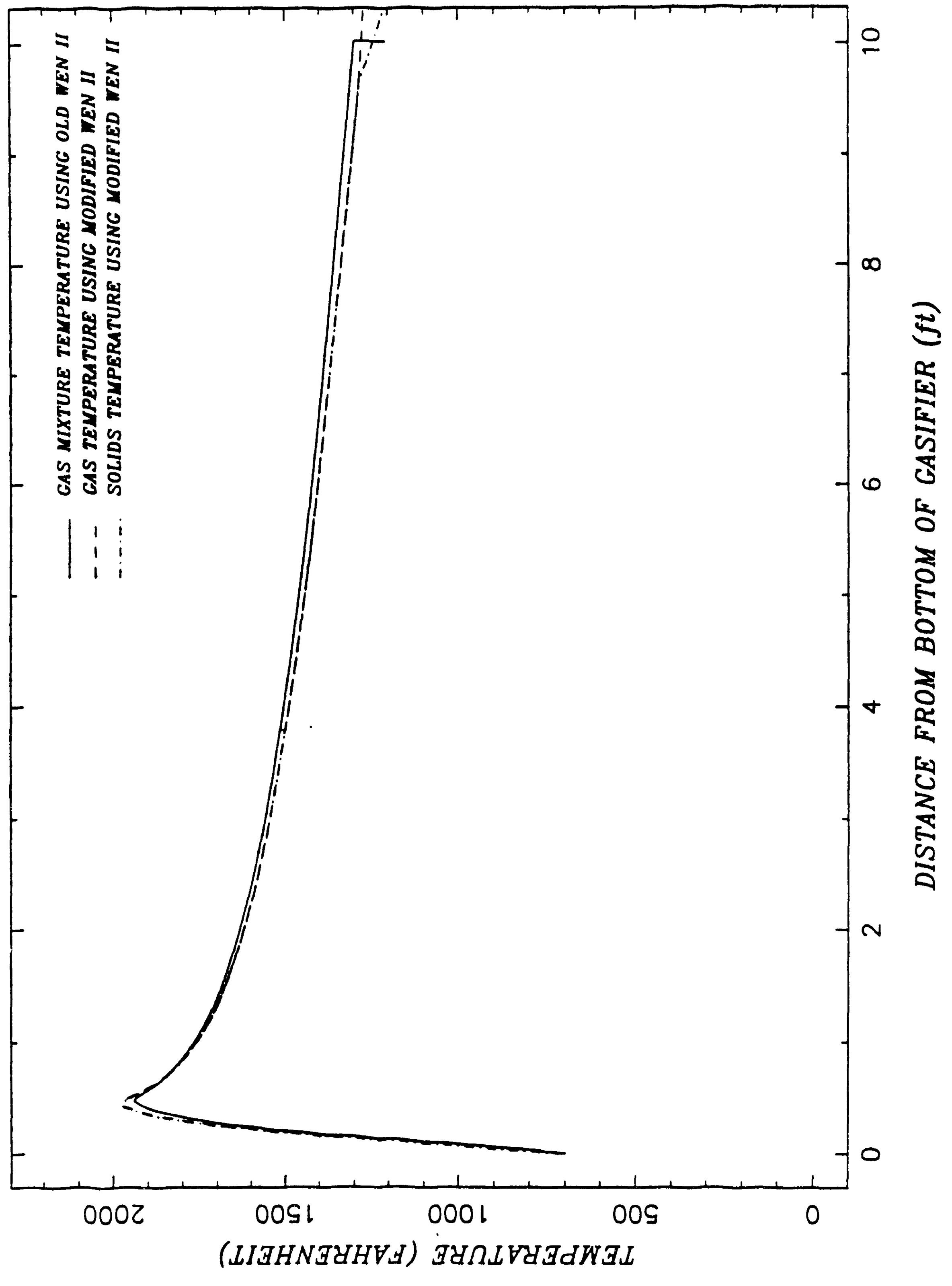


Figure 3.5: Comparison of Temperature Profiles.

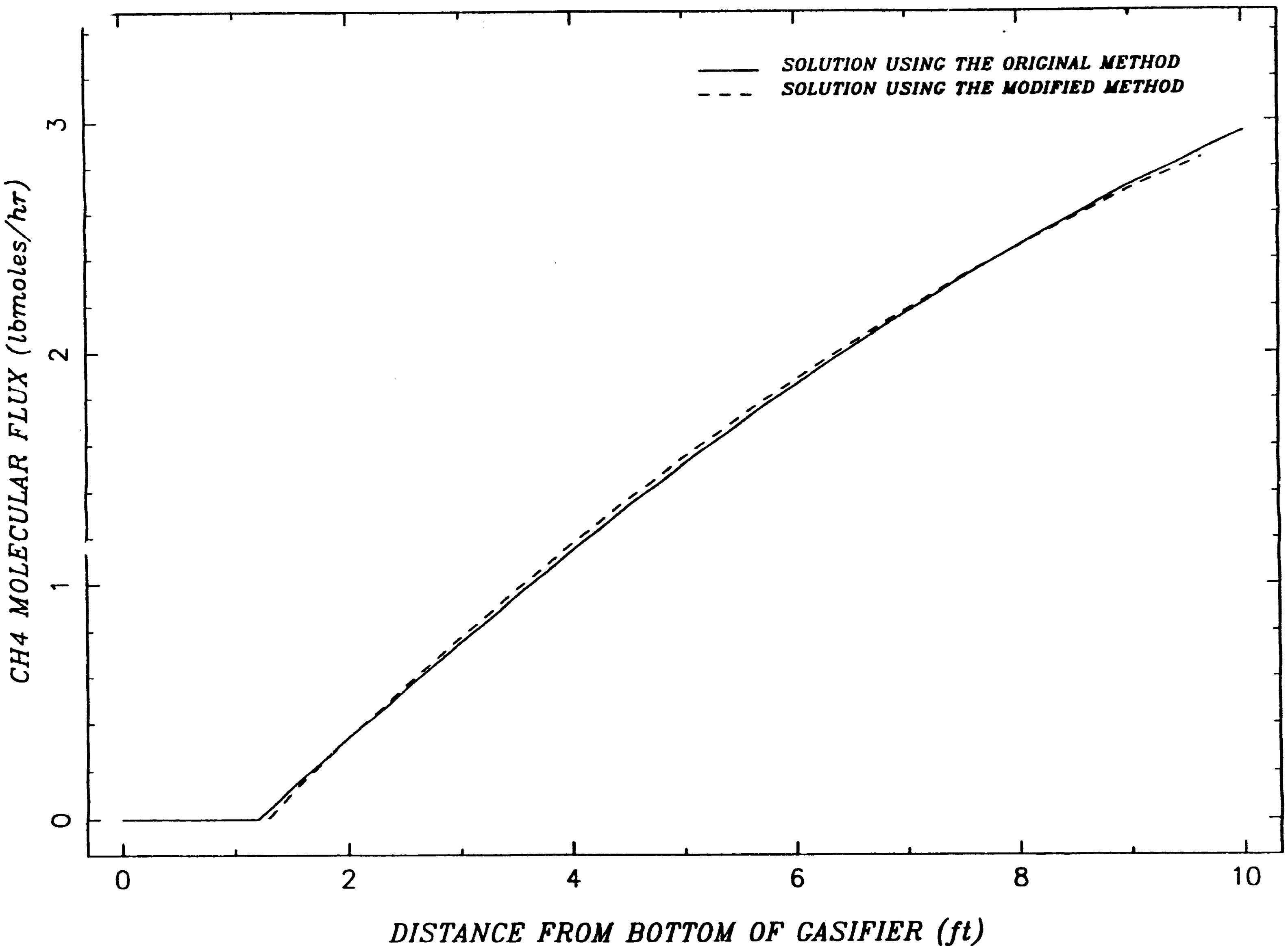
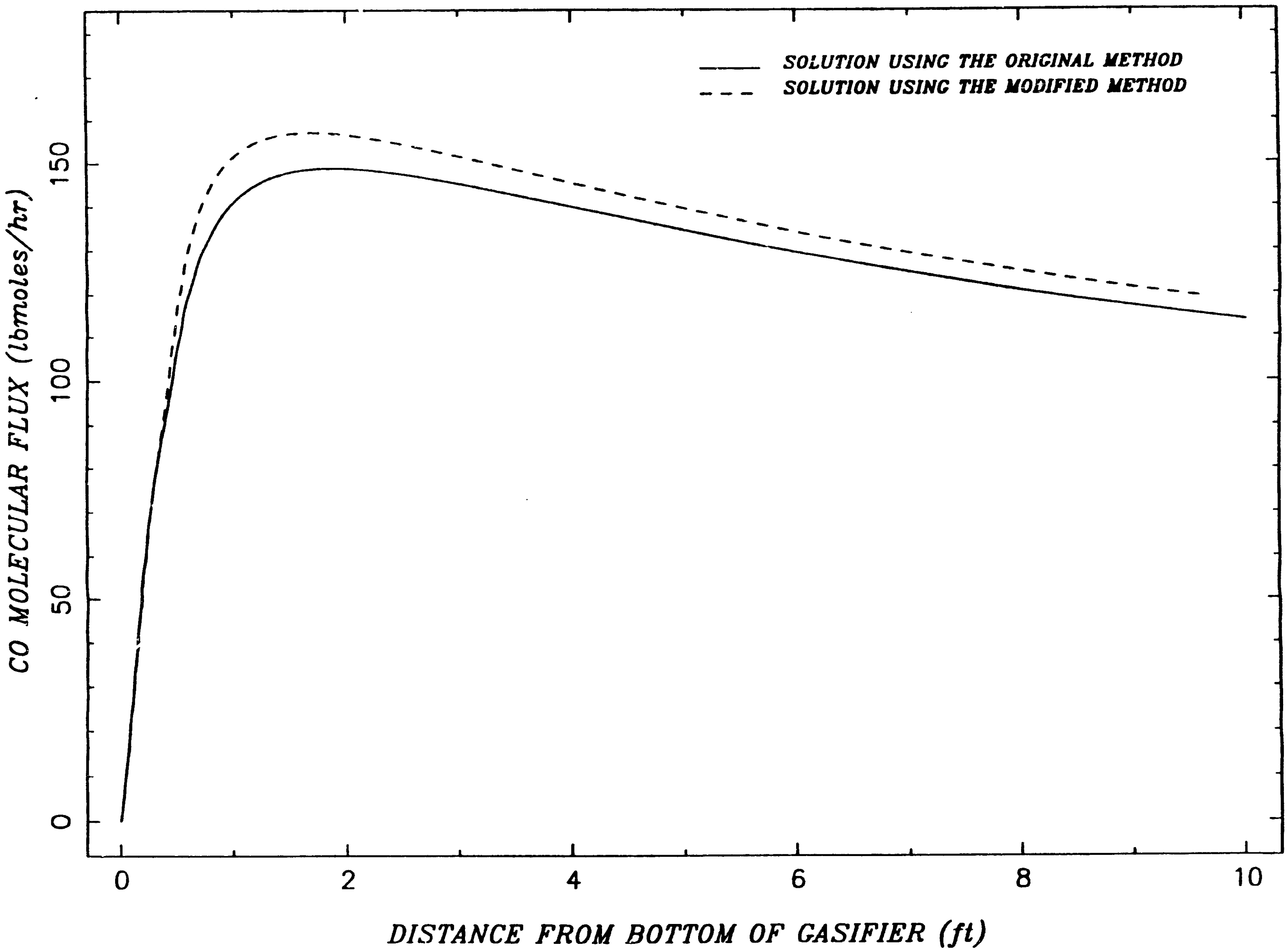


Figure 3.6: Comparision of Methane, CH_4, Profiles.



3.7: Comparison of Carbon Monozide, CO, Profiles.

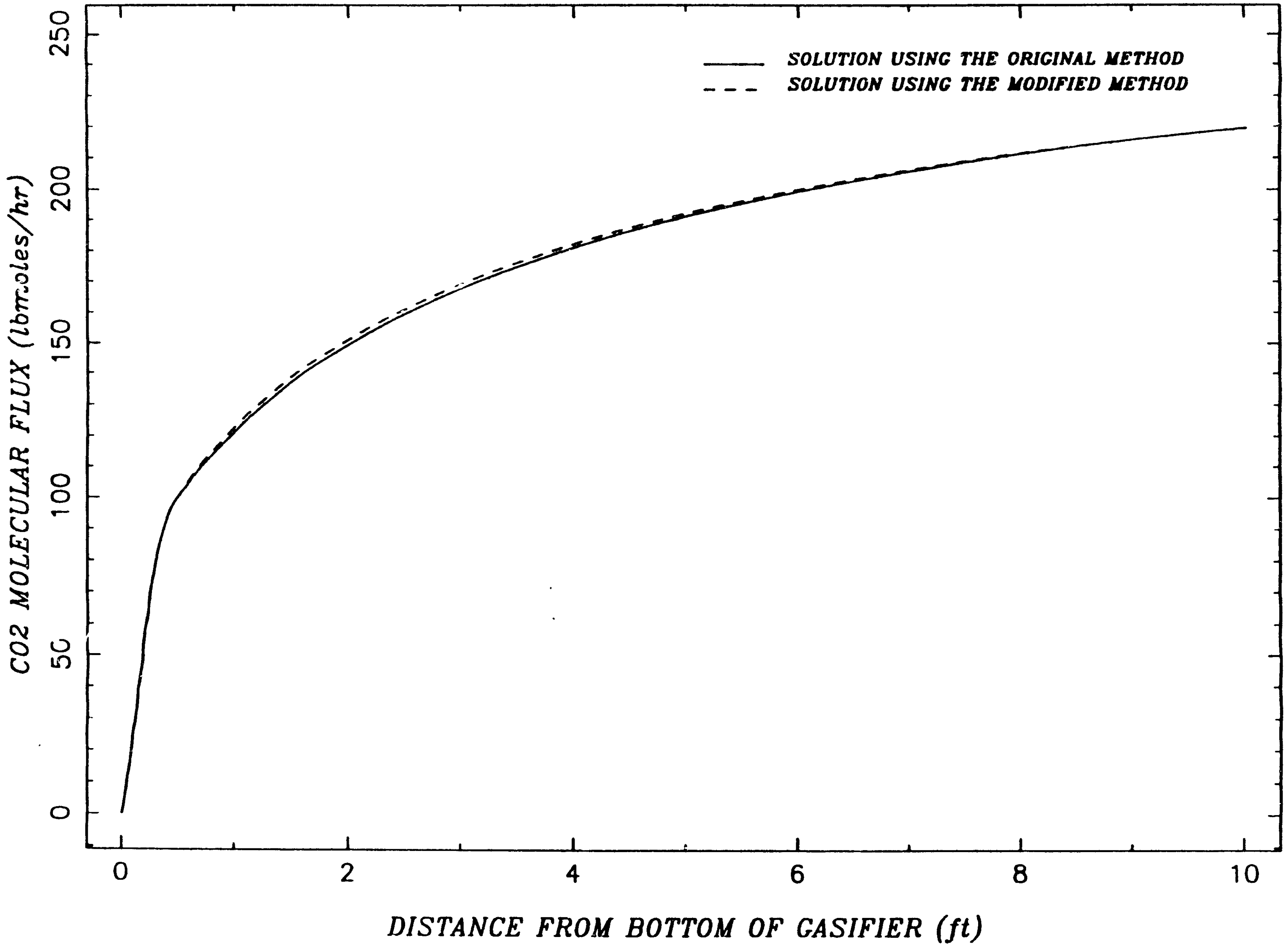


Figure 3.8: Comparison of Carbon Dioxide, CO_2, Profiles.

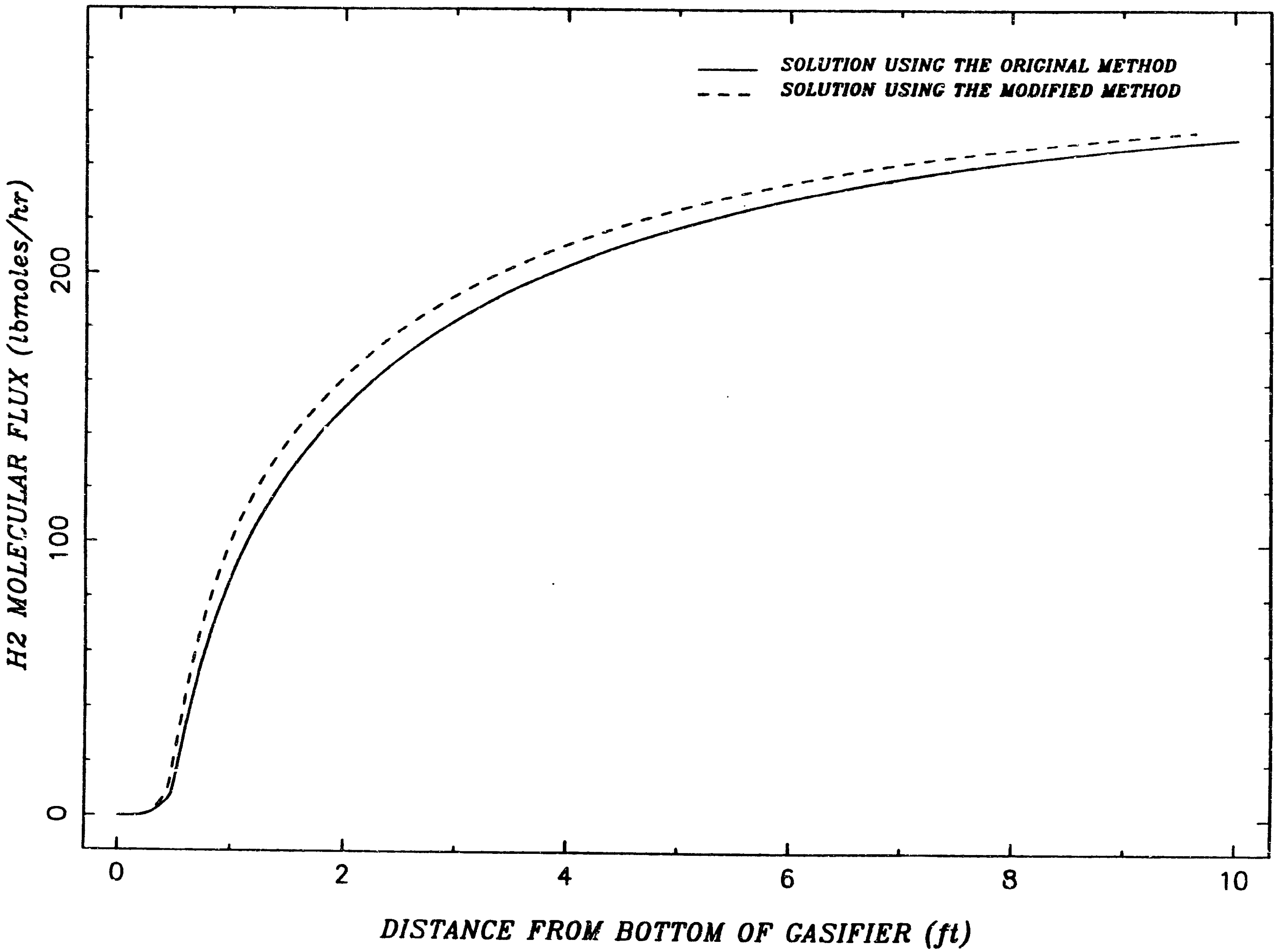


Figure 3.9: Comparison of Hydrogen, H_2, Profiles.

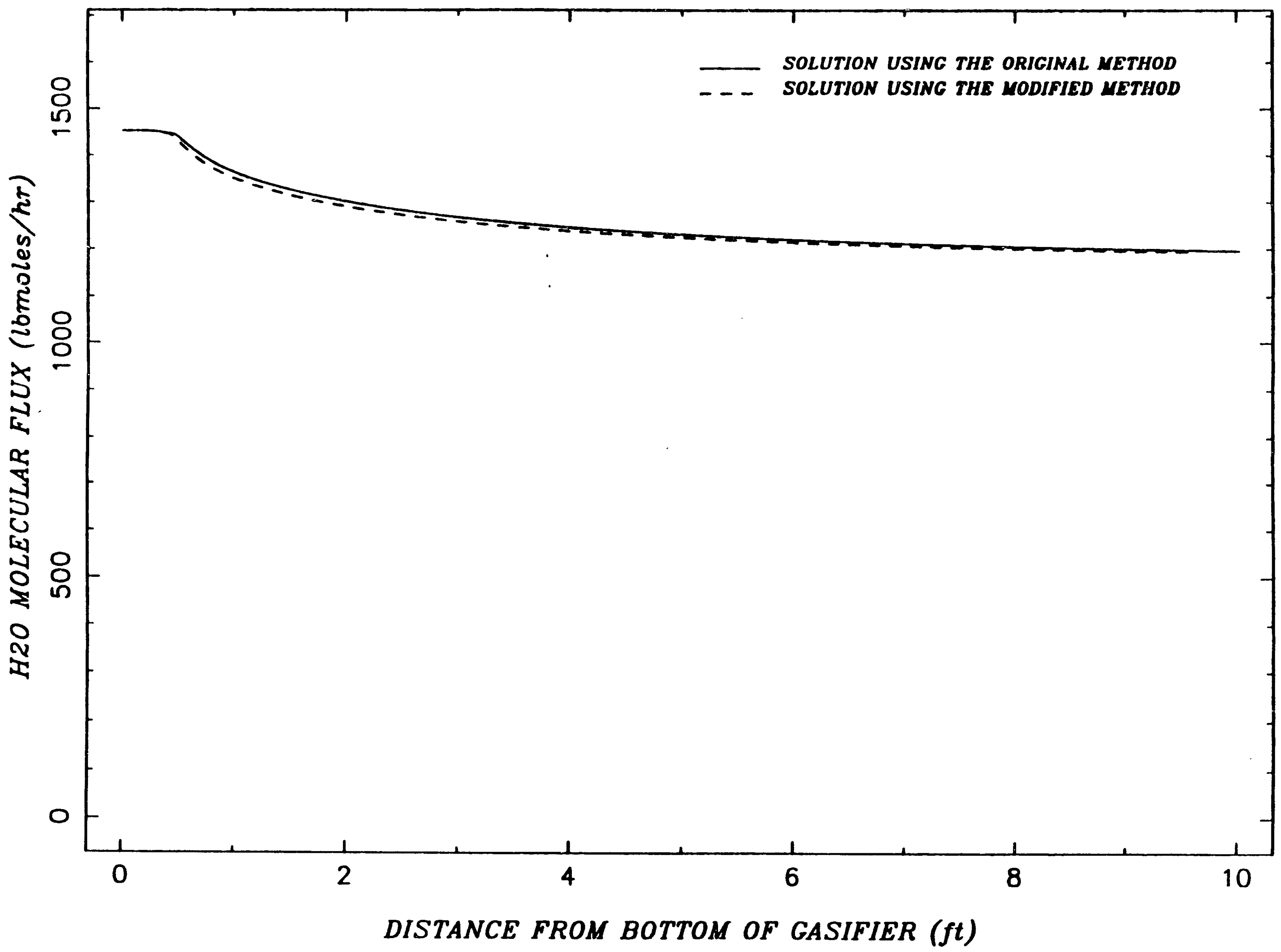


Figure 3.10: Comparison of Water/Steam, H_2O, Profiles.

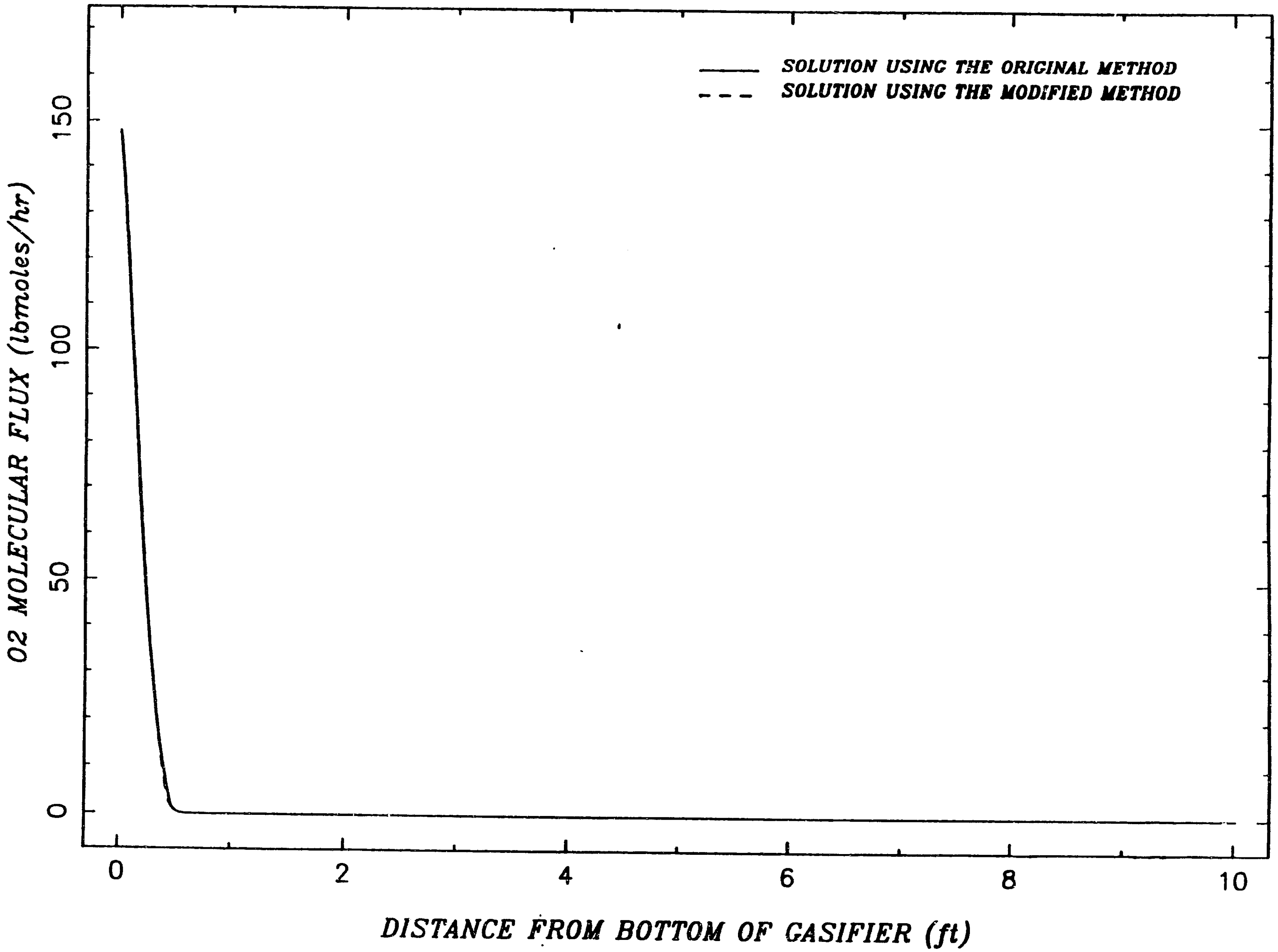


Figure 3.11: Comparison of Oxygen, O_2, Profiles.

Figures 3.12 through 3.15 show the total net tar plots and the instantaneous net tar generation plots for both versions. These plots compare the tar flow through the surface to the tar generated inside the particle. The original version of Wen II has a large discrepancy between the tar generated in the particle and the flow through the surface. Figures 3.14 and 3.15, which are the plots for the modified version, show very good agreement between the tar generated in the particle and tar flow through the surface.

Figures 3.16 through 3.27 show the tar, gas, and inerts mass fluxes and concentraions at various times for both versions. As seen in these figures, the time for devolatilization in the modified version is much longer than that of the original version. This time difference can be attributed facts the modified version used the actual coal diameter and accounted for coal particle heat up. As seen in Figure 3.25, the tar generation becomes zero in about a fourth of the time that it takes the particle to heat up to the gasification temperature. This time used in the heating of the particles affects the overall performance of the gasifier.

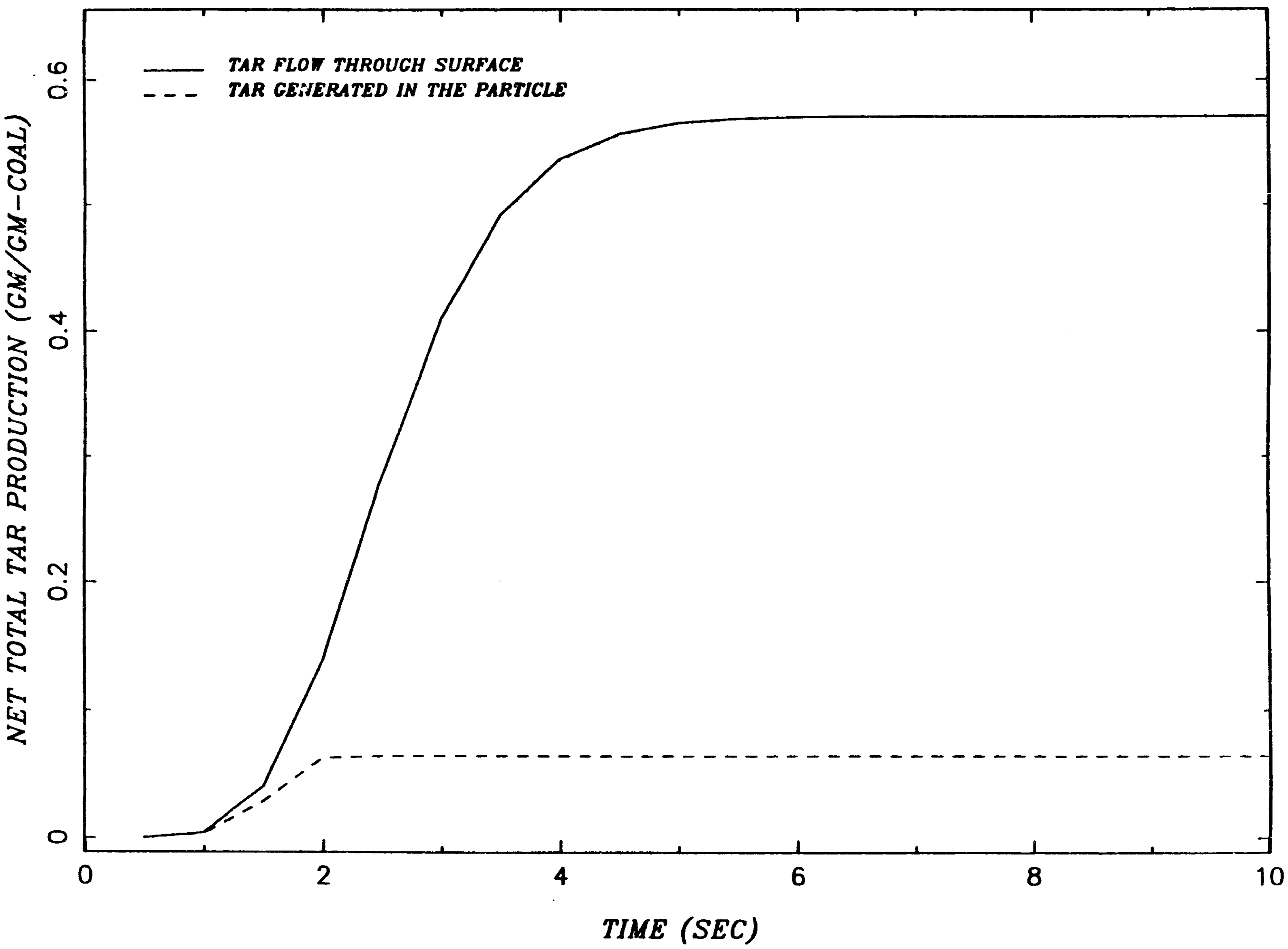


Figure 3.12: Comparison of Total Net Tar Generation for Flow through the Particle Surface Versus Generation Inside the Particle for the Original Wen II Model.

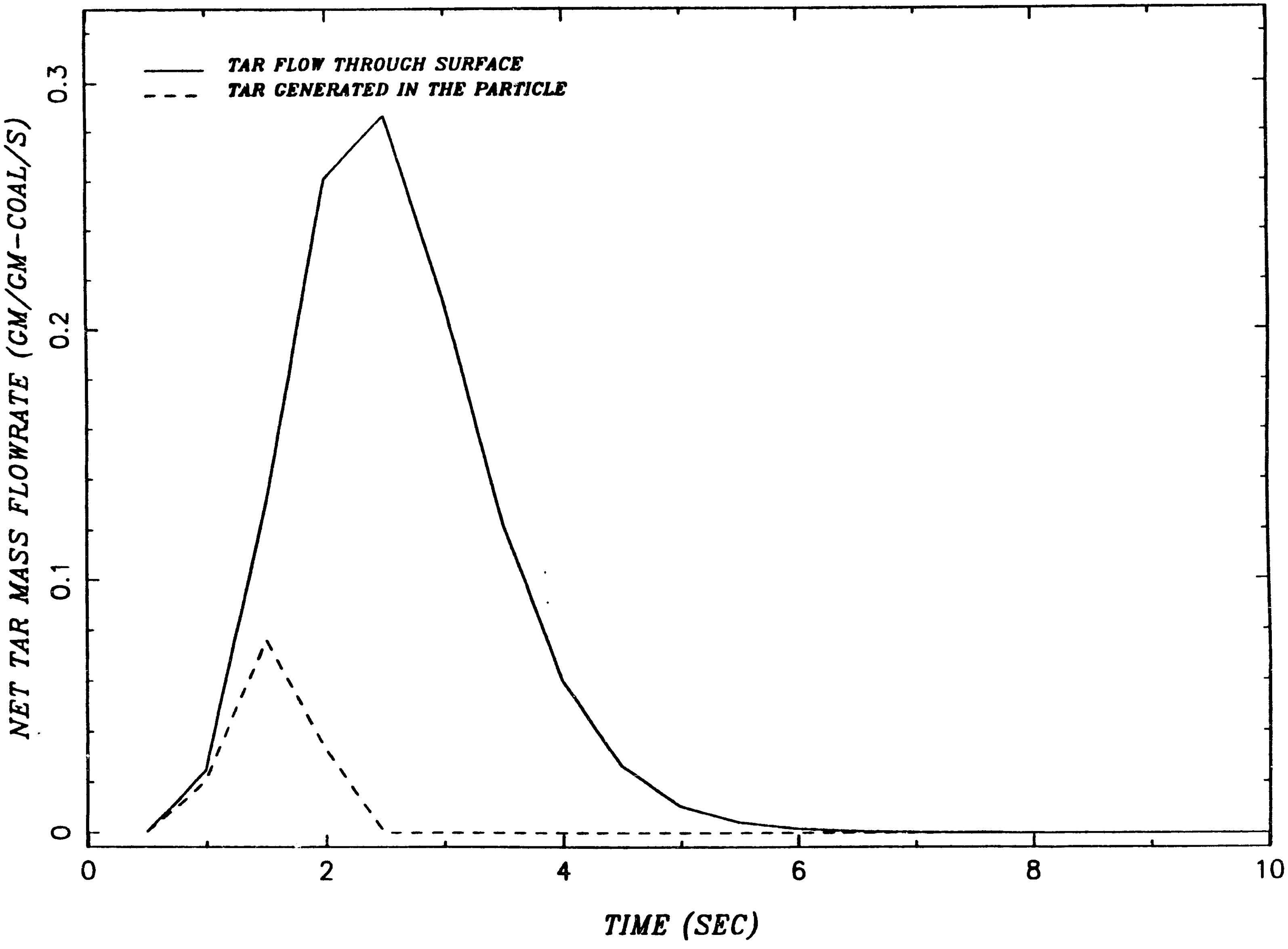


Figure 3.13: Comparison of Instantaneous Net Tar Generation for Flow through the Particle Surface Versus Generation Inside the Particle for the Original Wen II Model.

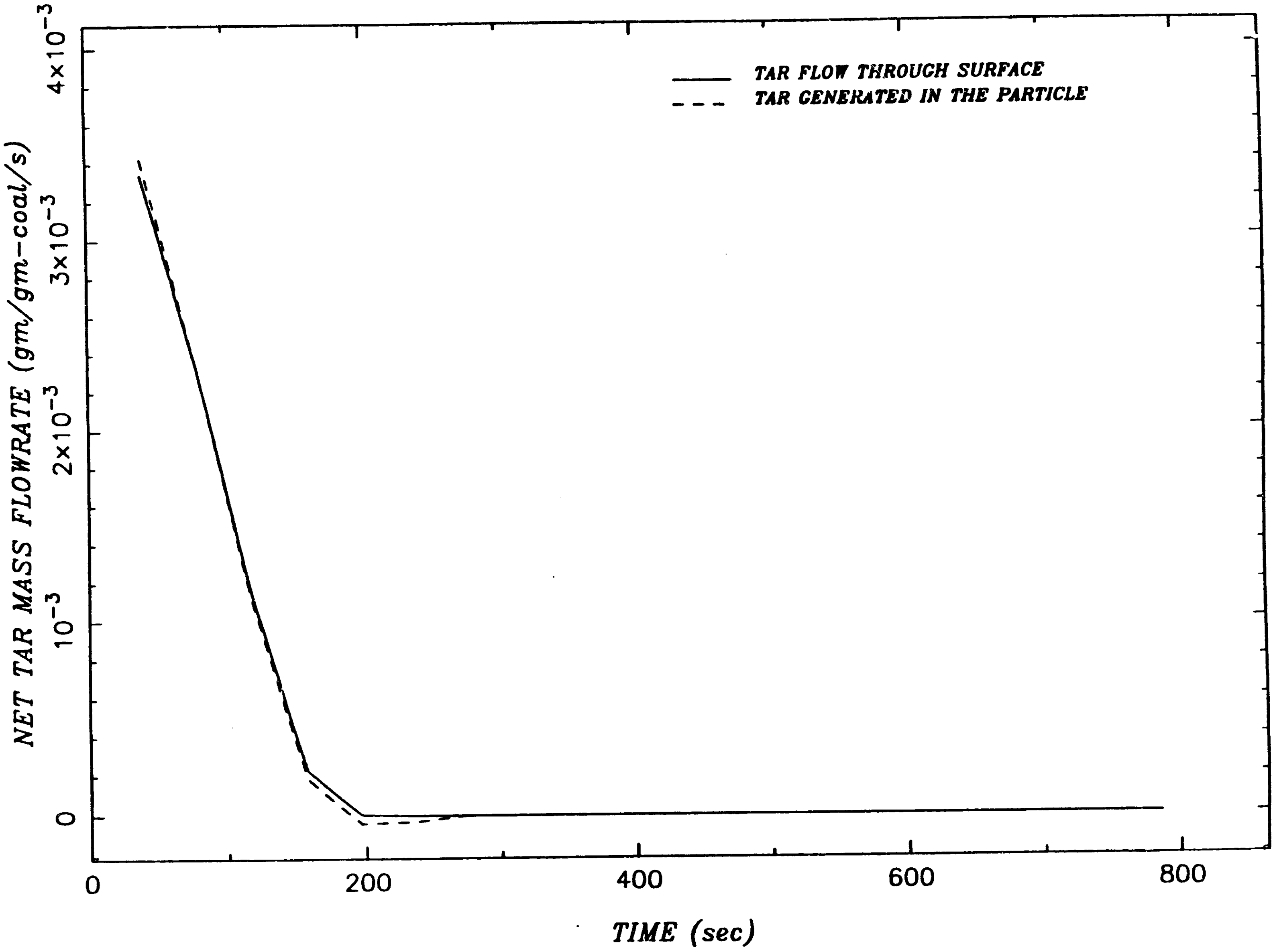


Figure 3.14: Comparison of Total Net Tar Generation for Flow through the Particle Surface Versus Generation Inside the Particle for the Modified Wen II Model.

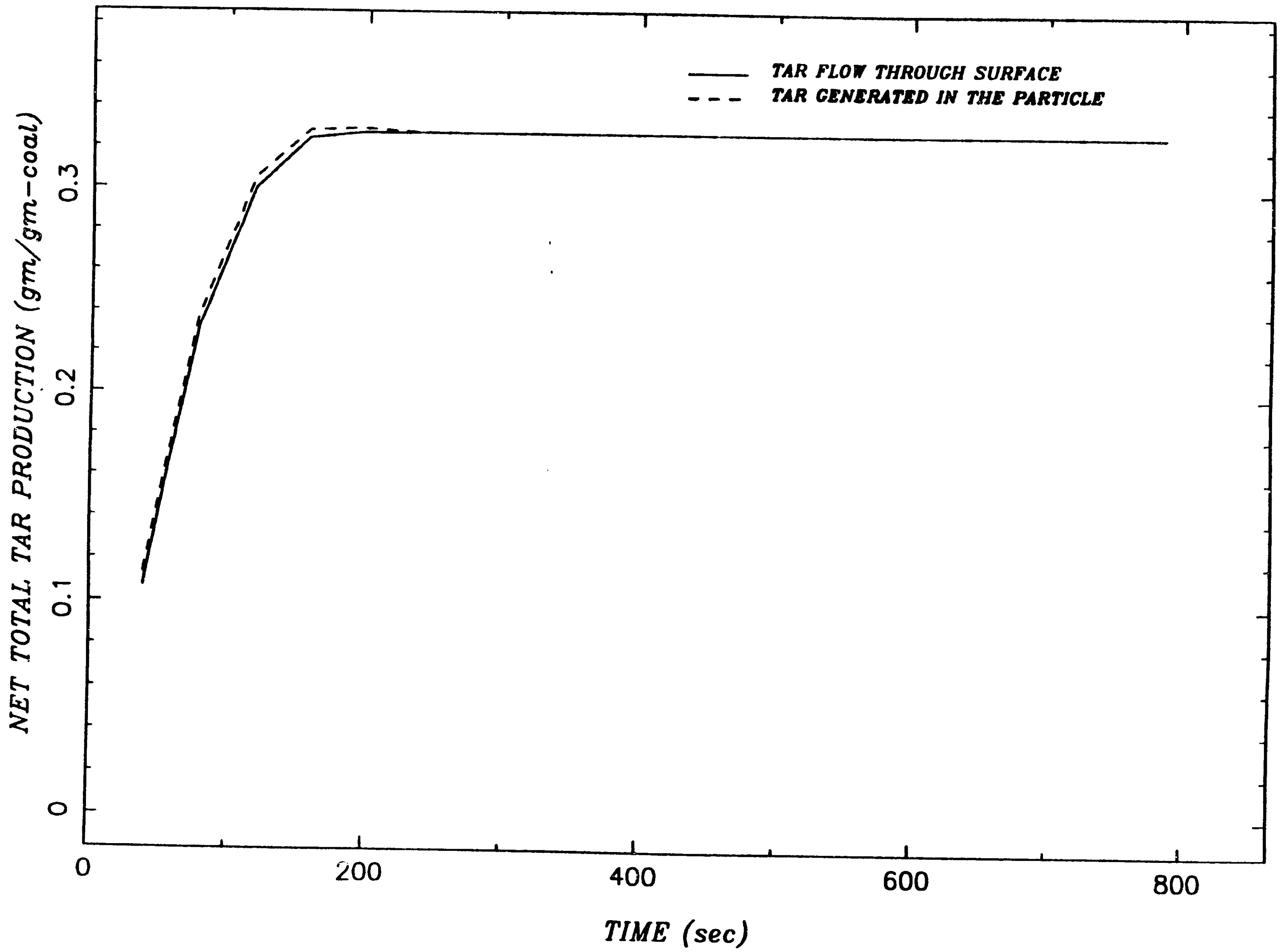


Figure 3.15: Comparison of Instantaneous Net Tar Generation for Flow through the Particle Surface Versus Generation Inside the Particle for the Modified Wen II Model.

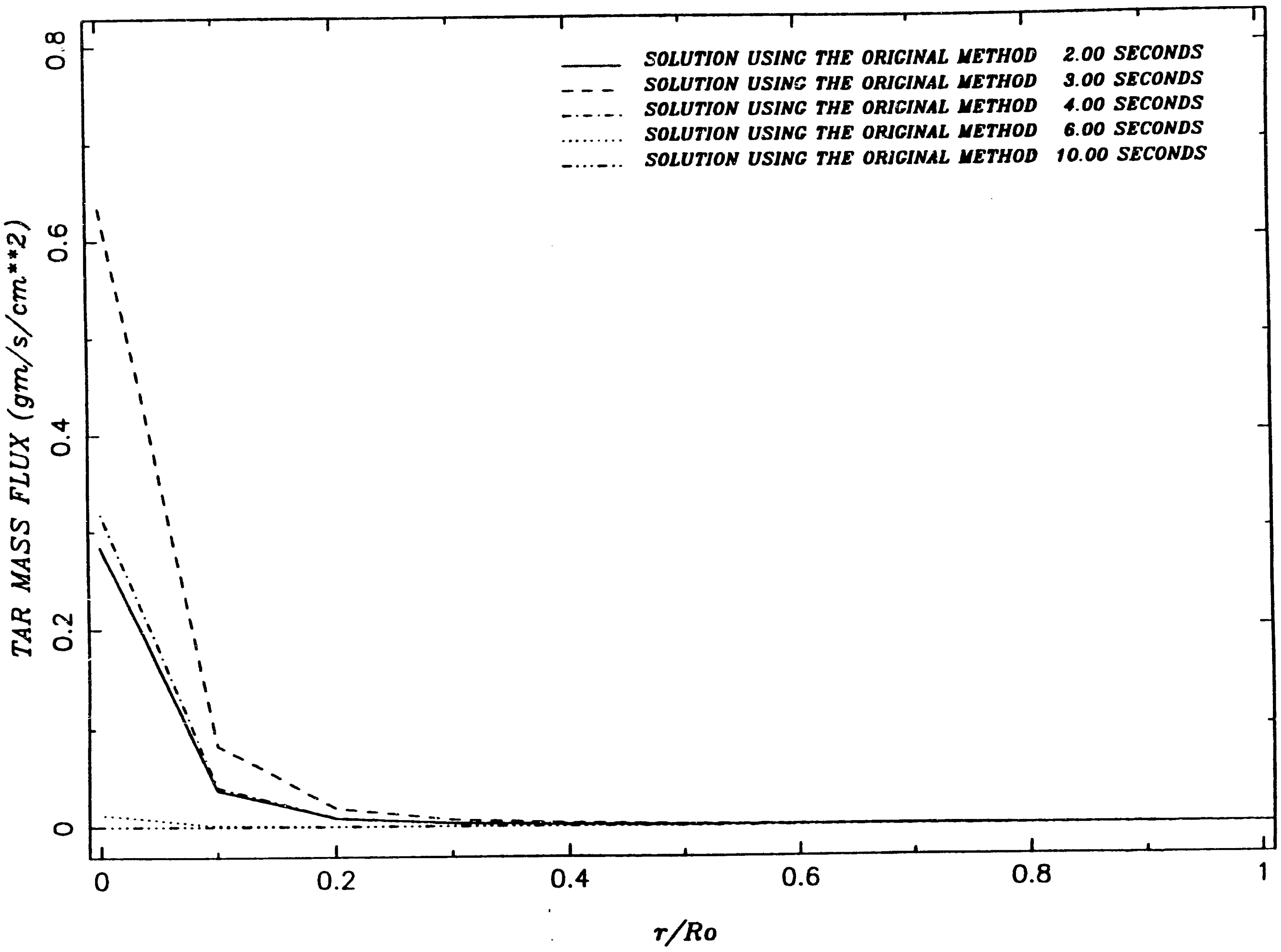


Figure 3.16: Comparison of Tar Mass Flux at Various Times for the Original Wen II Model.

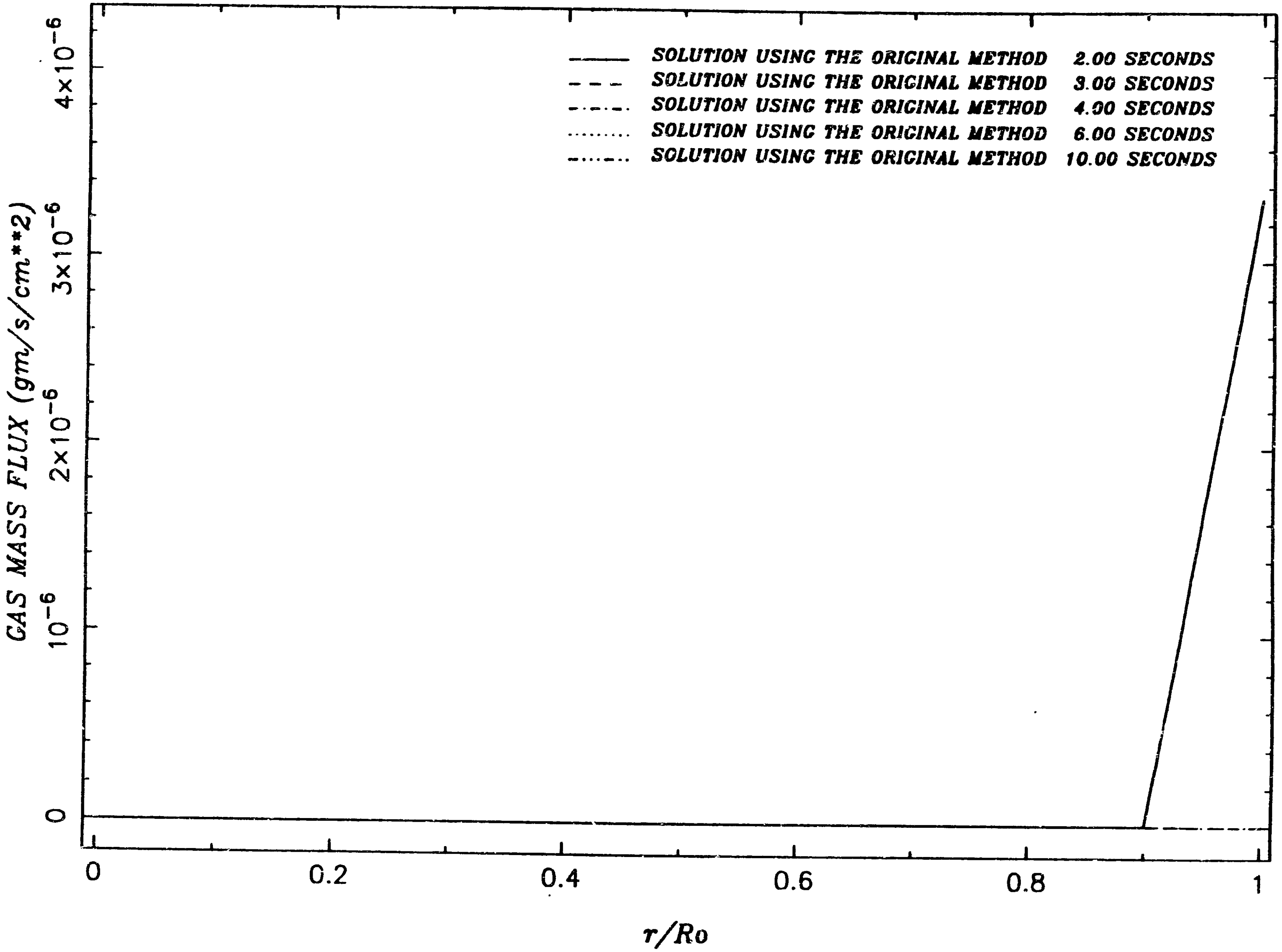


Figure 3.17: Comparison of Gas Mass Flux at Various Times for the Original Wen II Model.

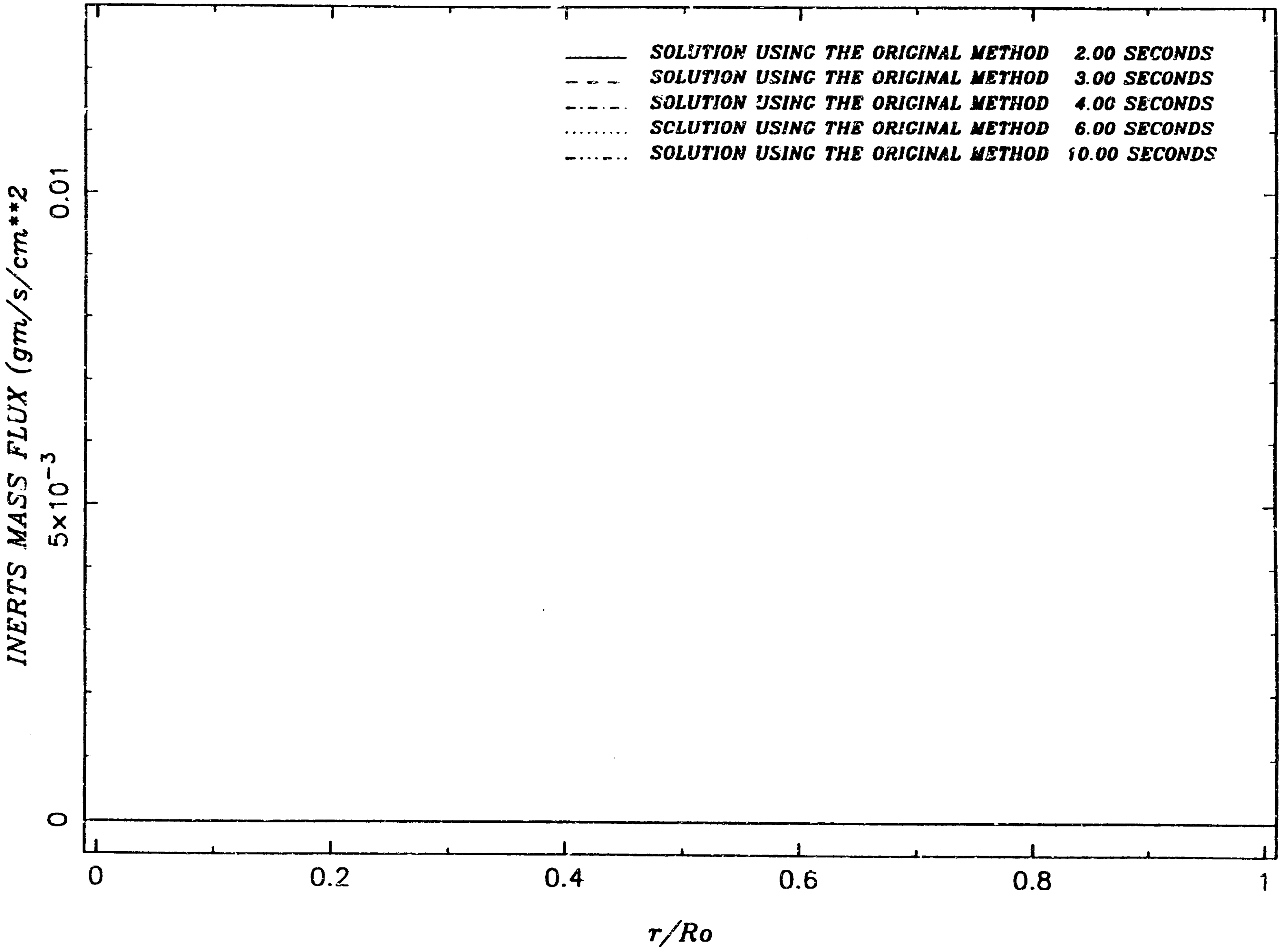


Figure 3.18: Comparison of Inerts Mass Flux at Various Times for the Original Wen II Model.

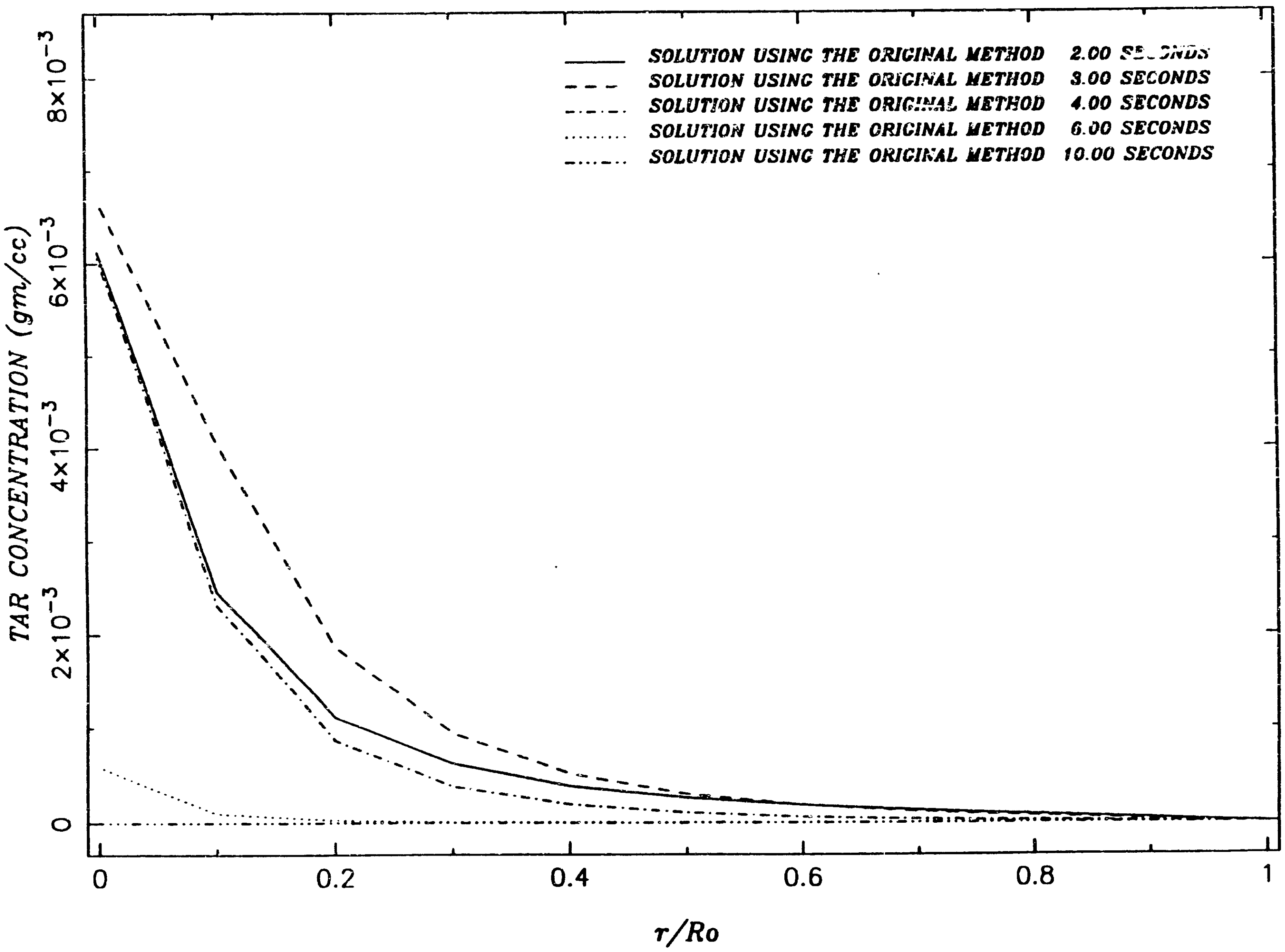


Figure 3.19: Comparison of Tar Concentration at Various Times for the Original Wen Model.

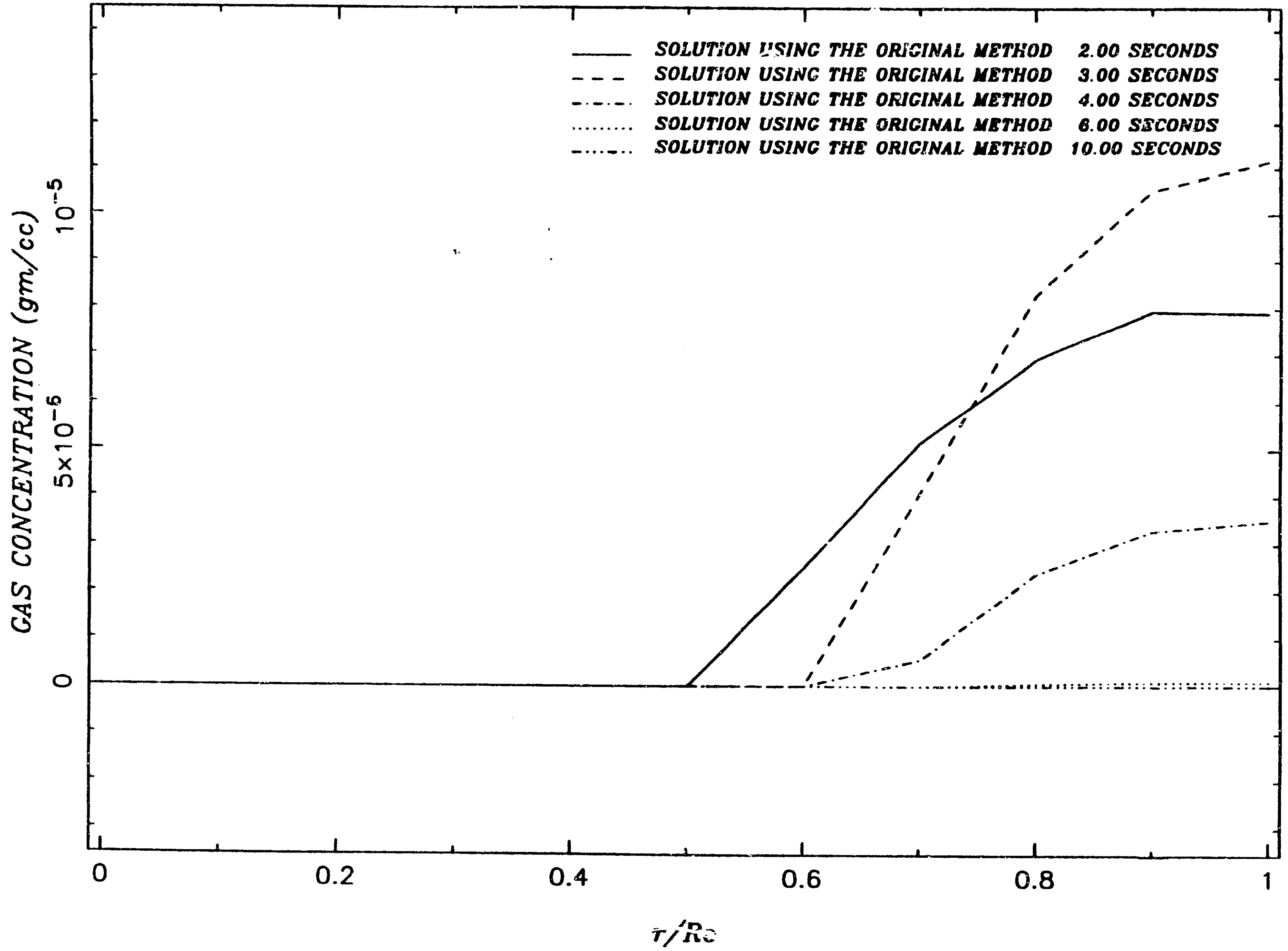


Figure 3.20: Comparison of Gas Concentration at Various Times for the Original Wen II Model.

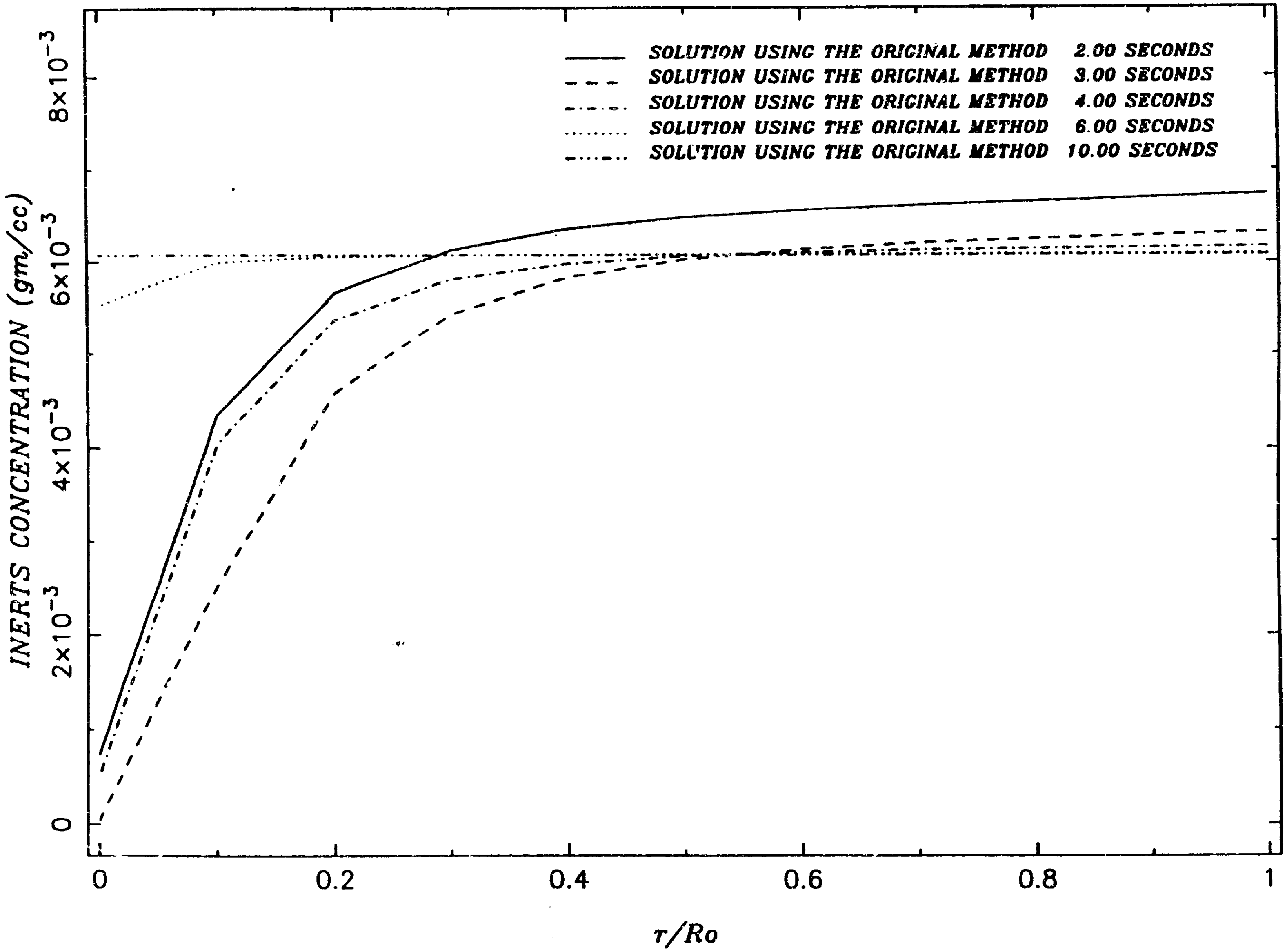


Figure 3.21: Comparison of Inerts Concentration at Various Times for the Original Wen II Model.

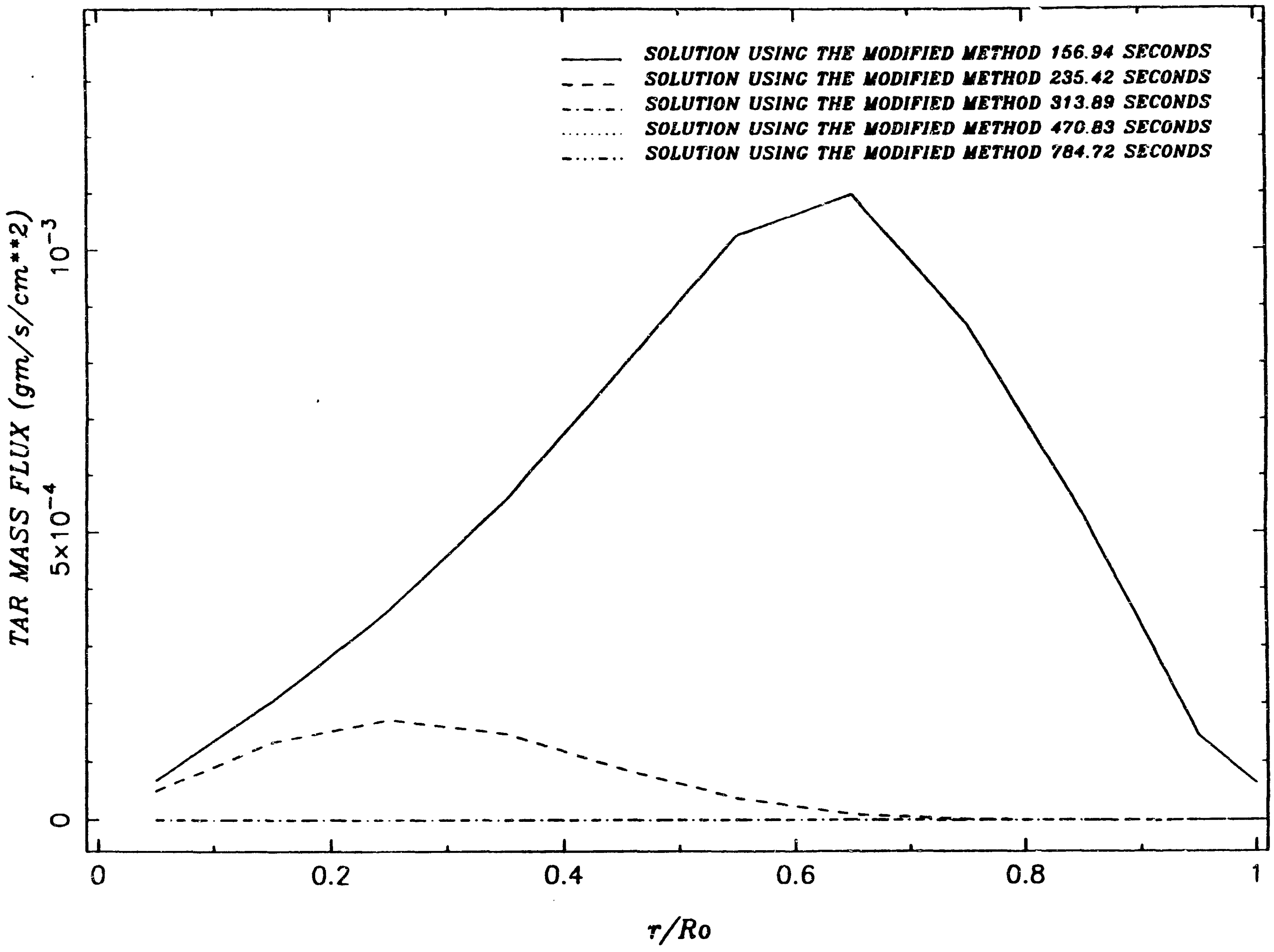


Figure 3.22: Comparison of Tar Mass Flux at Various Times for the Modified Wen II Model.

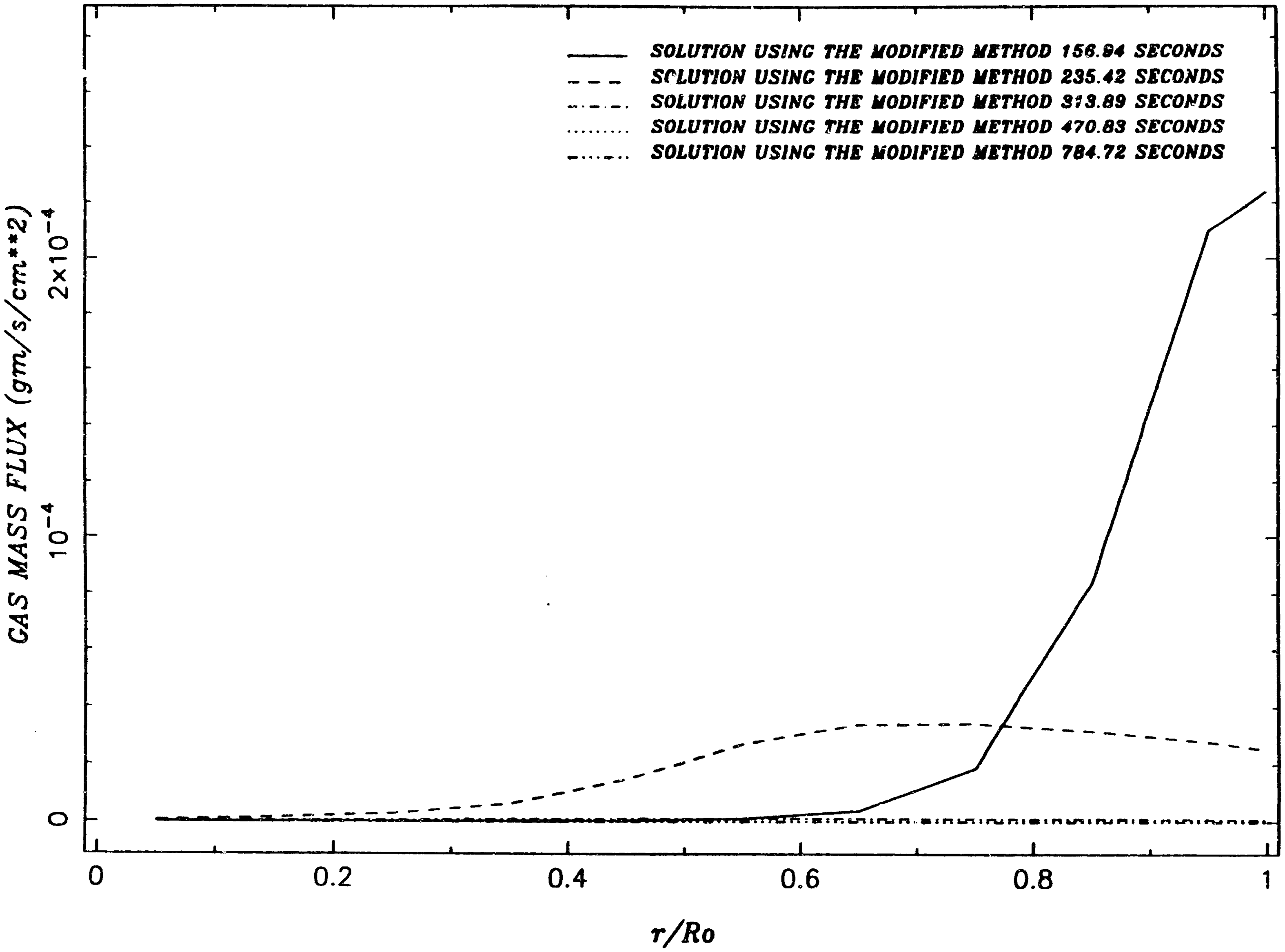


Figure 3.23: Comparison of Gas Mass Flux at Various Times for the Modified Wen II Model.

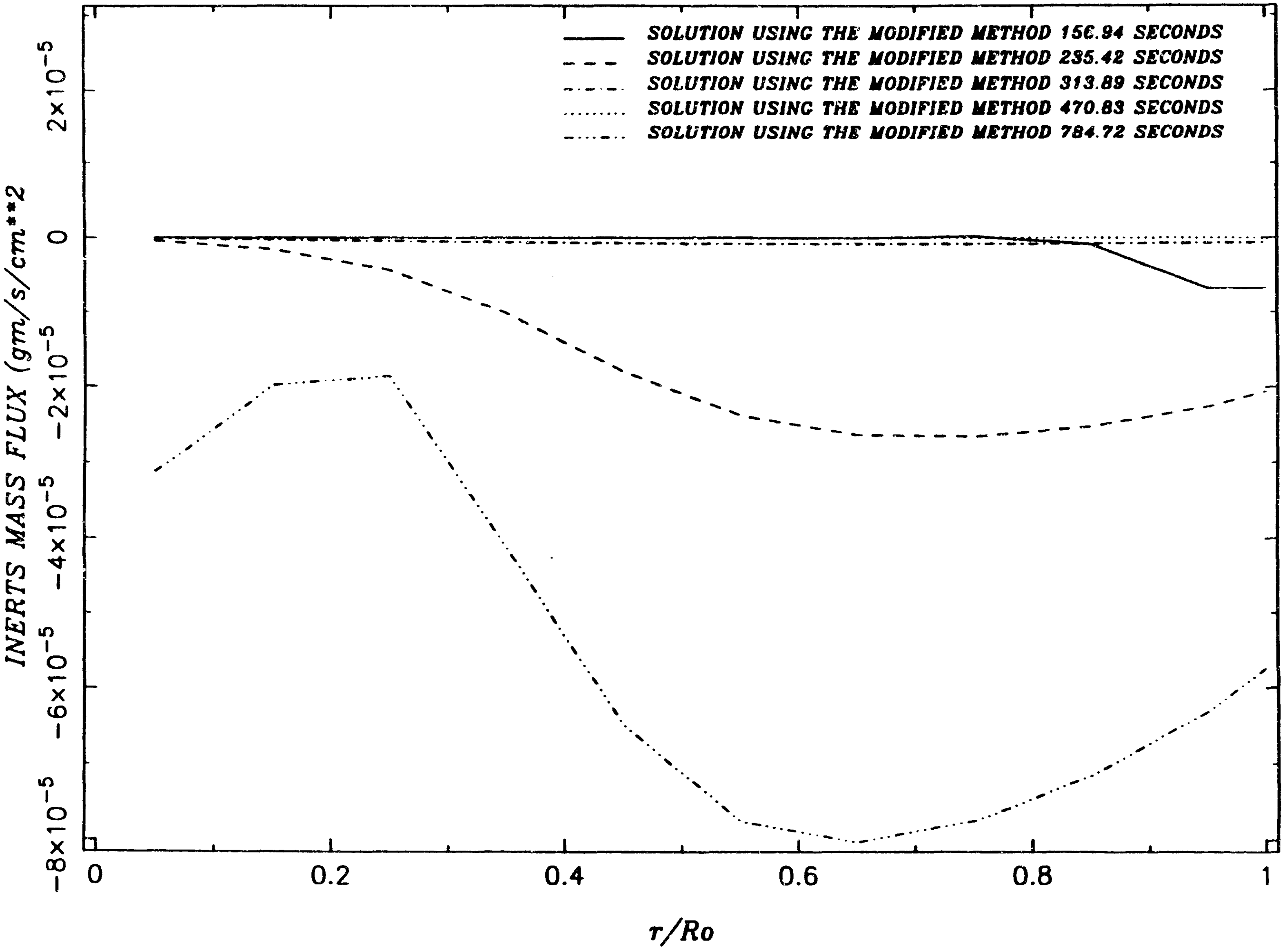


Figure 3.24: Comparison of Inerts Mass Flux at Various Times for Modified Wen II Model.

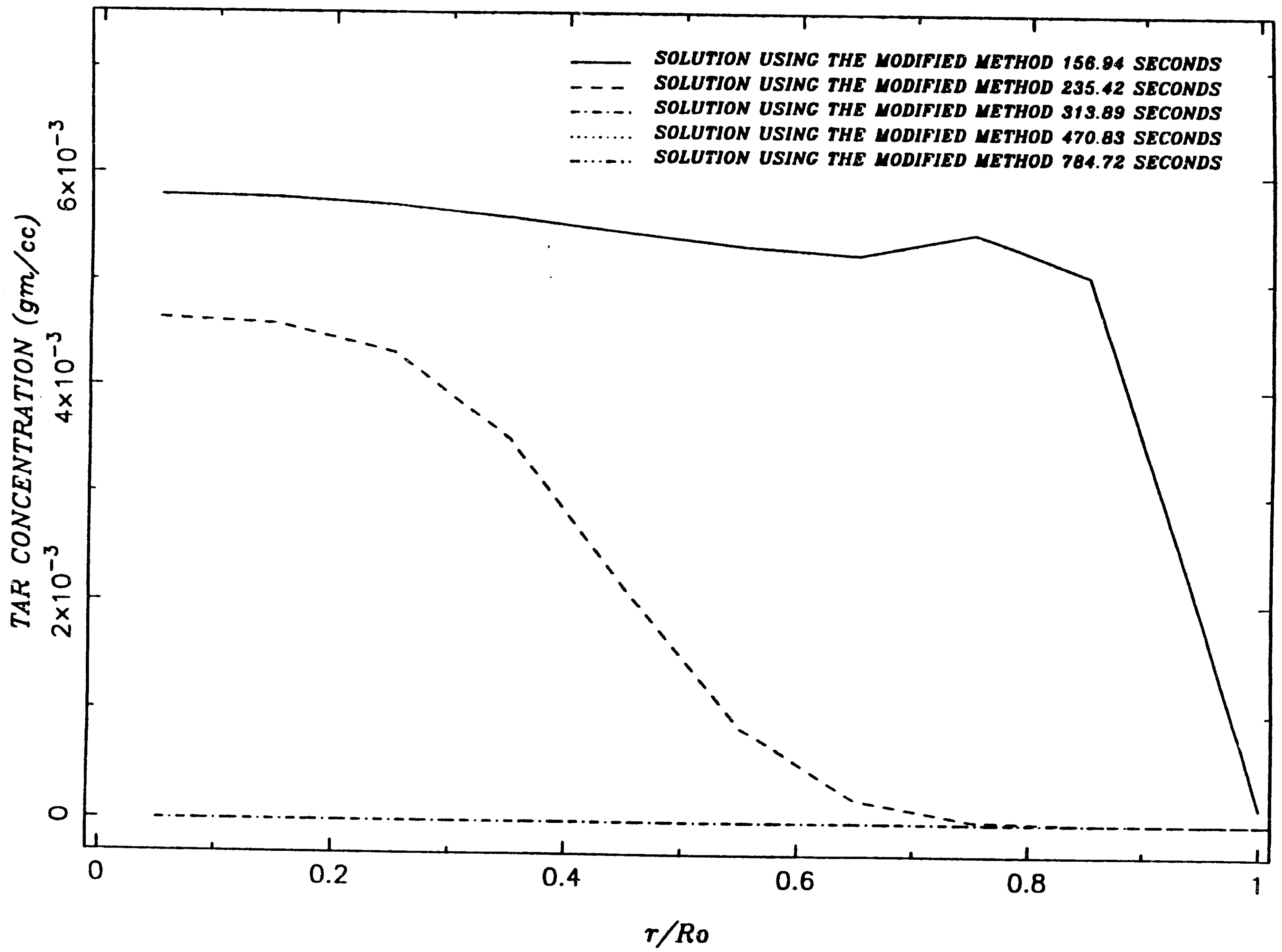


Figure 3.25: Comparison of Tar Concentration at Various Times for the Modified Wen II Model.

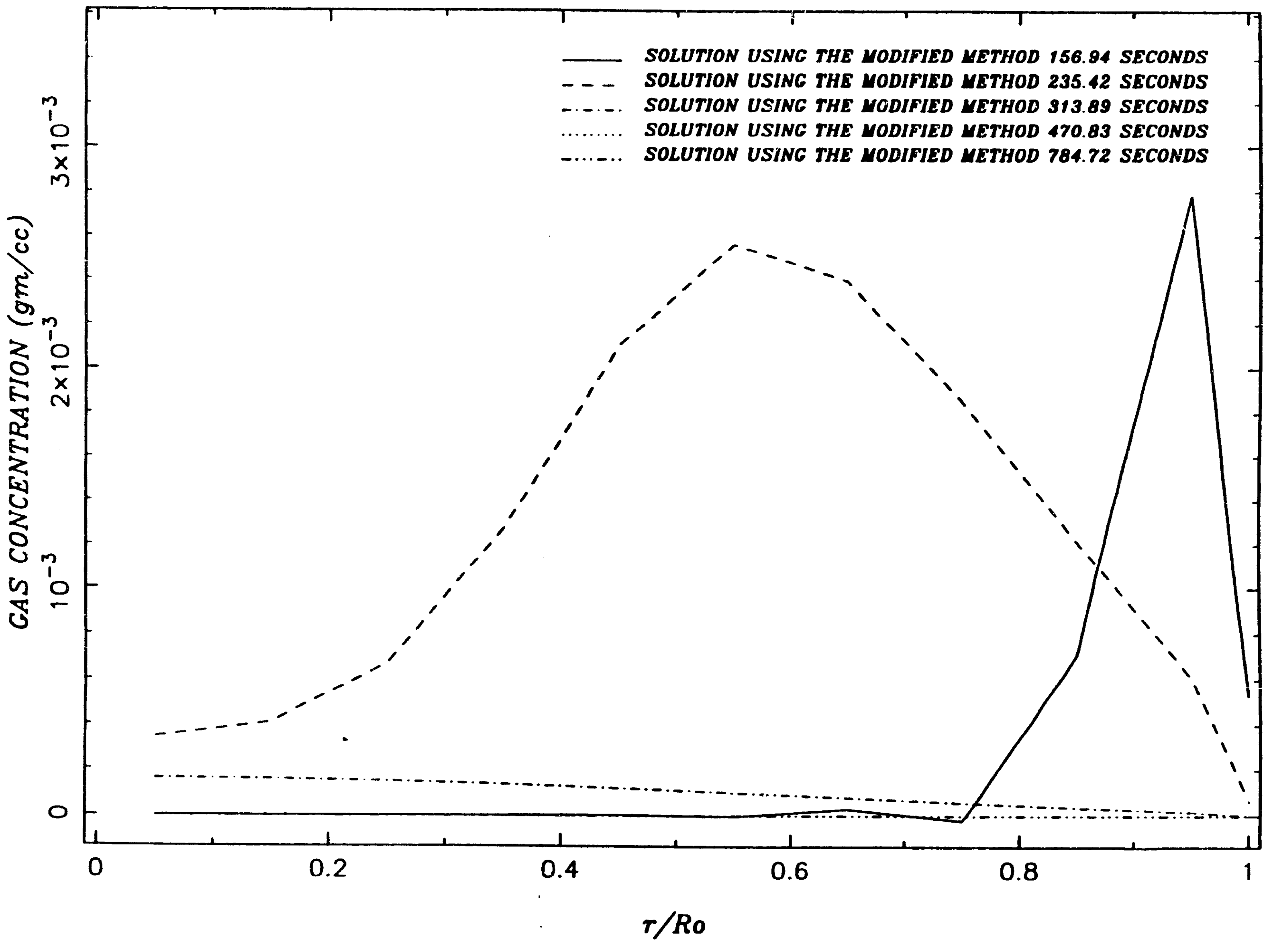


Figure 3.26: Comparison of Gas Concentration at Various Times for the Modified Wen II Model.

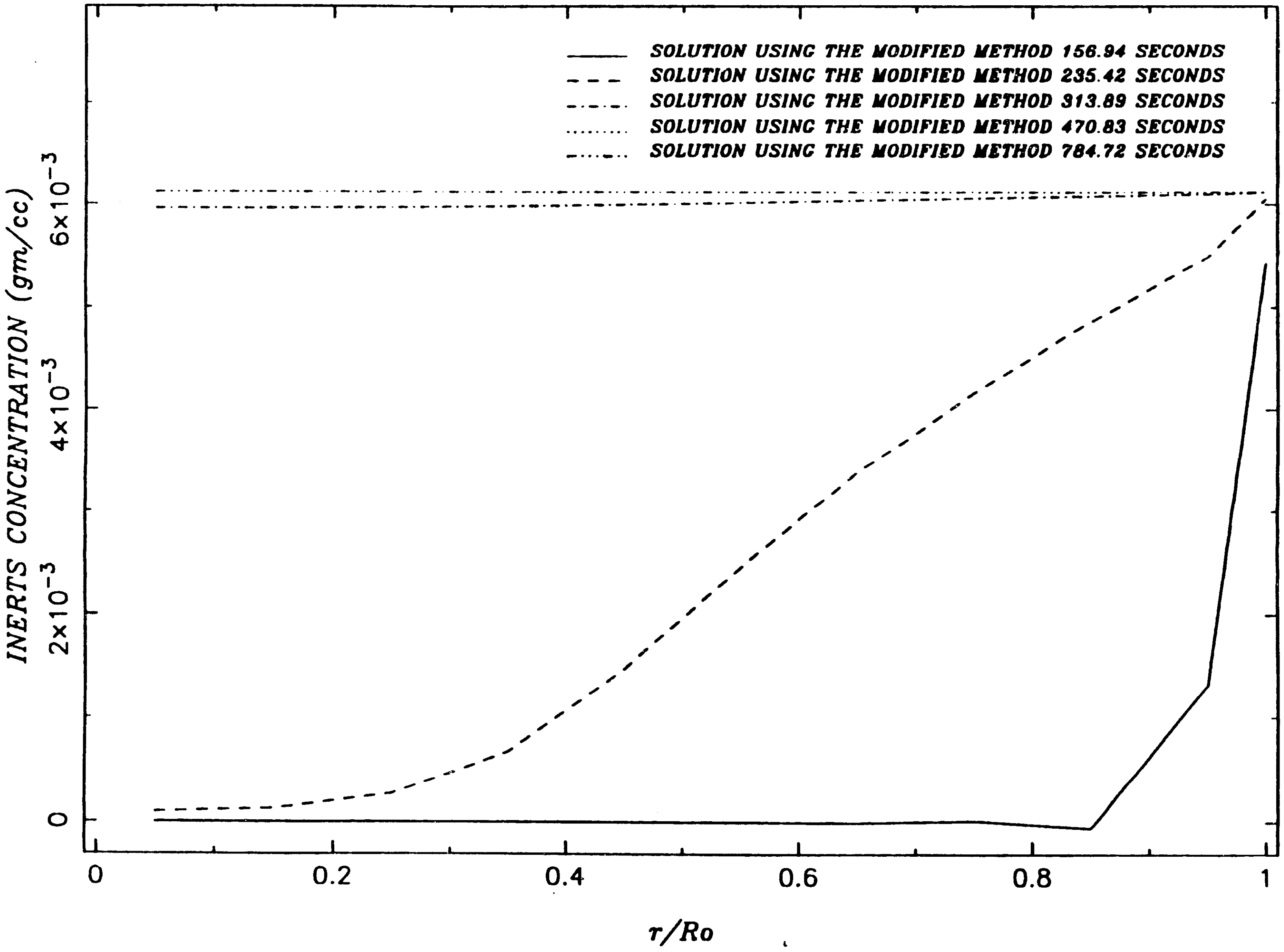


Figure 3.27: Comparison of Inerts Concentration at Various Times for the Modified Wen II Model.

3.4.2 GASIFIER PERFORMANCE

In Cases 3 through 12, an air-blown Lurgi Mark IV gasifier was modeled using Illinois #6 as the feed coal. These cases were run as a parametric study on the effect of feed coal size, gasifier bed height, air inlet temperature, and steam inlet temperature. Table 3.3 lists the common input data for Cases 3 to 12, specific to a Lurgi Mark IV and Illinois #6 coal.

Table 3.3 Coal Input Data for Cases 3 through 12

Coal Feed Rate, lbs/hr	24981.07

Proximate Analysis of Illinois #6 Coal, Wt %

Moisture	10.23	Volatile matter	34.70
Ash	9.91	Fixed Carbon	45.97

Ultimate Analysis of Illinois #6 Coal, Wt %

C	64.2	H_2	4.3	O_2	8.1
N_2	1.2	S	2.8	H_2O	10.23
Ash	9.10				

Heating Value of Coal, Btu/lb-wet coal	12397.00
Oxygen Content, mole ratio	0.21
Temperature of Coal, °F	70.00
Temperature of Wall, °F	700.00
Pressure, psig	300.00
Bed Diameter, ft	12.40
Heat Transfer Coefficient, Btu/(ft^2 $\cdot$ hr$\cdot$°R)	17.00
Bed Voidage	0.40

In Cases 3 to 7, the input parameters for steam feed rate in Table 3.4 were provided by our sponsor, CRS Sirrine, specific to their IGCC system. The inlet temperature of the steam is the saturation temperature at 300 psig, and the inlet air temperature was determined as if the air were compressed from atmospheric pressure to 300 psig with no intercooling. Table 3.4 list the results of this parametric case study.

In Table 3.5 it is worth noting that the size of the coal particle has a direct impact on the amount of tar produced. The larger particles of coal produced less tar than the smaller

Table 3.4 Input Data for Cases 3 through 7

Steam Feed Rate, lbs/hr					36472.36
Air Feed Rate, lbs/hr					48713.09
Temperature of Steam, °F					420.00
Temperature of Air, °F					900.00
	CASE NUMBER				
PARAMETERS	3	4	5	6	7
Initial Coal Particle Size, in	0.50	1.00	1.50	1.00	1.00
Bed Height, ft	8.5	8.5	8.5	7.0	10.00

ones. A reason for this effect is that the larger coal particles take longer to heat up, and more tar cracking occurs. Also, the size of the coal particles affects the heating value of the gas. The larger particles increased the heating value of the coalgas as an effect of the reduced tar production. However, the larger particles reduced the amount of carbon conversion for the gasifier. The larger particles take longer to heat up to the gasification temperatures, allowing less time for the gasification process to occur. The larger coal particles reduce the effective height of the gasifier. Table 3.5shows how the column height needed for devolatilization depends on the particle size. The additional time for the larger particles to devolatilize reduces the effective height of the gasifier. The devolatilization time will also be affected by the amount of moisture in the coal; i.e. wet coal will take longer to heat up than will dry coal.

The bed height affects the amount of carbon converted to coalgas and the amount of tar produced. The larger bed heights give the coal a longer time to react with the steam and air to produce the coalgas, increasing the carbon conversion efficiency. The amount of tar produced is related to the temperature in the devolatilization zone. For higher beds, the gas has more time to cool before reaching this zone, causing less tar to be cracked into gas.

In Cases 8 to 12, the input data was modified to simulate water injection into the air stream. The effect of the water injection is to cool the inlet air/steam mixture into the bottom of the gasifier. However, the inlet temperature can not be lowered below the dew point. In Cases 8 to 12 the inlet temperature is about 10 °F above the minimum allowable

Table 3.5 Comparison of Results Cases 3 through 7

COMPARISON PARAMETERS	CASE NUMBER				
Product Gas Composition, mole %	3	4	5	6	7
CO	9.78	10.90	11.80	11.40	10.46
CO_2	8.92	9.13	8.97	8.69	9.47
H_2	18.36	20.66	21.81	20.42	20.77
CH_4	0.07	0.06	0.05	0.05	0.07
H_2O	34.34	31.43	29.99	31.69	31.32
N_2	28.08	27.38	26.94	27.31	27.46
H_2S	0.46	0.44	0.44	0.44	0.45
Amount of Tar, lbs/hr	5444.84	4224.20	3277.89	4002.66	4420.93
Temperature of Exit Gas, $_o$F	1068.15	1108.92	1148.71	1137.76	1089.25
Maximum Temperature, $_o$F	1964.03	1961.63	1946.60	1958.75	1964.06
Carbon Conversion, %	95.72	95.96	94.93	95.15	96.45
Heating Value of Dry Gas, Btu/SCF	143.16	151.19	156.27	152.84	149.62
Heating Value of Wet Gas, Btu/SCF	94.70	104.29	109.80	104.91	103.03
Heat Loss, 10^6 Btu	4.11	3.81	3.40	3.15	4.45
Devolatilization Length, in	2.96	10.14	18.98	10.05	10.43
Devolatilization Time, min	4.47	15.31	28.64	15.17	15.74

temperature at 300 psig at which the air would be saturated. These cases were run making no additional changes to the input data in Cases 3 to 7. The steam flowrates were adjusted until the maximum temperature within the gasifier in this run was same as that of Case 4. The air flow rate was adjusted until the carbon conversion was also nearly the same. The adjusted values appear in Table 3.6as the input data for Cases 8 to 12. The primary purpose of Cases 8 to 12 was to investigate the possibility of reducing the amount of steam introduced into the system.

As seen in comparing Table 3.7 with Table ??, the results indicate that water injection does decrease the steam requirements, and also increases the heating value of the wet gas. The carbon conversion can be increased by increasing the air flow.

Table 3.6 Input Data for Cases 8 through 12

Steam Feed Rate, lbs/hr					27479.18
Air Feed Rate, lbs/hr					51960.63
Temperature of Steam, °F					365.00
Temperature of Air, °F					365.00
	CASE NUMBER				
PARAMETERS	8	9	10	11	12
Initial Coal Particle Size, in	0.50	1.00	1.50	1.00	1.00
Bed Height, ft	8.5	8.5	8.5	7.0	10.00

3.5 Suitability of Model for Predicting Lurgi Gasifier Performace

In this section we shall discuss some of the limitations of the current computer model with regards to its ability to provide accurate and relevant information needed to design an IGCC power plant. We shall begin by reviewing some specific information about a commercial fixed bed coal gasifier, known as the Lurgi Gasifier. An air blown Lurgi will probably be employed in the forthcoming IGCC demonstration plant. By reviewing the design of this gasifier, we wish to better define the requirements of the computer model and to point out potential problem areas which our computer model will not be capable of analyzing.

The Lurgi Gasifier reportedly [10 - 13] will take all types of coal feedstock, but requires an agitator and/or increased steam rate for strongly caking coals. The size of the coal is normally from 0.125 to 2.0 inches in diameter with up to 10% coal fines. The coal feed rate is in the range of 100 to 400 lb/hr-ft^2. Crushing and sizing may be required depending on the coal, and drying may be required to reduce the moisture content. Partial oxidation of the feed coal may also be required for strongly caking coals.

In oxygen-blown operation, 1.01 to 3.24 kg of steam per kg of coal are required, while as little as 0.6 kg of steam/kg- coal are required for air-blown operation. The gasifier requires from 0.23 to 0.61 kg of pure oxygen/kg-coal or from 1.3 to 1.9 kg of air/kg-coal for operation.

Table 3.7 Comparison of Results Cases 8 through 12

COMPARISON PARAMETERS	CASE NUMBER				
Product Gas Composition, mole %	8	9	10	11	12
CO	11.32	12.65	13.59	13.13	12.17
CO_2	9.24	9.43	9.31	9.03	9.76
H_2	18.68	21.31	22.67	21.15	21.34
CH_4	0.08	0.07	0.06	0.05	0.08
H_2O	27.53	24.33	22.75	24.52	24.32
N_2	32.66	31.72	31.14	31.63	31.83
H_2S	0.50	0.48	0.47	0.48	0.49
Amount of Tar, lbs/hr	5289.96	4051.60	3115.67	3835.77	4253.83
Temperature of Exit Gas, ${}_oF$	1056.18	1100.09	1141.47	1123.14	1079.46
Maximum Temperature, ${}_oF$	1990.97	1991.29	1986.60	1995.11	1986.41
Carbon Conversion, %	95.45	96.08	95.37	95.44	96.50
Heating Value of Dry Gas, Btu/SCF	139.03	148.04	153.30	149.55	146.36
Heating Value of Wet Gas, Btu/SCF	101.33	112.42	118.72	113.26	111.19
Heat Loss, 10^6 Btu	4.15	3.81	3.34	3.14	4.50

The coal residence time in the gasifier is approximately one hour. The operating pressure varies from 2.1 to 3.2 MPa with normal operating conditions of 2.1 MPa for air-blown and 3.0 MPa for oxygen-blown. The gas outlet temperature varies from 644 to 866 °K with a normal gas exit temperature of 744 °K [1].

The Lurgi Gasifier reportedly has many advantages. It can accept either caking or noncaking coals and use either oxygen or air as the oxidation media. The high pressure of the Lurgi favors the formation of methane in the gasifier, and high pressure is very advantageous for IGCC applications. The gasifier is highly developed and has been operated for many years.

On the other hand, the Lurgi Gasifier also has some disadvantages which become major concerns when we consider it for use in an IGCC system. One concern is the effect of the by-product tars and oils on the hot gas cleanup system, on gas turbine parts, and on components used for handling the by-products. The tars, which contain nitrogen, are also expected to contribute significantly to air pollution. The computer model described above does predict the amounts of tar produced depending on the coal properties and the gasifier operating conditions. However, the model predictions have not been checked against experimental data. We expect that the present model will have very limited value for defining problems due to tar in the product gas.

A second concern is the ability of the gasifier to operate with caking coals. It is known that the coal feed rate must be reduced for caking coals and that an agitator may be required. However we are not able to predict quantitatively how the swelling index of the coal affects the gasifiers performance. Our computer model does not even consider the swelling index of the coal.

The Lurgi Gasifier also has problems processing coal fines. The fines are swept out of the gasifier with the product gas and also tend to block the flow of gases through the bed of the gasifier, particularly when caking coals are used. Our computer model does not account for fines in the coal. It assumes a constant coal particle diameter and uniform flow through the gasifier bed.

The discussion above helps to define the way that the present computer model may be used in the IGCC system design study. Computer models are becoming increasingly useful for systems evaluation, but it is recognized that they have limitations. Operating experience often reveals the importance of simplifying assumptions in the models. In the case of the IGCC system, it is probable that coals will have to be selected so that caking is not a problem, and sized so that fines are kept at an acceptable level. The overall system design will have to be such that it can accomodate tars in the product gas. The computer models may still be valuable even though they do not account for some very important effects. However, the current gasifier model needs to be improved in several important areas. The devolatilization model needs updating. New rate equations should be programmed into the model so that it predicts quantities of methane and tar accurately. The model should account for more than one coal particle diameter.

4. Hot Gas Cleanup Model

4.1 Desulfurization Background

Zinc ferrite is formed by heating a mixture of zinc and iron oxide. Both zinc oxide and iron oxide have long histories of removing hydrogen sulfide from gas streams. Alone, iron oxide works well for hydrogen sulfide concentration above 150 parts per million, and is very easy to regenerate [14,15]. Zinc oxide by itself can perform to as low as 2 parts per million [14,16] but is more difficult to regenerate. However, together they combine the high sulfur affinity of zinc oxide with the good regenerability of iron oxide [14,17]. Zinc ferrite is a primary candidate for hot gas desulfurization in the integrated gasification combined cycle system [18]. The following are the governing chemical reactions:

Sulfidation,

$$3ZnFe_2O_4 + H_2 \longrightarrow 3ZnO + 2Fe_3O_4 + H_2O \tag{4.1}$$

$$Fe_3O_4 + 3H_2S + H_2 \longrightarrow 3FeS + 4H_2O \tag{4.2}$$

$$ZnO + H_2S \longrightarrow ZnS + H_2O \tag{4.3}$$

Regeneration,

$$2FeS + 7/2O_2 \longrightarrow Fe_2O_3 + 2SO_2 \tag{4.4}$$

$$ZnS + 3/2O_2 \longrightarrow ZnO + SO_2 \tag{4.5}$$

$$ZnO + Fe_2O_3 \longrightarrow ZnFe_2O_4 \tag{4.6}$$

It is important to operate zinc ferrite at the proper temperatures. Although the sulfidation temperature limitations are not agreed upon exactly, the general consensus is that the sorbent is most effective between 1000 °F and 1200 °F [14,19]. Within this range, magnetite (Fe_3O_4) is formed from the zinc ferrite and the sulfidation continues very well. Outside of the prescribed temperature range, species other than magnetite (iron/iron carbides or wustite) will be formed in the absorption bed, creating adverse effects. The sulfidation reaction is slightly exothermic and therefore will cause a rise in temperatures.

The regeneration is done by mixing air with the sorbent. This process is extremely exothermal and may be the cause of problems [14,19]. If the reaction is performed with pure air (21 % oxygen), temperatures may reach as high as 1700 °F. This is unacceptable because temperatures above 1500 °F will cause sintering of the sorbent, resulting in the loss of reactivity. This will render the sorbent potentially unusable for multi-cycles. There also exists a minimal temperature below which other unwanted process take place. At temperatures below 1200 °F considerable sulfate formation will occur. If the sulfate is not removed, a sulfidation cycle will start which emits high sulfur levels and contaminates the absorption cycle.

For the above reasons it is important to restrict the temperatures within 1200 °F and 1500 °F. This can be done by applying strict control to the stream of gases that react with the sorbent during the regeneration process. Inlet temperature, mass flow rate, and oxygen mole fraction of the reacting gases affect the temperatures in the regeneration cycle. Thus, these variables can be controlled to keep the reaction temperature within usable limits.

4.2 Regeneration Cycle System Design

The General Electric Company has developed [20,21] a system to provide oxygen in controlled amounts for proper regeneration of zinc ferrite. Figure 4.1 is a schematic of the system.

The General Electric design involves a three zone chamber. In the first zone 30 percent of the oxidation reaction that regenerates the sorbent is expected to occur. Oxygen levels in this zone start at 1 percent when the sorbent has been loaded, and then increases to about 2.5 percent to keep the reaction at 1250 °F. Although there is considerable sulfate formation in this zone, higher temperatures in the following zone will remove the sulfate. Gas inlet temperatures in this area range from 750 °F to 900 °F.

The second zone is where the completion of the reaction takes place. In this region a gas stream with 4 to 5 percent oxygen is input, allowing the reaction temperatures to be

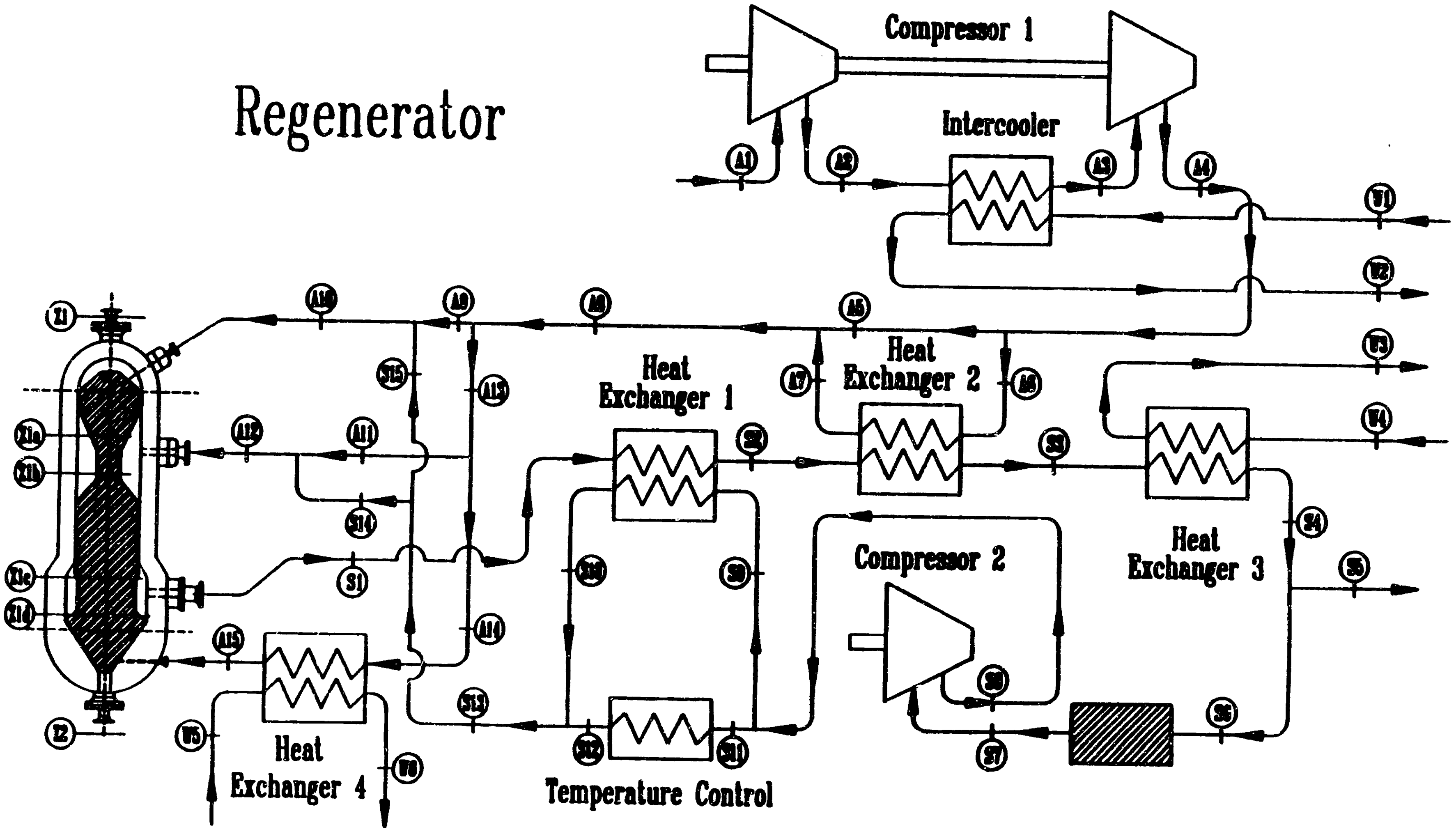


Figure 4.1 Closed Loop General Electric Regeneration Subsystem Design

kept at 1450 °F. This allows any sulfates created in the first zone to be destroyed without sintering the sorbent. Gas inlet temperatures are also kept between 750 °F and 900 °F in this zone. The flow rates are controlled so as to keep the excess oxygen to under 1 percent after exiting this area.

The purpose of the third zone is to cool the regenerated sorbent to between 800 °F and 1000 °F, while ensuring complete regeneration. This is done by introducing air (21 percent oxygen) at 600 °F to 800 °F in the bottom of the reactor, therefore purging any sulfur dioxide from the system. Mass flow rates in this area are controlled to ensure the needed sorbent exiting temperature. The following is a summary of inlet stream conditions required for the GE regeneration cycle.

Table 4.1 Inlet Conditions for GE Regeneration Cycle

	Percent Oxygen Inlet	Gas Inlet	Reaction @
Zone 1	1 - 2.5%	750 - 900 F	1250 F
Zone 2	4 - 5%	750 - 900 F	1450 F
Zone 3	21%	600 - 800 F	N / A

The flow system in Figure 4.1 provides the inlet streams at the conditions prescribed in the table. Air containing oxygen for regeneration of the zinc ferrite is compressed to about 20 atmospheres in compressor 1. In an IGCC system this air would probably be bled from the outlet line of the booster compressor so that compressor 1 would not be required. The air is preheated at heat exchanger 2 using waste heat from the exothermic reaction in the regenerator. The air is mixed with recirculating gases to provide oxygen concentrations at the inlet ports as specified in the above table. Heat exchanger 1 preheats the recirculating gases. The temperature controller insures that the gas temperatures remain within the limits prescribed, but is not required under nominal operating conditions. Heat exchanger 3 cools the exhaust gases to the temperatures required for the sulfur recovery process. If a direct sulfur recovery system is employed, heat exchanger 3 is not required. A filter and/or heat exchanger to cool the gases may be required upstream of compressor 2, which is needed to offset friction in the flow passages. Heat exchanger 4 cools the air entering the final stage of the regenerator.

4.3 Computer Model

A computer code was written for analyzing the requirements and performance of the system in Figure 4.1. The program determines flows required in all of the branches of the system, heat exchanger effectiveness requirements, and temperatures. The model incorporates energy balances, overall flow balances, and elemental component balances. It does not calculate pressure losses due to friction. Therefore, the requirements of compressor 2 can only be estimated.

The program is useful for determining how the system requirements depend on variables in the regeneration cycle. One variable is the concentration of SO_2 in the recirculating gases. The optimum concentration may change depending on the design of the sulfur recovery system. A second variable is the amount of sulfur loaded in the zinc ferrite sorbent. This may change with the operating conditions of the gasifier and with the age of the sorbent. Fluid temperatures such as the temperatures at A7 and the temperatures at S5 are variables that can be changed by sizing the heat exchangers or by adjusting the by-pass flow. It is important to know how the system requirements depend on the design variables since the system must function properly over a wide range of operating conditions. The computer model makes it easy to study the effects of changes in the operating conditions.

Parametric analysis described below were made for nominal gasifier operating conditions. In all cases, the flow of sorbent into the regenerator is calculated based on the following gasifier parameters:

Table 4.2 Conditions for Parametric Analysis

*	Illinois #6 7,258 lb/hr Sulfur in Coal 644,108 lb/hr Hot Gas

The input to the model can be easily adjusted to account for variations in the coal gas flow and composition.

4.4 Parametric Analysis

A parametric study was performed to determine the effects of the temperature at A7, the temperature at S5, the SO_2 mole fraction at S5, and the percent of reacted sorbent at the regenerator inlet. Flow rates and/or temperatures were adjusted to ensure that the reactor zone temperatures were kept at 1250 °F (zone 1) and 1450 °F (zone 2).

4.4.1 SO_2 Mole Fraction / O2 Mole Fraction at S5

The percentage of SO_2 in the sulfur rich stream became an important parameter for analysis because of the coupled relationship with the oxygen in the loop. From Figure 4.2 we can see that as the amount of oxygen decreases the amount of sulfur dioxide increases. This is due to the fact that sulfur dioxide is composed of oxygen. However, less obvious is the fact that a 13.2% increase in sulfur dioxide (.114 % $\longrightarrow$ .129 %) results in a 63.6% decrease in oxygen (.0360% $\longrightarrow$ .0131%). This relatively large change in oxygen can have a sizable effect on flow rates and required heat exchanger effectiveness.

From Figure 4.3 it can be seen that all the mass flow rates, with the exception of A15, increase as SO_2 mole fraction increases. Again, this is because higher SO_2 levels result in lower oxygen levels. These lower oxygen levels result in larger flow rates simply to allow the appropriate oxygen needed to complete the reaction. Also note that the flow rates A10, S1,

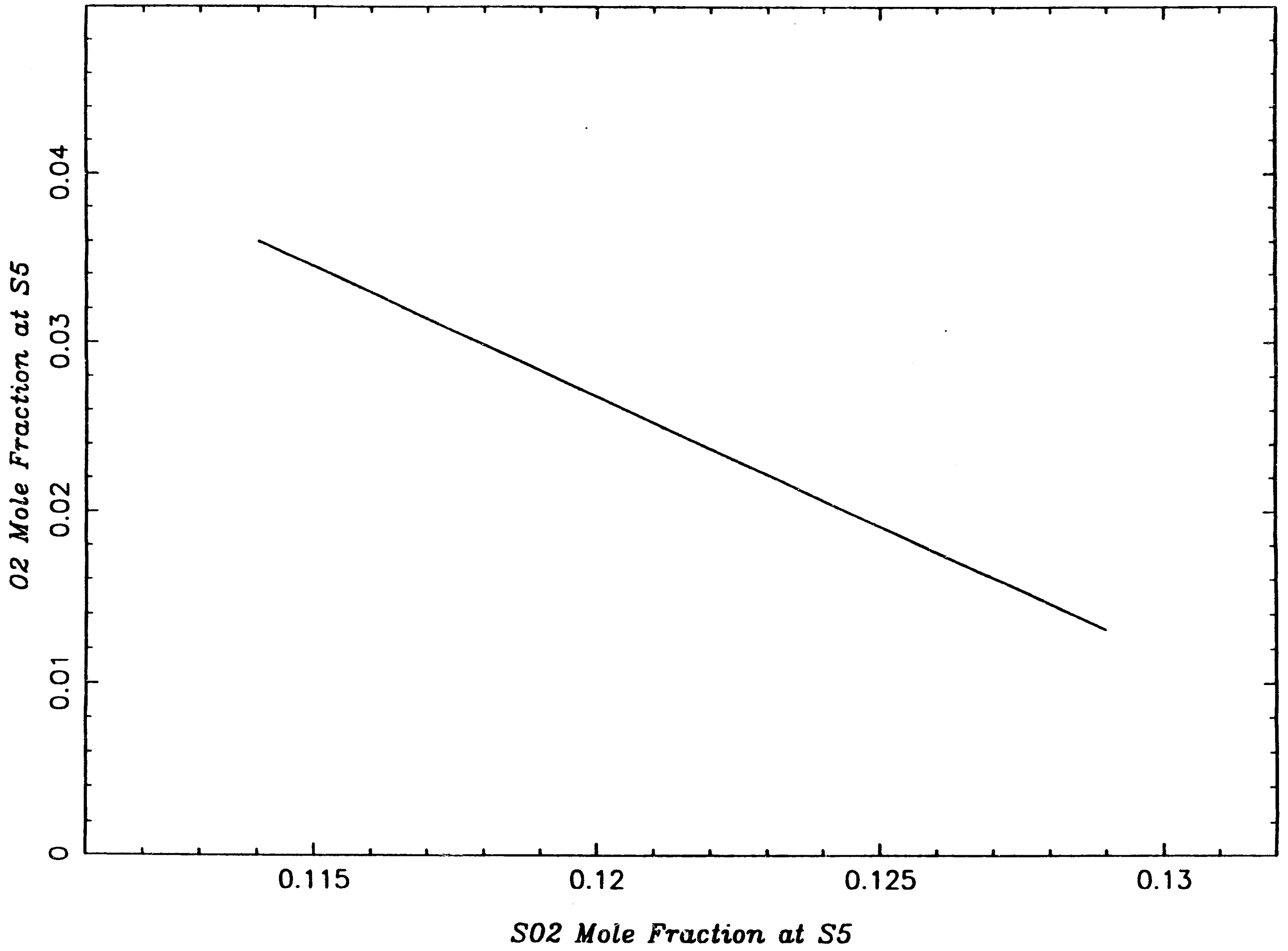


Figure 4.2 O_2 Mole Fraction at S5 versus SO_2 Mole Fraction at S5

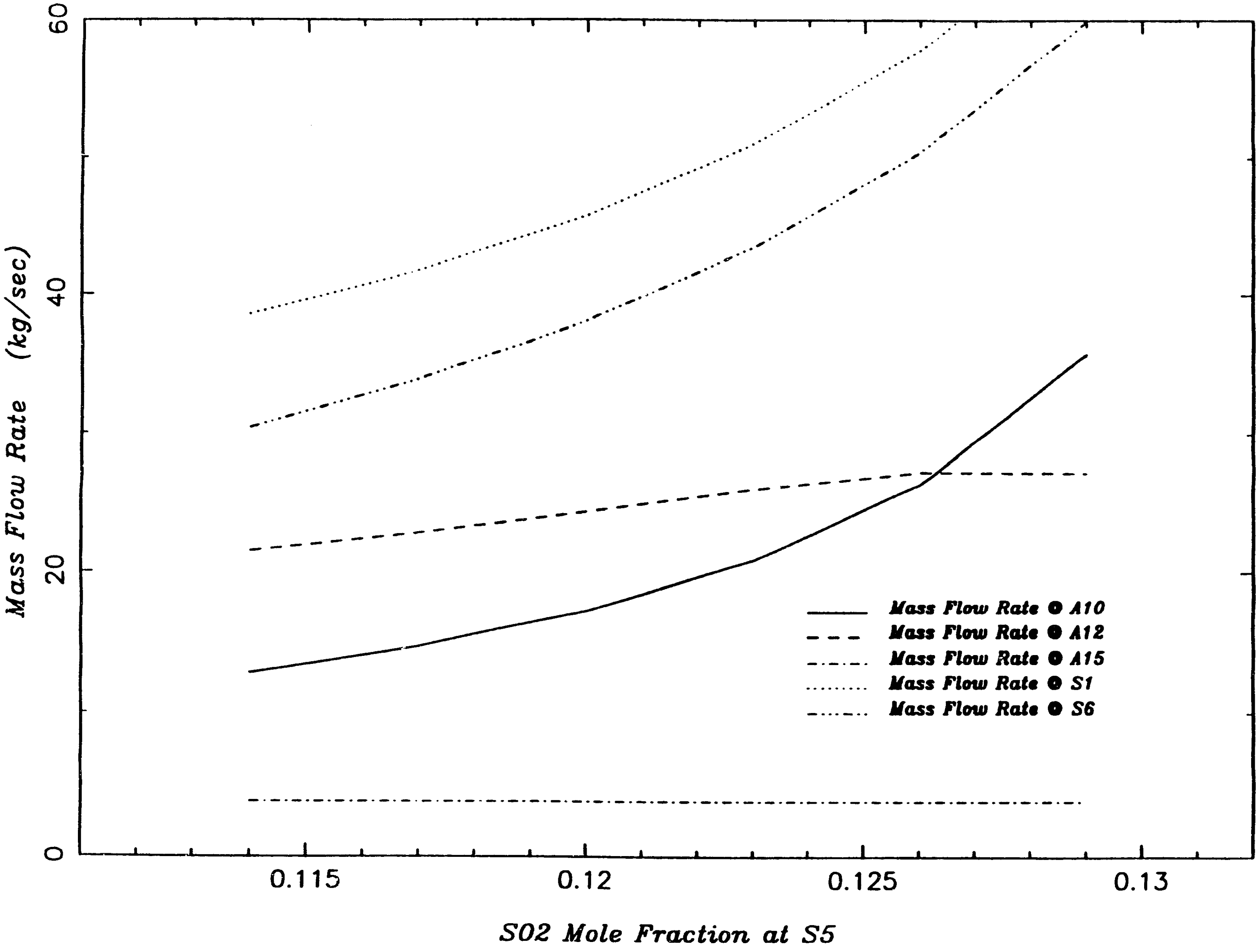


Figure 4.3 Mass Flow Rates of Regeneration Cycle verses SO_2 Mole Fraction at S5

and S6 increase at an increasing rate. Flow rates as high as 60 kg/sec can be very costly when considering compressor needs and therefore should be cautioned against. Mass flow rate A15 remains constant because it is used as a cooling stream and does not contribute to the oxidation reaction.

Figure 4.4 illustrates the change in effectiveness (i.e. size) of heat exchangers 1, 2, and 3 as the SO_2 mole fraction at S5 is varied. Heat exchanger 1 increases in needed effectiveness as the SO_2 mole fraction increases. This is mostly due to the increase in temperature of the S10-S13-S15-A10 stream needed to keep the first zone at 1250 °F. At an SO_2 mole fraction of .114, the temperature needed at A10 is 654.60 °F whereas an SO_2 mole fraction of .129 needs a temperature of 1036.60 °F. In the first case a lower temperature was needed to counter the effect of a higher O_2 mole fraction concentration (low SO_2 level). The lower needed temperatures consequently did not require the larger heat exchangers that would be needed for higher temperatures.

In the shadow of the same argument, heat exchanger 2 increases at an increasing rate as the SO_2 mole fraction at S5 increases (reducing O_2). As mentioned earlier, at lower SO_2 mole fractions higher temperatures are needed in the S10 stream. These higher temperatures cause the temperature at S2 to be reduced. However, a set amount of heat must be transferred in heat exchanger 2 to increase the temperature of A7 to the intended temperature. Therefore, a lower S2 temperature will cause heat exchanger 2 to increase in size to meet the temperature needs. Under these conditions it can be seen that SO_2 mole fractions higher than 12.6% may not be possible without reducing the load of heat exchanger 1 (i.e. adding heat in the S11-S12 stream).

Unlike heat exchangers 1 and 2, heat exchanger 3 slightly decreases in effectiveness as the SO_2 mole fraction increases. This is due to the decrease in temperature at the S3 location by the above arguments.

Finally, as seen in Figure 4.5, a change in the SO_2 mole fraction was also found to cause a change in the amount of excess oxygen at the end of zone 2. As the mole fraction of SO_2 increased (O_2 at S5 decreased), the amount of excess oxygen at the end of regeneration zone

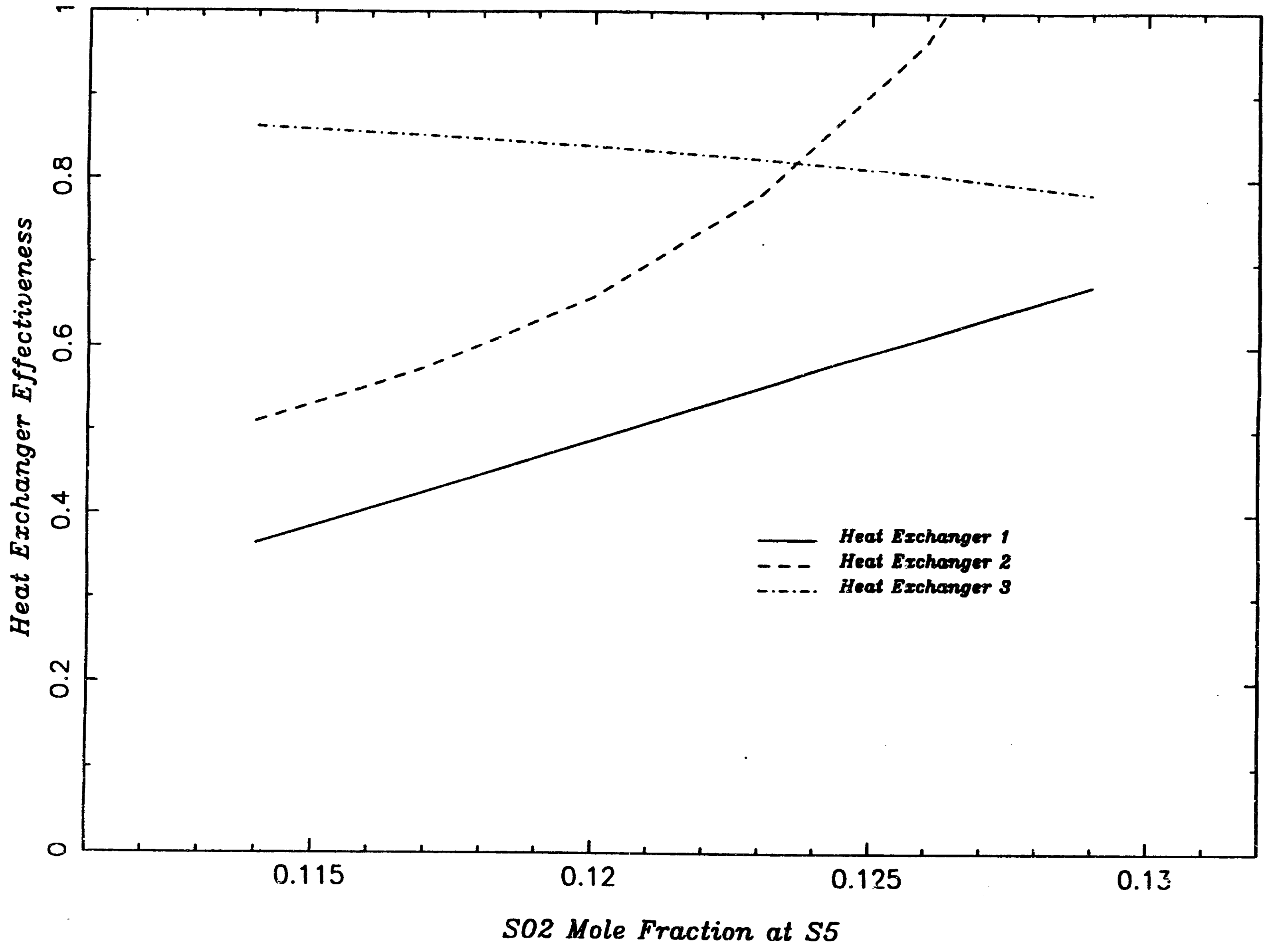


Figure 4.4 Heat Exchanger Effectiveness verses SO_2 Mole Fraction at S5

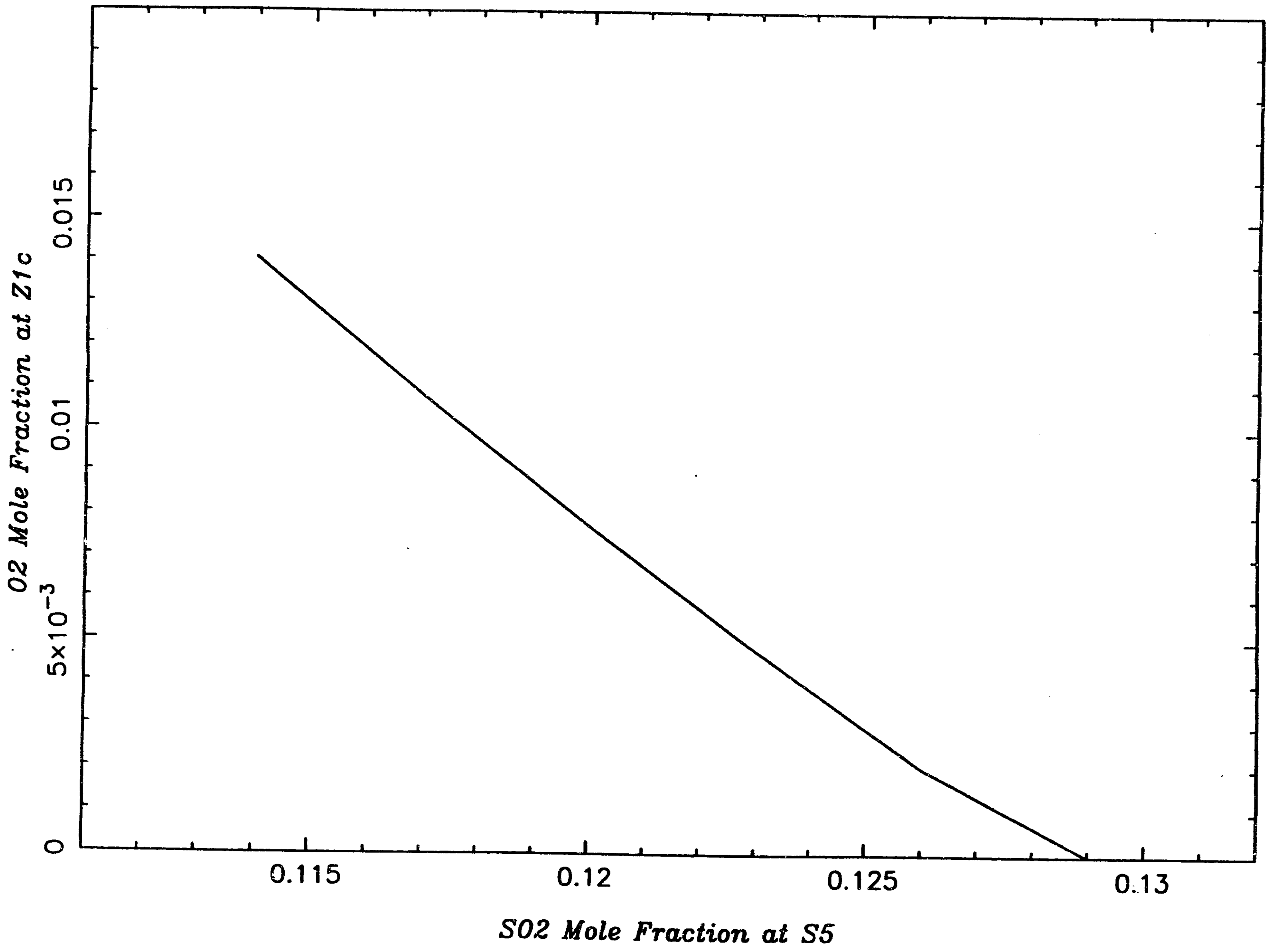


Figure 4.5 O_2 Mole Fraction at End of Zone 2 verses SO_2 Mole Fraction at S5

2 decreased. Note that the General Electric design called for about 1 percent excess oxygen at this location. Tables 4.3 through 4.8 show how variations in the SO_2 concentration at S5 affect flow variables at their locations in the system.

4.4.2 Percent Sorbent Reacted

A second parameter that was analyzed was the "percent of the sorbent reacted". This parameter is defined in the following equation:

$$ZnFe_2O_4 \longrightarrow xZnS + 2xFeS + (1-x)ZnFe_2O_4 \qquad (4.7)$$

where 'x' represents the percent of the sorbent reacted. If x equals zero there will be only $ZnFe_2O_4$. If x equals 1, there will be only ZnS and FeS entering the regeneration system. Note that this is written with respect to a sorbent with no inert binding material. The percent of the charged sorbent in Figure 4.6, 4.7, and 4.8 is related to 'x' by:

$$\%Charged\ Sorbent = x/(1 + \%\ Inerts) \qquad (4.8)$$

Figure 4.6 illustrates that the flow rates generally decrease as the percent sorbent reacted increases. This is largely due to the fact that less flow is needed to cool the reaction to the intended 1250 °F or 1450 °F because the mass flow rate of the sorbent is less. The flow rate of the sorbent is less because there is a larger percent of reacted sulfur. The flow rate of the A10 stream was unchanged, however. This is because the rate of this flow is dictated by a mandatory 30 percent reaction in zone 1. In the computer model this is found to be a function of the amount of inlet sulfur, which is a constant.

Figure 4.7 shows the required heat exchanger effectiveness verses the percent of sorbent reacted. There does not exist the extreme changes in heat exchanger effectiveness as found in the SO_2 mole fraction variations. However, it can be seen that the required effectiveness of heat exchanger 1 and 2 decrease as the percent of sorbent reacted increases. Conversely, the effectiveness of heat exchanger 3 increases as the sorbent has a larger percent of sulfur.

Table 4.3

SO2 Mole Fraction at S5
(y SO2 = .114)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.77	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.77	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.77	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.77	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.77	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.77	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.77	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	12.80	654.60	310.00	1.0097	0.0360	0.8500	0.1140
A11	3.92	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	21.54	675.61	310.00	1.0111	0.0707	0.8381	0.0913
A13	7.77	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	38.49	1423.71	306.00	1.0097	0.0360	0.8500	0.1140
S2	38.49	1076.14	302.00	1.0097	0.0360	0.8500	0.1140
S3	38.49	1011.40	298.00	1.0097	0.0360	0.8500	0.1140
S4	38.49	200.00	294.00	1.0097	0.0360	0.8500	0.1140
S5	8.07	200.00	294.00	1.0097	0.0360	0.8500	0.1140
S6	30.42	200.00	294.00	1.0097	0.0360	0.8500	0.1140
S7	30.42	200.00	294.00	1.0097	0.0360	0.8500	0.1140
S8	30.42	214.75	314.00	1.0097	0.0360	0.8500	0.1140
S9	30.42	214.75	314.00	1.0097	0.0360	0.8500	0.1140
S10	30.42	654.60	310.00	1.0097	0.0360	0.8500	0.1140
S11	0.00	214.75	314.00	1.0097	0.0360	0.8500	0.1140
S12	0.00	214.75	310.00	1.0097	0.0360	0.8500	0.1140
S13	30.42	654.60	310.00	1.0097	0.0360	0.8500	0.1140
S14	17.62	654.60	310.00	1.0097	0.0360	0.8500	0.1140
S15	12.80	654.60	310.00	1.0097	0.0360	0.8500	0.1140
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.75	NC	"			
W3	745.00	80.13	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	17.69	1249.93	314.00	0.9313	0.0000	0.7966	0.1270
Z1B	39.23	1249.93	314.00	0.9805	0.0436	0.8222	0.1050
Z1C	39.23	1449.87	314.00	0.9911	0.0138	0.8425	0.1261
Z1D	0.74	1449.87	314.00	0.9911	0.0138	0.8425	0.1261
Z2	4.58	900.00	314.00				

```
                                           Percent of Complete Reaction
Compressor 1:                                         0.500
   First Stages          0.850     N/A     Mass Flow Rate of Sulfur
   Last Stages           0.850     N/A            7258 lb/hr
Compressor 2             0.850     N/A
Intercooier               N/A     0.958    Errors:        8.88E-16 S balance
Heat Exchanger 1          N/A     0.364        -0.00000  0.00000 -0.00000
Heat Exchanger 2          N/A     0.510         0.00000 -0.00000  0.00000
Heat Exchanger 3          N/A     0.862        -0.00000  0.00000 -0.00000
Heat Exchanger 4          N/A     0.000         0.00000 above error
```

Table 4.4

SO2 Mole Fraction at S5
(y SO2 = .117)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.58	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.58	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.58	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.58	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.58	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.58	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.58	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	14.71	731.00	310.00	1.0096	0.0314	0.8516	0.1170
A11	3.74	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	22.89	737.37	310.00	1.0108	0.0635	0.8406	0.0960
A13	7.58	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	41.75	1425.23	306.00	1.0096	0.0314	0.8516	0.1170
S2	41.75	1006.54	302.00	1.0096	0.0314	0.8516	0.1170
S3	41.75	948.27	298.00	1.0096	0.0314	0.8516	0.1170
S4	41.75	200.00	294.00	1.0096	0.0314	0.8516	0.1170
S5	7.89	200.00	294.00	1.0096	0.0314	0.8516	0.1170
S6	33.86	200.00	294.00	1.0096	0.0314	0.8516	0.1170
S7	33.86	200.00	294.00	1.0096	0.0314	0.8516	0.1170
S8	33.86	214.75	314.00	1.0096	0.0314	0.8516	0.1170
S9	33.86	214.75	314.00	1.0096	0.0314	0.8516	0.1170
S10	33.86	731.00	310.00	1.0096	0.0314	0.8516	0.1170
S11	0.00	214.75	314.00	1.0096	0.0314	0.8516	0.1170
S12	0.00	214.75	310.00	1.0096	0.0314	0.8516	0.1170
S13	33.86	731.00	310.00	1.0096	0.0314	0.8516	0.1170
S14	19.15	731.00	310.00	1.0096	0.0314	0.8516	0.1170
S15	14.71	731.00	310.00	1.0096	0.0314	0.8516	0.1170
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.49	NC	"			
W3	745.00	80.13	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	19.60	1249.25	314.00	0.9406	0.0000	0.8045	0.1283
Z1B	42.49	1249.25	314.00	0.9827	0.0381	0.8261	0.1089
Z1C	42.49	1449.24	314.00	0.9925	0.0106	0.8448	0.1284
Z1D	0.74	1449.24	314.00	0.9925	0.0106	0.8448	0.1284
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.426
Heat Exchanger 2	N/A	0.574
Heat Exchanger 3	N/A	0.852
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
    -0.00000  0.00000 -0.00000
     0.00000 -0.00000  0.00000
    -0.00000  0.00000 -0.00000
     0.00000 above error
```

Table 4.5

SO2 Mole Fraction at S5
(y SO2 = .120)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	934.15	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	882.28	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.14	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

```
                                                  Percent of Complete Reaction
Compressor 1:                                                0.500
   First Stages         0.850        N/A          Mass Flow Rate of Sulfur
   Last Stages          0.850        N/A                  7258 lb/hr
Compressor 2            0.850        N/A
Intercooler              N/A        0.958         Errors:        0.00E+00 S balance
Heat Exchanger 1         N/A        0.489             -0.00000   0.00000   0.00000
Heat Exchanger 2         N/A        0.660              0.00000  -0.00000  -0.00000
Heat Exchanger 3         N/A        0.840             -0.00000   0.00000   0.00000
Heat Exchanger 4         N/A        0.000              0.00000 above error
```

Table 4.6

SO2 Mole Fraction at S5
(y SO2 = .123)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.24	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.24	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.24	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.24	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.24	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.24	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.24	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	20.89	885.00	310.00	1.0092	0.0222	0.8548	0.1230
A11	3.39	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	26.00	869.99	310.00	1.0103	0.0494	0.8454	0.1052
A13	7.24	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	51.04	1430.03	306.00	1.0092	0.0222	0.8548	0.1230
S2	51.04	858.89	302.00	1.0092	0.0222	0.8548	0.1230
S3	51.04	813.36	298.00	1.0092	0.0222	0.8548	0.1230
S4	51.04	200.00	294.00	1.0092	0.0222	0.8548	0.1230
S5	7.55	200.00	294.00	1.0092	0.0222	0.8548	0.1230
S6	43.49	200.00	294.00	1.0092	0.0222	0.8548	0.1230
S7	43.49	200.00	294.00	1.0092	0.0222	0.8548	0.1230
S8	43.49	214.75	314.00	1.0092	0.0222	0.8548	0.1230
S9	43.49	214.75	314.00	1.0092	0.0222	0.8548	0.1230
S10	43.49	885.00	310.00	1.0092	0.0222	0.8548	0.1230
S11	0.00	214.75	314.00	1.0092	0.0222	0.8548	0.1230
S12	0.00	214.75	310.00	1.0092	0.0222	0.8548	0.1230
S13	43.49	885.00	310.00	1.0092	0.0222	0.8548	0.1230
S14	22.61	885.00	310.00	1.0092	0.0222	0.8548	0.1230
S15	20.89	885.00	310.00	1.0092	0.0222	0.8548	0.1230
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.02	NC	•			
W3	745.00	80.15	NC	•			
W4	745.00	70.00	NC	•			
W5	1.80	70.00	NC	•			
W6	1.80	70.00	NC	•			
Z1	4.89	1000.00	310.00	•			
Z1A	25.78	1249.83	314.00	0.9596	0.0000	0.8207	0.1309
Z1B	51.78	1249.83	314.00	0.9874	0.0271	0.8343	0.1168
Z1C	51.78	1449.50	314.00	0.9954	0.0047	0.8495	0.1327
Z1D	0.74	1449.50	314.00	0.9954	0.0047	0.8495	0.1327
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.552
Heat Exchanger 2	N/A	0.782
Heat Exchanger 3	N/A	0.825
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:         0.00E+00 S balance
        0.00000 -0.00000  0.00000
       -0.00000  0.00000 -0.00000
        0.00000 -0.00000  0.00000
        0.00000 above error
```

Table 4.7

SO2 Mole Fraction at S5
(y SO2 = .126)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.08	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.08	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.08	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.08	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.08	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.08	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.08	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	26.38	961.10	310.00	1.0090	0.0176	0.8564	0.1260
A11	3.23	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	27.29	938.45	310.00	1.0100	0.0430	0.8476	0.1094
A13	7.08	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	57.83	1432.85	306.00	1.0090	0.0176	0.8564	0.1260
S2	57.83	781.85	302.00	1.0090	0.0176	0.8564	0.1260
S3	57.83	742.54	298.00	1.0090	0.0176	0.8564	0.1260
S4	57.83	200.00	294.00	1.0090	0.0176	0.8564	0.1260
S5	7.39	200.00	294.00	1.0090	0.0176	0.8564	0.1260
S6	50.44	200.00	294.00	1.0090	0.0176	0.8564	0.1260
S7	50.44	200.00	294.00	1.0090	0.0176	0.8564	0.1260
S8	50.44	214.75	314.00	1.0090	0.0176	0.8564	0.1260
S9	50.44	214.75	314.00	1.0090	0.0176	0.8564	0.1260
S10	50.44	961.10	310.00	1.0090	0.0176	0.8564	0.1260
S11	0.00	214.75	314.00	1.0090	0.0176	0.8564	0.1260
S12	0.00	214.75	310.00	1.0090	0.0176	0.8564	0.1260
S13	50.44	961.10	310.00	1.0090	0.0176	0.8564	0.1260
S14	24.06	961.10	310.00	1.0090	0.0176	0.8564	0.1260
S15	26.38	961.10	310.00	1.0090	0.0176	0.8564	0.1260
W1	60.00	70.00	NC	No Gas			
W2	60.00	79.79	NC	"			
W3	745.00	80.17	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	31.27	1249.92	314.00	0.9693	0.0000	0.8291	0.1322
Z1B	58.56	1249.92	314.00	0.9898	0.0217	0.8384	0.1207
Z1C	58.56	1449.95	314.00	0.9969	0.0020	0.8519	0.1347
Z1D	0.74	1449.95	314.00	0.9969	0.0020	0.8519	0.1347
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.613
Heat Exchanger 2	N/A	0.964
Heat Exchanger 3	N/A	0.807
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:          8.88E-16 S balance
    0.00000  0.00000 -0.00000
   -0.00000 -0.00000  0.00000
    0.00000  0.00000 -0.00000
    0.00000 above error
```

Table 4.8

SO2 Mole Fraction at S5
(y SO2 = .129)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	6.93	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	6.93	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	6.93	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	6.93	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	6.93	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	6.93	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	6.93	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	35.73	1036.60	310.00	1.0089	0.0131	0.8579	0.1290
A11	3.08	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	27.25	1006.44	310.00	1.0098	0.0379	0.8494	0.1127
A13	6.93	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	67.14	1435.30	306.00	1.0089	0.0131	0.8579	0.1290
S2	67.14	702.03	302.00	1.0089	0.0131	0.8579	0.1290
S3	67.14	668.89	298.00	1.0089	0.0131	0.8579	0.1290
S4	67.14	200.00	294.00	1.0089	0.0131	0.8579	0.1290
S5	7.24	200.00	294.00	1.0089	0.0131	0.8579	0.1290
S6	59.90	200.00	294.00	1.0089	0.0131	0.8579	0.1290
S7	59.90	200.00	294.00	1.0089	0.0131	0.8579	0.1290
S8	59.90	214.75	314.00	1.0089	0.0131	0.8579	0.1290
S9	59.90	214.75	314.00	1.0089	0.0131	0.8579	0.1290
S10	59.90	1036.60	310.00	1.0089	0.0131	0.8579	0.1290
S11	0.00	214.75	314.00	1.0089	0.0131	0.8579	0.1290
S12	0.00	214.75	310.00	1.0089	0.0131	0.8579	0.1290
S13	59.90	1036.60	310.00	1.0089	0.0131	0.8579	0.1290
S14	24.17	1036.60	310.00	1.0089	0.0131	0.8579	0.1290
S15	35.73	1036.60	310.00	1.0089	0.0131	0.8579	0.1290
W1	60.00	70.00	NC	No Gas			
W2	60.00	79.58	NC	•			
W3	745.00	80.20	NC	•			
W4	745.00	70.00	NC	•			
W5	1.80	70.00	NC	•			
W6	1.80	70.00	NC	•			
Z1	4.89	1000.00	310.00	•			
Z1A	40.62	1249.85	314.00	0.9792	0.0000	0.8375	0.1336
Z1B	67.87	1249.85	314.00	0.9924	0.0163	0.8426	0.1246
Z1C	67.87	1449.95	314.00	0.9984	-0.0006	0.8542	0.1366
Z1D	0.74	1449.95	314.00	0.9984	-0.0006	0.8542	0.1366
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.673
Heat Exchanger 2	N/A	1.271
Heat Exchanger 3	N/A	0.783
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
     0.500
Mass Flow Rate of Sulfur
      7258 lb/hr

Errors:       0.00E+00 S balance
   -0.00000  0.00000 -0.00000
    0.00000 -0.00000  0.00000
   -0.00000  0.00000 -0.00000
    0.00000 above error
```

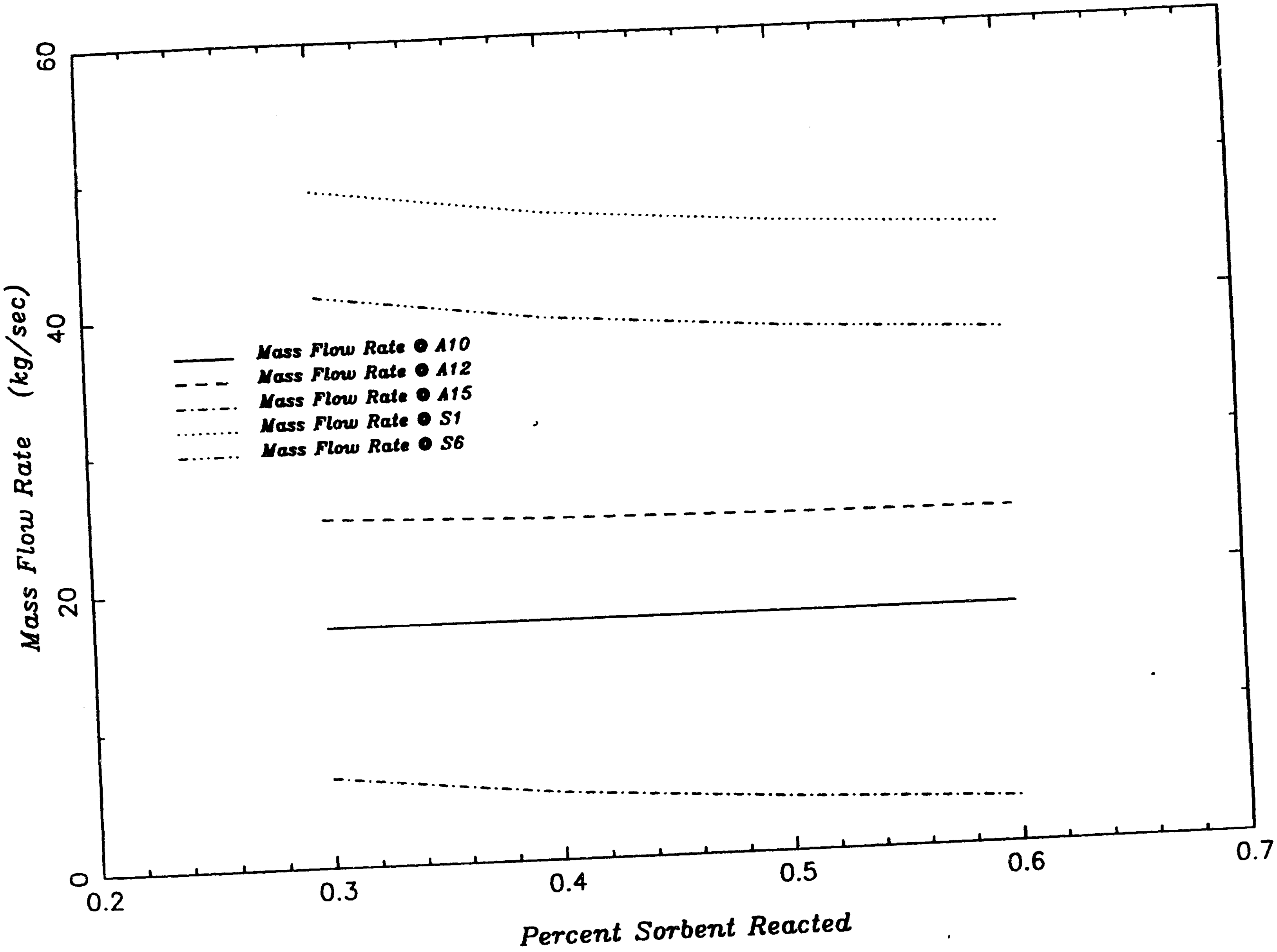


Figure 4.6 Mass Flow Rates of Regeneration Cycle Verses Percent of Inlet Sorbent Reacted

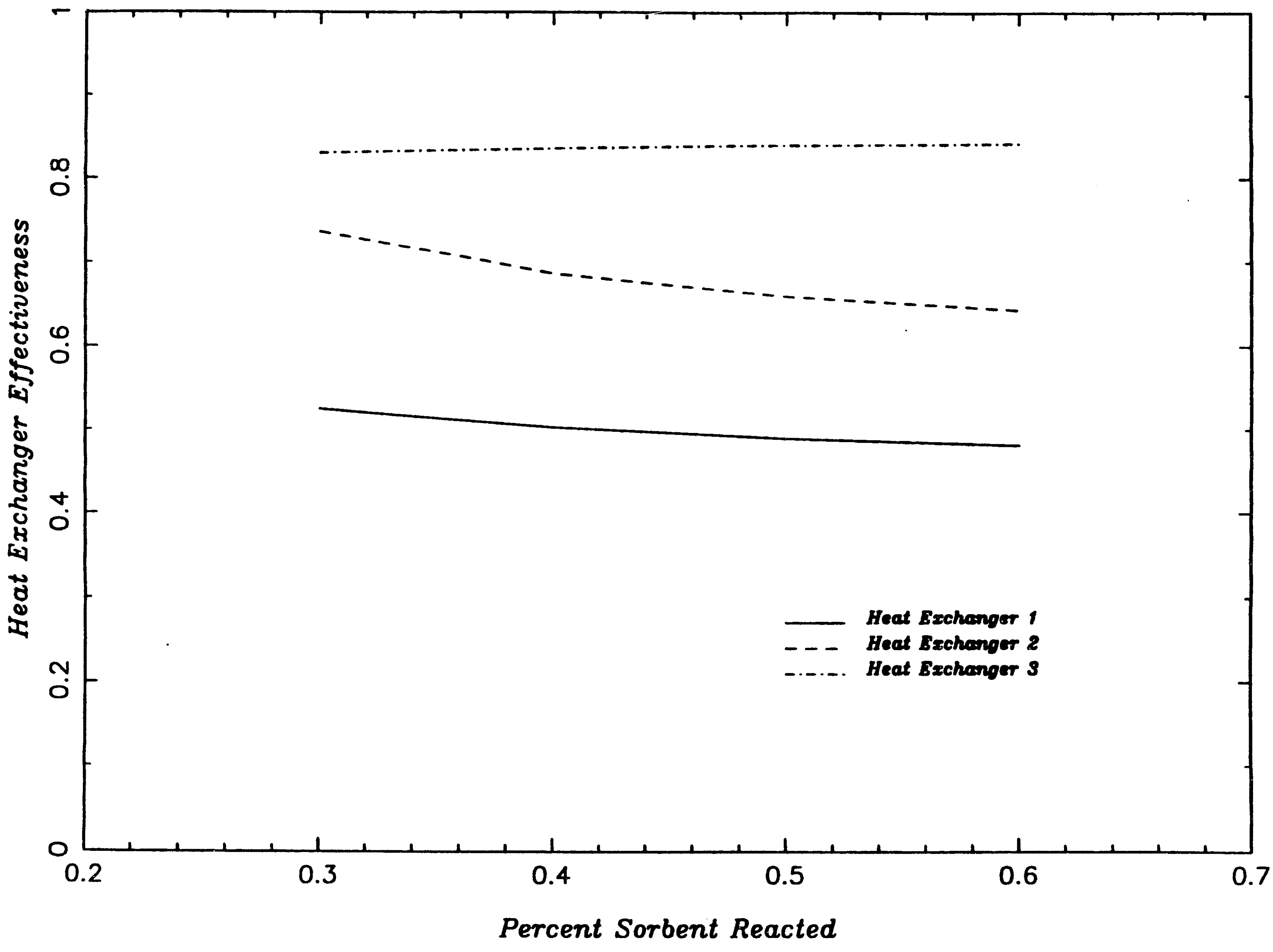


Figure 4.7 Heat Exchanger Effectiveness Verses Percent of Inlet Sorbent Reacted

The excess amount of oxygen at the end of zone 2 verses the percent of sorbent reacted can be seen in Figure 4.8. In this illustration the excess amount of oxygen increases at a decreasing rate as the percent sorbent reacted increases. Note that the excess amount of oxygen falls below zero when the percent sorbent reacted is around 0.36. This should not be taken as a limit due to the fact that many other parameters can also affect the percentage of excess oxygen. The purpose of this illustration is to analyze the results of a parameter change while all other independent variables are held constant. By changing other parameters, scenarios may be obtained that show excess oxygen at less than 0.30 percent sorbent reacted. Tables 4.9 through 4.12 show how the system flow variables depend on the percent of sorbent reacted.

4.4.3 Temperature at A7

The temperature at A7 is also a parameter that can influence the heat exchanger effectiveness and mass flow rates through the regeneration system. In Figure 4.9 it can be seen that the heat exchanger effectiveness at heat exchanger 2 increases greatly as the temperature at A7 is increased. However, heat exchangers 1 and 3 remain generally unchanged.

Figure 4.10 illustrates the changes in mass flow rates of important streams. It can be seen that the flow of stream A10 remains constant. Once again, this is due to the fact that the flow rate of this stream is dictated by oxygen requirements. The mass flow rates of streams A12 and A15 are slightly increased as the temperature of A7 increases. This is due to a more difficult job of cooling the reaction zones to 1250 °F and 1450 °F. The higher the inlet temperature, the larger the flow that is needed for cooling purposes. Finally, higher flow rates at streams S1 and S6 are a consequence of the higher flow rates needed earlier in the system. Tables 4.13 through 4.18 provide additional detailed information.

Table 4.9

Percent Sorbent Reacted
30 %

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	844.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	1.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	25.13	841.06	310.00	1.0097	0.0349	0.8504	0.1147
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	6.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	6.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	49.12	1414.23	306.00	1.0094	0.0268	0.8532	0.1200
S2	49.12	883.81	302.00	1.0094	0.0268	0.8532	0.1200
S3	49.12	835.42	298.00	1.0094	0.0268	0.8532	0.1200
S4	49.12	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	41.40	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	41.40	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	41.40	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	41.40	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	41.40	844.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	41.40	844.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	24.13	844.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	844.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.12	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	7.95	1000.00	310.00	"			
Z1A	25.22	1249.99	314.00	0.9290	0.0000	0.7945	0.1267
Z1B	50.35	1249.99	314.00	0.9755	0.0201	0.8267	0.1198
Z1C	50.35	1449.85	314.00	0.9840	-0.0046	0.8434	0.1373
Z1D	1.23	1449.85	314.00	0.9840	-0.0046	0.8434	0.1373
Z2	7.64	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.525
Heat Exchanger 2	N/A	0.737
Heat Exchanger 3	N/A	0.830
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
        0.300
Mass Flow Rate of Sulfur
         7258 lb/hr

Errors:          0.00E+00 S balance
      0.00000 -0.00000 -0.00000
     -0.00000  0.00000  0.00000
      0.00000 -0.00000 -0.00000
      0.00000 above error
```

Table 4.10

Percent Sorbent Reacted
40 %

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	822.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	2.60	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.63	816.51	310.00	1.0102	0.0483	0.8458	0.1059
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	4.81	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	4.81	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	47.01	1422.87	306.00	1.0094	0.0268	0.8532	0.1200
S2	47.01	915.25	302.00	1.0094	0.0268	0.8532	0.1200
S3	47.01	864.70	298.00	1.0094	0.0268	0.8532	0.1200
S4	47.01	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	39.30	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	39.30	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	39.30	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	39.30	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	39.30	822.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	39.30	822.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	22.03	822.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	822.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.13	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	6.04	1000.00	310.00	"			
Z1A	23.31	1250.00	314.00	0.9420	0.0000	0.8057	0.1285
Z1B	47.94	1250.00	314.00	0.9814	0.0279	0.8288	0.1155
Z1C	47.94	1449.94	314.00	0.9901	0.0029	0.8457	0.1331
Z1D	0.92	1449.94	314.00	0.9901	0.0029	0.8457	0.1331
Z2	5.73	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.503
Heat Exchanger 2	N/A	0.687
Heat Exchanger 3	N/A	0.836
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.400
Mass Flow Rate of Sulfur
7258 lb/hr

Errors: 0.00E+00 S balance
-0.00000 -0.00000 0.00000
0.00000 0.00000 -0.00000
-0.00000 -0.00000 0.00000
0.00000 above error

Table 4.11

Percent Sorbent Reacted
50 %

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	934.15	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	882.28	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.14	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.489
Heat Exchanger 2	N/A	0.660
Heat Exchanger 3	N/A	0.840
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
        0.500
Mass Flow Rate of Sulfur
         7258 lb/hr

Errors:        0.00E+00 S balance
     -0.00000  0.00000  0.00000
      0.00000 -0.00000 -0.00000
     -0.00000  0.00000  0.00000
      0.00000 above error
```

Table 4.12

Percent Sorbent Reacted
60 %

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	799.90	310.00	1.0094	0.0268	0.8532	0.1200
A11	4.20	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.27	794.72	310.00	1.0107	0.0617	0.8412	0.0971
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.21	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.21	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.05	1431.76	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.05	946.80	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.05	894.04	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.05	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	37.34	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	37.34	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	37.34	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	37.34	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	37.34	799.90	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	37.34	799.90	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.07	799.90	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	799.90	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.14	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.13	1000.00	310.00	"			
Z1A	21.40	1249.93	314.00	0.9554	0.0000	0.8172	0.1303
Z1B	45.67	1249.93	314.00	0.9875	0.0357	0.8311	0.1111
Z1C	45.67	1449.98	314.00	0.9964	0.0107	0.8482	0.1288
Z1D	0.61	1449.98	314.00	0.9964	0.0107	0.8482	0.1288
Z2	3.82	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.481
Heat Exchanger 2	N/A	0.643
Heat Exchanger 3	N/A	0.842
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
     0.600
Mass Flow Rate of Sulfur
     7258 lb/hr

Errors:      0.00E+00 S balance
   -0.00000 -0.00000  0.00000
    0.00000  0.00000 -0.00000
   -0.00000 -0.00000  0.00000
    0.00000 above error
```

Table 4.13

Temperature at A7
(T_{A7}=770 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	934.15	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	882.28	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.14	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.489
Heat Exchanger 2	N/A	0.660
Heat Exchanger 3	N/A	0.840
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

Errors: 0.00E+00 S balance
-0.00000 0.00000 0.00000
0.00000 -0.00000 -0.00000
-0.00000 0.00000 0.00000
0.00000 above error

Table 4.14

Temperature at A7
(T_{A7}=800 °F)

```
             Mdot      Temp      Press      Cp        O2        N2        SO2
             kg/s      deg F      psi     KJ/Kg*K

A1           7.41      70.00     14.70    1.0164    0.2100    0.7900    0.0000
A2           7.41     426.18     67.93    1.0164    0.2100    0.7900    0.0000
A3           7.41      85.00     67.93    1.0164    0.2100    0.7900    0.0000
A4           7.41     451.36    314.00    1.0164    0.2100    0.7900    0.0000
A5           0.00     451.36    310.00    1.0164    0.2100    0.7900    0.0000
A6           7.41     451.36    314.00    1.0164    0.2100    0.7900    0.0000
A7           7.41     800.00    310.00    1.0164    0.2100    0.7900    0.0000
A8           7.41     800.00    310.00    1.0164    0.2100    0.7900    0.0000
A9           0.00     800.00    310.00    1.0164    0.2100    0.7900    0.0000
A10         17.27     808.70    310.00    1.0094    0.0268    0.8532    0.1200
A11          3.33     800.00    310.00    1.0164    0.2100    0.7900    0.0000
A12         24.60     807.52    310.00    1.0104    0.0542    0.8437    0.1021
A13          7.41     800.00    310.00    1.0164    0.2100    0.7900    0.0000
A14          4.08     800.00    310.00    1.0164    0.2100    0.7900    0.0000
A15          4.08     800.00    310.00    1.0164    0.2100    0.7900    0.0000
S1          46.26    1427.72    306.00    1.0094    0.0268    0.8532    0.1200
S2          46.26     932.82    302.00    1.0094    0.0268    0.8532    0.1200
S3          46.26     876.60    298.00    1.0094    0.0268    0.8532    0.1200
S4          46.26     200.00    294.00    1.0094    0.0268    0.8532    0.1200
S5           7.71     200.00    294.00    1.0094    0.0268    0.8532    0.1200
S6          38.54     200.00    294.00    1.0094    0.0268    0.8532    0.1200
S7          38.54     200.00    294.00    1.0094    0.0268    0.8532    0.1200
S8          38.54     214.75    314.00    1.0094    0.0268    0.8532    0.1200
S9          38.54     214.75    314.00    1.0094    0.0268    0.8532    0.1200
S10         38.54     808.70    310.00    1.0094    0.0268    0.8532    0.1200
S11          0.00     214.75    314.00    1.0094    0.0268    0.8532    0.1200
S12          0.00     214.75    310.00    1.0094    0.0268    0.8532    0.1200
S13         38.54     808.70    310.00    1.0094    0.0268    0.8532    0.1200
S14         21.27     808.70    310.00    1.0094    0.0268    0.8532    0.1200
S15         17.27     808.70    310.00    1.0094    0.0268    0.8532    0.1200
W1          60.00      70.00      NC      No Gas
W2          60.00      80.25      NC        "
W3         745.00      80.15      NC        "
W4         745.00      70.00      NC        "
W5           1.80      70.00      NC        "
W6           1.80      70.00      NC        "
Z1           4.89    1000.00    310.00      "
Z1A         22.16    1249.93    314.00    0.9500    0.0000    0.8126    0.1296
Z1B         46.76    1249.93    314.00    0.9851    0.0314    0.8306    0.1136
Z1C         46.76    1449.47    314.00    0.9939    0.0065    0.8476    0.1313
Z1D          0.50    1449.47    314.00    0.9939    0.0065    0.8476    0.1313
Z2           4.58     900.00    314.00
                                             Percent of Complete Reaction
Compressor 1:                                           0.500
   First Stages        0.850      N/A        Mass Flow Rate of Sulfur
   Last Stages         0.850      N/A                7258 lb/hr
Compressor 2           0.850      N/A
Intercooler             N/A      0.958       Errors:          0.00E+00 S balance
Heat Exchanger 1        N/A      0.490           -0.00000  0.00000 -0.00000
Heat Exchanger 2        N/A      0.724            0.00000 -0.00000  0.00000
Heat Exchanger 3        N/A      0.839           -0.00000  0.00000 -0.00000
Heat Exchanger 4        N/A      0.000            0.00000 above error
```

Table 4.15

Temperature at A7
(T_{A7}=830 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	830.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	830.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	830.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.76	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.06	830.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.72	811.39	310.00	1.0104	0.0519	0.8445	0.1035
A13	7.41	830.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	4.35	830.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	4.35	830.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	46.64	1428.11	306.00	1.0094	0.0268	0.8532	0.1200
S2	46.64	932.35	302.00	1.0094	0.0268	0.8532	0.1200
S3	46.64	871.79	298.00	1.0094	0.0268	0.8532	0.1200
S4	46.64	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.93	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.93	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.93	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.93	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.93	808.76	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.93	808.76	310.00	1.0094	0.0268	0.8532	0.1200
S14	21.66	808.76	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.76	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.16	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.98	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.88	1249.98	314.00	0.9851	0.0302	0.8311	0.1145
Z1C	46.88	1449.90	314.00	0.9939	0.0053	0.8481	0.1321
Z1D	0.24	1449.90	314.00	0.9939	0.0053	0.8481	0.1321
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.490
Heat Exchanger 2	N/A	0.787
Heat Exchanger 3	N/A	0.838
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
     0.00000  0.00000 -0.00000
    -0.00000 -0.00000  0.00000
     0.00000  0.00000 -0.00000
     0.00000 above error
```

Table 4.16

Temperature at A7
(T_{A7}=860 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	860.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	860.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	860.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.78	310.00	1.0094	0.0268	0.8532	0.1200
A11	2.76	860.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.84	814.47	310.00	1.0103	0.0494	0.8454	0.1052
A13	7.41	860.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	4.65	860.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	4.65	860.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	47.06	1428.08	306.00	1.0094	0.0268	0.8532	0.1200
S2	47.06	931.42	302.00	1.0094	0.0268	0.8532	0.1200
S3	47.06	866.65	298.00	1.0094	0.0268	0.8532	0.1200
S4	47.06	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	39.35	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	39.35	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	39.35	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	39.35	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	39.35	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	39.35	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S14	22.08	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.78	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	•			
W3	745.00	80.17	NC	•			
W4	745.00	70.00	NC	•			
W5	1.80	70.00	NC	•			
W6	1.80	70.00	NC	•			
Z1	4.89	1000.00	310.00	•			
Z1A	22.16	1249.99	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	47.00	1249.99	314.00	0.9850	0.0287	0.8317	0.1154
Z1C	47.00	1449.91	314.00	0.9939	0.0039	0.8486	0.1330
Z1D	-0.06	1449.91	314.00	0.9939	0.0039	0.8486	0.1330
Z2	4.58	900.00	314.00				

```
                                              Percent of Complete Reaction
Compressor 1:                                            0.500
   First Stages        0.850      N/A         Mass Flow Rate of Sulfur
   Last Stages         0.850      N/A                  7258 lb/hr
Compressor 2           0.850      N/A
Intercooler             N/A      0.958        Errors:       0.00E+00 S balance
Heat Exchanger 1        N/A      0.490              0.00000  0.00000 -0.00000
Heat Exchanger 2        N/A      0.851             -0.00000 -0.00000  0.00000
Heat Exchanger 3        N/A      0.837              0.00000  0.00000 -0.00000
Heat Exchanger 4        N/A      0.000              0.00000 above error
```

Table 4.17

Temperature at A7
(T_{A7}=890 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	890.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	890.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	890.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.78	310.00	1.0094	0.0268	0.8532	0.1200
A11	2.41	890.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.93	816.64	310.00	1.0101	0.0465	0.8464	0.1071
A13	7.41	890.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	4.99	890.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	4.99	890.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	47.50	1427.95	306.00	1.0094	0.0268	0.8532	0.1200
S2	47.50	930.39	302.00	1.0094	0.0268	0.8532	0.1200
S3	47.50	861.51	298.00	1.0094	0.0268	0.8532	0.1200
S4	47.50	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	39.79	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	39.79	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	39.79	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	39.79	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	39.79	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	39.79	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S14	22.52	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.78	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.19	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.99	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	47.09	1249.99	314.00	0.9850	0.0271	0.8322	0.1165
Z1C	47.09	1449.84	314.00	0.9938	0.0022	0.8492	0.1341
Z1D	-0.41	1449.84	314.00	0.9938	0.0022	0.8492	0.1341
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.490
Heat Exchanger 2	N/A	0.916
Heat Exchanger 3	N/A	0.836
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
    -0.00000 -0.00000  0.00000
     0.00000  0.00000 -0.00000
    -0.00000 -0.00000  0.00000
     0.00000 above error
```

Table 4.18

Temperature at A7
(T_{A7}=920 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	920.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	920.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	920.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.78	310.00	1.0094	0.0268	0.8532	0.1200
A11	2.01	920.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.97	817.74	310.00	1.0100	0.0432	0.8475	0.1092
A13	7.41	920.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	5.40	920.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	5.40	920.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	47.94	1427.95	306.00	1.0094	0.0268	0.8532	0.1200
S2	47.94	929.51	302.00	1.0094	0.0268	0.8532	0.1200
S3	47.94	856.58	298.00	1.0094	0.0268	0.8532	0.1200
S4	47.94	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	40.22	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	40.22	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	40.22	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	40.22	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	40.22	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	40.22	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S14	22.95	808.78	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.78	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.21	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.99	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	47.13	1249.99	314.00	0.9849	0.0251	0.8329	0.1178
Z1C	47.13	1449.95	314.00	0.9937	0.0002	0.8498	0.1354
Z1D	-0.81	1449.95	314.00	0.9937	0.0002	0.8498	0.1354
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.490
Heat Exchanger 2	N/A	0.980
Heat Exchanger 3	N/A	0.835
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
        0.500
Mass Flow Rate of Sulfur
        7258 lb/hr

Errors:           0.00E+00 S balance
       0.00000  0.00000 -0.00000
      -0.00000 -0.00000  0.00000
       0.00000  0.00000 -0.00000
       0.00000 above error
```

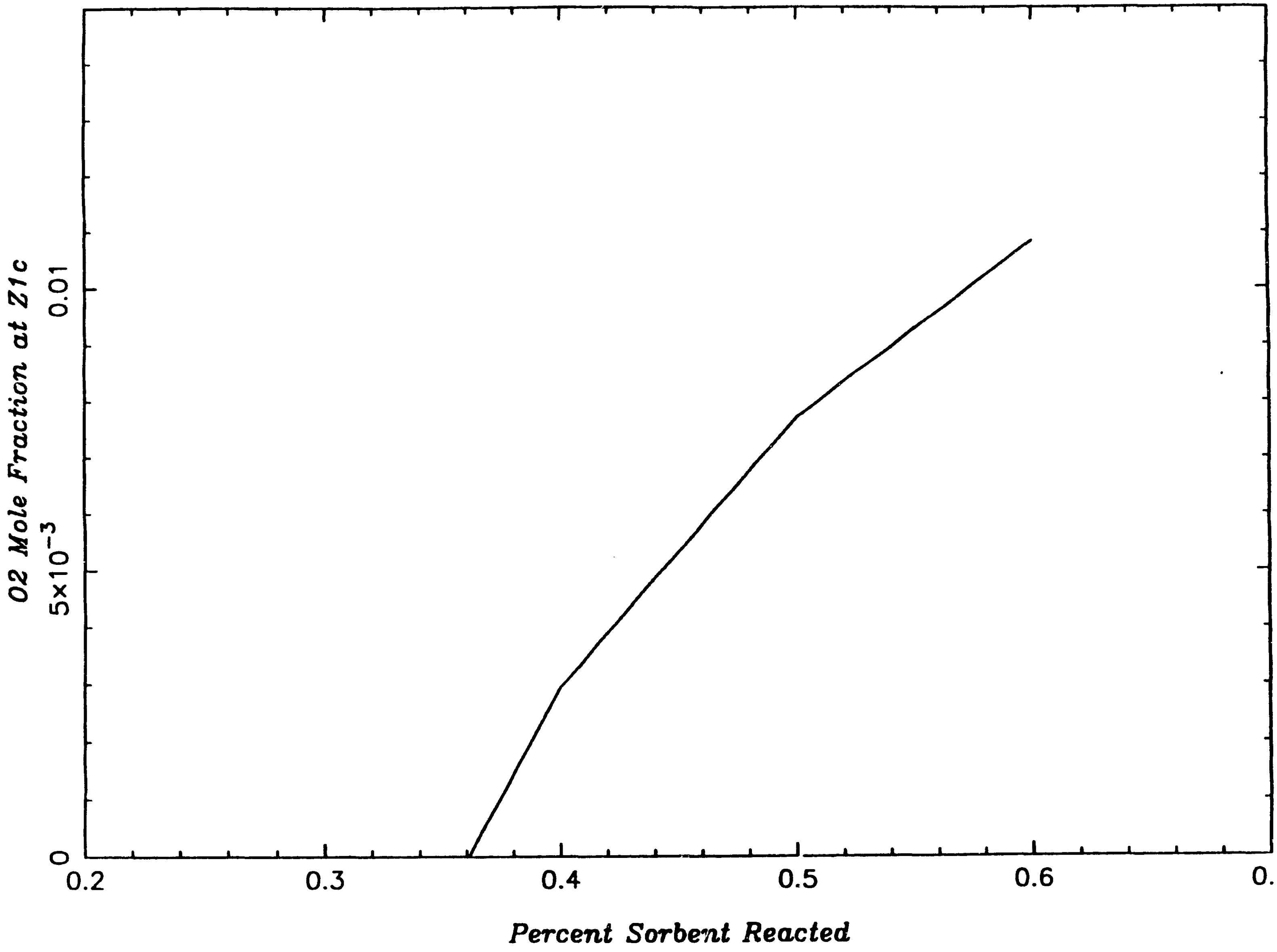


Figure 4.8 O_2 Mole Fraction at End of Zone 2 verses Percent of Inlet Sorbent Reacted

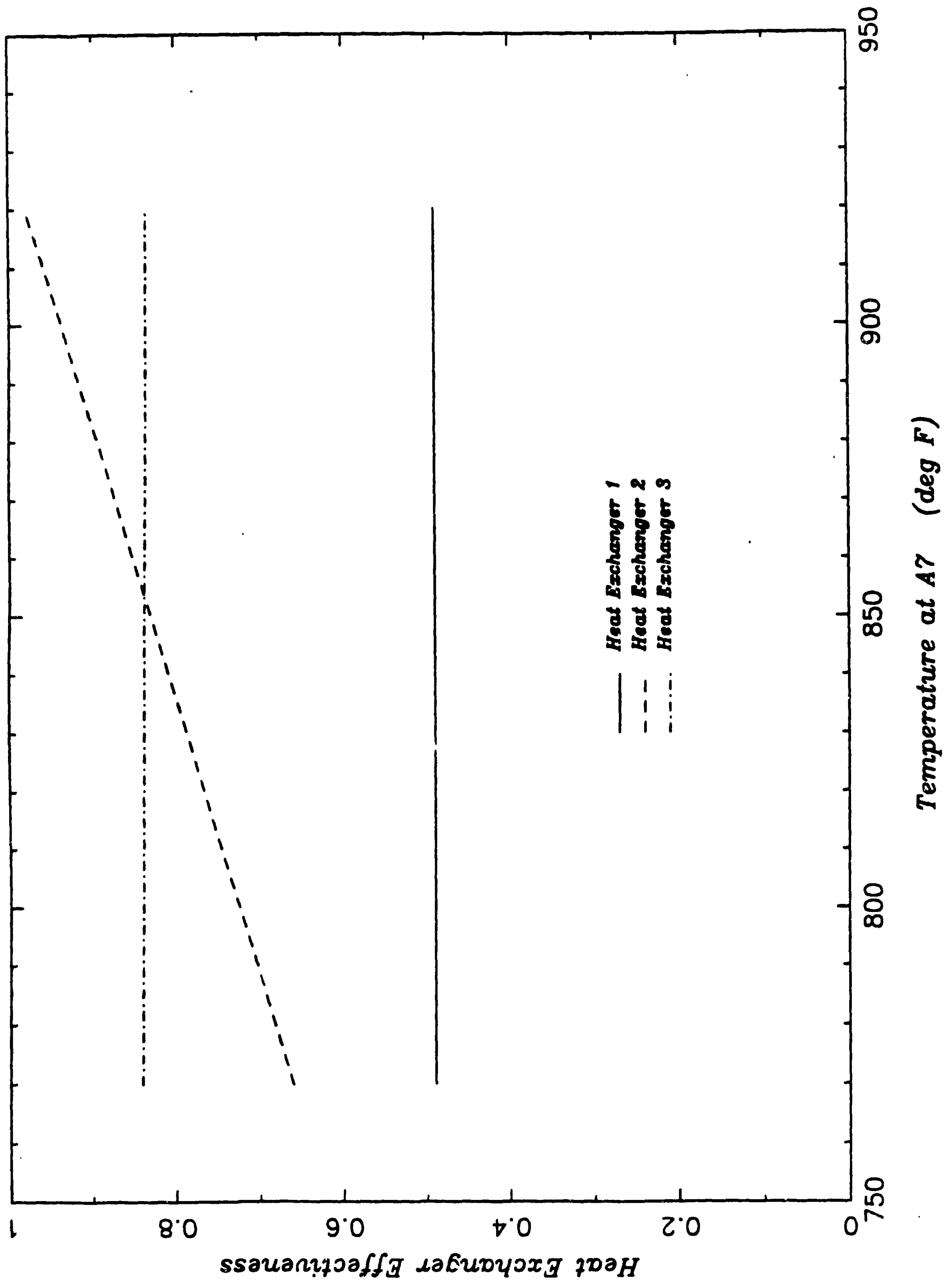


Figure 4.9 Heat Exchanger Effectiveness verses Temperature at A7

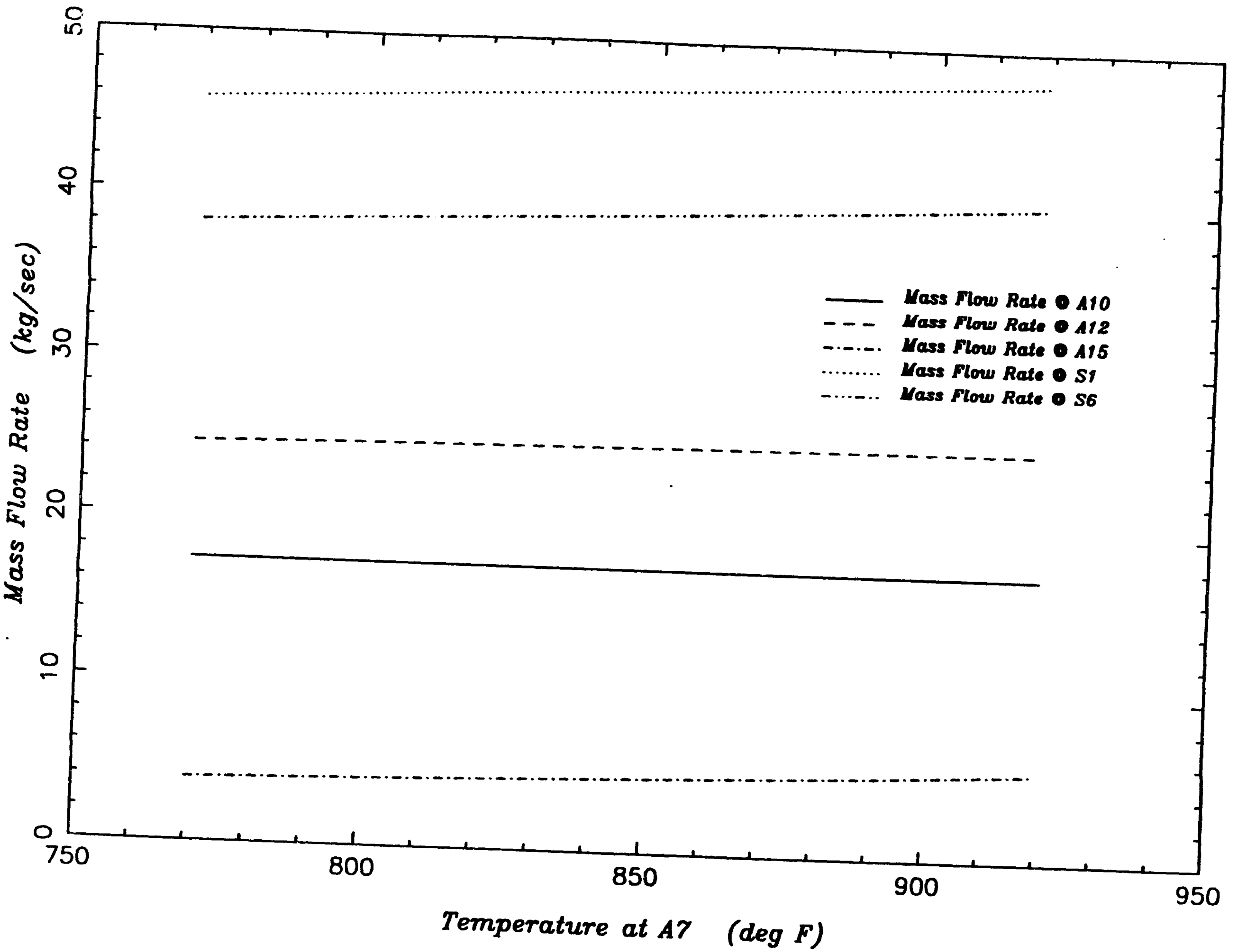


Figure 4.10 Mass Flow Rates of Regeneration Cycle verses Temperature at A7

4.4.4 Temperature at S5

Figure 4.11 illustrates the needed heat exchanger effectiveness as the temperature of the S5 stream is allowed to increase. As will be seen later, it is desirable to maintain higher temperatures at the S5 bleed stream. However, as can be seen in Figure 4.11, this is highly desirable with respect to heat exchangers. Heat exchangers 1, 2, and 3 decrease in needed effectiveness (i.e. size) as the temperature of S5 increases. Note that heat exchanger 1 decreases at a increasing rate and that at S5 temperatures higher than 780 °F a heat exchanger may not even be necessary. Note also that at this temperature heat exchangers 2 and 3 have effectiveness of only 32.6% and 45.6% respectively. Tables 4.19 through 4.31 provide additional information.

4.5 Direct Sulfur Removal

Research Triangle Institute (RTI) has been working on direct sulfur recovery under contract with the Department of Energy at Morgantown Energy Technology Center. Their work centers around tail-gasses produced by the regeneration of metal oxide sorbents (ie. Zinc Ferrite). Figure is a schematic of the system. Although experimental tests were preformed on gas streams with SO_2 concentrations around 1%-3%, not 10-13%, there appear to be only benefits when considering the more concentrated streams. In addition, RTI found that the yield of sulfur increased as temperatures were increased or when pressures increased [22]. Both of these facts are extremely beneficial to the General Electric design under consideration. Below are a few results obtained from the RTI experiments:

Table 4.32

At Constant Temperature (650 C)	
Pressure	Percentage Sulfur Removal
1 atm (14.7 psi)	20 %
10 atm (147.0 psi)	60 %
20 atm (294.0 psi)	90 %
40 atm (588.0 psi)	95 %

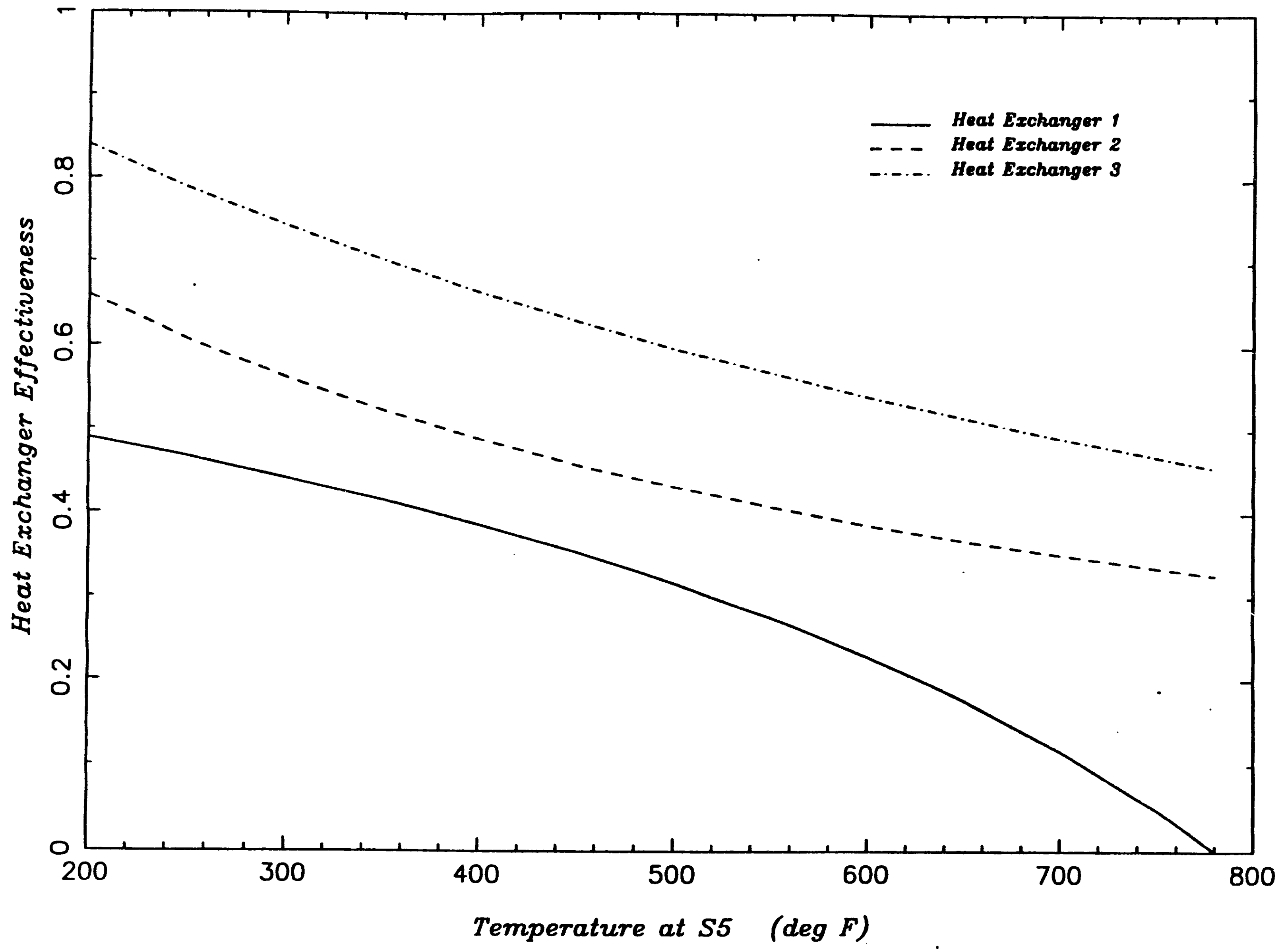


Figure 4.11 Heat Exchanger Effectiveness verses Temperature at S5

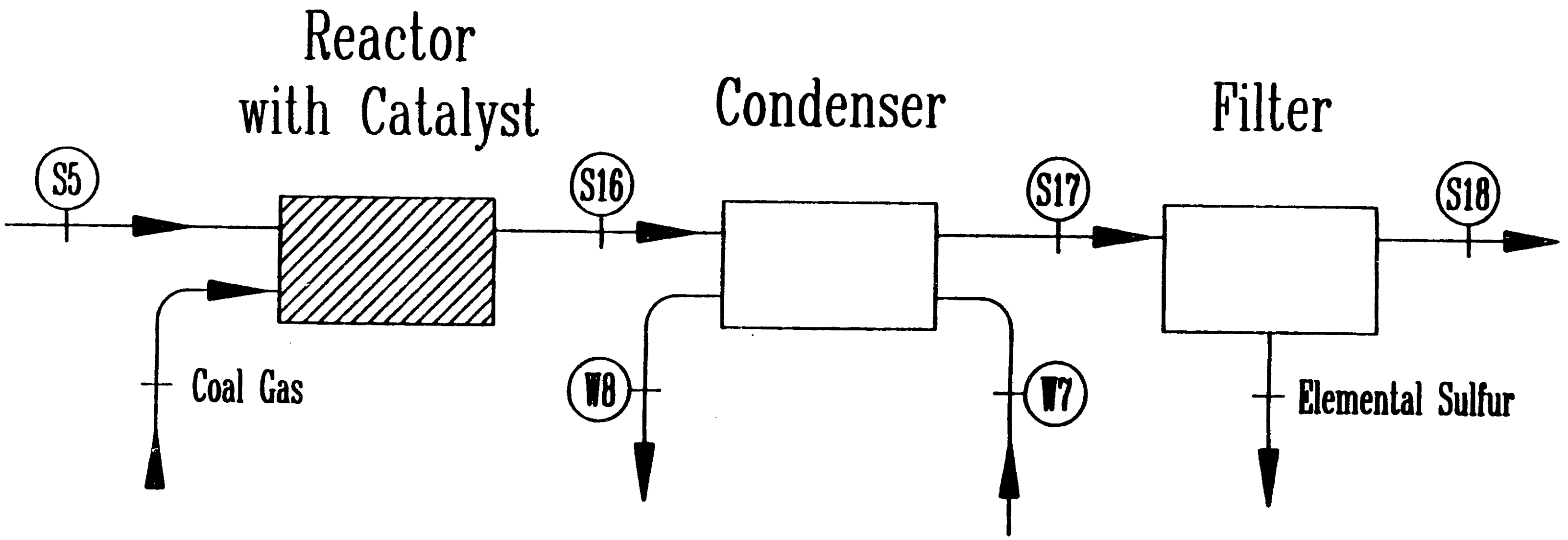


Figure 4.12 RTI Direct Surful Recovery Loop

Table 4.19

Temperature at S5

(T_{S5}=200 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	934.15	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	882.28	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	200.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	214.75	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	214.75	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.14	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.489
Heat Exchanger 2	N/A	0.660
Heat Exchanger 3	N/A	0.840
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
        0.500
Mass Flow Rate of Sulfur
        7258 lb/hr

Errors:          0.00E+00 S balance
     -0.00000  0.00000  0.00000
      0.00000 -0.00000 -0.00000
     -0.00000  0.00000  0.00000
      0.00000 above error
```

Table 4.20

Temperature at S5
(T_{S5}=250 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	976.67	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	924.79	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	250.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	250.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	250.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	250.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	265.87	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	265.87	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	265.87	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	265.87	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	80.03	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.467
Heat Exchanger 2	N/A	0.607
Heat Exchanger 3	N/A	0.789
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
     -0.00000  0.00000  0.00000
      0.00000 -0.00000 -0.00000
     -0.00000  0.00000  0.00000
      0.00000 above error
```

Table 4.21

Temperature at S5
(T_{S5}=300 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1019.18	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	967.31	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	300.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	300.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	300.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	300.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	316.99	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	316.99	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	316.99	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	316.99	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.92	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.442
Heat Exchanger 2	N/A	0.561
Heat Exchanger 3	N/A	0.744
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
    -0.00000  0.00000  0.00000
     0.00000 -0.00000 -0.00000
    -0.00000  0.00000  0.00000
     0.00000 above error
```

Table 4.22

Temperature at S5
(T_{S5}=350 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1061.69	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1009.82	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	350.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	350.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	350.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	350.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	368.11	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	368.11	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	368.11	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	368.11	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.80	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.415
Heat Exchanger 2	N/A	0.522
Heat Exchanger 3	N/A	0.702
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00  S balance
    -0.00000   0.00000   0.00000
     0.00000  -0.00000  -0.00000
    -0.00000   0.00000   0.00000
     0.00000  above error
```

Table 4.23

Temperature at S5
(T_{S5}=400 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1104.20	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1052.33	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	400.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	400.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	400.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	400.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	419.22	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	419.22	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	419.22	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	419.22	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.69	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.386
Heat Exchanger 2	N/A	0.488
Heat Exchanger 3	N/A	0.664
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
        0.500
Mass Flow Rate of Sulfur
        7258 lb/hr

Errors:        0.00E+00 S balance
    -0.00000  0.00000  0.00000
     0.00000 -0.00000 -0.00000
    -0.00000  0.00000  0.00000
     0.00000 above error
```

Table 4.24

Temperature at S5
(T_{S5}=450 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1146.72	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1094.85	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	450.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	450.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	450.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	450.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	470.34	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	470.34	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	470.34	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	470.34	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.58	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.353
Heat Exchanger 2	N/A	0.458
Heat Exchanger 3	N/A	0.629
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:       0.00E+00 S balance
    -0.00000  0.00000  0.00000
     0.00000 -0.00000 -0.00000
    -0.00000  0.00000  0.00000
     0.00000 above error
```

Table 4.25

Temperature at S5
(T_{S5}=500 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1189.23	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1137.36	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	500.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	500.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	500.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	500.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	521.46	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	521.46	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	521.46	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	521.46	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.47	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.316
Heat Exchanger 2	N/A	0.432
Heat Exchanger 3	N/A	0.597
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reaction
          0.500
Mass Flow Rate of Sulfur
         7258 lb/hr

Errors:          0.00E+00 S balance
    -0.00000  0.00000  0.00000
     0.00000 -0.00000 -0.00000
    -0.00000  0.00000  0.00000
     0.00000 above error
```

Table 4.26

Temperature at S5
(T_{S5}=550 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1231.74	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1179.87	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	550.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	550.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	550.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	550.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	572.58	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	572.58	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	572.58	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	572.58	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.36	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

```
                                                 Percent of Complete Reaction
Compressor 1:                                              0.500
   First Stages        0.850      N/A            Mass Flow Rate of Sulfur
   Last Stages         0.850      N/A                   7258 lb/hr
Compressor 2           0.850      N/A
Intercooler             N/A       0.958          Errors:        0.00E+00  S balance
Heat Exchanger 1        N/A       0.275              -0.00000   0.00000   0.00000
Heat Exchanger 2        N/A       0.408               0.00000  -0.00000  -0.00000
Heat Exchanger 3        N/A       0.568              -0.00000   0.00000   0.00000
Heat Exchanger 4        N/A       0.000               0.00000 above error
```

Table 4.27

Temperature at S5
(T_{S5}=600 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1274.26	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1222.38	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	600.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	600.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	600.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	600.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	623.70	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	623.70	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	623.70	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	623.70	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.25	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.229
Heat Exchanger 2	N/A	0.387
Heat Exchanger 3	N/A	0.540
Heat Exchanger 4	N/A	0.000

```
Percent of Complete Reactio
        0.500
Mass Flow Rate of Sulfur
          7258 lb/hr

Errors:          0.00E+00 S balance
      -0.00000  0.00000  0.00000
       0.00000 -0.00000 -0.00000
      -0.00000  0.00000  0.00000
       0.00000 above error
```

Table 4.28

Temperature at S5
(T_{S5}=650 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1316.77	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1264.90	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	650.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	650.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	650.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	650.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	674.82	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	674.82	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	674.82	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	674.82	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.14	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.177
Heat Exchanger 2	N/A	0.368
Heat Exchanger 3	N/A	0.515
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

Errors: 0.00E+00 S balance
-0.00000 0.00000 0.00000
0.00000 -0.00000 -0.00000
-0.00000 0.00000 0.00000
0.00000 above error

Table 4.29

Temperature at S5
(T_{S5}=700 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1359.28	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1307.41	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	700.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	700.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	700.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	700.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	725.93	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	725.93	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	725.93	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	725.93	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	79.03	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

```
                                                 Percent of Complete Reaction
Compressor 1:                                              0.500
   First Stages          0.850        N/A        Mass Flow Rate of Sulfur
   Last Stages           0.850        N/A                 7258 lb/hr
Compressor 2             0.850        N/A
Intercooler               N/A        0.958       Errors:        0.00E+00 S balance
Heat Exchanger 1          N/A        0.117           -0.00000  0.00000  0.00000
Heat Exchanger 2          N/A        0.351            0.00000 -0.00000 -0.00000
Heat Exchanger 3          N/A        0.491           -0.00000  0.00000  0.00000
Heat Exchanger 4          N/A        0.000            0.00000 above error
```

Table 4.30

Temperature at S5

(T_{S5}=750 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1401.79	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1349.92	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	750.00	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	750.00	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	750.00	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	750.00	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	777.05	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	777.05	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	777.05	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	777.05	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	•			
W3	745.00	78.91	NC	•			
W4	745.00	70.00	NC	•			
W5	1.80	70.00	NC	•			
W6	1.80	70.00	NC	•			
Z1	4.89	1000.00	310.00	•			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.958
Heat Exchanger 1	N/A	0.048
Heat Exchanger 2	N/A	0.335
Heat Exchanger 3	N/A	0.469
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500
Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
     -0.00000  0.00000  0.00000
      0.00000 -0.00000 -0.00000
     -0.00000  0.00000  0.00000
      0.00000 above error
```

Table 4.31

Temperature at S5
(T_{S5}=780.27 °F)

	Mdot kg/s	Temp deg F	Press psi	Cp KJ/Kg*K	O2	N2	SO2
A1	7.41	70.00	14.70	1.0164	0.2100	0.7900	0.0000
A2	7.41	426.18	67.93	1.0164	0.2100	0.7900	0.0000
A3	7.41	85.00	67.93	1.0164	0.2100	0.7900	0.0000
A4	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A5	0.00	451.36	310.00	1.0164	0.2100	0.7900	0.0000
A6	7.41	451.36	314.00	1.0164	0.2100	0.7900	0.0000
A7	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A8	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A9	0.00	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A10	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
A11	3.56	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A12	24.40	802.45	310.00	1.0105	0.0563	0.8430	0.1007
A13	7.41	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A14	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
A15	3.85	770.00	310.00	1.0164	0.2100	0.7900	0.0000
S1	45.82	1427.53	306.00	1.0094	0.0268	0.8532	0.1200
S2	45.82	1427.53	302.00	1.0094	0.0268	0.8532	0.1200
S3	45.82	1375.66	298.00	1.0094	0.0268	0.8532	0.1200
S4	45.82	780.27	294.00	1.0094	0.0268	0.8532	0.1200
S5	7.71	780.27	294.00	1.0094	0.0268	0.8532	0.1200
S6	38.11	780.27	294.00	1.0094	0.0268	0.8532	0.1200
S7	38.11	780.27	294.00	1.0094	0.0268	0.8532	0.1200
S8	38.11	808.00	314.00	1.0094	0.0268	0.8532	0.1200
S9	38.11	808.00	314.00	1.0094	0.0268	0.8532	0.1200
S10	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S11	0.00	808.00	314.00	1.0094	0.0268	0.8532	0.1200
S12	0.00	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S13	38.11	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S14	20.84	808.00	310.00	1.0094	0.0268	0.8532	0.1200
S15	17.27	808.00	310.00	1.0094	0.0268	0.8532	0.1200
W1	60.00	70.00	NC	No Gas			
W2	60.00	80.25	NC	"			
W3	745.00	78.85	NC	"			
W4	745.00	70.00	NC	"			
W5	1.80	70.00	NC	"			
W6	1.80	70.00	NC	"			
Z1	4.89	1000.00	310.00	"			
Z1A	22.16	1249.36	314.00	0.9500	0.0000	0.8126	0.1296
Z1B	46.56	1249.36	314.00	0.9850	0.0326	0.8302	0.1129
Z1C	46.56	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z1D	0.74	1449.31	314.00	0.9939	0.0076	0.8472	0.1306
Z2	4.58	900.00	314.00				

Compressor 1:		
First Stages	0.850	N/A
Last Stages	0.850	N/A
Compressor 2	0.850	N/A
Intercooler	N/A	0.953
Heat Exchanger 1	N/A	0.000
Heat Exchanger 2	N/A	0.326
Heat Exchanger 3	N/A	0.456
Heat Exchanger 4	N/A	0.000

Percent of Complete Reaction
0.500

Mass Flow Rate of Sulfur
7258 lb/hr

```
Errors:        0.00E+00 S balance
    -0.00000  0.00000  0.00000
     0.00000 -0.00000 -0.00000
    -0.00000  0.00000  0.00000
     0.00000 above error
```

Experimental tests at RTI indicate that over 90 percent of the direct sulfur removal can be achieved with this procedure. Higher percentages may be obtained by placing this system in series. For example, if 99% removal is desired, two systems may be placed together.

Under Research Triangle Institute's design, stoichiometric conditions are favorable for the best sulfur producing reaction. As an example [22].

$$SO_2 + 2H_2 \longrightarrow 2H_2O + S, \tag{4.9}$$

$$SO_2 + 2CO \longrightarrow 2CO_2 + S, \tag{4.10}$$

$$SO_2 + 2H_2S \longrightarrow 2H_2O + 3S, \text{ and} \tag{4.11}$$

$$H_2S + (1/2)O_2 \longrightarrow H_2O + S \tag{4.12}$$

Therefore, a reducing stream of coal gas will be needed for these reactions. With a sulfur percentage of about 4.04 % weight in the inlet coal, about 4.68% of the gasification gas (3.80 kg/sec) will need to be sent to the first direct sulfur recovery unit in order to achieve stoichiometric conditions. If two consecutive units are placed in series to achieve the 99 percent removal goal, a secondary stream of coal gas may need to be bled off. However, this stream should be at least an order of magnitude less than the first.

Table 4.33 is an example of flow rates and mole fractions that may occur in one stage of a direct sulfur recovery plant. Again, it can be seen that a mass flow rate of 3.8 kg/sec of coal gas is needed for a 12% SO_2 stream at 7.71 kg/sec. This preliminary direct sulfur recovery balance is done assuming that the reactions are thermally neutral.

Table 4.33

Direct Sulfur Recovery

	S5	Coal Gas Stream	S16	S17	S18	W7	W8
Mass Flow Rate (kg/sec)	7.71	3.80	11.51	11.51	10.66	NC	NC
Temp (F)	780.27	1020.00	859.40	320.00	320.00	70.00	NC
Pressure	NC	NC	NC	NC	NC	NC	NC
				y S	0.000043	Psat @ 320 F / P	
Mole Fraction							
O2	0.0268	0.0000	0.0158	0.0158	0.0169		
N2	0.8532	0.3851	0.6599	0.6599	0.7064		
SO2	0.1200	0.0000	0.0071	0.0071	0.0076		
CO	0.0000	0.1393	0.0057	0.0057	0.0061		
H2	0.0000	0.2003	0.0082	0.0082	0.0088		
CO2	0.0000	0.1134	0.0976	0.0976	0.1044		
H2O	0.0000	0.1215	0.1256	0.1256	0.1345		
CH4	0.0000	0.0333	0.0136	0.0136	0.0146		
C2H6	0.0000	0.0008	0.0003	0.0003	0.0003		
H2S	0.0000	0.0063	0.0003	0.0003	0.0003		
Ele S	0.0000	0.0000	0.0659	0.0659	0.0001		
Mass in one Mole (kg)							
O2	0.8576	0.0000	0.5054	0.5054	0.5410		
N2	23.9067	10.7905	18.4912	18.4912	19.7942		
SO2	7.6872	0.0000	0.4528	0.4528	0.4847		
CO	0.0000	3.9019	0.1594	0.1594	0.1707		
H2	0.0000	0.4038	0.0165	0.0165	0.0177		
CO2	0.0000	4.9908	4.2942	4.2942	4.5968		
H2O	0.0000	2.1889	2.2634	2.2634	2.4229		
CH4	0.0000	0.5342	0.2183	0.2183	0.2337		
C2H6	0.0000	0.0241	0.0098	0.0098	0.0105		
H2S	0.0000	0.2147	0.0088	0.0088	0.0094		
Total:	32.4515	23.0490	26.4200	26.4200	28.2816		
Mole Flow Rate (mole/sec)							
O2	0.0064	0.0000	0.0064	0.0064	0.0064		
N2	0.2028	0.0635	0.2663	0.2663	0.2663		
SO2	0.0285	0.0000	0.0029	0.0029	0.0029		
CO	0.0000	0.0230	0.0023	0.0023	0.0023		
H2	0.0000	0.0330	0.0033	0.0033	0.0033		
CO2	0.0000	0.0187	0.0394	0.0394	0.0394		
H2O	0.0000	0.0200	0.0507	0.0507	0.0507		
CH4	0.0000	0.0055	0.0055	0.0055	0.0055		
C2H6	0.0000	0.0001	0.0001	0.0001	0.0001		
H2S	0.0000	0.0010	0.0001	0.0001	0.0001		
Ele S	0.0000	0.0000	0.0266	0.0266	0.000043		
Total:	0.2377	0.1649	0.4036	0.4036	0.3770		

Elemental Balance Check	(Error)
S	-8.3E-19
O	-8.7E-19
C	-8.7E-19
H	-1.7E-18
N	-5.6E-17

Sulfur Removed
0.0266 mole/sec
0.8517 kg/sec

Sulfur NOT Removed
0.095980 kg/sec

89.87161 Percent Eff.

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APPENDICES – FORTRAN PROGRAM SOURCE CODES

A) IGCC System Model

B) Graphics Program

C) Fixed Bed Coal Gasifier Model

D) Coal Gasifier Devolatilization Subroutines

E) Tridiagonal Matrix Solver Subroutine

F) Packed Bed Convective Heat Transfer Coefficient Subroutine

G) HRSG Bottoming Cycle Subroutines

A) IGCC System Model

```
C
C
C
C                              by
C                   NORTH CAROLINA STATE UNIVERSITY
C
C
C ***************************
C ** INITIALIZE VARIABLES **
C ***************************
      DOUBLE PRECISION T(60),MDOT(60),P(60),V(60),CPAIR,CPPROD,KAIR,
     &  KPROD,TAMB,PAMB,MDOTAIR,VINLET,PIPEFF(30),NPC1,NPC2,NPT1,NPT2,
     &  P3P2,M5FRACT,PRESSGAS,WCOMP1,WCOMP2,WTURB1,CVPROD,MPROD,RPROD,
     &  ID(12),A(12),B(12),H298(12),S298(12),M(12),CP(12),NN2,NO2,
     &  NCO2,NCO,NH2O,NH2,NCH4,NC2H6,NSO2,NH2S,NNO,NOH,PRESS,TAIR,
     &  TREACT,TPROD,Z,TOTWORK,WTURB2,PEFF,TCEFFC,TCEFFT,FCOOL,EFF,HR,
     &  HHVCOAL,MC,MH2,MO2,MN2,MS,PERH2O,PERASH,NLIQH2O,TLIQ,NCO2G,
     &  NSTEAM,TSTEAM,GASEFF,Z1,MCOAL,NC1,NO21,NN21,NH21,NS1,SUMN,Z2,
     &  LHVCOAL,HHVGAS,LHVGAS,EFFCOAL,HRCOAL,LHV,COMEFF,TAVG,CP1,CP2,
     &  HHV2D,LHV2D,M2D,HHVPD,LHVPD,HHVPPD,LHVPPD,M1D,HHV2W,LHV2W,M2W,
     &  HHVPW,LHVPW,HHVPPW,LHVPPW,M1W,MDOTASH,MDOTH2O,GENEFF,MGAS,CPA,
     &  MASSGAS,MASSCOAL,MASSAIR,MASSH2O,RGAS,LVGAS,LVAIR,V1,V2,V3,
     &  MASH,MH2O,EFFGASW,HRGASW,EFGASW,CV,KA,NCOG,NH2G,NCH4G,NC2H6G,
     &  HRGW,EFCOAL,HRC,WTURB21,WTURB22,O,N,FLAG,EXIT,NN2G,NH2OG,COUNTR
      DOUBLE PRECISION NH2SG,ICPAIR,IKAIR,ITAMB,IPAMB,HHVC,DIFFH,
     &   IMDOTAIR,IVINLET,ITCEFFT,ITCEFFC,IPEFF,ICOMEFF,IGASEFF,
     &   IGENEFF,IM5FRACT,IFCOOL,IPRESSGAS,IMC,IMH2,IMO2,IMN2,IMS,
     &   IHHVCOAL,IPERH2O,IPERASH,IZ1,IZ2,INN2,INCO2,INCO,INH2,
     &   INCH4,INC2H6,MDOTA(2),RPM,X,Y,XO,MDOTT(2),DIFF2(2),KT,WTURBR,
     &   MCF,MH2F,MO2F,MN2F,MSF,RAT(2),MAIR,PEREXTRAS,MFINES,MEXTRAS,
     &   MC1,MH21,MO21,MN21,MS1,NN2S,NO2S,NCO2S,NCOS,NH2OS,NH2SE,NCH4S,
     &   NC2H6S,NSO2S,NH2SS,NNOS,NOHS,DIFFY(2),WNET,WPUMPR1,WPUMPR2,
     &   WPUMPR3,WTURBR1,WTURBR2,WTURBR3,WTURBR4,QSUPER,QHPBOIL,
     &   QCONDENSER,QPIPELOSS,QLPBOIL,TOT1WORK,TOT2WORK,EFFGASW1,
     &   HRGASW1,EFFCOAL1,EFF1,HRCOAL1,HR1,EFGASW1,HRGW1,EFCOAL1,HRC1,
     &   EFFGASW2,HRGASW2,EFFCOAL2,EFF2,HRCOAL2,HR2,EFGASW2,HRGW2,
     &   EFCOAL2,HRC2,EFFGASW3,HRGASW3,EFFCOAL3,EFF3,HRCOAL3,HR3,
     &   EFGASW3,HRGW3,EFCOAL3,HRC3,EFFGASW4,HRGASW4,EFFCOAL4,EFF4,
     &   HRCOAL4,HR4,EFGASW4,HRGW4,EFCOAL4,HRC4,MDOTASH2,MDOTH2O2,
     &   XMASS,TOT4WORK,TOT3WORK,INH2S,INH2O,INO2,INSO2
      INTEGER I,J,TEST,FLAG2,L,K,TFACT,ITEST,IFLAG2,ITFACT,I2,COUNT2,
     &   IFLAG,TEST2
      CHARACTER QUEST*1,QS*1
C  Set Compound Constants
      A(1)=32.901
      A(2)=36.599
      A(3)=60.329
      A(4)=33.672
      A(5)=42.020
      A(6)=30.131
      A(7)=86.864
      A(8)=152.596
      A(9)=61.390
      A(10)=42.020
      A(11)=29.895
      A(12)=34.671
      B(1)=1434.17
      B(2)=2521.26
      B(3)=7488.88
```

```
      B(4)=1695.05
      B(5)=3050.70
      B(6)=413.611
      B(7)=15214.7
      B(8)=29845.7
      B(9)=7441.58
      B(10)=3050.70
      B(11)=99.4481
      B(12)=1823.22
      H298(1)=0
      H298(2)=0
      H298(3)=-393522
      H298(4)=-110529
      H298(5)=-241827
      H298(6)=0
      H298(7)=-74873
      H298(8)=-84667
      H298(9)=-296847
      H298(10)=-20142
      H298(11)=39463
      H298(12)=90592
      S298(1)=191.611
      S298(2)=205.142
      S298(3)=213.795
      S298(4)=197.653
      S298(5)=188.833
      S298(6)=130.684
      S298(7)=186.256
      S298(8)=229.602
      S298(9)=248.488
      S298(10)=205.609
      S298(11)=183.703
      S298(12)=210.761
      M(1)=28.013
      M(2)=32.000
      M(3)=44.010
      M(4)=28.010
      M(5)=18.015
      M(6)=2.016
      M(7)=16.043
      M(8)=28.054
      M(9)=64.066
      M(10)=34.076
      M(11)=17.007
      M(12)=30.006
C
C                          COMPOUNDS
C
C                            1   N2
C                            2   O2
C                            3   CO2
C                            4   CO
C                            5   H2O
C                            6   H2
C                            7   CH4
C                            8   C2H6
C                            9   SO2
C                           10   H2S
C                           11   OH
C                           12   NO
C
C
C
C
C
```

```
C
C
      DO 10 J=1,12
         ID(J)=J
 10   CONTINUE
C
      OPEN(UNIT=13,FILE='DATA',STATUS='UNKNOWN')
      ITFACT=1
      ITEST=0
      ICPAIR=1.0035
      IKAIR=1.400
      ITAMB=298.15
      IPAMB=101.325
      IMDOTAIR=633.*.4536
      IVINLET=10.
      ITCEFFT=.92
      ITCEFFC=.86
      IPEFF=.95
      ICOMEFF=.95
      IGASEFF=.96
      IGENEFF=.96
      IM5FRACT=.088
      IFCOOL=.05
      IPRESSGAS=2068.428
      IMC=81.3d0
      IMH2=5.3d0
      IMO2=9.8d0
      IMN2=1.7d0
      IMS=1.9d0
      IHHVCOAL=33725.0d0
      IPERH2O=.10d0
      IPERASH=.10d0
      IFLAG2=0
      IZ1=.5
      IZ2=.215
      INN2=.435d0
      INCO2=.103d0
      INCO=.212d0
      INH2=.201d0
      INCH4=.046d0
      INC2H6=.003d0
c
 98   CONTINUE
      DO 799 K=1,2
      IF(K.EQ.1) L=6
      IF(K.EQ.2) L=13
      DO 97 I=1,8
         WRITE(L,*) ' '
 97   CONTINUE
      WRITE(L,*) '                      **********************'
      WRITE(L,*) '                      **   COMMAND MENU   **'
      WRITE(L,*) '                      **********************'
      WRITE(L,*) ' '
      WRITE(L,*) '    Please type the number or letter of the variable'
      WRITE(L,*) '  you wish to change and PRESS ENTER.'
      WRITE(L,*) '       ---------------------------------------------'
      WRITE(L,*) '                        (TOGGLE VALUES)'
      WRITE(L,301)
      IF(ITEST.EQ.0) THEN
         WRITE(L,*) '                            COALGAS'
      ENDIF
      IF(ITEST.EQ.1) THEN
         WRITE(L,*) '                            METHANE'
         IM5FRACT=0.
         INCO2=0.
```

```
   INCO=0.
   INH2=0.
   INCH4=1.
   INC2H6=0.
   INH2O=0.
   INN2=0.
   INH2S=0.
   INSO2=0.
   INO2=0.
ENDIF
IF(ITEST.EQ.0) THEN
   WRITE(L,302)
   IF(IFLAG2.EQ.0) THEN
     WRITE(L,*) '                            EXPERIMENTAL'
   ENDIF
   IF(IFLAG2.EQ.1) THEN
      WRITE(L,*) '                   THEORETICAL -> (EQUILIBRIUM)'
   ENDIF
ENDIF
WRITE(L,*) '        ---------------------------------------------'
WRITE(L,*) '                         (INPUT VALUES)'
WRITE(L,303) ITAMB
WRITE(L,304) IPAMB
WRITE(L,305) IMDOTAIR
WRITE(L,306) IFCOOL
WRITE(L,307) ITCEFFC
WRITE(L,308) ITCEFFT
WRITE(L,309) ICONEFF
WRITE(L,310) IPEFF
WRITE(L,311) IGENEFF
IF(ITEST.EQ.0) THEN
   WRITE(L,401) IGASEFF
   WRITE(L,402) IPRESSGAS
   WRITE(L,403) IM5FRACT
   WRITE(L,*) ' F)                    COAL STATISTICS'
   WRITE(L,*) '                  (Amounts in MASS FRACTIONS)'
   WRITE(L,404) IMC
   WRITE(L,405) IMH2
   WRITE(L,406) IMO2
   WRITE(L,407) IMN2
   WRITE(L,408) IMS
   WRITE(L,409) IHHVCOAL
   WRITE(L,410) IPERH2O
   WRITE(L,411) IPERASH
   WRITE(L,412) IZ1
ENDIF
IF(IFLAG.EQ.0) THEN
   WRITE(L,*) ' I)                  PRODUCT STATISTICS'
   WRITE(L,*) '           (Amounts in moles - DRY & Sulfur FREE)'
   WRITE(L,414) INCO2
   WRITE(L,415) INCO
   WRITE(L,416) INH2
   WRITE(L,417) INCH4
   WRITE(L,418) INC2H6
   WRITE(L,419) INN2
ENDIF
IF(IFLAG.EQ.1) THEN
   WRITE(L,413) IZ2
ENDIF
IF(ITEST.EQ.0) THEN
   WRITE(L,*) ' '
   WRITE(L,505)
   IF(ITFACT.EQ.1) THEN
      WRITE(L,507)
   ENDIF
```

```
         IF(ITFACT.EQ.0) THEN
            WRITE(L,506)
         ENDIF
      ENDIF
C
C
 301  FORMAT(54H  1)               Fuel used in power system          )
 302  FORMAT(54H  2)      Method of finding products leaving gasifier )
 303  FORMAT(54H  3)  Temperature of air at inlet (Location 1)......  ,
     &   F6.2,2H K)
 304  FORMAT(54H  4)  Pressure of air at inlet (Location 1).........  ,
     &   F6.2,4H KPA)
 305  FORMAT(53H  5)  Mass flow rate of air at inlet (Location 1)... ,
     &   F7.2,7H KG/SEC)
 306  FORMAT(54H  6)  Fraction of air used to cool blades...........  ,
     &   F5.3)
 307  FORMAT(54H  7)  Efficiency of air compressors.................  ,
     &   F5.3)
 308  FORMAT(54H  8)  Efficiency of gas turbines....................  ,
     &   F5.3)
 309  FORMAT(54H  9)  Efficiency of combustor.......................  ,
     &   F5.3)
 310  FORMAT(54H  A)  Efficiency of pipes...........................  ,
     &   F5.3)
 311  FORMAT(54H  B)  Efficiency of generator and drive.............  ,
     &   F5.3)
 401  FORMAT(54H  C)  Efficiency of gasifier........................  ,
     &   F5.3)
 402  FORMAT(52H  D)  Pressure in gasifier..........................,
     &   F9.2,4H KPA)
 403  FORMAT(54H  E)  Fraction of air sent to gasifier..............  ,
     &   F5.3)
 404  FORMAT(33H                     Carbon....  ,F7.3)
 405  FORMAT(33H                    Hydrogen...  ,F7.3)
 406  FORMAT(33H                     Oxygen....  ,F7.3)
 407  FORMAT(33H                    Nitrogen...  ,F7.3)
 408  FORMAT(33H                     Sulfur....  ,F7.3)
 409  FORMAT(41H               Heating value of coal...  ,F7.1)
 410  FORMAT(49H           Percent WATER in coal as received...  ,
     &   F5.3)
 411  FORMAT(48H            Percent ASH in coal as received...  ,F5.3)
 412  FORMAT(54H  G)  Amount of water added per mole of dry coal....  ,
     &   F5.3)
 413  FORMAT(54H  H)  Amount of air added per mole of dry coal......  ,
     &   F5.3)
 414  FORMAT(31H                      CO2....  ,F8.5)
 415  FORMAT(31H                      CO.....  ,F8.5)
 416  FORMAT(31H                      H2.....  ,F8.5)
 417  FORMAT(31H                      CH4....  ,F8.5)
 418  FORMAT(31H                      CnHm...  ,F8.5)
 419  FORMAT(31H                      N2.....  ,F8.5)
 503  FORMAT(40H       Please input the new value ..... )
 505  FORMAT(41H  J)             AUXILIARY TURBINE STATUS)
 506  FORMAT(41H                    ---> THROTTLE <---   )
 507  FORMAT(44H                ---> AUXILIARY TURBINE <--- )
      WRITE(L,*) ' '
      WRITE(L,*) '              ----->  INPUT SELECTION  <-----'
      WRITE(L,*) '             (ENTER -> 0 <- TO CONTINUE ONWARD)'
      WRITE(L,*) ' '
 799  CONTINUE
      READ (5,'(A1)') QUEST
      IF(QUEST.EQ.'0') GO TO 96
      IF(QUEST.EQ.'1') THEN
         EXIT=0
         IF(ITEST.EQ.0) THEN
```

```
            ITEST=1
            EXIT=1
         ENDIF
         IF(ITEST.EQ.1.AND.EXIT.EQ.0) THEN
            ITEST=0
         ENDIF
      ENDIF
      IF(QUEST.EQ.'2') THEN
         EXIT=0
         IF(IFLAG2.EQ.0) THEN
            IFLAG2=1
            EXIT=1
         ENDIF
         IF(IFLAG2.EQ.1.AND.EXIT.EQ.0) THEN
            IFLAG2=0
         ENDIF
      ENDIF
      IF(QUEST.EQ.'3') THEN
         WRITE(6,503)
         READ(5,*) ITAMB
      ENDIF
      IF(QUEST.EQ.'4') THEN
         WRITE(6,503)
         READ(5,*) IPAMB
      ENDIF
      IF(QUEST.EQ.'5') THEN
         WRITE(6,503)
         READ(5,*) IMDOTAIR
      ENDIF
      IF(QUEST.EQ.'6') THEN
         WRITE(6,503)
         READ(5,*) IFCOOL
      ENDIF
      IF(QUEST.EQ.'7') THEN
         WRITE(6,503)
         READ(5,*) ITCEFFC
      ENDIF
      IF(QUEST.EQ.'8') THEN
         WRITE(6,503)
         READ(5,*) ITCEFFT
      ENDIF
      IF(QUEST.EQ.'9') THEN
         WRITE(6,503)
         READ(5,*) ICOMEFF
      ENDIF
      IF(QUEST.EQ.'A') THEN
         WRITE(6,503)
         READ(5,*) IPEFF
      ENDIF
      IF(QUEST.EQ.'B') THEN
         WRITE(6,503)
         READ(5,*) IGENEFF
      ENDIF
      IF(QUEST.EQ.'C') THEN
         WRITE(6,503)
         READ(5,*) IGASEFF
      ENDIF
      IF(QUEST.EQ.'D') THEN
         WRITE(6,503)
         READ(5,*) IPRESSGAS
      ENDIF
      IF(QUEST.EQ.'E') THEN
         WRITE(6,503)
         READ(5,*) IM5FRACT
      ENDIF
```

```
      IF(QUEST.EQ.'F') THEN
         WRITE(6,*)'                Input the new amount of CARBON.....'
         READ(5,*) INC
         WRITE(6,*)'                Input the new amount of HYDROGEN...'
         READ(5,*) INH2
         WRITE(6,*)'                Input the new amount of OXYGEN.....'
         READ(5,*) INO2
         WRITE(6,*)'                Input the new amount of NITROGEN...'
         READ(5,*) INN2
         WRITE(6,*)'                Input the new amount of SULFUR.....'
         READ(5,*) INS
      ENDIF
      IF(QUEST.EQ.'G') THEN
         WRITE(6,503)
         READ(5,*) IZ1
      ENDIF
      IF(QUEST.EQ.'H') THEN
         WRITE(6,503)
         READ(5,*) IZ2
      ENDIF
      IF(QUEST.EQ.'I') THEN
         WRITE(6,*)'                Input the new amount of CO2....'
         READ(5,*) INCO2
         WRITE(6,*)'                Input the new amount of CO.....'
         READ(5,*) INCO
         WRITE(6,*)'                Input the new amount of H2.....'
         READ(5,*) INH2
         WRITE(6,*)'                Input the new amount of CH4....'
         READ(5,*) INCH4
         WRITE(6,*)'                Input the new amount of CnHm...'
         READ(5,*) INC2H6
         WRITE(6,*)'                Input the new amount of N2.....'
         READ(5,*) INN2
      ENDIF
      IF(QUEST.EQ.'J') THEN
         EXIT=0
         IF(ITFACT.EQ.0) THEN
            ITFACT=1
            EXIT=1
         ENDIF
         IF(ITFACT.EQ.1.AND.EXIT.EQ.0) THEN
            ITFACT=0
         ENDIF
      ENDIF
      GO TO 98
 96   CONTINUE
      WRITE(6,*) 'Is a desulfurization plant in'
      READ (5,'(A1)') QS
C
      COUNT2=1
      MDOTA(1)=633.*.4536*.99
      MDOTA(2)=633.*.4536
 902  COUNT2=COUNT2+1
      DO 901 I2=1,2
      TFACT=ITFACT
      TEST=ITEST
      CPAIR=ICPAIR
      KAIR=IKAIR
      TAMB=ITAMB
      PAMB=IPAMB
      MDOTAIR=MDOTA(I2)
      VINLET=IVINLET
      TCEFFT=ITCEFFT
      TCEFFC=ITCEFFC
      PEFF=IPEFF
```

```
      COMEFF=ICOMEFF
      GASEFF=IGASEFF
      GENEFF=IGENEFF
      M5FRACT=IM5FRACT
      FCOOL=IFCOOL
      PRESSGAS=IPRESSGAS
      MC=IMC
      MH2=IMH2
      MO2=IMO2
      MN2=IMN2
      MS=IMS
      HHVCOAL=IHHVCOAL
      PERH2O=IPERH2O
      PERASH=IPERASH
      FLAG2=IFLAG2
      Z1=IZ1
      Z2=IZ2
      NN2=INN2
      NCO2=INCO2
      NCO=INCO
      NH2=INH2
      NCH4=INCH4
      NC2H6=INC2H6
      NH2O=0.
      NH2S=0.
      NSO2=0.
      NO2=0.
C ****************************
C ** PARAMETER ASSIGNMENT **
C ****************************
      PIPEFF(1)=PEFF
      PIPEFF(2)=PEFF
      PIPEFF(3)=PEFF
      PIPEFF(4)=PEFF
      PIPEFF(5)=PEFF
      PIPEFF(6)=PEFF
      NPC1=TCEFFC
      NPC2=TCEFFC
      NPT1=TCEFFT*TFACT
      NPT2=TCEFFT
      P3P2=11.7
C  *****************
C  ** MAIN SYSTEM **
C  *****************
C  --> INPUT INITIAL CONDITIONS <--
      T(1)=TAMB
      P(1)=PAMB
      MDOT(1)=MDOTAIR
C  --> 1 TO 2 (ADJUSTING FOR INCREASE IN SPEED OF GAS) <--
      V(2)=VINLET
      T(2)=T(1)-(V(2)**2./(2000.*CPAIR))
      P(2)=P(1)*(T(2)/T(1))**(KAIR/(KAIR-1.))
      MDOT(2)=MDOT(1)
C  --> 2 TO 3 (ACROSS FIRST COMPRESSOR) <--
      RPM=3600.
      X=MDOTA(I2)/122.55
      Y=RPM/(RPM/.9979)
      XO=2.33*Y**3.
      P3P2=1.+7.5*(X/Y)**2.-(X/(Y*Y))**4.
      NPC1=.5125005*(1.+.25*DEXP(-25.*(Y-.9)**2.)+.5*
     &   DEXP(-50.*(X-XO)**2.))
      V(3)=V(2)
      T(3)=T(2)*P3P2**((KAIR-1.)/(NPC1*KAIR))
      DO 589 I=1,3
         TAVG=(T(2)+T(3))/2.
```

```
         CP1=32.901-1434.17/TAVG
         CP2=36.599-2521.26/TAVG
         CPA=(CP2+3.77*CP1)/(4.77*28.97)
         CV=CPA-.287
         KA=CPA/CV
         T(3)=T(2)*P3P2**((KA-1.)/(NPC1*KA))
         WCOMP1=MDOT(2)*CPA*(T(2)-T(3))
 589  CONTINUE
      P(3)=P3P2*P(2)
      MDOT(3)=MDOT(2)
C  --> 3 TO 4 (PRESSURE LOSS IN PIPES) <--
      V(4)=V(3)
      T(4)=T(3)
      P(4)=PIPEFF(1)*P(3)
      MDOT(4)=MDOT(3)
C  --> 4 TO 13 (DIVISION OF STEAM TO COMBUSTOR) <--
      V(13)=V(4)
      T(13)=T(4)
      P(13)=P(4)
      MDOT(13)=(1.-M5FRACT-FCOOL)*MDOT(4)
C  --> 13 TO 14 (PRESSURE LOSS IN PIPES) <--
      V(14)=V(13)
      T(14)=T(13)
      P(14)=PIPEFF(6)*P(13)
      MDOT(14)=MDOT(13)
c *** branch ***
      IF(TEST.EQ.1) GO TO 14
C  --> 4 TO 5 (DIVISION OF STEAM TO SECOND COMPRESSOR) <--
      V(5)=V(4)
      T(5)=T(4)
      P(5)=P(4)
      MDOT(5)=M5FRACT*MDOT(4)
C  --> 5 TO 6 (PRESSURE LOSS IN PIPES) <--
      V(6)=V(5)
      T(6)=T(5)
      P(6)=PIPEFF(2)*P(5)
      MDOT(6)=MDOT(5)
C  --> 6 TO 7 TO 8 (ACROSS SECOND COMPRESSOR & LOSS IN PIPES) <--
      P(8)=PRESSGAS
      P(7)=P(8)/PIPEFF(3)
      V(7)=V(6)
      T(7)=T(6)*(P(7)/P(6))**((KAIR-1.)/(NPC2*KAIR))
      DO 588 I=1,3
         TAVG=(T(6)+T(7))/2.
         CP1=32.901-1434.17/TAVG
         CP2=36.599-2521.26/TAVG
         CPA=(CP2+3.77*CP1)/(4.77*28.97)
         CV=CPA-.287
         KA=CPA/CV
         T(7)=T(6)*(P(7)/P(6))**((KA-1.)/(NPC2*KA))
         WCOMP2=MDOT(6)*CPA*(T(6)-T(7))
 588  CONTINUE
      MDOT(7)=MDOT(6)
      V(8)=V(7)
      T(8)=1(7)
      MDOT(8)=MDOT(7)
C  --> 8 TO 9 (GASIFIER) <--
      V(9)=V(8)
      TAIR=T(8)
      TLIQ=25.d0
      TSTEAM=573.15d0
      MDOT(21)=.083744*Z1*MDOT(8)/Z2
      MDOT(22)=.5625*MDOT(21)
      IF(FLAG2.EQ.0) THEN
         CALL GASTEMP(MC,MH2,MO2,MN2,MS,PERH2O,PERASH,HHVCOAL,NN2,NO2,
```

```
     &      NCO2,NCO,NH2O,NH2,NCH4,NC2H6,NSO2,NH2S,NOH,NNO,NLIQH2O,
     &      TLIQ,NSTEAM,TSTEAM,GASEFF,TPROD,Z1,Z2,TAIR,MASH,MH2O)
      ENDIF
      IF(FLAG2.EQ.1) THEN
         CALL GASIFIER(MC,MH2,MO2,MN2,MS,PERH2O,PERASH,HHVCOAL,NN2,NO2,
     &      NCO2,NCO,NH2O,NH2,NCH4,NC2H6,NSO2,NH2S,NOH,NNO,NLIQH2O,
     &      TLIQ,NSTEAM,TSTEAM,GASEFF,TPROD,Z1,Z2,TAIR,MASH,MH2O)
      ENDIF
      NCO2G=NCO2
      NCOG=NCO
      NH2G=NH2
      NCH4G=NCH4
      NC2H6G=NC2H6
      NN2G=NN2
      NH2OG=NH2O
      NH2SG=NH2S
      T(20)=25.0
      T(21)=TSTEAM
      T(22)=TLIQ
      T(9)=TPROD
      NC1=MC/12.01
      NH21=MH2/2.016
      NO21=MO2/32.000
      NN21=MN2/28.013
      NS1=MS/32.06
      SUMN=NC1+NH21+NO21+NN21+NS1
      NC1=NC1/SUMN
      NH21=NH21/SUMN
      NO21=NO21/SUMN
      NN21=NN21/SUMN
      NS1=NS1/SUMN
      MCOAL=NC1*12.011+NH21*2.016+NO21*31.999+NN21*28.013+NS1*32.064
      LHVCOAL=HHVCOAL-(NH21-NS1)*44000./MCOAL
      MGAS=(NCO*28.011+NCO2*44.01+NH2*2.016+NH2O*18.015+NN2*28.013+
     &      NH2S*34.0760+NCH4*16.043+NC2H6*30.070+NSO2*64.0588)/
     &     (NCO+NCO2+NH2+NH2O+NN2+NH2S+NCH4+NC2H6+NSO2)
      MASSGAS=NCO*28.011+NCO2*44.01+NH2*2.016+NH2O*18.015+NN2*28.013+
     &      NH2S*34.0760+NCH4*16.043+NC2H6*30.070+NSO2*64.0588
      MASSCOAL=MCOAL+MASH+MH2O
      MASSAIR=Z2*(3.77*28.013+32.0)
      MASSH2O=Z1*18.015
      RGAS=1545./MGAS
      LVGAS=(RGAS*536.67)/(14.6959*144.)
      LVAIR=(53.3*536.67)/(14.6959*144.)
      V1=(LVGAS*MASSGAS)/MASSCOAL
      V2=MASSH2O/(LVGAS*MASSGAS)
      V3=(LVAIR*MASSAIR)/(LVGAS*MASSGAS)
      LHVCOAL=HHVCOAL-NH21*44011/MCOAL
      MDOT(20)=MCOAL*MDOT(8)/(137.56*Z2)
      DO 11 I=1,12
         CP(I)=A(I)-B(I)/900.
11    CONTINUE
      CALL GASPROP(NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,NO2
     &   ,CPPROD,MPROD,RPROD,CVPROD,KPROD,CP)
      HHVGAS = (NCH4*((-74873)-(-393522)-
     &   2.*(-285838))+NC2H6*((-84667)-2.*(-393522)-3.*(-285838))+
     &   NH2*(0.-(-285838))+NCO*((-110529)-(-393522))+
     &   NH2S*((-20142)-(-285838)-(-296847)))/(NCH4+NC2H6+
     &   NH2+NCO+NH2S+NCO2+NN2)
      HHVGAS=HHVGAS/MPROD
      LHVGAS = (NCH4*((-74873)-(-393522)-
     &   2.*(-241827))+NC2H6*((-84667)-2.*(-393522)-3.*(-241827))+
     &   NH2*(0.-(-241827))+NCO*((-110529)-(-393522))+
     &   NH2S*((-20142)-(-241827)-(-296847)))/(NCH4+NC2H6+NH2+NCO+
     &   NH2S+NCO2+NN2)
```

```
      LHVGAS=LHVGAS/MPROD
      HHV2D=NCO*282993.+NH2*285838.+NCH4*890322.+NC2H6*1559881.+
     &   NH2S*562543.+NH2O*44000.
      LHV2D=NCO*282993.+NH2*241827.+NCH4*802310.+NC2H6*1427844.+
     &   NH2S*518543.
      M1D=(NCO*28.01+NCO2*44.01+NH2*2.016+NCH4*16.043+NC2H6*30.07+
     &   NN2*28.013+NH2S*34.22)
      M2D=M1D/(NCO+NCO2+NH2+NCH4+NC2H6+NN2+NH2S)
      HHVPD=HHV2D/M1D
      LHVPD=LHV2D/M1D
      HHVPPD=(1.1127D-3)*M2D*HHVPD
      LHVPPD=(1.1127D-3)*M2D*LHVPD
      HHV2W=NCO*282993.+NH2*285838.+NCH4*890322.+NC2H6*1559881.+
     &   NH2S*562543.+NH2O*44000.
      LHV2W=NCO*282993.+NH2*241827.+NCH4*802310.+NC2H6*1427844.+
     &   NH2S*518543.
      M1W=(NCO*28.01+NCO2*44.01+NH2*2.016+NCH4*16.043+NC2H6*30.07+
     &   NN2*28.013+NH2O*18.015+NH2S*34.22)
      M2W=M1W/(NCO+NCO2+NH2+NCH4+NC2H6+NN2+NH2O+NH2S)
      HHVPW=HHV2W/M1W
      LHVPW=LHV2W/M1W
      HHVPPW=(1.1127D-3)*M2W*HHVPW
      LHVPPW=(1.1127D-3)*M2W*LHVPW
      P(9)=PRESSGAS
      MDOTASH=((PERASH*MDOT(20))/(1.-PERASH)+(PERASH*PERH2O*MDOT(20))/
     &   ((1.-PERH2O)*(1.-PERASH)))/(1.-((PERASH*PERH2O)/((1.-PERASH)*
     &   (1.-PERH2O))))
      MDOTH2O=(PERH2O*MDOT(20)+PERH2O*MDOTASH)/(1.-PERH2O)
      MDOT(23)=MDOTASH
      MDOT(9)=MDOT(8)+MDOT(20)+MDOT(21)+MDOT(22)+MDOTH2O
      MDOT(20)=MDOT(20)+MDOTASH+MDOTH2O
C  --> 9 TO 10 (PRESSURE LOSS IN PIPES) <--
      V(10)=V(9)
      T(10)=T(9)
      P(10)=PIPEFF(4)*P(9)
      MDOT(10)=MDOT(9)
C  --> 10 TO 11 TO 12 (ACROSS FIRST TURBINE & LOSS IN PIPES) <--
      P(12)=P(14)
      P(11)=P(12)/PIPEFF(5)
      V(11)=V(10)
      T(11)=T(10)*(P(11)/P(10))**((NPT1*(KPROD-1.))/KPROD)
      MDOT(11)=MDOT(10)
      WTURB1=MDOT(11)*CPPROD*(T(10)-T(11))
      V(12)=V(11)
      T(12)=T(11)
      MDOT(12)=MDOT(11)
C  --> 12 & 14 TO 15 (THROUGH COMBUSTOR) <--
      Z=MDOT(13)*(NCO*28.011+NCO2*44.01+NH2*2.016+NH2O*18.015+
     &    NN2*28.013+NH2S*34.0760+NCH4*16.043+NC2H6*30.070+
     &    NSO2*64.0588)/(137.61*MDOT(11))
      xmass=(NCO*28.011+NCO2*44.01+NH2*2.016+NH2O*18.015+
     &    NN2*28.013+NH2S*34.0760+NCH4*16.043+NC2H6*30.070+
     &    NSO2*64.0588)
 14   IF(TEST.EQ.1) THEN
         Z=6.37
         P(12)=P(14)
         P(11)=150.
         T(11)=300.
         V(11)=V(2)
         MDOT(11)=MDOT(13)*.1166/Z
         DO 13 I=1,12
            CP(I)=A(I)-B(I)/450.
 13      CONTINUE
         CALL GASPROP(NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,NO2
     &      ,CPPROD,MPROD,RPROD,CVPROD,KPROD,CP)
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```
         V(12)=V(11)
         T(12)=T(11)*(P(12)/P(11))**((KPROD-1.)/(.9*KPROD))
         MDOT(12)=MDOT(11)
         WCOMP2=MDOT(12)*CPPROD*(T(11)-T(12))
      ENDIF
      TAIR=T(14)
      TREACT=T(12)
      PRESS=P(14)
      LHV=LHVGAS
      IF(TEST.EQ.1) THEN
         LHV=50010.
      ENDIF
      IF(QS.EQ.'Y'.OR.QS.EQ.'y') NH2S=NH2S*.050
      CALL COMBUSTOR(NN2,Z,NCO2,NCO,NH2O,NH2,NCH4,NC2H6,
     &   NSO2,NH2S,TAIR,TREACT,TPROD,PRESS,N,NO2,LHV,COMEFF)
      V(15)=V(14)
      T(15)=TPROD
      P(15)=P(14)
      MDOT(15)=MDOT(14)+MDOT(12)
      N=7
C  --> 15 TO 16 (ACROSS SECOND TURBINE)
      DO 12 I=1,12
         CP(I)=A(I)-B(I)/1200.
 12   CONTINUE
      CALL GASPROP(NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,NO2
     &   ,CPPROD,MPROD,RPROD,CVPROD,KPROD,CP)
      P(18)=102.000
      P(16)=(P(18)/P(15))**.3333333333*P(15)
      KT=(277.77*(T(15)**.5))/P(15)
      MDOTT(I2)=((KT*P(15))/(T(15)**.5))
      DIFF2(I2)=MDOTT(I2)-MDOT(15)
 901  CONTINUE
      MDOTA(2)=(MDOTA(2)*DIFF2(1)-MDOTA(1)*DIFF2(2))/
     &   (DIFF2(1)-DIFF2(2))
      MDOTA(1)=.99*MDOTA(2)
      TEST2=ABS(DIFF2(2))
      IF(TEST2.GT..001) GO TO 902
      P(17)=P(16)
      V(16)=V(15)
      T(16)=T(15)*(P(16)/P(15))**((NPT2*(KPROD-1.))/KPROD)
      MDOT(16)=MDOT(15)
      WTURB21=MDOT(16)*CPPROD*(T(15)-T(16))
      MDOT(17)=MDOT(16)+MDOT(4)*FCOOL
      T(17)=(FCOOL*MDOT(4)*T(4)+MDOT(16)*T(16))/(FCOOL*MDOT(4)+
     &       MDOT(16))
      V(17)=V(16)
      V(18)=V(17)
      T(18)=T(17)*(P(18)/P(17))**((NPT2*(KPROD-1.))/KPROD)
      MDOT(18)=MDOT(17)
      WTURB22=MDOT(17)*CPPROD*(T(17)-T(18))
      WTURB2=WTURB21+WTURB22
C ** SECOND COMBUSTOR **
      RAT(1)=.020
      RAT(2)=.018
 829  COUNTR=COUNTR+1.
      DO 849 I=1,2
         HHVC=HHVCOAL
         TREACT=T(18)
         TPROD=0.
         PRESS=P(18)
         MC1=MC*RAT(I)/12.01
         MH21=MH2*RAT(I)/2.016
         MO21=MO2*RAT(I)/32.000
         MN21=MN2*RAT(I)/28.013
         MS1=MS*RAT(I)/32.06
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```
         MCF=MC1
         MH2F=MH21
         MO2F=MO21
         MN2F=MN21
         MSF=MS1
         NN2S=NN2
         NO2S=NO2
         NCO2S=NCO2
         NCOS=NCO
         NH2OS=NH2O
         NH2SE=NH2
         NCH4S=NCH4
         NC2H6S=NC2H6
         NSO2S=NSO2
         NH2SS=NH2S
         NOHS=NOH
         NNOS=NNO
         MFINES=MCF*12.011+MH2F*2.016+MO2F*31.999+MN2F*28.013+
     &      MSF*32.064
         MGAS=NN2S*28.013+NO2S*32.000+NCO2S*44.010+NCOS*28.010+
     &      NH2OS*18.015+NH2SE*2.016+NCH4S*16.043+NC2H6S*28.054+
     &      NSO2S*64.066+NH2SS*34.076+NOHS*17.007+NNOS*30.006
         PEREXTRAS=PERH2O+PERASH
         MEXTRAS=(PEREXTRAS*MFINES)/(1.-PEREXTRAS)
         MASH=(PERASH/PEREXTRAS)*MEXTRAS
         MH2O=(PERH2O/PEREXTRAS)*MEXTRAS
         NH2OS=NH2OS+MH2O/18.015
         MAIR=MGAS*FCOOL*MDOT(4)/MDOT(15)
         NO2S=NO2S+MAIR/137.56
         NN2S=NN2S+MAIR*3.77/137.56
         CALL COMBUSTOR2(NN2S,NO2S,NCO2S,NCOS,NH2OS,NH2SS,NCH4S,NC2H6S,
     &     NSO2S,NH2SS,NNOS,NOHS,MCF,MH2F,MO2F,MN2F,MSF,HHVC,MASH,
     &     TREACT,TPROD,PRESS,COMEFF,MFINES,DIFFH)
      DIFFY(1)=DIFFH
 849  CONTINUE
      RAT(2)=(RAT(2)*DIFFY(1)-RAT(1)*DIFFY(2))/(DIFFY(1)-DIFFY(2))
      RAT(1)=1.05*RAT(2)
      TEST2=ABS(DIFFY(2))
      IF(TEST2.GT..1) GO TO 829
      MDOT(50)=MDOT(15)*MFINES/MGAS
      T(50)=298.15
      P(50)=101.325
      MDOT(51)=MDOT(15)*MASH/MGAS
      T(51)=TPROD
      P(51)=PRESS
      MDOT(19)=MDOT(50)+MDOT(18)-MDOT(51)
      T(19)=TPROD
      P(19)=P(18)
      MDOTASH2=((PERASH*MDOT(50))/(1.-PERASH)+(PERASH*PERH2O*MDOT(50))/
     &   ((1.-PERH2O)*(1.-PERASH)))/(1.-((PERASH*PERH2O)/((1.-PERASH)*
     &   (1.-PERH2O))))
      MDOTH2O2=(PERH2O*MDOT(50)+PERH2O*MDOTASH2)/(1.-PERH2O)
C
      IF (TEST.EQ.1) THEN
         TOT2WORK=WTURB2+WCOMP1
         TOTWORK=TOT2WORK
      ENDIF
      IF (TEST.EQ.0) THEN
         TOT1WORK=WTURB1+WTURB2+WCOMP1+WCOMP2
         TOT2WORK=WTURB2+WCOMP1+WCOMP2
         IF(TFACT.EQ.0) THEN
            TOTWORK=TOT2WORK
         ENDIF
         IF(TFACT.EQ.1) THEN
            TOTWORK=TOT1WORK
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         ENDIF
         T(23)=1000.
         P(20)=P(8)
         P(21)=P(8)
         P(22)=P(8)
         P(23)=P(8)
      ENDIF
      T(20)=T(20)+273.15
      T(22)=T(22)+273.15
      TOTWORK=TOTWORK*GENEFF
      TOT1WORK=TOT1WORK*GENEFF
      TOT2WORK=TOT2WORK*GENEFF
C
      CALL GASPROP(NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,NO2
     &   ,CPPROD,MPROD,RPROD,CVPROD,KPROD,CP)
      CALL HEATRECOVERY(T,P,MDOT,WNET,WPUMPR1,WPUMPR2,WPUMPR3,
     &   WTURBR1,WTURBR2,WTURBR3,WTURBR4,QSUPER,QHPBOIL,QLPBOIL,
     &   QCONDENSER,QPIPELOSS,CPPROD)
      WTURBR=WNET
      TOT3WORK=TOT1WORK+WTURBR
      TOT4WORK=TOT2WORK+WTURBR
C
C  ** GAS TURBINE - THROTTLE AFTER GASIFIER
      EFFGASW2=TOT2WORK/(MDOT(9)*LHVPW)
      HRGASW2=3413./EFFGASW2
      EFFCOAL2=TOT2WORK/((MDOT(20)-MDOTASH-MDOTH2O)*LHVCOAL)
      EFF2=TOT2WORK/(MDOT(12)*50010)
      HRCOAL2=3413./EFFCOAL2
      HR2=3413./EFF2
      EFGASW2=TOT2WORK/(MDOT(9)*HHVFW)
      HRGW2=3413./EFGASW2
      EFCOAL2=TOT2WORK/((MDOT(20)-MDOTASH-MDOTH2O)*HHVCOAL)
      HRC2=3413./EFCOAL2
      EFF=EFF2
      HR=HR2
C
C  ** GAS TURBINE - RECOVERY TURBINE - THROTTLE AFTER GASIFIER **
      EFFGASW4=TOT4WORK/(MDOT(9)*LHVPW)
      HRGASW4=3413./EFFGASW4
      EFFCOAL4=TOT4WORK/((MDOT(20)-MDOTASH-MDOTH2O+MDOT(50)-MDOTASH2-
     &   MDOTH2O2)*LHVCOAL)
      EFF4=TOT4WORK/(MDOT(12)*50010)
      HRCOAL4=3413./EFFCOAL4
      HR4=3413./EFF4
      EFGASW4=TOT4WORK/(MDOT(9)*HHVPW)
      HRGW4=3413./EFGASW4
      EFCOAL4=TOT4WORK/((MDOT(20)-MDOTASH-MDOTH2O+MDOT(50)-MDOTASH2-
     &   MDOTH2O2)*HHVCOAL)
      HRC4=3413./EFCOAL4
C
C  ** GAS TURBINE - TURBINE AFTER GASIFIER **
      EFFGASW1=TOT1WORK/(MDOT(9)*LHVPW)
      HRGASW1=3413./EFFGASW1
      EFFCOAL1=TOT1WORK/((MDOT(20)-MDOTASH-MDOTH2O)*LHVCOAL)
      EFF1=TOT1WORK/(MDOT(12)*50010)
      HRCOAL1=3413./EFFCOAL1
      HR1=3413./EFF1
      EFGASW1=TOT1WORK/(MDOT(9)*HHVPW)
      HRGW1=3413./EFGASW1
      EFCOAL1=TOT1WORK/((MDOT(20)-MDOTASH-MDOTH2O)*HHVCOAL)
      HRC1=3413./EFCOAL1
C
C  ** GAS TURBINE - RECOVERY TURBINES - TURBINE AFTER GASIFER **
      EFFGASW3=TOT3WORK/(MDOT(9)*LHVPW)
      HRGASW3=3413./EFFGASW3
```

```
      EFFCOAL3=TOT3WORK/((MDOT(20)-MDOTASH-MDOTH2O+MDOT(50)-MDOTASH2-
     &   MDOTH2O2)*LHVCOAL)
      EFF3=TOT3WORK/(MDOT(12)*50010)
      HRCOAL3=3413./EFFCOAL3
      HR3=3413./EFF3
      EFGASW3=TOT3WORK/(MDOT(9)*HHVPW)
      HRGW3=3413./EFGASW3
      EFCOAL3=TOT3WORK/((MDOT(20)-MDOTASH-MDOTH2O+MDOT(50)-MDOTASH2-
     &   MDOTH2O2)*HHVCOAL)
      HRC3=3413./EFCOAL3
C
c
C  **************
C  ** PRINTING **
C  **************
      DO 797 K=1,2
      IF(K.EQ.1) L=6
      IF(K.EQ.2) L=13
      IF(FLAG2.EQ.1) THEN
         WRITE(L,*) ' '
         WRITE(L,*) '              GASIFIER PRODUCTS'
         ssum=NCO2G+NCOG+NH2G+NCH4G+NC2H6G+NN2G+NH2OG+NH2SG
         WRITE(L,701) NCO2G/ssum
         WRITE(L,702) NCOG/ssum
         WRITE(L,703) NH2G/ssum
         WRITE(L,704) NCH4G/ssum
         WRITE(L,705) NC2H6G/ssum
         WRITE(L,706) NN2G/ssum
         WRITE(L,707) NH2OG/ssum
         WRITE(L,708) NH2SG/ssum
701      FORMAT(27H        CO2 ----------->  ,F9.7)
702      FORMAT(27H        CO ------------>  ,F9.7)
703      FORMAT(27H        H2 ------------>  ,F9.7)
704      FORMAT(27H        CH4 ----------->  ,F9.7)
705      FORMAT(27H        C2H6 ---------->  ,F9.7)
706      FORMAT(27H        N2 ------------>  ,F9.7)
707      FORMAT(27H        H2O ----------->  ,F9.7)
708      FORMAT(27H        H2S ----------->  ,F9.7)
      ENDIF
      WRITE(L,*) ' '
      WRITE(L,*) '                    ENGLISH UNITS'
      WRITE(L,*) 'location   degrees F       psi        lbm/sec'
      DO 20 I=1,51
           WRITE(L,32) I,(T(I)*1.8-460.),(P(I)*.145),
     &     (MDOT(I)*2.204585538)
20    CONTINUE
      WRITE(L,*) ' '
      WRITE(L,*) '                    METRIC UNITS'
      WRITE(L,*) 'location   degrees K      KPA        kg/sec'
      DO 21 I=1,51
           WRITE(L,32) I,T(I),P(I),MDOT(I)
21    CONTINUE
32    format(2x,i4,5x,f8.2,5x,f8.2,5x,f8.2)
      WRITE(L,*) ' '
      WRITE(L,*) '              COMBUSTOR 1 PRODUCTS'
      sssum=NN2+NO2+NCO2+NCO+NH2O+NH2+NCH4+NC2H6+NSO2+NH2S+NOH+NNO
      WRITE(L,601) NN2/sssum
      WRITE(L,602) NO2/sssum
      WRITE(L,603) NCO2/sssum
      WRITE(L,604) NCO/sssum
      WRITE(L,605) NH2O/sssum
      WRITE(L,606) NH2/sssum
      WRITE(L,607) NCH4/sssum
      WRITE(L,608) NC2H6/sssum
      WRITE(L,609) NSO2/sssum
```

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      WRITE(L,610) NH2S/sssum
      WRITE(L,611) NOH/sssum
      WRITE(L,612) NNO/sssum
      WRITE(L,*) ' '
      WRITE(L,*) '                COMBUSTOR 2 PRODUCTS'
      ssssum=NN2S+NO2S+NCO2S+NCOS+NH2OS+NH2S+NCH4S+
     +     NC2H6S+NSO2S+NH2SS+NOHS+NNOS
      WRITE(L,601) NN2S/ssssum
      WRITE(L,602) NO2S/ssssum
      WRITE(L,603) NCO2S/ssssum
      WRITE(L,604) NCOS/ssssum
      WRITE(L,605) NH2OS/ssssum
      WRITE(L,606) NH2S/ssssum
      WRITE(L,607) NCH4S/ssssum
      WRITE(L,608) NC2H6S/ssssum
      WRITE(L,609) NSO2S/ssssum
      WRITE(L,610) NH2SS/ssssum
      WRITE(L,611) NOHS/ssssum
      WRITE(L,612) NNOS/ssssum
 601  FORMAT(27H            N2   --------> ,F11.5)
 602  FORMAT(27H            O2   --------> ,F11.5)
 603  FORMAT(27H            CO2  --------> ,F11.5)
 604  FORMAT(27H            CO   --------> ,F11.5)
 605  FORMAT(27H            H2O  --------> ,F11.5)
 606  FORMAT(27H            H2   --------> ,F11.5)
 607  FORMAT(27H            CH4  --------> ,F11.5)
 608  FORMAT(27H            C2H6 --------> ,F11.5)
 609  FORMAT(27H            SO2  --------> ,F11.5)
 610  FORMAT(27H            H2S  --------> ,F11.5)
 611  FORMAT(27H            OH   --------> ,F11.5)
 612  FORMAT(27H            NO   --------> ,F11.5)
      WRITE(L,*) ' '
      WRITE(L,*) '               WORK INPUT/OUTPUT (KW)'
      WRITE(L,*) ' '
      WRITE(L,*) '  WORK FROM MAIN GAS TURBINE (GE MS7001 HEAVY DUTY)'
      WRITE(L,621) WCOMP1
      WRITE(L,622) WCOMP2
      WRITE(L,623) WTURB1
      WRITE(L,624) WTURB2
      WRITE(L,*) ' '
      WRITE(L,626) TOTWORK
      WRITE(L,625) WTURBR
      WRITE(L,627) (WTURBR+TOTWORK)
 621  FORMAT(41H     Work of FIRST COMPRESSOR ---------> ,F9.1)
 622  FORMAT(41H     Work of SECOND COMPRESSOR --------> ,F9.1)
 623  FORMAT(41H     Work of FIRST TURBINE ------------> ,F9.1)
 624  FORMAT(41H     Work of SECOND TURBINE (optional)-> ,F9.1)
 625  FORMAT(41H  Net Work of RECOVERY TURBINES -------> ,F9.1)
 626  FORMAT(46H   TOTAL OUTPUT OF GAS TURBINE (GE MS7001)--> ,F9.1)
 627  FORMAT(46H    ******* TOTAL OUTPUT OF SYSTEM ******* -> ,F9.1)
      IF(TEST.EQ.0) THEN
         WRITE(L,*) ' '
         WRITE(L,*) '                HIGHER HEATING VALUES'
         WRITE(L,*) '                  KJ/KG           BTU/SCF'
         WRITE(L,631) HHVPD,HHVPPD
         WRITE(L,632) HHVPW,HHVPPW
 631     FORMAT(2X,10HDRY BASIS ,4X,F7.2,11X,F6.2)
 632     FORMAT(2X,10HWET BASIS ,4X,F7.2,11X,F6.2)
         WRITE(L,*) ' '
         WRITE(L,*) '                LOWER HEATING VALUES'
         WRITE(L,*) '                  KJ/KG           BTU/SCF'
         WRITE(L,633) LHVPD,LHVPPD
         WRITE(L,634) LHVPW,LHVPPW
 633     FORMAT(2X,10HDRY BASIS ,4X,F7.2,11X,F6.2)
 634     FORMAT(2X,10HWET BASIS ,4X,F7.2,11X,F6.2)
```

```
      WRITE(L,*) ' '
      WRITE(L,*) '             HEAT RATES & EFFICIENCIES'
      IF(TFACT.EQ.0) THEN
      WRITE(L,*) ' '
      WRITE(L,*) '        GAS TURBINE-THROTTLE AFTER GASIFIER'
      WRITE(L,*) '              (HIGHER HEATING VALUES)'
      WRITE(L,641) EFCOAL2
      WRITE(L,642) HRC2
      WRITE(L,643) EFGASW2
      WRITE(L,644) HRGW2
      WRITE(L,*) '               (LOWER HEATING VALUES)'
      WRITE(L,641) EFFCOAL2
      WRITE(L,642) HRCOAL2
      WRITE(L,643) EFFGASW2
      WRITE(L,644) HRGASW2
      WRITE(L,*) ' '
      WRITE(L,*) ' '
     WRITE(L,*)'GAS TURBINE-RECOVERY TURBINE-THROTTLE AFTER GASIFIER'
      WRITE(L,*) '              (HIGHER HEATING VALUES)'
      WRITE(L,641) EFCOAL4
      WRITE(L,642) HRC4
      WRITE(L,*) '               (LOWER HEATING VALUES)'
      WRITE(L,641) EFFCOAL4
      WRITE(L,642) HRCOAL4
      WRITE(L,*) ' '
      ENDIF
      IF(TFACT.EQ.1) THEN
      WRITE(L,*) ' '
      WRITE(L,*) '        GAS TURBINE-TURBINE AFTER GASIFIER'
      WRITE(L,*) '              (HIGHER HEATING VALUES)'
      WRITE(L,641) EFCOAL1
      WRITE(L,642) HRC1
      WRITE(L,643) EFGASW1
      WRITE(L,644) HRGW1
      WRITE(L,*) '               (LOWER HEATING VALUES)'
      WRITE(L,641) EFFCOAL1
      WRITE(L,642) HRCOAL1
      WRITE(L,643) EFFGASW1
      WRITE(L,644) HRGASW1
      WRITE(L,*) ' '
      WRITE(L,*) ' '
     WRITE(L,*)'GAS TURBINE-RECOVERY TURBINE-TURBINE AFTER GASIFIER'
      WRITE(L,*) '              (HIGHER HEATING VALUES)'
      WRITE(L,641) EFCOAL3
      WRITE(L,642) HRC3
      WRITE(L,*) '               (LOWER HEATING VALUES)'
      WRITE(L,641) EFFCOAL3
      WRITE(L,642) HRCOAL3
      WRITE(L,*) ' '
      ENDIF
      WRITE(L,*) '                  RELATIVE FLOWS'
      WRITE(L,645) (MDOT(21)/MDOT(20))
      WRITE(L,646) ((MDOT(21)+MDOT(22))/MDOT(20))
      WRITE(L,647) (MDOT(8)/MDOT(20))
      WRITE(L,648) V1
      WRITE(L,649) V2
      WRITE(L,650) V3
641   FORMAT(30H  COAL EFFICIENCY ----------> ,F5.4)
642   FORMAT(30H  COAL HEAT RATE -----------> ,F7.1)
643   FORMAT(30H  GAS EFFICIENCY -----------> ,F5.4)
644   FORMAT(30H  GAS HEAT RATE ------------> ,F7.1)
645   FORMAT(30H   LBM STEAM / LBM COAL ----> ,F7.4)
646   FORMAT(30H LBM STEAM&WATER / LBM COAL > ,F7.4)
647   FORMAT(30H     LMB AIR / LBM COAL  ---> ,F7.4)
648   FORMAT(F8.4,30H   STD FT^3 GAS OUT / LBM COAL)
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```
649     FORMAT(F8.5,30H   LBM H2O / STD FT^3 GAS OUT )
650     FORMAT(F8.5,30H   STD FT^3 AIR / STD FT^3 GAS)
      ENDIF
      IF(TEST.EQ.1) THEN
         WRITE(L,*) ' '
         WRITE(L,*) '      (BASED ON LOWER HEATING VALUE)'
         WRITE(L,*) '           Efficiency ---> ',EFF
         WRITE(L,*) '           Heat Rate ----> ',HR
      ENDIF
 797  CONTINUE
      CLOSE(13)
      END
C
      SUBROUTINE GASPROP(NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,NO2
     &   ,CPPROD,MPROD,RPROD,CVPROD,KPROD,CP)
      DOUBLE PRECISION NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,NO2,
     &   CPPROD,MPROD,RPROD,CVPROD,KPROD,CP(12)
      CPPROD=(NN2*CP(1)+NCO2*CP(3)+NCO*CP(4)+NH2O*CP(5)+NH2*CP(6)+
     &    NCH4*CP(7)+NC2H6*CP(8)+NSO2*CP(9)+NH2S*CP(10)+NO2*CP(2))/
     &    (NCO+NCO2+NH2+NH2O+NN2+NH2S+NCH4+NC2H6+NSO2+NO2)
      MPROD=(NCO*28.011+NCO2*44.01+NH2*2.016+NH2O*18.015+NN2*28.013+
     &      NH2S*34.0760+NCH4*16.043+NC2H6*30.070+NSO2*64.0588+NO2*
     &      31.999)/(NCO+NCO2+NH2+NH2O+NN2+NH2S+NCH4+NC2H6+NSO2+NO2)
      CPPROD=CPPROD/MPROD
      RPROD=8.3144/MPROD
      CVPROD=CPPROD-RPROD
      KPROD=CPPROD/CVPROD
      RETURN
      END
C
      SUBROUTINE GASIFIER(MC,MH2,MO2,MN2,MS,PERH2O,PERASH,HHV,NN2,NO2,
     &   NCO2,NCO,NH2O,NH2,NCH4,NC2H6,NSO2,NH2S,NOH,NNO,NLIQH2O,TLIQ,
     &   NSTEAM,TSTEAM,GASEFF,TPROD,Z1,Z2,TAIR,MASH,MH2O)
      DOUBLE PRECISION NCO2,NCO,NN2,NNO,
     &   A(11),B(11),T(2),X(5),H(11),S(11),G(11),ECONST(5),
     &   DIFF(3),NCH4,NC2H6,NSO2,NH2S,NC,NS,Z1,Z2,ID(11),H298(11),
     &   S298(11),M(11),NLIQH2O,NAIR,TLIQ,TSTEAM,TAIR,NC1,NH21,NO21,
     &   NS1,SUMN,NSTEAM,NN21,MC,MH2,MO2,MN2,MS,NH2O,NH2,NO2,HHV,
     &   DIF1,DIF2,DIF3,DIF4,DIF5,DIF6,NCOAL,MASH,PERASH,
     &   PERH2O,MH2O,MEXTRAS,PEREXTRAS,NFACT,
     &   GASEFF,NOH,TPROD,DIF7,SUM1,P
      INTEGER I,J,TEST,COUNT
      OPEN(UNIT=11,FILE='DATA1',STATUS='UNKNOWN')
      DO 10 J=1,10
         READ(11,*) ID(J),A(J),B(J),H298(J),S298(J),M(J)
 10   CONTINUE
      CLOSE(11)
      T(1)=1000.
      T(2)=860.
      NFACT=1
      COUNT=0.
C  ****************
C  ** MAIN LOOP **
C  ****************
      P=20.*101.325
      NC=MC/12.01
      NH2=MH2/2.016
      NO2=MO2/32.000
      NN2=MN2/28.013
      NS=MS/32.06
      SUMN=NC+NH2+NO2+NN2+NS
      SUM1=SUMN
      NC=NC/SUMN
      NC1=NC
      NH2=NH2/SUMN
```

```
      NH21=NH2
      NO2=NO2/SUMN
      NO21=NO2
      NN2=NN2/SUMN
      NN21=NN2
      NS=NS/SUMN
      NS1=NS
      NAIR=Z2
      NLIQH2O=.36d0*Z1
      NSTEAM=(1.0d0-.36d0)*Z1
      MCOAL=NC*12.011+NH2*2.016+NO2*31.999+NN2*28.013+NS*32.064
      PEREXTRAS=PERH2O+PERASH
      IF(PEREXTRAS.EQ.0) GO TO 25
      MEXTRAS=(PEREXTRAS*MCOAL)/(1.0d0-PEREXTRAS)
      MASH=(PERASH/PEREXTRAS)*MEXTRAS
      MH2O=(PERH2O/PEREXTRAS)*MEXTRAS
      Z1=Z1+MH2O/18.
25    CONTINUE
20    COUNT=COUNT+1.
      DO 40 I=1,2
         DO 30 J=1,12
            H(J)=H298(J)+A(J)*(T(I)-298.)-B(J)*DLOG(T(I)/298.)
            S(J)=S298(J)+A(J)*DLOG(T(I)/298.)+B(J)*(1./T(I)-1./298.)
            G(J)=H(J)-T(I)*S(J)
30       CONTINUE
         ECONST(1)=((G(6)+G(3)-G(5)-G(4))/(8.31434*T(I)))
         ECONST(2)=((G(4)+3*G(6)-G(7)-G(5))/(8.31434*T(I)))
         ECONST(3)=((2*G(4)+5*G(6)-G(8)-2.*G(5))/(8.31434*T(I)))
         ECONST(4)=((G(10)+2*G(5)-G(9)-3*G(6))/(8.31434*T(I)))
         CALL EQUIL(ECONST,P,X,Z1,Z2,NC1,NH21,NO21,NN21,NS1,T(I),NFACT)
         NCO=NC1-2.*Z2-2.*NO21+X(1)-X(2)-2.*X(3)
         NCO2=2*Z2+2*NO21-X(1)
         NH2=NH21+NC1-NS1-X(1)-3.*X(2)-5.*X(3)+3.*X(4)
         NH2O=Z1-NC1+X(1)+X(2)+2.*X(3)-2.*X(4)
         NN2=NFACT*3.77*Z2+NN21
         NH2S=NS1-X(4)
         NCH4=X(2)
         NC2H6=X(3)
         NSO2=X(4)
         NO2=0.D0
         DIF1=-(1.-GASEFF)*MCOAL*HHV
         DIF2=(NLIQH2O+MH2O/18.)*(-285838.+(72.8815*(TLIQ-25)+
     &      .026086*(TLIQ**2.-625.)))
         DIF3=NSTEAM*(-241827+42.02*(TSTEAM-298.)-
     &      3050.7*DLOG(TSTEAM/298.))
         DIF4=(NC1*(-393522)+NH21*(-285838)+NS1*(-296847)+
     &      HHV*(NC1*12.011+NH21*2.016+NO21*31.999+NN21*28.013+
     &      NS1*32.06))
         DIF5=-(NCO*H(4)+NCO2*H(3)+NH2*H(6)+NH2O*H(5)+NN2*H(1)+
     &      NH2S*H(10)+NCH4*H(7)+NC2H6*H(8)+NSO2*H(9))
         DIF6=-MASH*1.100*(1000-298.15)
         DIF7=NAIR*(0.+A(2)*(TAIR-298.)-B(2)*DLOG(TAIR/298.))+
     &      3.77*NAIR*(0.+A(1)*(TAIR-298.)-B(1)*DLOG(TAIR/298.))
         DIFF(I)=DIF1+DIF2+DIF3+DIF4+DIF5+DIF6+DIF7
40    CONTINUE
      T(2)=(T(2)*DIFF(1)-T(1)*DIFF(2))/(DIFF(1)-DIFF(2))
      TEST=ABS(DIFF(2))
      IF(TEST.GT..1) GO TO 20
      TPROD=T(2)
      RETURN
      END
C
      SUBROUTINE EQUIL(ECONST,P,X,Z1,Z2,NC1,NH21,NO21,NN21,NS1,T,NFACT)
      DOUBLE PRECISION ECONST(4),X(4),A(4,4),B(4),F(4),FO(4),
     &   DX(4),Z1,Z2,NC1,NH21,NO21,NN21,NS1,T,NFACT,ACON,BCON,
```

```
     &   NH22,NH2O2,P,DELX
      INTEGER J,TEST,I
      IF(T.GT.950.) THEN
         ACON=2.77528D-1
         BCON=-9.97464D-1
         X(1)=ACON*DEXP(-ECONST(1)*BCON)
         ACON=3.27707D-1
         BCON=-2.18632D-1
         X(2)=ACON*DEXP(-ECONST(2)*BCON)
         ACON=4.47123D-4
         BCON=-1.99404D-1
         X(3)=ACON*DEXP(-ECONST(3)*BCON)
         ACON=1.18176D-7
         BCON=-4.24760D-1
         X(4)=ACON*DEXP(-ECONST(4)*BCON)
      ENDIF
      IF(T.LE.950) THEN
         ACON=2.16083D-1
         BCON=-6.72486D-1
         X(1)=ACON*DEXP(-ECONST(1)*BCON)
         ACON=2.41669D-1
         BCON=4.10778D-2
         X(2)=ACON*DEXP(-ECONST(2)*BCON)
         ACON=3.41324D-5
         BCON=8.61858D-3
         X(3)=ACON*DEXP(-ECONST(3)*BCON)
         ACON=5.56312D-8
         BCON=-3.80523D-1
         X(4)=ACON*DEXP(-ECONST(4)*BCON)
      ENDIF
 10   CALL KSUB(X,P,FO,Z1,Z2,NC1,NH21,NO21,NN21,NS1,NFACT)
      DO 30 I=1,4
         DELX=.01*X(I)
         X(I)=X(I)+DELX
         CALL KSUB(X,P,F,Z1,Z2,NC1,NH21,NO21,NN21,NS1,NFACT)
         DO 20 J=1,4
            A(J,I)=(F(J)-FO(J))/DELX
 20      CONTINUE
         X(I)=X(I)-DELX
         B(I)=ECONST(I)-FO(I)
 30   CONTINUE
      CALL GAUSS(A,DX,B,4)
      TEST=0.
      DO 40 I=1,4
         X(I)=X(I)+DX(I)
         TEST=TEST+ABS(DX(I)/X(I))
 40   CONTINUE
      NH22=NH21+NC1-NS1-X(1)-3.*X(2)-5.*X(3)+3.*X(4)
      NH2O2=Z1-NC1+X(1)+X(2)+2.*X(3)-2.*X(4)
      IF(NH22.LT.0) THEN
         X(2)=(-.01+NH22+3.*X(2))/3.
      ENDIF
      IF(NH2O2.LT.0) THEN
         X(1)=.01-Z1-NC1-X(2)-2.*X(3)+2.*X(4)
      ENDIF
      IF(TEST.GT.0.00001) GO TO 10
      RETURN
      END
C
      SUBROUTINE KSUB(X,P,F,Z1,Z2,NC1,NH21,NO21,NN21,NS1,NFACT)
      DOUBLE PRECISION X(4),F(4),Z1,Z2,NC1,NH21,NO21,NN21,NS1,NFACT,
     &   YCO,YCO2,YH2,YH2O,YN2,YH2S,YCH4,YC2H6,YSO2,SUMN,P
      SUMN=NC1-2.*Z2-2.*NO21+X(1)-X(2)-2.*X(3)+2.*Z2+2.*NO21-X(1)+NH21+
     & NC1-NS1-X(1)-3.*X(2)-5.*X(3)+3.*X(4)+Z1-NC1+X(1)+X(2)+2.*X(3)-
     & 2.*X(4)+NFACT*3.77*Z2+NN21+NS1-X(4)+X(2)+X(3)+X(4)
```

```
      YCO=(NC1-2.*Z2-2.*NO21+X(1)-X(2)-2.*X(3))/SUMN
      YCO2=(2.*Z2+2.*NO21-X(1))/SUMN
      YH2=(NH21+NC1-NS1-X(1)-3.*X(2)-5.*X(3)+3.*X(4))/SUMN
      YH2O=(Z1-NC1+X(1)+X(2)+2.*X(3)-2.*X(4))/SUMN
      YN2=(NFACT*3.77*Z2+NN21)/SUMN
      YH2S=(NS1-X(4))/SUMN
      YCH4=X(2)/SUMN
      YC2H6=X(3)/SUMN
      YSO2=X(4)/SUMN
      F(1)=DLOG(((YH2O*P/100.)*(YCO*P/100.))/
     &       ((YH2*P/100.)*(YCO2*P/100.)))
      F(2)=DLOG(((YCH4*P/100.)*(YH2O*P/100.))/
     &       ((YCO*P/100.)*(YH2*P/100.)**3.))
      F(3)=DLOG(((YC2H6*P/100.)*(YH2O*P/100.)**2.)/
     &       ((YCO*P/100.)**2.*(YH2*P/100.)**5.))
      F(4)=DLOG(((YSO2*P/100.)*(YH2*P/100.)**3.)/
     &       ((YH2S*P/100.)*(YH2O*P/100.)**2.))
      RETURN
      END
C
      SUBROUTINE COMBUSTOR(NN2,Z,NCO2,NCO,NH2O,NH2,NCH4,NC2H6,
     &   NSO2,NH2S,TAIR,TREACT,TPROD,P,N,NO2,HHV,COMEFF)
      DOUBLE PRECISION NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,
     &   NO2,NNO,NOH,A(12),B(12),T(2),X(7),H(12),
     &   S(12),G(12),ECONST(12),DIFF(2),ID(12),H298(12),S298(12),
     &   M(12),TAIR,TREACT,TPROD,NCO21,NCO1,NH21,NCH41,NC2H61,
     &   NH2O1,NN21,NH2S1,NSO21,NO21,NNO1,NOH1,DIF1,DIF2,DIF3,DIF4,
     &   NFACT,P,HR(12),HA(12),TR,TA,Z,COMEFF,HHV,MPROD
      INTEGER N,TEST,I,COUNT,J
      OPEN(UNIT=12,FILE='DATA1',STATUS='UNKNOWN')
      DO 10 J=1,12
         READ(12,*) ID(J),A(J),B(J),H298(J),S298(J),M(J)
 10   CONTINUE
      CLOSE(12)
      NN21=NN2
      NCO21=NCO2
      NCO1=NCO
      NH2O1=NH2O
      NH21=NH2
      NCH41=NCH4
      NC2H61=NC2H6
      NSO21=NSO2
      NH2S1=NH2S
      NFACT=1.0d0
      DO 12 J=1,12
         TR=TREACT
         TA=TAIR
         HR(J)=H298(J)+A(J)*(TR-298.)-B(J)*DLOG(TR/298.)
         HA(J)=H298(J)+A(J)*(TA-298.)-B(J)*DLOG(TA/298.)
 12   CONTINUE
      T(1)=1300.
      T(2)=1350.
      MPROD=(NCO*28.011+NCO2*44.01+NH2*2.016+NH2O*18.015+NN2*28.013+
     &      NH2S*34.0760+NCH4*16.043+NC2H6*30.070+NSO2*64.0588+NO2*
     &      31.999)/(NCO+NCO2+NH2+NH2O+NN2+NH2S+NCH4+NC2H6+NSO2+NO2)
      HHV=HHV*MPROD
      COUNT=0.
C  ****************
C  ** MAIN LOOP **
C  ****************
 20   COUNT=COUNT+1.
      DO 40 I=1,2
         DO 30 J=1,12
            H(J)=H298(J)+A(J)*(T(I)-298.)-B(J)*DLOG(T(I)/298.)
            S(J)=S298(J)+A(J)*DLOG(T(I)/298.)+B(J)*(1./T(I)-1./298.)
```

```
            G(J)=H(J)-T(I)*S(J)
 30        CONTINUE
           ECONST(1)=(2.*G(3)-2.*G(4)-G(2))/(8.31434*T(I))
           ECONST(2)=(2.*G(9)+2.*G(5)-2.*G(10)-3.*G(2))/(8.31434*T(I))
           ECONST(3)=(2.*G(5)-2.*G(6)-G(2))/(8.31434*T(I))
           ECONST(4)=(2.*G(5)-G(6)-2.*G(11))/(8.31434*T(I))
           ECONST(5)=(G(1)+G(2)-2.*G(12))/(8.31434*T(I))
           ECONST(6)=(G(3)+2.*G(5)-2.*G(2)-G(7))/(8.31434*T(I))
           ECONST(7)=(2.*G(3)+3.*G(5)-3.5*G(2)-G(8))/(8.31434*T(I))
           X(1)=0.
           X(2)=0.
           X(3)=0.
           X(4)=0.
           X(5)=0.
           X(6)=0.
           X(7)=0.
           NN2=Z*3.77*NFACT+NN21-X(5)
           NO2=Z-.5*NCO1-.5*NH21-2.*NCH41-3.5*NC2H61-1.5*NH2S1+X(1)+
     &        3.*X(2)+X(3)-X(5)+2.*X(6)+3.5*X(7)
           NCO2=NCO21+NCO1+NCH41+2.*NC2H61-2.*X(1)-X(6)-2.*X(7)
           NCO=2.*X(1)
           NH2O=NH21+NH2O1+2.*NCH41+3.*NC2H61+NH2S1-2.*X(2)-2.*X(3)-
     &        2.*X(4)-2.*X(6)-3.*X(7)
           NH2=2.*X(3)+X(4)
           NCH4=X(6)
           NC2H6=X(7)
           NSO2=NH2S1+NSO21-2.*X(2)
           NH2S=2.*X(2)
           NOH=2.*X(4)
           NNO=2.*X(5)
           DIF1=(COMEFF-1.)*HHV
           DIF2=NCO21*HR(3)+NCO1*HR(4)+NH21*HR(6)+NCH41*HR(7)+
     &       NC2H61*HR(8)+NH2O1*HR(5)+NN21*HR(1)+NH2S1*HR(10)+
     &       NSO21*HR(9)+NO21*HR(2)+NNO1*HR(12)+NOH1*HR(11)
           DIF3=Z*3.77*HA(1)+Z*HA(2)
           DIF4=-(NCO*H(4)+NCO2*H(3)+NH2*H(6)+NH2O*H(5)+NN2*H(1)+
     &       NH2S*H(10)+NCH4*H(7)+NC2H6*H(8)+NSO2*H(9)+NNO*H(12)+
     &       NOH*H(11)+NO2*H(2))
           DIFF(I)=DIF1+DIF2+DIF3+DIF4
 40     CONTINUE
        T(2)=(T(2)*DIFF(1)-T(1)*DIFF(2))/(DIFF(1)-DIFF(2))
        T(1)=.95*T(2)
        TEST=ABS(DIFF(2))
        IF(TEST.GT..1) GO TO 20
 50     TPROD=T(2)
        RETURN
        END
C
        SUBROUTINE COMBUSTOR2(NN2,NO2,NCO2,NCO,NH2O,NH2,NCH4,NC2H6,
     &  NSO2,NH2S,NNO,NOH,MCF,MH2F,MO2F,MN2F,MSF,HHVC,MASH,TREACT,
     &  TPROD,P,COMEFF,MFINES,DIFF)
        DOUBLE PRECISION NCO2,NCO,NH2,NCH4,NC2H6,NH2O,NN2,NH2S,NSO2,
     &   NO2,NNO,NOH,A(12),B(12),X(7),H(12),MFINES,
     &   S(12),G(12),ECONST(12),DIFF,ID(12),H298(12),S298(12),
     &   M(12),TAIR,TREACT,TPROD,NCO21,NCO1,NH21,NCH41,NC2H61,
     &   NH2O1,NN21,NH2S1,NSO21,NO21,NNO1,NOH1,DIF1,DIF2,DIF3,DIF4,
     &   P,HR(12),TR,COMEFF,HHVC,MPROD,TEMP,MC,MH2,MO2,MN2,MH2O1,
     &   MS,MC1,MH21,MO21,MN21,MS1,MASH,MCF,MH2F,MO2F,MN2F,MSF
        INTEGER TEST,I,J
        OPEN(UNIT=12,FILE='DATA1',STATUS='UNKNOWN')
        DO 10 J=1,12
           READ(12,*) ID(J),A(J),B(J),H298(J),S298(J),M(J)
 10     CONTINUE
        CLOSE(12)
        TEMP=949.8167
```

```
      NN21=NN2
      NO21=NO2
      NCO21=NCO2
      NCO1=NCO
      NH2O1=NH2O
      NH21=NH2
      NCH41=NCH4
      NC2H61=NC2H6
      NSO21=NSO2
      NH2S1=NH2S
      NNO1=NNO
      NOH1=NOH
      MC1=MCF
      MH21=MH2F
      MO21=MO2F
      MN21=MN2F
      MS1=MSF
C
      DO 12 J=1,12
         TR=TREACT
         HR(J)=H298(J)+A(J)*(TR-298.)-B(J)*DLOG(TR/298.)
         H(J)=H298(J)+A(J)*(TEMP-298.)-B(J)*DLOG(TEMP/298.)
         G(J)=H(J)-TEMP*S(J)
 12   CONTINUE
C
      ECONST(1)=(2.*G(3)-2.*G(4)-G(2))/(8.31434*TEMP)
      ECONST(2)=(2.*G(9)+2.*G(5)-2.*G(10)-3.*G(2))/(8.31434*TEMP)
      ECONST(3)=(2.*G(5)-2.*G(6)-G(2))/(8.31434*TEMP)
      ECONST(4)=(2.*G(5)-G(6)-2.*G(11))/(8.31434*TEMP)
      ECONST(5)=(G(1)+G(2)-2.*G(12))/(8.31434*TEMP)
      ECONST(6)=(G(3)+2.*G(5)-2.*G(2)-G(7))/(8.31434*TEMP)
      ECONST(7)=(2.*G(3)+3.*G(5)-3.5*G(2)-G(8))/(8.31434*TEMP)
      X(1)=0.
      X(2)=0.
      X(3)=0.
      X(4)=0.
      X(5)=0.
      X(6)=0.
      X(7)=0.
      NN2=NN21+MN21-X(5)
      NO2=NO21+MO21-.5*NCO1-2.*NCH41-3.5*NC2H61-1.5*NH2S1-.5*NH21-
     &    MC1-.5*MH21-MS1+X(1)+3.*X(2)+X(3)-X(5)+2.*X(6)+3.5*X(7)
      NCO2=NCO21+NCO1+NCH41+2.*NC2H61+MC1-2.*X(1)-X(6)-2.*X(7)
      NCO=2.*X(1)
      NH2O=NH21+NH2O1+2.*NCH41+3.*NC2H61+NH2S1+MH21+MH2O1-2.*X(2)
     &     -2.*X(3)-2.*X(4)-2.*X(6)-3.*X(7)
      NH2=2.*X(3)+X(4)
      NCH4=X(6)
      NC2H6=X(7)
      NSO2=NH2S1+NSO21+MS1-2.*X(2)
      NH2S=2.*X(2)
      NOH=2.*X(4)
      NNO=2.*X(5)
      DIF1=(COMEFF-1.)*MFINES*HHVC
      DIF2=NCO21*HR(3)+NCO1*HR(4)+NH21*HR(6)+NCH41*HR(7)+
     &   NC2H61*HR(8)+NH2O1*HR(5)+NN21*HR(1)+NH2S1*HR(10)+
     &   NSO21*HR(9)+NO21*HR(2)+NNO1*HR(12)+NOH1*HR(11)
      DIF3=-(NCO*H(4)+NCO2*H(3)+NH2*H(6)+NH2O*H(5)+NN2*H(1)+
     &   NH2S*H(10)+NCH4*H(7)+NC2H6*H(8)+NSO2*H(9)+NNO*H(12)+
     &   NOH*H(11)+NO2*H(2))
      DIF4=-MASH*1.100*(949.8-298.15)
      DIFF=DIF1+DIF2+DIF3+DIF4
      TPROD=949.8
      RETURN
      END
```

```
C
      SUBROUTINE GAUSS(A,X,B,N)
      DOUBLE PRECISION A(N,N),X(N),B(N),T
      INTEGER I,M,J,NM,N,KP,K
      NM=N-1
      DO 20 K=1,NM
      KP=K+1
      DO 20 I=KP,N
      T=A(I,K)/A(K,K)
      DO 10 J=K,N
 10   A(I,J)=A(I,J)-T*B(K)
 20   B(I)=B(I)-T*B(K)
      X(N)=B(N)/A(N,N)
      K=N
      DO 40 M=1,NM
      K=K-1
      KP=K+1
      X(K)=B(K)
      DO 30 J=KP,N
 30   X(K)=X(K)-A(K,J)*X(J)
 40   X(K)=X(K)/A(K,K)
      RETURN
      END
C
      SUBROUTINE GASTEMP(MC,MH2,MO2,MN2,MS,PERH2O,PERASH,HHV,NN2,NO2,
     &   NCO2,NCO,NH2O,NH2,NCH4,NC2H6,NSO2,NH2S,NOH,NNO,NLIQH2O,TLIQ,
     &   NSTEAM,TSTEAM,GASEFF,TPROD,Z1,Z2,TAIR,MASH,MH2O)
      DOUBLE PRECISION MC,MH2,MO2,MN2,MS,PERH2O,PERASH,HHV,NN2,NO2,
     &   NCO2,NCO,NH2O,NH2,NCH4,NC2H6,NSO2,NH2S,NOH,NNO,NLIQH2O,TLIQ,
     &   NSTEAM,TSTEAM,T(2),MCOAL,PEREXTRAS,MEXTRAS,MASH,MH2O,GASEFF,
     &   NC1,NH21,NO21,NN21,NS1,DIF1,DIF2,DIF3,DIF4,DIF5,DIF6,DIFF(2),
     &   TEST,TPROD,AMOUNTC,RATIO,DIF7,ID(12),A(12),B(12),H298(12),
     &   S298(12),M(12),H(12),TAIR,Z1,Z2,NAIR,SUMN
      INTEGER COUNT,I,J
      OPEN(UNIT=11,FILE='DATA1',STATUS='UNKNOWN')
      DO 10 J=1,10
         READ(11,*) ID(J),A(J),B(J),H298(J),S298(J),M(J)
 10   CONTINUE
      CLOSE(11)
      T(1)=800.
      T(2)=900.
      NC1=MC/12.01
      NH21=MH2/2.016
      NO21=MO2/32.000
      NN21=MN2/28.013
      NS1=MS/32.06
      SUMN=NC1+NH21+NO21+NN21+NS1
      NC1=NC1/SUMN
      NH21=NH21/SUMN
      NO21=NO21/SUMN
      NN21=NN21/SUMN
      NS1=NS1/SUMN
      AMOUNTC=NCO2+NCO+NCH4+2.*NC2H6
      RATIO=NC1/AMOUNTC
      NN2=NN2*RATIO
      NCO2=NCO2*RATIO
      NCO=NCO*RATIO
      NH2=NH2*RATIO
      NCH4=NCH4*RATIO
      NC2H6=NC2H6*RATIO
      NH2S=NS1
      Z2=(NN2-NN21)/3.77
      NAIR=Z2
      NLIQH2O=.36*Z1
      NSTEAM=(1.-.36)*Z1
```

```
      MCOAL=NC1*12.011+NH21*2.016+NO21*31.999+NN21*28.013+NS1*32.064
      PEREXTRAS=PERH2O+PERASH
      IF(PEREXTRAS.EQ.0) GO TO 25
      MEXTRAS=(PEREXTRAS*MCOAL)/(1.-PEREXTRAS)
      MASH=(PERASH/PEREXTRAS)*MEXTRAS
      MH2O=(PERH2O/PEREXTRAS)*MEXTRAS
      Z1=Z1+MH2O/18.
      NH2O=NH21+Z1-NH2-2.*NCH4-3.*NC2H6-NS1
25    CONTINUE
20    COUNT=COUNT+1.
      DO 40 I=1,2
         DO 30 J=1,12
            H(J)=H298(J)+A(J)*(T(I)-298.)-B(J)*DLOG(T(I)/298.)
30       CONTINUE
         DIF1=-(1.-GASEFF)*MCOAL*HHV
         DIF2=(NLIQH2O+MH2O/18.)*(-285838.+(72.8815*(TLIQ-25)+
     &     .026086*(TLIQ**2.-625.)))
         DIF3=NSTEAM*(-241827+42.02*(TSTEAM-298.)-
     &     3050.7*DLOG(TSTEAM/298.))
         DIF4=(NC1*(-393522)+NH21*(-285838)+NS1*(-296847)+
     &     HHV*(NC1*12.011+NH21*2.016+NO21*31.999+NN21*28.013+
     &     NS1*32.06))
         DIF5=-(NCO*H(4)+NCO2*H(3)+NH2*H(6)+NH2O*H(5)+NN2*H(1)+
     &     NH2S*H(10)+NCH4*H(7)+NC2H6*H(8)+NSO2*H(9))
         DIF6=-MASH*1.100*(1000-298.15)
         DIF7=NAIR*(0.+A(2)*(TAIR-298.)-B(2)*DLOG(TAIR/298.))+
     &     3.77*NAIR*(0.+A(1)*(TAIR-298.)-B(1)*DLOG(TAIR/298.))
         DIFF(I)=DIF1+DIF2+DIF3+DIF4+DIF5+DIF6+DIF7
40    CONTINUE
      T(2)=(T(2)*DIFF(1)-T(1)*DIFF(2))/(DIFF(1)-DIFF(2))
      T(1)=1.05*T(2)
      TEST=ABS(DIFF(2))
      IF(TEST.GT..1) GO TO 20
      TPROD=T(2)
      RETURN
      END
C
      SUBROUTINE HEATRECOVERY(T,P,MDOT,WNET,WPUMPR1,WPUMPR2,WPUMPR3,
     &   WTURBR1,WTURBR2,WTURBR3,WTURBR4,QSUPER,QHPBOIL,QLPBOIL,
     &   QCONDENSER,QPIPELOSS,CPPROD)
      DOUBLE PRECISION WNET,TA1,TA2,TA3,TA4,P1,P2,P3,P4,P5,P6,P7,P8,P9,
     &   P10,P11,P12,P13,P14,P15,P16,
     &   CPAIR,MDOTAIR,NP,NT,
     &   MDOTGAS,CPWATER,CPWATER1,CPWATER2,UABOIL1,UABOIL2,WTURBR1,UA1,
     &   WTURBR2,WTURBR3,WTURBR4,WTURB,WPUMP,WPUMP1,WPUMP2,WPUMP3,C1,C2,
     &   DIFFA3,DIFFA4,RCRIT1,RCRIT2,RCRIT3,RCRIT4,R1,R2,R3,R4,MDOTB1,
     &   MDOTB2,MDOTF,
     &   COUNTA2,COUNTA3,COUNTA4,VF1,VG1,HF1,HG1,SF1,SG1,VF3,VG3,HF3,
     &   HG3,SF3,SG3,VF5,VG5,HF5,HG5,SF5,SG5,UA2,RSTAR1,RSTAR2,V6,H6,S6,
     &   V12,H12,S12,VF12,VG12,HF12,HG12,SF12,SG12,V10,H10,S10,VF10,
     &   VG10,HF10,HG10,SF10,SG10,X10,V16,H16,S16,VF16,VG16,HF16,HG16,
     &   SF16,SG16,H2,H4,V7,H7,S7,T12T,T16T,H8,S8,H9,S9,H11,S11,
     &   TESTA2,TESTA3,TESTA4,DIFFA2,UASUPER,DTMEAN,TA2PRIME,VF15,VG15,
     &   HF15,HG15,SF15,SG15,H13,S13,H14,QIN,T1,T2,T3,T4,T5,T6,T7,T8,T9,
     &   T10,T11,T12,T13,T14,T15,T16,MDOTGASE,QPIPELOSS,MDOT,T,P,QREJ,
     &   CPPROD,QCONDENSER,QSUPER,QHPBOIL,QLPBOIL,WTURB1,WTURB2,WTURB3,
     &   WTURB4,WPUMPR1,WPUMPR2,WPUMPR3,QGAS,QBD
      INTEGER I
      DIMENSION C1(2),DIFFA3(2),C2(2),DIFFA4(2),MDOT(60),T(60),P(60)
      P1=10.0D0
      P2=140.0D0
      P3=140.0D0
      P4=6276.0D0
      P5=P4
      P6=P4
```

```
      P14=1207.0D0
      P7=.95D0*P6
      P8=2172.0D0
      P9=P14*.95D0
      P10=P14*.95D0
      P11=140.0D0/.95D0
      P12=140.0D0
      P13=10.0D0
      P15=P14
      P16=P14*.95D0
      TA1=T(19)
      T6=838.70D0
      T7=T6-3.0D0
      NP=.6D0
      NT=.75D0
      UABOIL1=1082.7D0
      UABOIL2=700.0D0
      MDOTAIR=.985D0*MDOT(19)
      MDOTGAS=MDOT(22)
      CPAIR=CPPROD
      CPWATER=4.167D0
      CALL DSAT(T1,P1,VF1,VG1,HF1,HG1,SF1,SG1,2)
      WPUMP1=VF1*(P2-P1)/NP
      T2=WPUMP1/CPWATER+T1
      H2=WPUMP1+HF1
      CALL DSAT(T3,P3,VF3,VG3,HF3,HG3,SF3,SG3,2)
      WPUMP2=VF3*(P4-P3)/NP
      T4=WPUMP2/CPWATER+T3
      H4=WPUMP2+HF3
      WPUMP3=VF3*(P14-P3)/NP
      T14=WPUMP3/CPWATER+T3
      H14=WPUMP3+HF3
      TA2=480.0D0+273.15D0
      CALL DSAT(T5,P5,VF5,VG5,HF5,HG5,SF5,SG5,2)
      CALL DSUPER(T6,P6,V6,H6,S6,1)
      COUNTA2=0.0D0
10    COUNTA2=COUNTA2+1.0D0
      COUNTA3=0.0D0
      CPWATER1=(HF5-H4)/(T5-T4)
      RCRIT1=(HG5-HF5)/CPWATER1/(TA2-T5)
      RCRIT2=CPWATER1*(TA2-T4)/(HG5-HF5+CPWATER1*(T5-T4))
      IF(RCRIT1.GE.RCRIT2)THEN
        RSTAR1=RCRIT1
       ELSE
        RSTAR1=RCRIT2
      ENDIF
      R1=RSTAR1/(1.D0-DEXP(-UABOIL1/MDOTAIR/CPAIR))
      R2=R1+(UABOIL1/MDOTAIR/CPAIR)*(R1-RSTAR1)
      C1(1)=1/R1
      C1(2)=1/R2
20    COUNTA3=COUNTA3+1.0D0
      DO 30 I=1,2
        UA1=MDOTAIR*CPAIR*(C1(I)/(C1(I)-1.0D0)*DLOG((TA2-T5-C1(I)*(HG5-
     &      HF5)/CPWATER1)/(TA2-T4-C1(I)*((HG5-HF5)/CPWATER1+T5-T4)))+
     &      DLOG((TA2-T5)/(TA2-T5-C1(I)*((HG5-HF5)/CPWATER1))))
30      DIFFA3(I)=UA1-UABOIL1
      TESTA3=DABS(DIFFA3(2))
      C1(2)=(C1(2)*DIFFA3(1)-C1(1)*DIFFA3(2))/(DIFFA3(1)-DIFFA3(2))
      C1(1)=.97*C1(2)
      IF(COUNTA3.GT.20.0D0)GO TO 99
      IF(TESTA3-.1)40,40,20
40    MDOTB1=C1(2)*CPAIR/CPWATER1*MDOTAIR
      TA3=TA2-C1(2)*(T5-T4+(HG5-HF5)/CPWATER1)
      TA2PRIME=TA1-.97D0*MDOTB1*(H6-HG5)/CPAIR/MDOTAIR
      DIFFA2=TA2-TA2PRIME
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```
      TESTA2=DABS(DIFFA2)
      TA2=(TA2+TA2PRIME)/2.0D0
      IF(COUNTA2.GT.90.0D0)GO TO 99
      IF(TESTA2-.1D0)50,50,10
50    DTMEAN=(TA1-T6-TA2+T5)/DLOG((TA1-T6)/(TA2-T5))
      UASUPER=MDOTAIR*CPAIR*(TA1-TA2)/DTMEAN
      COUNTA4=0.0D0
      CALL DSAT(T15,P15,VF15,VG15,HF15,HG15,SF15,SG15,2)
      CPWATER2=(HF15-H14)/(T15-T14)
      RCRIT3=(HG15-HF15)/CPWATER2/(TA3-T15)
      RCRIT4=CPWATER2*(TA3-T14)/(HG15-HF15+CPWATER2*(T15-T14))
      IF(RCRIT3.GE.RCRIT4)THEN
        RSTAR2=RCRIT3
       ELSE
        RSTAR2=RCRIT4
      ENDIF
      R3=RSTAR2/(1.0D0-DEXP(-UABOIL2/CPAIR/MDOTAIR))
      R4=R3+(UABOIL2/MDOTAIR/CPAIR)*(R1-RSTAR2)
      C2(1)=1/R3
      C2(2)=1/R4
60    COUNTA4=COUNTA4+1.0D0
      DO 70 I=1,2
        UA2=MDOTAIR*CPAIR*(C2(I)/(C2(I)-1.0D0)*DLOG((TA3-T15-C2(I)*(HG15
     &      -HF15)/CPWATER2)/(TA3-T14-C2(I)*((HG15-HF15)/CPWATER2+T15-
     &      T14)))+DLOG((TA3-T15)/(TA3-T15-C2(I)*((HG15-HF15)/
     &      CPWATER2))))
70      DIFFA4(I)=UA2-UABOIL2
      TESTA4=DABS(DIFFA4(2))
      C2(2)=(C2(2)*DIFFA4(1)-C2(1)*DIFFA4(2))/(DIFFA4(1)-DIFFA4(2))
      C2(1)=.97D0*C2(2)
      IF(COUNTA4.GT.90.D0)GO TO 98
      IF(TESTA4-.1)80,80,60
80    MDOTB2=C2(2)*CPAIR/CPWATER2*MDOTAIR
      TA4=TA3-C2(2)*(T15-T14+(HG15-HF15)/CPWATER2)
      CALL DSUPER(T7,P7,V7,H7,S7,1)
      CALL DTURBINE(NT,P7,P8,T7,T8,H7,H8,S7,S8,WTURB1)
      CALL DTURBINE(NT,P8,P9,T8,T9,H8,H9,S8,S9,WTURB2)
      CALL DSAT(T16T,P16,VF16,VG16,HF16,HG16,SF16,SG16,2)
      T16=T15-3.0D0
      IF(T16.GT.T16T)THEN
        CALL DSUPER(T16,P16,V16,H16,S16,1)
       ELSE
        CALL DSAT(T16,P16,VF16,VG16,HF16,HG16,SF16,SG16,2)
        H16=HG16
        S16=SG16
      END IF
      H10=((.97D0*MDOTB1-MDOTGAS)*H9+.97D0*MDOTB2*H16)/(.97D0*MDOTB1+
     &    .97D0*MDOTB2-MDOTGAS)
      CALL DSAT(T10,P10,VF10,VG10,HF10,HG10,SF10,SG10,2)
      IF(H10.GT.HG10)THEN
        CALL DSUPER(T10,P10,V10,H10,S10,3)
       ELSE
        X10=(H10-HF10)/(HG10-HF10)
        S10=X10*SG10+(1.0D0-X10)*SF10
      END IF
      CALL DTURBINE(NT,P10,P11,T10,T11,H10,H11,S10,S11,WTURB3)
      CALL DTURBINE(NT,P11,P13,T11,T13,H11,H13,S11,S13,WTURB4)
      CALL DSAT(T12T,P12,VF12,VG12,HF12,HG12,SF12,SG12,2)
      IF(T12.GT.T12T)THEN
        CALL DSUPER(T12,P12,V12,H12,S12,1)
       ELSE
        H12=HG12
        S12=SG12
        T12=T12T
      END IF
```

```
 MDOTF=(MDOTB1+MDOTB2)*(HF3-H2)/(H12-H2)
 WTURB=.97D0*MDOTB1*WTURB1+(.97D0*MDOTB1-MDOTGAS)*WTURB2+(.97D0*
& MDOTB1+.97D0*MDOTB2-MDOTGAS)*WTURB3+(.97D0*MDOTB1+.97D0*MDOTB2-
& MDOTGAS-MDOTF)*WTURB4
 WPUMP=(MDOTB1+MDOTB2-MDOTF)*WPUMP1+MDOTB1*WPUMP2+MDOTB2*WPUMP3
 WNET=WTURB-WPUMP
 MDOT(39)=MDOTF
 MDOT(24)=MDOT(18)
 MDOT(25)=MDOT(18)
 MDOT(26)=MDOT(18)
 MDOT(27)=.97D0*MDOTB1+.97D0*MDOTB2-MDOTF-MDOTGAS
 MDOT(28)=MDOTB1+MDOTB2-MDOTF
 MDOT(29)=MDOT(28)+MDOT(39)
 MDOT(30)=MDOTB1
 MDOT(31)=MDOTB1
 MDOT(32)=.97D0*MDOTB1
 MDOT(33)=MDOT(32)
 MDOT(34)=MDOT(33)
 MDOT(35)=MDOT(34)-MDOT(21)
 MDOT(36)=MDOT(35)
 MDOT(37)=MDOT(36)+.97D0*MDOTB2
 MDOT(38)=MDOT(37)
 MDOT(40)=MDOT(38)-MDOT(39)
 MDOT(41)=MDOT(40)
 MDOT(42)=.03D0*MDOTB1+.03D0*MDOTB2+MDOTGAS
 MDOT(43)=MDOT(27)+MDOT(42)
 MDOT(44)=MDOTB2
 MDOT(45)=MDOTB2
 MDOT(46)=.97D0*MDOTB2
 MDOT(47)=MDOT(46)
 MDOT(48)=.03D0*MDOTB1
 MDOT(49)=.03D0*MDOTB2
 P(27)=P1
 P(28)=P2
 P(29)=P3
 P(30)=P4
 P(31)=P5
 P(32)=P6
 P(33)=P7
 P(34)=P8
 P(35)=P8
 P(36)=P9
 P(37)=P10
 P(38)=P11
 P(39)=P12
 P(40)=P11
 P(41)=P13
 P(42)=P1
 P(43)=P1
 P(44)=P14
 P(45)=P15
 P(46)=P15
 P(47)=P16
 P(48)=P5
 P(49)=P15
 P(24)=P(18)
 P(25)=P(18)
 P(26)=P(18)
 T(24)=TA2
 T(25)=TA3
 T(26)=TA4
 T(27)=T1
 T(28)=T2
 T(29)=T3
 T(30)=T4
```

```
      T(31)=T5
      T(32)=T6
      T(33)=T7
      T(34)=T8
      T(35)=T8
      T(36)=T9
      T(37)=T10
      T(38)=T11
      T(39)=T12
      T(40)=T11
      T(41)=T13
      T(42)=T1
      T(43)=T1
      T(44)=T14
      T(45)=T15
      T(46)=T15
      T(47)=T16
      T(48)=T5
      T(49)=T15
      WTURBR1=MDOT(33)*WTURB1
      WTURBR2=MDOT(35)*WTURB2
      WTURBR3=MDOT(37)*WTURB3
      WTURBR4=MDOT(40)*WTURB4
      WPUMPR1=MDOT(28)*WPUMP1
      WPUMPR2=MDOT(30)*WPUMP2
      WPUMPR3=MDOT(44)*WPUMP3
      QREJ=(.97D0*MDOTB1+.97D0*MDOTB2-MDOTF-MDOTGAS)*H13
     &  -(.97D0*MDOTB1+.97D0*MDOTB2-MDOTF-MDOTGAS)*HF1
      QCONDENSER=QREJ
      QBD=.03D0*MDOTB1*(HG5-HF1)+.03D0*MDOTB2*(HG15-HF1)
      QGAS=MDOTGAS*(H8-HF1)-MDOTGAS*(H7-H8)
      QPIPELOSS=.97D0*MDOTB1*(H6-H7)+.97D0*MDOTB2*(HG15-H16)
      QIN=MDOTAIR*CPAIR*(TA1-TA4)
      QSUPER=MDOT(24)*(T(18)-T(24))*CPAIR
      QHPBOIL=MDOT(25)*(T(24)-T(25))*CPAIR
      QLPBOIL=MDOT(26)*(T(25)-T(26))*CPAIR
      RETURN
 98   WRITE(6,*)'THE TA3 IS WRONG FOR SOME REASON'
      WRITE(6,119)TA3,TA3E
 119  FORMAT(1X,'TEMP OF AIR AT BOILER #2 IS ',6X,F10.3,1X,'K',1X,'|',
     &1X,F10.3,1X,'F')
      RETURN
 99   WRITE(6,*)'GUESS ANOTHER TA2'
      RETURN
      END
C
C
      SUBROUTINE DTURBINE(NT,PENTER,PEXIT,TENTER,TEXIT,HENTER,HEXIT,
     &SENTER,SEXIT,WORKTURB)
      DOUBLE PRECISION NT,PENTER,PEXIT,TENTER,TEXIT,HENTER,HEXIT,
     &   SENTER,SEXIT,
     &   WORKTURB,XS,XR,VFX,VGX,HFX,HGX,SFX,SGX,TXS,VXS,HXS,VEXIT
      CALL DSAT(TEXIT,PEXIT,VFX,VGX,HFX,HGX,SFX,SGX,2)
      IF(SENTER.GE.SGX)THEN
        CALL DSUPER(TXS,PEXIT,VXS,HXS,SENTER,2)
        WORKTURB=NT*(HENTER-HXS)
        HEXIT=HENTER-WORKTURB
        CALL DSUPER(TEXIT,PEXIT,VEXIT,HEXIT,SEXIT,3)
       ELSE
        XS=(SENTER-SFX)/(SGX-SFX)
        HXS=XS*HGX+(1.0D0-XS)*HFX
        WORKTURB=NT*(HENTER-HXS)
        HEXIT=HENTER-WORKTURB
        XR=(HEXIT-HFX)/(HGX-HFX)
        SEXIT=XR*SGX+(1.0D0-XR)*SFX
```

```
      ENDIF
      RETURN
      END
C
C
C     SATURATED AND SUPERHEATED STEAM TABLES
C
C
      subroutine dlook(x1,x2,y1,y2,m,n,prop)
      implicit double precision (a-h,o-z)
      dimension prop(5),prop0(5)
      count=0.
 10   count=count+1
      call dsuperprop(x1,x2,prop0)
      b1=y1-prop0(m)
      b2=y2-prop0(n)
      dx=.01d0*x1
      x1=x1+dx
      call dsuperprop(x1,x2,prop)
      a11=(prop(m)-prop0(m))/dx
      a21=(prop(n)-prop0(n))/dx
      x1=x1-dx
      dx=.01d0*x2
      x2=x2+dx
      call dsuperprop(x1,x2,prop)
      a12=(prop(m)-prop0(m))/dx
      a22=(prop(n)-prop0(n))/dx
      x2=x2-dx
      dx2=(b2-a21*b1/a11)/(a22-a21*a12/a11)
      dx1=(b1-a12*dx2)/a11
      test=dabs(dx2/x2)+dabs(dx1/x1)
      x2=x2+dx2
      x1=x1+dx1
      if(count.gt.10.d0) go to 20
      if(test.gt..00001d0) go to 10
      go to 30
 20   write(6,600) x1,x2
600   format(" no converge, t=",e14.7,"   rho=",e14.7)
 30   call dsuperprop(x1,x2,prop)
      return
      end
      function drhoz(tr,pr)
      implicit double precision (a-h,o-z)
      if(tr-1.d0) 20,10,10
 10   x=(pr/tr**3)**2
      z=1.d0-x*(1.289d0/tr-.532d0*tr*x)
      go to 30
 20   z=1.d0-.7d0*(pr/tr)**2
 30   drhoz=73.94d0*pr/z/tr
      return
      end
      subroutine dsatprop(t,p,dpdt,rhol)
      implicit double precision (a-h,o-z)
      dimension d(8),f(8)
      data (d(i),i=1,8)/3.6711257,-28.512396,222.6524,-882.43852,
     *2000.276,-2612.2557,1829.7674,-533.5052/
      data(f(i),i=1,8)/-7.41924,.29721,-.1155286,8.685635e-3,
     * 1.094098e-3,-4.39993e-3,2.520658e-3,-5.218684e-4/
      data a,tp,tc,pc,rhoc/.01,338.15,647.286,22089.,317./
      x=a*(t-tp)
      y=f(1)+x*(f(2)+x*(f(3)+x*(f(4)+x*(f(5)+x*(f(6)+x*(f(7)+
     *x*f(8)))))))
      dydx=f(2)+x*(2.*f(3)+x*(3.*f(4)+x*(4.*f(5)+x*(5.*f(6)+
     *x*(6.*f(7)+x*7.*f(8))))))
      p=pc*dexp((tc/t-1.)*y)
```

```
      dpdt=p*(-y*tc/t/t+(tc/t-1.)*dydx*a)
      x=(1.-t/tc)**(1./3.)
      x3=x*x*x
      rhol=rhoc*(1.+x*(d(1)+x3*(d(4)+d(7)*x3)+x*(d(2)+x3*(d(5)+
     *d(8)*x3)+x*(d(3)+d(6)*x3))))
      return
      end
      subroutine dsat(t,p,vf,vg,hf,hg,sf,sg,n)
      implicit double precision (a-h,o-z)
      if(n-1) 10,10,20
10    call dsatprop(t,p,dpdt,rhol)
      go to 30
20    t=4900./(17.572-dlog(p))
      count=0.
25    count=count+1
      call dsatprop(t,p0,dpdt,rhol)
      t=t+(p-p0)/dpdt
      err=dabs((p-p0)/p)
      if(count.gt.10d0) go to 26
      if(err.gt..00001d0) go to 25
      go to 30
26    write(6,610) t
610   format("  no converge at tsat=",e14.7)
30    vf=1./rhol
      call dsuper(t,p,vg,hg,sg,1)
      hfg=t*(vg-vf)*dpdt
      hf=hg-hfg
      sf=sg-hfg/t
      return
      end
      subroutine dsuper (t,p,v,h,s,n)
      implicit double precision (a-h,o-z)
      dimension prop(5),x(2),diff(2)
      pr=p/22089.
      if(n-2) 10,20,30
10    tr=t/647.29d0
      x(1)=drhoz(tr,pr)
      x(2)=.98*x(1)
      count=0
15    count=count+1
      do 16 i=1,2
      call dsuperprop(t,x(i),prop)
16    diff(i)=prop(3)-p
      x(2)=(x(2)*diff(1)-x(1)*diff(2))/(diff(1)-diff(2))
      x(1)=.98*x(2)
      if(count.gt.10) go to 17
      test=dabs(diff(2)/p)
      if(test.gt..00001d0) go to 15
      h=prop(4)
      s=prop(5)
      go to 40
17    write(6,600) t,p
600   format("  did not converge at t=",e14.7,"  p=",e14.7)
      go to 40
20    b=8.57-s-.4615*dlog(p/101.35)
      c=-.2652-.4615*pr
      xi=(-b+dsqrt(b*b-.8136*c))/.4086
      tr=xi**.33333
      t=tr*647.29
      rho=drhoz(tr,pr)
      v=1./rho
      call dlook(t,rho,p,s,3,5,prop)
      t=prop(1)
      h=prop(4)
      go to 40
```

```
30    b=3072.3-h
      c=-418.2119*pr-130.2
      xi=(-b+dsqrt(b*b-1210.6*c))/605.3
      tr=xi**.4
      t=tr*647.29
      rho=drhoz(tr,pr)
      v=1./rho
      call dlook(t,rho,p,h,3,4,prop)
      t=prop(1)
      s=prop(5)
40    v=1./prop(2)
      return
      end
      subroutine dsuperprop(t,rho,prop)
      implicit double precision (a-h,o-z)
      dimension prop(5),a(10,7),rhoa(7),c(7),g(6),cp(7),h(7),hi(7)
      data(a(i,1),i=1,10)/2.9492937e-2,-1.3213917e-4,2.7464632e-7,
     *-3.6093828e-10,3.4218431e-13,-2.4450042e-16,1.5518535e-19,
     *5.9728487e-24,-.41030848,-4.1605860e-4/
      data(a(i,2),i=1,10)/-5.198586e-3,7.7779182e-6,-3.3301902e-8,
     *-1.6254622e-11,-1.7731074e-13,1.2748742e-16,1.3746153e-19,
     *1.5597836e-22,.3373118,-2.0988866e-4/
      data(a(i,3),i=1,10)/6.8335354e-3,-2.6149751e-5,6.532639e-8,
     * -2.6181978e-11,0.,0.,0.,0.,-1.3746618e-1,-7.3396848e-4/
      data(a(i,4),i=1,10)/-1.5641040e-4,-7.2546108e-7,-9.2734289e-9,
     *4.3125840e-12,0.,0.,0.,0.,6.7874983e-3,1.0401717e-5/
      data(a(i,5),i=1,10)/-6.3972405e-3,2.6409282e-5,-4.7740374e-8,
     *5.6323130e-11,0.,0.,0.,0.,.13687317,6.4581880e-4/
      data(a(i,6),i=1,10)/-3.9661401e-3,1.5453061e-5,-2.9142470e-8,
     *2.9568796e-11,0.,0.,0.,0.,7.9847970e-2,3.9917570e-4/
      data(a(i,7),i=1,10)/-6.9048554e-4,2.7407416e-6,-5.1028070e-9,
     *3.9636085e-12,0.,0.,0.,0.,1.3041253e-2,7.1531353e-5/
      data(rhoa(j),j=1,7)/634.,1000.,1000.,1000.,1000.,1000.,1000./
      data(g(i),i=1,6)/4.6e4,1.011249e3,.83893,-2.19989e-4,
     *2.46619e-7,-9.7047e-11/
      data e,ta,xm,tc,pc,rhoc,t0/.0048,1000.,18.016,647.286,22.089,
     *317.,273.16/
      r=8314.34/xm
      s=6696.5776-g(1)/t+g(2)*dlog(t/t0)+t*(g(3)+t*(g(4)/2.+t*(g(5)/3.
     *+t*g(6)/4.)))+g(1)/t0-t0*(g(3)+t0*(g(4)/2.+t0*(g(5)/3.+t0*g(6)
     */4.)))
      u=2375020.7+g(1)*dlog(t/t0)+t*(g(2)+t*(g(3)/2.+t*(g(4)/3.+t*(
     *g(5)/4.+t*g(6)/5.))))-t0*(g(2)+t0*(g(3)/2.+t0*(g(4)/3.+t0*
     *(g(5)/4.+t0*g(6)/5.))))
      tau=ta/t
      tauc=ta/tc
      c(1)=r*t
      c(2)=c(1)*(tau-tauc)
      cp(1)=r
      temp=r*tau
      cp(2)=c(2)/t-temp
      do 10 i=3,7
      c(i)=c(i-1)*(tau-2.5)
      cp(i)=c(i)/t-temp*(tau-2.5+(i-2)*(tau-tauc))
10    temp=temp*(tau-2.5)
      te=dexp(-e*rho)
      do 40 j=1,7
      temp=rho-rhoa(j)
      h(j)=a(1,j)+a(2,j)*(temp+rho)
      hi(j)=rho*(a(1,j)+a(2,j)*temp)
      do 30 i=3,8
      h(j)=h(j)+a(i,j)*temp*(rho-rhoa(j)+(i-1.)*rho)
      temp=temp*(rho-rhoa(j))
30    hi(j)=hi(j)+a(i,j)*rho*temp
      h(j)=h(j)+(a(9,j)+rho*(2.*a(10,j)-e*a(9,j)-e*a(10,j)*rho))*te
```

```
      h(j)=h(j)*rho*rho
40    hi(j)=hi(j)+rho*(a(9,j)+a(10,j)*rho)*te
      p=rho*r*t
      do 50 j=1,7
      p=p+c(j)*h(j)
      u=u+(c(j)-t*cp(j))*hi(j)
50    s=s-cp(j)*hi(j)
      s=s-r*dlog(rho)
      prop(1)=t
      prop(2)=rho
      prop(3)=p/1000.
      prop(4)=u/1000.+prop(3)/rho
      prop(5)=s/1000.
      return
      end
```

Graphics Program Listing

```
      PROGRAM GRAPH3
      INTEGER NAR
      PARAMETER(NAR=20000)
C
C      **************************
C      **  Program Variables   **
C      **************************
      REAL XLOCAL(20),YLOCAL(20),XMIN,XMAX,YMIN,YMAX,POINTS(NAR,3),
     +   X(NAR),Y(NAR),XHORZ(2),YHORZ(2),XVERT(2),YVERT(2),
     +   ORIG(NAR,4),TMAT(4,4),TEMP(NAR,4),TEST1(2,2),TEST2(2,2),
     +   TMAT1(4,4),TMAT2(4,4),TMAT3(4,4),TMAT4(4,4),TMAT5(4,4),
     +   TMAT6(4,4),TMAT7(4,4),TMAT8(4,4),ZLOCAL(20),PLOT(NAR,4),
     +   PROJ(4,4),PLOT1(NAR,4),PLOT2(NAR,4),ZCMIN,ZCMAX,CLOW(255),
     +   CHIGH(255),CFRACT,COLOR(255),PLOT3(NAR,4),PLOT4(NAR,4),
     +   XSPOT,YSPOT,DELTAY,DELTAX,VAL2,VAL3,VAL4,VAL,PERCENT,DX,DY,
     +   VAL1,VAL5,XCMIN,XCMAX,YCMAX,AVGXY,YCMIN,FACTOR,SCFACT,ANGLE,
     +   BSHEAR,CSHEAR,DSHEAR,FSHEAR,HSHEAR,ISHEAR,RMAT,QMAT,MMAT,
     +   LMAT,PMAT,NMAT
      INTEGER ICOMP_NUM(NAR),IFIRST,ILAST,IDSEQ_NUM(NAR),CH,COL,LEG,
     +   IDSEQ(NAR),OLD,HORZ_PTS,VERT_PTS,IPOINT_NUM,FOUR,NUMCOLOR,
     +   PRI,BX,N,I,M,P,FLAG2,L,J,FLAG1,NUM_DSEQ,NUM_COMPS,PLT1,PLT2
      CHARACTER QUEST*32,QUEST2*32,HEADER_CORD*32,CHAR*9,TITLE*50,
     +   HEADER_DSEQ*32,FILE1*32,FILE2*32,QUEST3*32,QUEST4*32,
     +   TEXT*32,XAXIS*50,YAXIS*50,QUEST5*32,QUEST6*32
C  ************************
C  ** LOAD IN COLOR DATA **
C  ************************
      OPEN(UNIT=11,FILE='color.dat',STATUS='OLD')
      READ(11,*) NUMCOLOR
      DO 10 I=1,NUMCOLOR
         READ(11,*) COLOR(I)
 10   CONTINUE
      CLOSE(11)
C---->  Initial settings
      FOUR=NAR
      CH=0
      COL=0
C
C      *****************************************
C      **  Prompts for different functions   **
C      *****************************************
100   DO 42 N=1,8
         WRITE(6,*) ' '
42    CONTINUE
      WRITE(6,*) '                 Would you like to.....'
      WRITE(6,*) ' '
      WRITE(6,*) '               A) Load object from files'
      WRITE(6,*) '               B)     Modify object'
      WRITE(6,*) '               C)     Adjust window'
      WRITE(6,*) '               D)      Color option'
      WRITE(6,*) '               E)   View/Print objects'
      WRITE(6,*) ' '
      WRITE(6,*) '              (Or "QUIT" to exit program)'
      DO 43 N=1,8
         WRITE(6,*) ' '
43    CONTINUE
      READ(5,'(A32)') QUEST
C
C      *****************************************
```

```
C       **  Get points entered from a file  **
C       ************************************
      IF (QUEST.EQ.'A'.OR.QUEST.EQ.'a') THEN
504        WRITE(6,*) ' '
           WRITE(6,*) ' Input the Coordinate File....'
           WRITE(6,*) '   Example:   HOUSE.CORD'
           READ(5,'(A32)') FILE1
           OPEN(UNIT=10,FILE=FILE1,STATUS='OLD',ERR=504)
           READ(10,'(A32)') HEADER_CORD
           READ(10,*) NUM_COMPS
           DO 200 I=1,NUM_COMPS
              READ(10,*) ICOMP_NUM(I),XLOCAL(I),YLOCAL(I),ZLOCAL(I)
200        CONTINUE
           READ(10,*) IFIRST,ILAST
           DO 210 I=IFIRST,ILAST
              READ(10,*) IPOINT_NUM,POINTS(I,1),POINTS(I,2),
     +           POINTS(I,3),ICOMP_NUM(I)
210        CONTINUE
           CLOSE(10)
505        WRITE(6,*) ' '
           WRITE(6,*) ' Input the Sequence File'
           WRITE(6,*) '   Example:   HOUSE.DSEQ'
           READ(5,'(A32)') FILE2
           OPEN(UNIT=11,FILE=FILE2,STATUS='OLD',ERR=505)
           READ(11,'(A32)') HEADER_DSEQ
           READ(11,*) NUM_DSEQ
           DO 220 I=1,NUM_DSEQ
              READ(11,*) IDSEQ_NUM(I),IDSEQ(I)
220        CONTINUE
           CLOSE(11)
C     **--->   BECAUSE A DATA POINT IS REQUIRED TO BE IN THE FORM
C          [X,Y,Z,1] AND OUR DATA IS IN THE FORM [X,Y,Z,COMPONENT#],
C          THE LIST OF POINTS MUST BE CONVERTED.
           DO 81 I=IFIRST,ILAST
              ORIG(I,1)=POINTS(I,1)+XLOCAL(ICOMP_NUM(I))
              ORIG(I,2)=POINTS(I,2)+YLOCAL(ICOMP_NUM(I))
              ORIG(I,3)=POINTS(I,3)+ZLOCAL(ICOMP_NUM(I))
              ORIG(I,4)=1
              TEMP(I,1)=POINTS(I,1)+XLOCAL(ICOMP_NUM(I))
              TEMP(I,2)=POINTS(I,2)+YLOCAL(ICOMP_NUM(I))
              TEMP(I,3)=POINTS(I,3)+ZLOCAL(ICOMP_NUM(I))
              TEMP(I,4)=1
81         CONTINUE
           FLAG1=1
C     *****************
C     ** FIND LIMITS **
C     *****************
           XCMAX=-1000000000
           XCMIN=+1000000000
           DO 20 I=IFIRST,ILAST
              IF(ORIG(I,1).GT.XCMAX) XCMAX=ORIG(I,1)
              IF(ORIG(I,1).LT.XCMIN) XCMIN=ORIG(I,1)
 20        CONTINUE
           YCMAX=-1000000000
           YCMIN=+1000000000
           DO 23 I=IFIRST,ILAST
              IF(ORIG(I,2).GT.YCMAX) YCMAX=ORIG(I,2)
              IF(ORIG(I,2).LT.YCMIN) YCMIN=ORIG(I,2)
 23           CONTINUE
           ZCMAX=-1000000000
           ZCMIN=+1000000000
           DO 22 I=IFIRST,ILAST
              IF(ORIG(I,3).GT.ZCMAX) ZCMAX=ORIG(I,3)
              IF(ORIG(I,3).LT.ZCMIN) ZCMIN=ORIG(I,3)
 22        CONTINUE
```

```
         WRITE(6,*) '   Do you wish to input your own color limits?'
         WRITE(6,*) '                  (Y or N)'
         READ(5,'(A32)') QUEST6
         IF (QUEST6.EQ.'Y'.OR.QUEST6.EQ.'y') THEN
            WRITE(6,*) 'Please input the MINimum Z value ...'
            READ(5,*) ZCMIN
            WRITE(6,*) 'Please input the MAXimum Z value ...'
            READ(5,*) ZCMAX
         ENDIF
C     ******************
C     ** SCALE Z AXIS **
C     ******************
         AVGXY=(YCMAX+XCMAX-YCMIN-XCMIN)/2.
         FACTOR=.2*(AVGXY/ZCMAX)
         DO 24 I=IFIRST,ILAST
            ORIG(I,3)=ORIG(I,3)*FACTOR
            TEMP(I,3)=TEMP(I,3)*FACTOR
 24      CONTINUE
C     *********************
C     ** SET COLOR RANGE **
C     *********************
         CFRACT=(ZCMAX-ZCMIN)/NUMCOLOR
         DO 30 I=1,NUMCOLOR
            CLOW(I)=ZCMIN+((I-1)*CFRACT)
            CHIGH(I)=ZCMIN+(I*CFRACT)
 30      CONTINUE
C     *****************************
C     ** SET INITIAL WINDOW SIZE **
C     *****************************
         XMIN=-.5
         XMAX=2
         YMIN=-1
         YMAX=.5
      ENDIF
C
C      ***************************
C      **  Object Modification  **
C      ***************************
      IF (QUEST.EQ.'B'.OR.QUEST.EQ.'b') THEN
         IF (FLAG1.NE.1) THEN
            WRITE(6,*) ' '
            WRITE(6,*) '   You have attempted to make modifications'
            WRITE(6,*) 'to an object.  However, because no object is'
            WRITE(6,*) 'in memory, you will be sent back to the'
            WRITE(6,*) 'main menu.'
            WRITE(6,*) ' '
            WRITE(6,*) '          (PRESS RETURN TO CONTINUE)'
            READ(5,*)
            FLAG2=1
         ENDIF
         IF (FLAG2.EQ.1) GOTO 21
         WRITE(6,*) '                MODIFY OBJECT'
         WRITE(6,*) ' '
         WRITE(6,*) '  You have chosen to make modifications to'
         WRITE(6,*) 'the object in memory.  Please select the'
         WRITE(6,*) 'type of modification to be done.....'
         WRITE(6,*) ' '
         WRITE(6,*) '            A)   Local Scaling'
         WRITE(6,*) '            B)  Overall Scaling'
         WRITE(6,*) '            C)      Shear'
         WRITE(6,*) '            D)     Rotation'
         WRITE(6,*) '            E)    Reflection'
         WRITE(6,*) '            F)    Translation'
         WRITE(6,*) '            G)    Projection'
         WRITE(6,*) ' '
```

```
        WRITE(6,*) ' '
        READ(5,'(A32)') QUEST2
C
C     *********************
C     **  Local Scaling  **
C     *********************
         IF (QUEST2.EQ.'A'.OR.QUEST2.EQ.'a') THEN
            CALL IDENT(TMAT1,4)
            WRITE(6,*) ' '
            WRITE(6,*) '               ---> LOCAL SCALING <---'
            WRITE(6,*) ' '
            WRITE(6,*) '   Within local scaling, objects can be
     + stretched (scaled) in either the X, Y or Z axis.  Please enter
     + the axis to which you wish to scale...'
            WRITE(6,*) ' '
            WRITE(6,*) '  (NOTE: a value of zero will make no change)'
            WRITE(6,*) ' '
            WRITE(6,*) '         (Please type "X", "Y", or "Z")'
            READ(5,'(A32)') QUEST3
            IF (QUEST3.EQ.'X'.OR.QUEST3.EQ.'x') THEN
               WRITE(6,*) ' '
               WRITE(6,*) '   What is the scale factor?'
               READ(6,*) SCFACT
               TMAT1(1,1)=SCFACT
            ENDIF
            IF (QUEST3.EQ.'Y'.OR.QUEST3.EQ.'y') THEN
               WRITE(6,*) ' '
               WRITE(6,*) '   What is the scale factor?'
               READ(6,*) SCFACT
               TMAT1(2,2)=SCFACT
            ENDIF
            IF (QUEST3.EQ.'Z'.OR.QUEST3.EQ.'z') THEN
               WRITE(6,*) ' '
               WRITE(6,*) '   What is the scale factor?'
               READ(6,*) SCFACT
               TMAT1(3,3)=SCFACT
            ENDIF
            CALL TYPE(QUEST4)
            IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
              CALL IDENT(TMAT,4)
               CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
               CALL MULT(TEMP,FOUR,4,TMAT1,4,4)
            ENDIF
            IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
               CALL MULT(TEMP,FOUR,4,TMAT1,4,4)
            ENDIF
            CALL MULT(TMAT,4,4,TMAT1,4,4)
            CALL NORMAL(TEMP,FOUR,4)
         ENDIF
C
C     ***********************
C     **  Overall Scaling  **
C     ***********************
         IF (QUEST2.EQ.'B'.OR.QUEST2.EQ.'b') THEN
            CALL IDENT(TMAT2,4)
            WRITE(6,*) ' '
            WRITE(6,*) '             ---> OVERALL SCALING <---'
            WRITE(6,*) ' '
            WRITE(6,*) '   Within overall scaling, objects can be
     + stretched (scaled) in the X, Y, and Z axis at the same time.
     +  Please enter the constant to which you wish to scale...'
            WRITE(6,*) ' '
            READ (6,*) SCFACT
            SCFACT=1.0/SCFACT
            TMAT2(4,4)=SCFACT
```

```
           CALL TYPE(QUEST4)
           IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
              CALL IDENT(TMAT,4)
              CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
              CALL MULT(TEMP,FOUR,4,TMAT2,4,4)
           ENDIF
           IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
              CALL MULT(TEMP,FOUR,4,TMAT2,4,4)
           ENDIF
           CALL MULT(TMAT,4,4,TMAT2,4,4)
           CALL NORMAL(TEMP,FOUR,4)
        ENDIF
C
C      ****************
C      **  Shearing  **
C      ****************
        IF (QUEST2.EQ.'C'.OR.QUEST2.EQ.'c') THEN
           CALL IDENT(TMAT3,4)
           WRITE(6,*) ' '
           WRITE(6,*) '               ---> SHEARING <---'
           WRITE(6,*) ' '
           WRITE(6,*) '  Within shearing, objects can be distorted
     + with respect to the X, Y, or Z axis.  These constants are in the
     + form...'
           WRITE(6,*) ' '
           WRITE(6,*) '              |  1  B  C  0 |'
           WRITE(6,*) '              |  D  1  F  0 |'
           WRITE(6,*) '              |  H  I  1  0 |'
           WRITE(6,*) '              |  0  0  0  1 |'
           WRITE(6,*) ' '
           WRITE(6,*) ' (NOTE: a value of zero will make no change.)'
           WRITE(6,*) ' '
           WRITE(6,*) '   What is the new "B" value'
           READ(5,*) BSHEAR
           WRITE(6,*) '   What is the new "C" value'
           READ(5,*) CSHEAR
           WRITE(6,*) '   What is the new "D" value'
           READ(5,*) DSHEAR
           WRITE(6,*) '   What is the new "F" value'
           READ(5,*) FSHEAR
           WRITE(6,*) '   What is the new "H" value'
           READ(5,*) HSHEAR
           WRITE(6,*) '   What is the new "I" value'
           READ(5,*) ISHEAR
           TMAT3(1,2)=BSHEAR
           TMAT3(1,3)=CSHEAR
           TMAT3(2,1)=DSHEAR
           TMAT3(2,3)=FSHEAR
           TMAT3(3,1)=HSHEAR
           TMAT3(3,2)=ISHEAR
           CALL TYPE(QUEST4)
           IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
              CALL IDENT(TMAT,4)
              CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
              CALL MULT(TEMP,FOUR,4,TMAT3,4,4)
           ENDIF
           IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
              CALL MULT(TEMP,FOUR,4,TMAT3,4,4)
           ENDIF
           CALL MULT(TMAT,4,4,TMAT3,4,4)
           CALL NORMAL(TEMP,FOUR,4)
        ENDIF
C
C      ****************
C      **  Rotating  **
```

```
C      ****************
          IF (QUEST2.EQ.'D'.OR.QUEST2.EQ.'d') THEN
            CALL IDENT(TMAT4,4)
            WRITE(6,*) ' '
            WRITE(6,*) '                    ---> ROTATING <---'
            WRITE(6,*) ' '
            WRITE(6,*) ' Please enter the axis to which you wish
     + to rotate about (Type "X", "Y", or "Z")'
            WRITE(6,*) ' '
            READ(5,'(A32)') QUEST3
            WRITE(6,*) '  Please enter the angle (in degrees) to
     + which you want to rotate this object...'
            WRITE(6,*) ' '
            WRITE(6,*) 'NOTE:    a possitive angle will result in a
     + counter-clockwise rotation.  Also, a value of zero will make
     + no change.'
            WRITE(6,*) ' '
            READ (5,*) ANGLE
            ANGLE=ANGLE*(3.14159/180)
            IF (QUEST3.EQ.'X'.OR.QUEST3.EQ.'x') THEN
               TMAT4(2,2)=COS(ANGLE)
               TMAT4(2,3)=SIN(ANGLE)
               TMAT4(3,2)=-SIN(ANGLE)
               TMAT4(3,3)=COS(ANGLE)
            ENDIF
            IF (QUEST3.EQ.'Y'.OR.QUEST3.EQ.'y') THEN
               TMAT4(1,1)=COS(ANGLE)
               TMAT4(1,3)=-SIN(ANGLE)
               TMAT4(3,1)=SIN(ANGLE)
               TMAT4(3,3)=COS(ANGLE)
            ENDIF
            IF (QUEST3.EQ.'Z'.OR.QUEST3.EQ.'z') THEN
               TMAT4(1,1)=COS(ANGLE)
               TMAT4(1,2)=SIN(ANGLE)
               TMAT4(2,1)=-SIN(ANGLE)
               TMAT4(2,2)=COS(ANGLE)
            ENDIF
            CALL TYPE(QUEST4)
            IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
               CALL IDENT(TMAT,4)
               CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
               CALL MULT(TEMP,FOUR,4,TMAT4,4,4)
            ENDIF
            IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
               CALL MULT(TEMP,FOUR,4,TMAT4,4,4)
            ENDIF
            CALL MULT(TMAT,4,4,TMAT4,4,4)
            CALL NORMAL(TEMP,FOUR,4)
          ENDIF
C
C      ******************
C      **  Reflection  **
C      ******************
          IF (QUEST2.EQ.'E'.OR.QUEST2.EQ.'e') THEN
            CALL IDENT(TMAT5,4)
            WRITE(6,*) ' '
            WRITE(6,*) '                ---> REFLECTION <---'
            WRITE(6,*) ' '
            WRITE(6,*) '  Within reflection, objects can be
     + reflected in either the X axis, Y axis, or Z axis.  Please enter
     + the axis to which you wish to reflect about...'
            WRITE(6,*) ' '
            WRITE(6,*) '           (Please type "X", "Y", or "Z")'
            READ(5,'(A32)') QUEST3
            IF (QUEST3.EQ.'X'.OR.QUEST3.EQ.'x') TMAT5(1,1)=-1
```

```
           IF (QUEST3.EQ.'Y'.OR.QUEST3.EQ.'y') TMAT5(2,2)=-1
           IF (QUEST3.EQ.'Z'.OR.QUEST3.EQ.'z') TMAT5(3,3)=-1
           CALL TYPE(QUEST4)
           IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
              CALL IDENT(TMAT,4)
              CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
              CALL MULT(TEMP,FOUR,4,TMAT5,4,4)
           ENDIF
           IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
              CALL MULT(TEMP,FOUR,4,TMAT5,4,4)
           ENDIF
           CALL MULT(TMAT,4,4,TMAT5,4,4)
           CALL NORMAL(TEMP,FOUR,4)
        ENDIF
C
C      *******************
C      **  Translation  **
C      *******************
        IF (QUEST2.EQ.'F'.OR.QUEST2.EQ.'f') THEN
           CALL IDENT(TMAT6,4)
           WRITE(6,*) ' '
           WRITE(6,*) '               ---> TRANSLATION <---'
           WRITE(6,*) ' '
           WRITE(6,*) '        Within translation, objects can be
     + moved up, down, right, or left.  The relative constants are
     + in the form...'
           WRITE(6,*) ' '
           WRITE(6,*) '              |  1  0  0  0  |'
           WRITE(6,*) '              |  0  1  0  0  |'
           WRITE(6,*) '              |  0  0  1  0  |'
           WRITE(6,*) '              |  L  M  N  1  |'
           WRITE(6,*) ' '
           WRITE(6,*) ' (NOTE: a value of zero will make no change.)'
           WRITE(6,*) ' '
           WRITE(6,*) '       What is the new "L" value'
           READ(5,*) LMAT
           WRITE(6,*) '       What is the new "M" value'
           READ(5,*) MMAT
           WRITE(6,*) '       What is the new "N" value'
           READ(5,*) NMAT
           TMAT6(4,1)=LMAT
           TMAT6(4,2)=MMAT
           TMAT6(4,3)=NMAT
           CALL TYPE(QUEST4)
           IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
              CALL IDENT(TMAT,4)
              CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
              CALL MULT(TEMP,FOUR,4,TMAT6,4,4)
           ENDIF
           IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
              CALL MULT(TEMP,FOUR,4,TMAT6,4,4)
           ENDIF
           CALL MULT(TMAT,4,4,TMAT6,4,4)
           CALL NORMAL(TEMP,FOUR,4)
        ENDIF
C
C      *******************
C      **  Projection   **
C      *******************
        IF (QUEST2.EQ.'G'.OR.QUEST2.EQ.'g') THEN
           CALL IDENT(TMAT7,4)
           WRITE(6,*) ' '
           WRITE(6,*) '               ---> PROJECTION <---'
           WRITE(6,*) ' '
           WRITE(6,*) '    Within projection, the object can take
```

```
     + on a variety of scewed looks.  These constants are in
     + the form...'
           WRITE(6,*) ' '
           WRITE(6,*) '              |  1  C  0  P  |'
           WRITE(6,*) '              |  0  1  0  Q  |'
           WRITE(6,*) '              |  0  0  1  R  |'
           WRITE(6,*) '              |  0  0  0  1  |'
           WRITE(6,*) ' '
           WRITE(6,*) ' (NOTE: a value of zero will make no change.)'
           WRITE(6,*) ' '
           WRITE(6,*) '          What is the new "P" value'
           READ(5,*) PMAT
           WRITE(6,*) '          What is the new "Q" value'
           READ(5,*) QMAT
           WRITE(6,*) '          What is the new "R" value'
           READ(5,*) RMAT
           TMAT7(1,4)=PMAT
           TMAT7(2,4)=QMAT
           TMAT7(3,4)=RMAT
           CALL TYPE(QUEST4)
           IF (QUEST4.EQ.'A'.OR.QUEST4.EQ.'a') THEN
              CALL IDENT(TMAT,4)
              CALL CONVERT(ORIG,FOUR,4,TEMP,FOUR,4)
              CALL MULT(TEMP,FOUR,4,TMAT7,4,4)
           ENDIF
           IF (QUEST4.EQ.'B'.OR.QUEST4.EQ.'b') THEN
              CALL MULT(TEMP,FOUR,4,TMAT7,4,4)
           ENDIF
           CALL MULT(TMAT,4,4,TMAT7,4,4)
           CALL NORMAL(TEMP,FOUR,4)
         ENDIF
21    FLAG2=0
      ENDIF
C
C      *********************
C      **  Change Window  **
C      *********************
      IF (QUEST.EQ.'C'.OR.QUEST.EQ.'c') THEN
390      WRITE(6,*) ' '
         WRITE(6,*) '   The present values of the world coordinates'
         WRITE(6,*) 'in the form (1,XMIN,XMAX,YMIN,YMAX) are...'
         WRITE(6,*) '             XMIN=',XMIN
         WRITE(6,*) '             XMAX=',XMAX
         WRITE(6,*) '             YMIN=',YMIN
         WRITE(6,*) '             YMAX=',YMAX
         WRITE(6,*) ' '
         WRITE(6,*) '       Would you like to change these ?'
         WRITE(6,*) '      (Type "Y" for yes or "N" to exit)'
         READ(5,'(A32)') QUEST2
         IF (QUEST2.EQ.'Y'.OR.QUEST2.EQ.'y') THEN
            WRITE(6,*) ' '
            WRITE(6,*) '  What is the new "XMIN" value'
            READ(5,*) XMIN
            WRITE(6,*) '  What is the new "XMAX" value'
            READ(5,*) XMAX
            WRITE(6,*) '  What is the new "YMIN" value'
            READ(5,*) YMIN
            WRITE(6,*) '  What is the new "YMAX" value'
            READ(5,*) YMAX
         ENDIF
         IF (QUEST2.EQ.'N'.OR.QUEST2.EQ.'n') GOTO 400
         GOTO 390
400     ENDIF
C
C     ******************
```

```
C     ** COLOR OPTION **
C     ******************
      CH=0
      IF (QUEST.EQ.'D'.OR.QUEST.EQ.'d') THEN
         IF(COL.EQ.0) THEN
            WRITE(6,*) '     COLOR IS NOW ON'
            COL=1
            CH=1
         ENDIF
         IF(COL.EQ.1.AND.CH.EQ.0) THEN
            WRITE(6,*) '     COLOR IS NOW OFF'
            COL=0
            CH=1
         ENDIF
         CH=0
      ENDIF
C
C      ***********************************
C      **  Drawing of objects and Text  **
C      ***********************************
      IF (QUEST.EQ.'E'.OR.QUEST.EQ.'e') THEN
         WRITE(6,*) ' '
         WRITE(6,*) ' '
         WRITE(6,*) ' '
         WRITE(6,*) '    Please enter the way in which you wish to
     + view this object...'
         WRITE(6,*) ' '
         WRITE(6,*) ' '
         WRITE(6,*) '                     A)     Front View'
         WRITE(6,*) '                     B)      Top View'
         WRITE(6,*) '                     C)   Right Side View'
         WRITE(6,*) '                     D)    Dimetric View'
         WRITE(6,*) '                     E)   Isometric View'
         WRITE(6,*) ' '
         WRITE(6,*) ' '
         WRITE(6,*) ' '
         READ(5,'(A32)') QUEST3
         CALL IDENT(PROJ,4)
         CALL CONVERT(ORIG,FOUR,4,PLOT1,FOUR,4)
         CALL CONVERT(TEMP,FOUR,4,PLOT2,FOUR,4)
         IF(QUEST3.EQ.'A'.OR.QUEST3.EQ.'a') THEN
            PROJ(1,1)=0
            PLT1=2
            PLT2=3
         ENDIF
         IF(QUEST3.EQ.'B'.OR.QUEST3.EQ.'b') THEN
            PROJ(3,3)=0
            PLT1=2
            PLT2=1
            DO 501 I=1,ILAST
               PLOT1(I,1)=-PLOT1(I,1)
               PLOT2(I,1)=-PLOT2(I,1)
501         CONTINUE
         ENDIF
         IF(QUEST3.EQ.'C'.OR.QUEST3.EQ.'c') THEN
            PROJ(2,2)=0
            PLT1=1
            PLT2=3
            DO 502 I=1,ILAST
               PLOT1(I,1)=-PLOT1(I,1)
               PLOT2(I,1)=-PLOT2(I,1)
502         CONTINUE
         ENDIF
         IF(QUEST3.EQ.'D'.OR.QUEST3.EQ.'d') THEN
            PROJ(1,1)=.9428
```

```
           PROJ(1,2)=.2425
           PROJ(1,3)=-.2287
           PROJ(2,1)=-.2357
           PROJ(2,2)=.9701
           PROJ(2,3)=.0572
           PROJ(3,1)=.2357
           PROJ(3,3)=.9718
           PLT1=2
           PLT2=3
        ENDIF
        IF(QUEST3.EQ.'E'.OR.QUEST3.EQ.'e') THEN
           PROJ(1,1)=.577
           PROJ(1,2)=.707
           PROJ(1,3)=-.408
           PROJ(2,1)=-.577
           PROJ(2,2)=.707
           PROJ(2,3)=.408
           PROJ(3,1)=.577
           PROJ(3,3)=.816
           PLT1=2
           PLT2=3
        ENDIF
       PRI=0
       WRITE(6,*) '     Do you want to print this out?'
       WRITE(6,*) '                (Y or N)'
        READ(5,'(A32)') QUEST4
        IF(QUEST4.EQ.'Y'.OR.QUEST4.EQ.'y') THEN
           PRI=1
           WRITE(6,*) 'Please input the TITLE'
           READ(5,'(A40)') TITLE
           WRITE(6,*) 'Please input the X-Axis lable'
           READ(5,'(A40)') XAXIS
           WRITE(6,*) 'Please input the Y-Axis lable'
           READ(5,'(A40)') YAXIS
           WRITE(6,*) 'Do you want the BOX drawn?'
           WRITE(6,*) '       (Y OR N)'
           READ(5,'(A32)') QUEST5
           BX=0
            IF(QUEST5.EQ.'N'.OR.QUEST5.EQ.'n') THEN
              BX=0
           ENDIF
            IF(QUEST5.EQ.'Y'.OR.QUEST5.EQ.'y') THEN
              BX=1
           ENDIF
       ENDIF
       IF(QUEST4.EQ.'N'.OR.QUEST4.EQ.'n') THEN
          PRI=0
       ENDIF
c       WRITE(6,*) '     Do you want the Z-Axis drawn?'
c       WRITE(6,*) '                 (Y or N)'
c       READ(5,'(A32)') QUEST4
c       IF(QUEST4.EQ.'N'.OR.QUEST4.EQ.'n') THEN
c          ZA=0
c       ENDIF
c       IF(QUEST4.EQ.'Y'.OR.QUEST4.EQ.'y') THEN
c          ZA=1
c       ENDIF
       CALL MULT(PLOT1,FOUR,4,PROJ,4,4)
       CALL MULT(PLOT2,FOUR,4,PROJ,4,4)
       CALL NORMAL(PLOT1,FOUR,4)
       CALL NORMAL(PLOT2,FOUR,4)
       CALL CONVERT(PLOT2,FOUR,4,PLOT3,FOUR,4)
       CALL CONVERT(PLOT2,FOUR,4,PLOT4,FOUR,4)
C      *************
C      **  PRINT  **
```

```
C     *************
      IF (PRI.EQ.1) THEN
         CALL PGBEGIN(0,'post.ps/ps',1,1)
         IF(BX.EQ.0) THEN
            CALL PGENV(XMIN,XMAX,YMIN,YMAX,1,-2)
         ENDIF
         IF(BX.EQ.1) THEN
            CALL PGENV(XMIN,XMAX,YMIN,YMAX,1,0)
         ENDIF
         CALL PGSCH(1.5)
         XSPOT=(XMIN+XMAX)/2.0
         YSPOT=YMAX+.07*(YMAX-YMIN)
         CALL PGPTEXT (XSPOT,YSPOT,0.0,0.5,TITLE)
         CALL PGSCH(1.0)
         XSPOT=XMIN-.05*(XMAX-XMIN)
         YSPOT=(YMAX+YMIN)/2.0
         CALL PGPTEXT (XSPOT,YSPOT,90.0,0.5,YAXIS)
         XSPOT=(XMIN+XMAX)/2.0
         YSPOT=YMIN-.11*(YMAX-YMIN)
         CALL PGSCH(1.0)
         CALL PGPTEXT (XSPOT,YSPOT,0.0,0.5,XAXIS)
         CALL PGSCI(1)
         CALL PGSHLS(1,100.,1.,1.)
         OLD=0
         DO 509 I=1,NUM_DSEQ
            X(I-OLD)=PLOT4(ABS(IDSEQ(I)),PLT1)
            Y(I-OLD)=PLOT4(ABS(IDSEQ(I)),PLT2)
            IF(IDSEQ(I+1).GT.0..OR.IDSEQ(I).EQ.0.) GOTO 509
            CALL PGLINE((I-OLD),X,Y)
            OLD=I
509      CONTINUE
         CALL PGEND
      ENDIF
C
C     ***************************
C     ** OPEN PLOTTING PACKAGE **
C     ***************************
      CALL PGBEGIN(0,'/x',1,1)
      IF(BX.EQ.0) THEN
         CALL PGENV(XMIN,XMAX,YMIN,YMAX,1,-2)
      ENDIF
      IF(BX.EQ.1) THEN
         CALL PGENV(XMIN,XMAX,YMIN,YMAX,1,0)
      ENDIF
      IF(PRI.EQ.1) THEN
         CALL PGSCH(1.5)
         XSPOT=(XMIN+XMAX)/2.0
         YSPOT=YMAX+.07*(YMAX-YMIN)
         CALL PGPTEXT (XSPOT,YSPOT,0.0,0.5,TITLE)
         CALL PGSCH(1.0)
         XSPOT=XMIN-.05*(XMAX-XMIN)
         YSPOT=(YMAX+YMIN)/2.0
         CALL PGPTEXT (XSPOT,YSPOT,90.0,0.5,YAXIS)
         XSPOT=(XMIN+XMAX)/2.0
         YSPOT=YMIN-.11*(YMAX-YMIN)
         CALL PGSCH(1.0)
         CALL PGPTEXT (XSPOT,YSPOT,0.0,0.5,XAXIS)
      ENDIF
C
C     ************************************
C     **  Graphics part of the program  **
C     ************************************
      IF(COL.EQ.0) THEN
         CALL PGSCI(1)
         CALL PGSHLS(1,100.,1.,1.)
```

```
            OLD=0
            DO 508 I=1,NUM_DSEQ
               X(I-OLD)=PLOT3(ABS(IDSEQ(I)),PLT1)
               Y(I-OLD)=PLOT3(ABS(IDSEQ(I)),PLT2)
               IF(IDSEQ(I+1).GT.0..OR.IDSEQ(I).EQ.0.) GOTO 508
               CALL PGLINE((I-OLD),X,Y)
               OLD=I
 508        CONTINUE
         ENDIF
         IF(COL.EQ.1) THEN
            WRITE(6,*) 'Do you wish to use the LEGEND?'
            WRITE(6,*) '       (Y OR N)'
            READ(5,'(A32)') QUEST5
            IF(QUEST5.EQ.'N'.OR.QUEST5.EQ.'n') THEN
               LEG=0
            ENDIF
            IF(QUEST5.EQ.'Y'.OR.QUEST5.EQ.'y') THEN
               LEG=1
            ENDIF
            IF(LEG.EQ.1) THEN
C              ************
C              ** LEGEND **
C              ************
               CALL PGSLW(2)
               DELTAX=XMAX-XMIN
               DELTAY=YMAX-YMIN
               DX=DELTAX*.05
               PERCENT=.3
               DY=(DELTAY-PERCENT*DELTAY)/NUMCOLOR
               DO 60 I=1,NUMCOLOR
                  Y(1)=(YMAX-.5*PERCENT*DELTAY)-(I-1)*DY
                  Y(2)=(YMAX-.5*PERCENT*DELTAY)-(I-1)*DY
                  Y(3)=(YMAX-.5*PERCENT*DELTAY)-(I)*DY
                  Y(4)=(YMAX-.5*PERCENT*DELTAY)-(I)*DY
                  X(1)=XMAX-.2*DELTAX
                  X(2)=XMAX-.2*DELTAX+DX
                  X(3)=XMAX-.2*DELTAX+DX
                  X(4)=XMAX-.2*DELTAX
                  L=NUMCOLOR+1-I
                  VAL5=COLOR(L)
                  CALL PGSHLS(L,VAL5,.5,1.0)
                  CALL PGSCI(L)
                  CALL PGSFS(1)
                  CALL PGPOLY(4,X,Y)
                  CALL PGLINE(4,X,Y)
                  WRITE(CHAR,'(F8.3)') CHIGH(L)
                  VAL1=X(2)+.5*DX
                  VAL2=Y(2)-.2*DY
                  CALL PGSCH(.8)
                  CALL PGTEXT(VAL1,VAL2,CHAR)
 60            CONTINUE
               WRITE(CHAR,'(F8.3)') CLOW(L)
               VAL1=X(2)+.5*DX
               VAL2=Y(3)-.3*DY
               CALL PGTEXT(VAL1,VAL2,CHAR)
            ENDIF
C           *************
C           ** DRAWING **
C           *************
            L=2
            CALL PGSCI(2)
            CALL PGSLW(1)
            CALL PGSHLS(2,100.,1.,1.)
            OLD=0
            DO 507 I=1,NUM_DSEQ
```

```
               X(I-OLD)=PLOT2(ABS(IDSEQ(I)),PLT1)
               Y(I-OLD)=PLOT2(ABS(IDSEQ(I)),PLT2)
               IF(IDSEQ(I+1).GT.0..OR.IDSEQ(I).EQ.0.) GOTO 507
               IF(L.GT.250) L=2
               VAL1=ORIG(ABS(IDSEQ(I-3)),3)
               VAL2=ORIG(ABS(IDSEQ(I-2)),3)
               VAL3=ORIG(ABS(IDSEQ(I-1)),3)
               VAL4=ORIG(ABS(IDSEQ(I)),3)
               VAL=(VAL1+VAL2+VAL3+VAL4)/(4.*FACTOR)
               DO 50 J=1,NUMCOLOR
                  IF (VAL.LE.CHIGH(J).AND.VAL.GT.CLOW(J))
     +               VAL5=COLOR(J)
 50            CONTINUE
               CALL PGSHLS(L,VAL5,.5,1.0)
               CALL PGSCI(L)
               CALL PGSFS(1)
               CALL PGPOLY((I-OLD),X,Y)
               CALL PGLINE((I-OLD),X,Y)
               L=L+1
               OLD=I
507         CONTINUE
         ENDIF
C        ****************************
C        ** CLOSE PLOTTING PACKAGE **
C        ****************************
         CALL PGEND
      ENDIF
      IF (QUEST.EQ.'QUIT'.OR.QUEST.EQ.'quit') GOTO 999
      GOTO 100
999   END
C
C      *******************
C      **  Subroutines  **
C      *******************
C
      SUBROUTINE IDENT(MATRIX,SIZE)
      INTEGER SIZE,I,J
      REAL MATRIX(SIZE,SIZE)
      DO 10 I=1,SIZE
         DO 20 J=1,SIZE
            MATRIX(I,J)=0
20       CONTINUE
10    CONTINUE
      DO 30 I=1,SIZE
         MATRIX(I,I)=1
30    CONTINUE
      RETURN
      END
C
      SUBROUTINE TYPE(TYPE_MOD)
      CHARACTER TYPE_MOD*32
10    WRITE(6,*) ' '
      WRITE(6,*) 'Do you wish to....'
      WRITE(6,*) '    A) Modify original object'
      WRITE(6,*) '    B) Modify current edited object'
      WRITE(6,*) ' '
      READ(5,'(A32)') TYPE_MOD
      IF (TYPE_MOD.EQ.'A'.OR.TYPE_MOD.EQ.'a') RETURN
      IF (TYPE_MOD.EQ.'B'.OR.TYPE_MOD.EQ.'b') RETURN
      WRITE(6,*) 'Something other than "A" or "B" has been entered.'
      WRITE(6,*) '           Please try again....'
      GOTO 10
      END
C
      SUBROUTINE MULT(FIRST,ROW1,COL1,SECOND,ROW2,COL2)
```

```
      INTEGER ROW1,ROW2,COL1,COL2,I,J,K
      REAL FIRST(ROW1,COL1),SECOND(ROW2,COL2),THIRD(20000,4)
      DO 50 I=1,ROW1
         DO 60 J=1,COL2
            THIRD(I,J)=0
60       CONTINUE
50    CONTINUE
      IF (COL1.NE.ROW2) GOTO 10
      DO 20 K=1,COL1
         DO 30 I=1,ROW1
            DO 40 J=1,COL2
               THIRD(I,J)=THIRD(I,J)+FIRST(I,K)*SECOND(K,J)
40          CONTINUE
30       CONTINUE
20    CONTINUE
      DO 70 I=1,ROW1
         DO 80 J=1,COL2
            FIRST(I,J)=THIRD(I,J)
80       CONTINUE
70    CONTINUE
      RETURN
10    WRITE (6,*) ' '
      WRITE (6,*) '  Because the length of column 1 does not equal the
     + length of row 2 these two matricies can not be multiplied
     + together!'
      WRITE(6,*) ' '
      WRITE (6,*) '                  FATAL ERROR!'
      END
C
      SUBROUTINE PRARR2(POINTS,ROW,COL)
      INTEGER ROW,COL,I,J
      REAL POINTS(ROW,COL)
      DO 10 I=1,ROW
         DO 20 J=1,COL
            WRITE(6,*) '      ROW',I,'   COL',J
            WRITE(6,*) POINTS(I,J)
            WRITE(6,*) ' '
20       CONTINUE
10    CONTINUE
      RETURN
      END
C
      SUBROUTINE CONVERT(FIRST,ROW1,COL1,SECOND,ROW2,COL2)
      INTEGER ROW1,COL1,ROW2,COL2,I,J
      REAL FIRST(ROW1,COL1),SECOND(ROW2,COL2)
      DO 10 I=1,ROW1
         DO 20 J=1,COL1
            SECOND(I,J)=FIRST(I,J)
20       CONTINUE
10    CONTINUE
      RETURN
      END
C
      SUBROUTINE NORMAL(MAT,ROW,COL)
      INTEGER ROW,COL,I,J
      REAL MAT(ROW,COL)
      DO 20 I=1,ROW
         DO 30 J=1,COL
            IF (MAT(I,COL).NE.0) THEN
               MAT(I,J)=MAT(I,J)/MAT(I,COL)
            ENDIF
30       CONTINUE
20    CONTINUE
10    RETURN
      END
```

C) Fixed Bed Coal Gasifier Model

MAIN PROGRAM

```
C
      LOGICAL DEB, MON, OK, FPLOT, TPLOT
C
      COMMON / D1 / RMOIST, VM, FIXC, ASH
      COMMON / D2 / FC, FH, FO, FN, FS, FASH
      COMMON / D3 / COAL, STEAM, AIR, OAIR, TCOAL, TSTEAM, TAIR
      COMMON / D4 / IND, ITYPE
      COMMON / D5 / HVCOAL, P, DIA, DP, VMD, PA
      COMMON / D6 / EP, HTC, TW
      COMMON / RR / RATE(6)
      COMMON / XX / XCO, XCO2, XO2, XH2, XCH4, XH2O, XCAR, XASH
      COMMON / FF / F(8), AREA
      COMMON / HE / H(9), CP(9)
      COMMON / RHO / RHOC
      COMMON / RD / C, CCOM, AC, YNUMBER
      COMMON / DEB / OK, DEB, MON, FPLOT, TPLOT, METHOD
      COMMON / PPP / FN2
      COMMON / DE / THK, FR, DH, DENSO, CPP, DENW, CPW, HOVW
      COMMON / DV / DGAS,HFTARV,HFTARL,HFGAS,CPTAR,CPGAS,DVTIME,HOV
      IMPLICIT REAL*8 (A-H,O-Z)
      CHARACTER ICHAR*7
      DIMENSION X1(350),X3(350),X4(350),X5(350),X6(350),X7(350),X8(350)
      DIMENSION Y1(350), ICHAR(7), X10(350)
      DIMENSION PGAS(8), CS(350,10), HV(6), TAR(3), HR(6)
      DIMENSION DF(8), X11(350), X12(350)
C
      DATA (ICHAR(I),I=1,7) / '3333','4444','5555','6666','7777','8888',
     & 'TTTT' /
      DATA DZ, TB, NSF, ISW, N, N154 /1.0, 0.0, 3, 2, 8, 180 /
      DATA PI, R / 3.14159, 82.057 /
      DATA HV / 67636.0, 0.0, 0.0, 57798.0, 191759.0, 0.0 /
      II=0
C   1 = T      2 = C      3 = CO      4 = CO2     5 = O2
C   6 = H2     7 = CH4    8 = H2O     9 = N2
C
      NPLOT = 0
      IRT = 0
111   IRT = IRT + 1
      IF ( IRT .GT. 1 ) STOP
      CALL INPUT
      IF ( DEB ) WRITE (6,68)
C
C CONVERSION OF UNITS TO CGS SYSTEM
```

```
C
      COAL = COAL * 453.6 / 3600.0
      AIR = AIR * 453.6 / ( 3600.0 * ( ( 1.0 - OAIR ) * 28.0  +
     + OAIR * 32.0 ) )
      STEAM = STEAM * 453.6 / ( 3600.0 * 18.0 )
      TCOAL = ( TCOAL + 460.0 ) / 1.8
      TSTEAM = ( TSTEAM + 460.0 ) / 1.8
      TAIR = ( TAIR + 460.0 ) / 1.8
      TW = ( TW + 460.0 ) / 1.8
      P = ( P + 14.7 ) / 14.7
      HTC = HTC * 252.0 * 1.8 / ( 3600.0 * 30.48 * 30.48 )
      DP = DP * 2.54
      WRITE (6,1)COAL,AIR,STEAM,TCOAL,TSTEAM,TAIR,TW,P,HTC,DP
1     FORMAT (//,5X,'COAL,AIR,STEAM,TCOAL,TSTEAM,TAIR,TW,P,HTC,DP',
     1/,5X,5G12.4,/,5X,5G12.4)
C
      IF ( DEB ) WRITE (6,10) COAL, STEAM, AIR, TCOAL, TSTEAM, TAIR,
     + P, HTC, TW
C
C TO EVALUATE OTHER CONSTANTS
C
      AREA = DIA * DIA * 30.48 * 30.48 * PI / 4.0
      CIR = PI * DIA * 30.48
      AC = ( 100.0 - VM * VMD - RMOIST - ASH ) / ( 100.0 * FC )
      FASH = ASH / 100.0
C
      IF ( DEB ) WRITE (6,12) AREA, CIR, AC
C
      DTTOP = 0.0D0
      DEVOLL = 0.0D0
C
C     DO 2 ITERATIONS :
C       FIRST ASSUME THE DEVOLATILIZATION LENGTH = 0.0 CM
C       SECOND USE THE VALUE FOR DEVOL LENGTH OBTAINED IN THE FIRST CASE
C
      DO 550 IDEV=1,2
      C = COAL * FC
      AF = COAL * FASH
      CCOM = AIR * OAIR * 12.0
      CC = C * AC
      FN2 = AIR * ( 1.0 - OAIR )
      IF ( IND .EQ. 1 ) XC = PA
      IF ( IND .EQ. 2 ) HT = PA * 30.48
      IF ( IND .EQ. 2 ) XC = 0.99
C
```

```
C INLET GAS TEMPERATURE
C
      CALL CPH ( 9, TAIR )
      CALL CPH ( 5, TAIR )
      CALL CPH ( 8, TSTEAM )
C
      CPGIN = ( 1.0 - OAIR ) * CP(9) + OAIR * CP(5)
      CPMGIN = AIR * CPGIN + STEAM * CP(8)
      TGIN = ( AIR * CPGIN * TAIR + STEAM * CP(8) * TSTEAM ) / CPMGIN
C
      IF ( DEB ) WRITE (6,16) TGIN
C
C INITIALIZATION
C
      IT = 0
C
C BEGINNING OF OUTER LOOP OF ADJUSTING XC
C
100   IT = IT + 1
C
C     DO THREE ITERATIONS ON THE GAS-SOLID TEMPERATURE DIFFERENCE
C
      DO 495 IC=1,3
      TMAX = 0.0
      THL = 0.0
      Z = 0.0
      J = 1
      COUT = C * ( 1.0 - XC )
      RTG = 0.0
      RTS = 0.0
C
      F(1) = TGIN
      F(2) = COUT
      F(3) = 0.0
      F(4) = 0.0
      F(5) = AIR * OAIR
      F(6) = 0.0
      F(7) = 0.0
      F(8) = STEAM
      FRAC = 1.0D0
      SUMHR=0.0
C
      IF ( MON ) WRITE (6,20) IT , IC
      IF ( DEB ) WRITE (6,32) FI
C
```

```
C GRAPHICAL AND TABLE OUTPUT
C
      SUMG = AIR + STEAM
      Y1(J) = 0.0
      X1(J) = TGIN
      X3(J) = 0.0
      X4(J) = 0.0
      X5(J) = F(5) / SUMG
      X6(J) = 0.0
      X7(J) = 0.0
      X8(J) = STEAM / SUMG
      CF = F(2)
      CPS = CPSOL (TGIN,CF,AF)
      CALL CONV (TGIN,DP,HC)
      X11(J)=HC*6.0D0*(1.0D0-EP)*AREA/DP/CPS/(CF+AF)
      X12(J)=(1.0D0-FRAC)*SUMHR/CPS/(CF+AF)
C
      DO 120 K = 2, 8
120   CS(J,K) = F(K) * 3600.0 / 453.6
      CS(J,1) = F(1) * 1.8 - 460.0
      CS(J,10) = X10(J) * 1.8D0 - 460.0D0
140   CALL RUNGE( 8, F, DF, Z, DZ, KEY )
      IF( KEY.NE.1 ) GO TO 340
C
C TOTAL GAS FLOW RATE
C
      SUMG = FN2
C
      DO 160 K = 3, 6
      IF ( F(K) .LT. 1.0E-10 ) F(K) = 0.0
160   SUMG = SUMG + F(K)
C
      IF ( F(8) .LT. 1.0E-10 ) F(8) = 0.0
      SUMG = SUMG + F(7) + F(8)
C
C MOLE FRACTION OF GAS
C
      XCO = F(3) / SUMG
      XCO2 = F(4) / SUMG
      XO2 = F(5) / SUMG
      XH2 = F(6) / SUMG
      XCH4 = F(7) / SUMG
      XH2O = F(8) / SUMG
C
C TOTAL SOLID FLOW RATE
```

```
C
      SUMS = AF + F(2)
C
C MASS FRACTION OF SOLID
C
      XCAR = F(2) / SUMS
      XASH = AF / SUMS
C
C EVALUATE RATE CONSTANTS
C
      T = F(1)
      XJ = (J-1)*DZ
      TC = X10(J)+(Z-XJ)*(X10(J+1)-X10(J))/DZ
      IF(IC.EQ.1)TC=T
      CALL RATES1 ( TC , T)
C
      DO 180 K = 1, 2
180   IF ( RATE(K) .LT. 0.0 ) RATE(K) = 0.0
      DO 200 K = 4, 6
200   IF ( RATE(K) .LT. 0.0 ) RATE(K) = 0.0
C
C  CO2
C
      T4 = 0.0
      IF ( RATE(3) .LE. 0.0 ) T4 = -RATE(3)
      TEST4 = ( RATE(5) + T4 ) * AREA * DZ
      IF ( TEST4 .LE. F(4) ) GO TO 220
      IF ( TEST4 .LE. 0.00001 ) GO TO 220
      RATE(5) = RATE(5) * F(4) / TEST4
      IF ( T4 .EQ. 0.0 ) GO TO 220
      RATE(3) = - T4 * F(4) / TEST4
C
C  H2
C
220   TEST6 = ( T4 + RATE(4) + 2.0 * RATE(6) ) * AREA * DZ
      IF ( TEST6 .LE. F(6) ) GO TO 240
      IF ( TEST6 .LE. 0.00001 ) GO TO 240
      RATE(4) = RATE(4) * F(6) / TEST6
      RATE(6) = RATE(6) * F(6) / TEST6
      IF ( T4 .GT. 0.0 ) RATE(3) = RATE(3) * F(6) / TEST6
C
C  CO
C
240   TEST3 = RATE(3) * AREA * DZ
      IF ( TEST3 .LE. F(3) ) GO TO 260
```

```
      IF ( TEST3 .LE. 0.00001 ) GO TO 260
      RATE(3) = F(3) * RATE(3) / TEST3
C
C  H2O
C
260   TEST8 = ( RATE(2) + RATE(3) ) * AREA * DZ
      IF ( TEST8 .LE. F(8) ) GO TO 280
      IF ( TEST8 .LE. 0.00001 ) GO TO 280
      RATE(2) = F(8) * RATE(2) / TEST8
      RATE(3) = F(8) * RATE(3) / TEST8
C
C O2
C
280   RATIO = 1.0
      A5 = ( RATIO + 2.0 ) / ( 2.0 + 2.0 * RATIO )
      TEST5 = ( A5 * RATE(1) + RATE(4) / 2.0 ) *AREA* DZ
      IF ( TEST5 .LE. F(5) ) GO TO 300
      IF ( TEST5 .LE. 0.00001 ) GO TO 300
      RATE(1) = RATE(1) * F(5) / TEST5
      RATE(4) = RATE(4) * F(5) / TEST5
C
C SPECIFIC HEAT OF COAL
C
300   CP(2) = 2.673 + 0.002617 * T - 116900.0 / ( T * T )
      H(2) = 2.673*(T-298.) + 0.002617*(T*T-298.*298.)/2.
     + + 116900./T  - 116900./298.
C
C CPMG = SUM OF ( MOLAR FLOW RATE * CP )
C
      CALL CPH ( 9, T )
      CPMG = CP(9) * FN2
C
      DO 320 K = 3, 8
      CALL CPH ( K, T )
      CPMG = CPMG + CP(K) * F(K)
320   CONTINUE
C
C HEAT OF REACTION
C
      RATIO = 1.0
      HR(1) = ( H(4) + H(3) * RATIO - H(5) * ( 1.0 + RATIO/2.))
     + / ( 1.0 + RATIO ) - H(2)
      HR(2) = H(3) + H(6) - H(8) - H(2)
      HR(3) = H(4) + H(6) - H(3) - H(8)
      HR(4) = H(8) - H(5) / 2.0 - H(6)
```

```
      HR(5) = 2.0 * H(3) - H(4) - H(2)
      HR(6) = H(7) - 2.0 * H(6) - H(2)
C
C DF
C
      DF(2) = AREA * ( RATE(1) + RATE(2) + RATE(5) + RATE(6) ) * 12.0
      DF(3) = AREA * ( RATE(1) * RATIO / ( 1.0 + RATIO ) + RATE(2)
     + - RATE(3) + 2.0 * RATE(5) )
      DF(4) = AREA * ( RATE(1) / ( 1.0 + RATIO ) + RATE(3)
     + - RATE(5) )
      DF(5) = AREA * ( - RATE(1) * ( 1.0 + RATIO / 2.0 ) / ( 1.0
     + + RATIO ) - RATE(4) / 2.0 )
      DF(6) = AREA * ( RATE(2) + RATE(3) - RATE(4) - 2.0 * RATE(6) )
      DF(7) = AREA * RATE(6)
      DF(8) = AREA * ( RATE(4) - RATE(2) - RATE(3) )
C
C HEAT GENERATION
C
      A8 = ( -HR(1) * RATE(1) - HR(3) * RATE(3) - HR(6) * RATE(6) )
     + * AREA
      A9 = ( -HR(2) * RATE(2) - HR(5) * RATE(5) ) * AREA
      A10 = - HR(4) * RATE(4) * AREA
C
C HEAT LOSS
C
      HLOS = HTC * CIR * ( T - TW )
      IF ( HLOS .LT. 0.0 ) HLOS = 0.0
C
C SPECIFIC HEAT OF SOLID
C
      CF = F(2)
      CPS = CPSOL (T,CF,AF)
C
C OVERALL HEAT TRANSFER COEFFICIENT
C
      CALL CONV(T,DP,HC)
      HASH=2.0D0*THK/DP*(YNUMBER/(1.0D0-YNUMBER))
      HAC=1.0D0/(1.0D0/HC+1.0D0/HASH)
      HTRANS = HAC*6.0D0*(1.0D0-EP)*AREA/DP*(T-TC)
C
C DF   (1)
C
      SUMHR = A8 + A9 +A10
      TERM = DF(2)*CPS*(TC-T)
      SUMHR = SUMHR + TERM
```

```
      DF(1) = ( -HTRANS - HLOS + FRAC * SUMHR) / CPMG
      GO TO 140
340   HLOS1= HTC * CIR * (F(1)-TW)
      THL = THL + (HTC * CIR * (F(1)-TW)) * DZ
C
      J = J + 1
      X11(J)=HAC*6.0D0*(1.0D0-EP)*AREA/DP/SUMS/CPS
      X12(J)=(1.0D0-FRAC)*SUMHR/SUMS/CPS
C
C DEBUGGING
C
      IF ( .NOT. DEB ) GO TO 360
      WRITE (6,88) J, Z
      WRITE (6,86) RATE
      WRITE (6,84) HR
      WRITE(6,92) F
C
C TOTAL GAS FLOW RATE
C
360   SUMG = FN2
      DO 380 K = 3, 8
      IF ( F(K) .LT. 0.0 ) F(K) = 0.0
380   SUMG = SUMG + F(K)
C
      T = F(1)
      IF ( T .GT. TMAX ) TMAX = T
      VEL = SUMG * 22400.0 * T / ( P * 273.0 * AREA )
      RTG = DZ / VEL + RTG
C
C TOTAL SOLID FLOW RATE
C
      SUMS = AF + F(2)
      VEL = SUMS / ( RHOC * ( 1.0 - EP ) * AREA )
      RTS = DZ / VEL + RTS
C
C FOR GRAPHICAL OUTPUT
C
400   Y1(J) = Z / 30.48
C
      X1(J) = T
      X3(J) = F(3) / SUMG
      X4(J) = F(4) / SUMG
      X5(J) = F(5) / SUMG
      X6(J) = F(6) / SUMG
      X7(J) = F(7) / SUMG
```

```
      X8(J) = F(8) / SUMG
C
C TABLE OUTPUT
C
      DO 420 K = 2, 8
420   CS(J,K) = F(K) * 3600.0 / 453.6
C
      CS(J,1) = F(1) * 1.8 - 460.0
      CS(J,10)= X10(J) * 1.8D0 - 460.0D0
C
      IF ( J .LT. 348 ) GO TO 460
C
C MAXIMUM LENGTH EXCEEDED
C
      Z = Z / 30.48
      WRITE (6,56) Z
      IF ( MON ) WRITE (6,60)
      WRITE (6,22) F
      WRITE (6,24) J, Z, SUMG, RTS, RTG, THL, TMAX
C
      GO TO 111
C
C TERMINATION CRITERION
C
460   IF ( IND .EQ. 2 ) GO TO 480
      IF ( F(2) .LT. CC ) GO TO 140
      GO TO 500
C
480   TESTZ=(HT-DEVOLL-Z)/DZ
      IF(TESTZ.GT..5)GO TO 140
      JS=J
      X10(J)=X1(J)-DTTOP
490   TERM1=(X11(J)+X11(J-1))*DZ/2.0D0
      TERM2=(X1(J-1)-X1(J))/TERM1-(X12(J)+X12(J-1))/2.0D0
      X10(J-1) = X1(J-1)-TERM2+(X10(J)-X1(J)+TERM2)/DEXP(TERM1)
C      WRITE(6,*)'X10(J-1) = ',X10(J-1)
      J=J-1
      IF(J.GT.1)GO TO 490
      J=JS
495   CONTINUE
      WRITE(6,*) IT
C
C END OF INNER LOOP
C
C DEBUGGING
```

```
C
500   IF ( .NOT. MON ) GO TO 520
      WRITE (6,22) F
      WRITE (6,24) J, Z, SUMG, RTS, RTG, THL, TMAX
      WRITE (6,23) CC ,F(2)
C
C TERMINATION CRITERION FOR OUTER LOOP
C
520   IF(IND.EQ.1) GO TO 540
      ER = CC - F(2)
      IF ( MON ) WRITE (6,38) IT, XC, ER
      IF(ABS(ER).LT.1.0) GO TO 540
      CALL CRECT ( IT, XC, ER )
      IF ( .NOT. OK ) GO TO 111
      IF ( MON ) WRITE (6,26) XC
      IF ( IT .LT. 15 ) GO TO 100
      WRITE (6,40) IT
      GO TO 111
C
C END OF OUTER LOOP
C
C DEVOLATILIZATION
C
540   WMI = 28.0 * F(3) + 44.0 * F(4) + 32.0 * F(5) + 2.0 * F(6) +
     + 16.0 * F(7) + 18.0 * F(8) + 28.0 * FN2
      WMI = WMI / SUMG
      IF ( MON ) WRITE (6,62) T, WMI
C
      CALL DEV01 ( WMI, T, CMET, DCO, DCO2, DH2, DCH4, DH2O, DN2,
     + DH2S, DTAR, TAR, COUNT )
      IF ( COUNT .GT. 10.0 ) GO TO 111
      IF ( MON ) WRITE (6,18) DCO, DCO2, DH2, DCH4, DH2O, DN2,
     + DH2S, DTAR, TAR
      DMOIST = COAL * RMOIST / ( 100.0 * 18.0)
      DCARBO = ( DCO + DCO2 + DCH4 ) * 12.0
      AMW=78.0
C
C GAS FLOW RATE AT TOP OF GASIFIER
C
      F(3) = F(3) + DCO
      F(4) = F(4) + DCO2
      F(6) = F(6) + DH2
      F(7) = F(7) + DCH4
      F(8) = F(8) + DMOIST + DH2O
      F(2) = F(2) + DCARBO + TAR(1) + CMET * 12.0
```

```
C
C
C GAS EXIT TEMPERATURE
C
      CF = C
      CPS = CPSOL ( TCOAL, CF, AF )
C
      CALL CPH ( 9, T )
      CPMG = CP(9) * ( FN2 + DN2 )
      DO 580 K = 3, 8
      CALL CPH ( K, T )
580   CPMG = CPMG + F(K) * CP(K)
      TO = TCOAL
      TF = T
      HFG = 578.0D0
      CALL CPH ( 8 , TO )
      CPH2O = CP(8)/18.0D0
      DMOIST = RMOIST * COAL/100.0D0
      A1 = DTAR *(HFTARV-HFTARL-CPTAR*TO) + DGAS*(HFGAS-HFTARL-CPGAS*TO)
     &     + DMOIST*(HFG - CPH2O * TO) + (DTAR + DGAS + DMOIST - COAL)
     &     * CPS * TO
      B1 = DTAR*CPTAR + DGAS*CPGAS + DMOIST*CPH2O
      C1 = (COAL - DTAR -DGAS - DMOIST ) * CPS
      DEVOLL = COAL * DVTIME / AREA
      HA = 6.0D0 * DEVOLL * AREA * (1.0D0 - EP) * HOV / DP
      CC = (CF+AF)*CPS/CPMG
      XNTU = HA/(CF +AF)/CPS
      GAMA = DEXP((CC-1.0D0)*XNTU)
      EFF = (1.0D0 - GAMA)/(1.0D0-CC*GAMA)
      TCTOP = TO - EFF * (TO -TF)
      TE = (CPMG * TF -A1-C1*TCTOP)/(B1+CPMG)
C


C
      DTTOP = TF-TCTOP
      WRITE(6,*)'DVTIME = ',DVTIME,'SEC  COAL   = ',COAL ,'GM PER SEC'
      WRITE(6,*)'TO     = ',TO    ,'K    TE     = ',TE   ,'K'
      WRITE(6,*)'TCTOP  = ',TCTOP ,'K    TF     = ',TF   ,'K'
      WRITE(6,*)'DEVOLL = ',DEVOLL,'CM   DTTOP = ',DTTOP,'DELTA K'
550   CONTINUE
C
      OPEN(UNIT=22,FILE='NEWTEMP',STATUS='NEW')
      JTERP = J + 1
      TDEVOLL = DEVOLL/30.48D0
      Y1(JTERP)=Y1(J)+DEVOLL
```

```
      DO 543, I=1,J
         X1(I)=X1(I)*1.8-460.0D0
 543     X10(I)=X10(I)*1.8-460.0D0
      WRITE(22,*)JTERP,'     ! temperatures in F'
      DO 541 I = 1,J
 541    WRITE(22,*)Y1(I),' ',X1(I)
      TEXIT = TE *1.8D0 - 460.0D0
      WRITE(22,*)Y1(JTERP),' ',TEXIT
      WRITE(22,*)JTERP
      DO 542 I=1,J
 542    WRITE(22,*)Y1(I),' ',X10(I)
      TENTER = TO *1.8D0 - 460.0D0
      WRITE(22,*)Y1(JTERP),' ',TENTER
      CLOSE(22)
C
C
      SUMG = FN2 + DN2 + DH2S + DTAR / AMW
      DO 560 K = 3, 8
 560  SUMG = SUMG + F(K)
      F(1) = TE
      T = TE
C
C GRAPHICAL OUTPUT
C
      J = J + 1
      Y1(J) = ( Z + DEVOLL ) / 30.48
C
      SUMG = SUMG - DTAR / AMW
      X1(J) = T * 1.8 - 460.0
      X3(J) = F(3) / SUMG
      X4(J) = F(4) / SUMG
      X5(J) = F(5) / SUMG
      X6(J) = F(6) / SUMG
      X7(J) = F(7) / SUMG
      X8(J) = F(8) / SUMG
C
C TABLE OUTPUT
C
      DO 660 K = 2, 8
660   CS(J,K) = F(K) * 3600.0 / 453.6
      CS(J,1) = T * 1.8 -460.0
C
C EVALUATION OF EFFICIENCY, ETC.
C
      STDE = 1.0 - ( F(8) - DMOIST - DH2O ) / STEAM
```

```
C
      SUMG = SUMG - F(8) + DTAR / AMW
      HVG = ( 94052.0 * TAR(1) + 57798.0 * TAR(2) ) / ( SUMG * AMW )
      DO 680 K = 1, 6
 680  HVG = HVG + HV(K) * F(K+2) / SUMG
      HVG = HVG * 537.0 / ( 252.0 * 0.791 * 520.0 )
C
      HVG1 = HVG * SUMG / ( SUMG + F(8) )
      SUMG = SUMG - DTAR / AMW + F(8)
      DO 700 K = 1, 6
      PGAS(K) = F(K+2) * 100.0 / SUMG
 700  CONTINUE
C
      PGAS(7) = ( FN2 + DN2 ) * 100.0 / SUMG
      PGAS(8) = DH2S * 100.0 / SUMG
C
C CPS = CPSOL ( TGIN )
C
      SUMG = SUMG * 3600.0 / 453.6
      SOUT = ( COUT + AF ) * 3600.0 / 453.6
      COAL = COAL * 3600.0 / 453.6
      THL = THL * 3600.0 / 252.0
      T = T * 1.8 - 460.0
      TGIN = TGIN * 1.8 - 460.0
      TMAX = TMAX * 1.8 - 460.0
      COLDE = HVG * SUMG * 347.46 * 100.0 / ( HVCOAL * COAL )
      DO 720 K = 1, 4
 720  TAR(K) = TAR(K) * 100.0 / DTAR
      DTAR = DTAR * 3600.0 / 453.6
      IF ( IND .EQ. 1 ) HT = Z / 30.48
      SEXIT = X10(1) * 1.8 - 460.0
C
C OUTPUT
C
      WRITE (6,66)
      WRITE (6,44)
C
      IF ( .NOT. TPLOT ) GO TO 145
      OPEN(UNIT=11,FILE='NEWCO',STATUS='NEW')
      OPEN(UNIT=12,FILE='NEWCO2',STATUS='NEW')
      OPEN(UNIT=13,FILE='NEWO2',STATUS='NEW')
      OPEN(UNIT=14,FILE='NEWH2',STATUS='NEW')
      OPEN(UNIT=15,FILE='NEWCH4',STATUS='NEW')
      OPEN(UNIT=16,FILE='NEWH2O',STATUS='NEW')
      WRITE(11,*)'     ',J
```

```
      WRITE(12,*)'     ',J
      WRITE(13,*)'     ',J
      WRITE(14,*)'     ',J
      WRITE(15,*)'     ',J
      WRITE(16,*)'     ',J
C
      DO 741 K=1,J,1
        WRITE(11,144)Y1(K),CS(K,3)
        WRITE(12,144)Y1(K),CS(K,4)
        WRITE(13,144)Y1(K),CS(K,5)
        WRITE(14,144)Y1(K),CS(K,6)
        WRITE(15,144)Y1(K),CS(K,7)
741     WRITE(16,144)Y1(K),CS(K,8)
144     FORMAT(1X,F6.3,4X,E20.6)
C
      CLOSE(11)
      CLOSE(12)
      CLOSE(13)
      CLOSE(14)
      CLOSE(15)
      CLOSE(16)
C
145   DO 740 K = 1, J, 5
        WRITE (6,46) Y1(K)
        WRITE (6,48) ( CS(K,M), M = 1, 8 )
740   CONTINUE
C
      IF ( K .EQ. J ) GO TO 760
      WRITE (6,46) Y1(J)
      WRITE (6,48) ( CS(J,M), M = 1, 8 )
C
760   WRITE (6,50) PGAS
      WRITE (6,54) TAR
      WRITE (6,52) SUMG, HVG, HVG1, T, DTAR, SOUT, SEXIT, THL,
     + COLDE, STDE, TMAX
      IF ( IND .EQ. 1 ) WRITE (6,58) HT
      IF ( IND .EQ. 2 ) WRITE (6,64) XC
C
      IF ( NPLOT .NE. 1 ) GO TO 780
C
C      WRITE (6,70)
C      CALL FPPLOT ( X1, Y1, J, ICHAR(7), 1, J )
C      WRITE (6,72)
C      CALL FPPLOT ( X3, Y1, J, ICHAR(1), 1, J )
C      WRITE (6,74)
```

```
C       CALL FPPLOT ( X4, Y1, J, ICHAR(2), 1, J )
C       WRITE (6,76)
C       CALL FPPLOT ( X5, Y1, J, ICHAR(3), 1, J )
C       WRITE (6,78)
C       CALL FPPLOT ( X6, Y1, J, ICHAR(4), 1, J )
C       WRITE (6,82)
C       CALL FPPLOT ( X7, Y1, J, ICHAR(5), 1, J )
C       WRITE (6,80)
C       CALL FPPLOT ( X8, Y1, J, ICHAR(6), 1, J )
C
780   GO TO 111
10    FORMAT (' COAL, STEAM, AIR, TCOAL, TSTEAM, TAIR '/
     + 1X, 6E20.6 / ' P, HTC, TW = ', 3E20.6 )
12    FORMAT (' AREA, CIR, AC  ', 3E20.6 )
16    FORMAT (' TGIN = ', E20.6 )
18    FORMAT (' DEVOLATILIZATION RESULT - CO, CO2, H2, CH4, H2O,',
     + ' N2, H2S '/ 7E15.6 / 27X, ' TAR, C, H, O, N '/ 5E15.6 )
20    FORMAT (/'OUTER LOOP ITERATION',I5,4X,'TEMPERATURE ITERATION ',I1)
22    FORMAT (' F ', 8E15.6 )
23    FORMAT ( 'CC=  ',E15.6,10X,'F(2)= ',E15.6 )
24    FORMAT (' J, Z, SUMG, RTS, RTG, THL, TMAX' / I5, 6E15.6 )
26    FORMAT ( ' UPDATED XC = ', E15.6 )
32    FORMAT (' FI ', 8E15.6 )
38    FORMAT ( ' OUTER LOOP ITERATION - IT, XC, ER ', I5, 2E15.6 )
40    FORMAT ( // ' OUTER LOOP LIMIT OF ', I5, ' ITERATIONS EXCEEDED ' )
44    FORMAT (/' PROFILES OF FLOW RATES AND TEMPERATURES ',
     + '(UNITS ARE F (1), LB/HR (2), LBMOLE/HR (3-8) ) ' /
     + 5X, 'Z', 11X, 'T', 19X, 'C', 18X, 'CO', 17X, 'CO2' /
     + 16X, 'O2', 18X, 'H2', 17X, 'CH4', 17X, 'H2O' )
46    FORMAT (1X, F6.3 )
48    FORMAT (6X, 4E20.6 / 6X, 4E20.6 )
50    FORMAT (/' PERCENTAGE OF GAS PRODUCT '/ 4X, 'CO',
     + 7X, 'CO2', 8X, 'O2', 8X, 'H2', 7X, 'CH4',7X, 'H2O', 8X, 'N2',
     + 7X, 'H2S'  / 8F10.5 )
52    FORMAT (/' TOTAL GAS OUTPUT            = ', E15.6, ' LBMOLE/HR' /
     + ' HEATING VALUE OF GAS (DRY) = ', E15.6, ' BTU/SCF' /
     + ' HEATING VALUE OF GAS (WET) = ', E15.6, ' BTU/SCF' /
     + ' GAS EXIT TEMPERATURE       = ', E15.6, ' F' /
     + ' AMOUNT OF TAR              = ', E15.6, ' LB/HR' //
     + ' TOTAL SOLID OUTPUT         = ', E15.6, ' LB/HR ' /
     + ' SOLID EXIT TEMP            = ', E15.6, ' F ' //
     + ' TOTAL HEAT LOSS            = ', E15.6, ' BTU/HR ' /
     + ' THERMAL EFFICIENCY         = ', E15.6, ' PERCENT'  //
     + ' STEAM DECOMPOSITION        = ', E15.6, /
     + ' MAXIMUM TEMPERATURE        = ', E15.6, ' F'  // )
```

```
54    FORMAT ( / ' PERCENTAGE OF TAR PRODUCT ' / 4X, 'C', 9X, 'H',
     + 9X, 'O', 9X, 'N' / 4F10.4 )
56    FORMAT ( // ' MAXIMUM LENGTH OF ', F6.1, ' FT EXCEEDED. ',
     + 'INCREASE BED DIAMETER OR DECREASE CARBON CONVERSION ',
     + 'AND TRY AGAIN. ' )
58    FORMAT ( ' BED HEIGHT           = ', E15.6, ' HT ' )
60    FORMAT (' THE FOLLOWINGS ARE THE VALUES AT THE LAST COMPARTMENT')
62    FORMAT ( ' DEVOLATILIZATION - T, WMI = ', 2E15.6 )
64    FORMAT ( ' CARBON CONVERSION    = ', E15.6 )
66    FORMAT ( / 1X, 11('*') // 1X, 'OUTPUT DATA' // 1X, 11('*') // )
68    FORMAT ( // 1X, 9('*') // 1X, 'DEBUGGING' // 1X, 9('*') // )
70    FORMAT ( 1H1, 20X, 'TEMPERATURE (F) VS. DISTANCE (FT) ' )
72    FORMAT ( 1H1, 20X, 'MOLE FRACTION OF CO VS. DISTANCE (FT) ' )
74    FORMAT ( 1H1, 20X, 'MOLE FRACTION OF CO2 VS. DISTANCE (FT) ' )
76    FORMAT ( 1H1, 20X, 'MOLE FRACTION OF O2 VS. DISTANCE (FT) ' )
78    FORMAT ( 1H1, 20X, 'MOLE FRACTION OF H2 VS. DISTANCE (FT) ')
80    FORMAT ( 1H1, 20X, 'MOLE FRACTION OF H2O VS. DISTANCE (FT) ')
82    FORMAT ( 1H1, 20X, 'MOLE FRACTION OF CH4 VS. DISTANCE (FT) ' )
84    FORMAT ( ' HR   ', 6E15.6 )
86    FORMAT ( ' RATE ', 6E15.6 )
88    FORMAT ( ' J ', I5, ' Z ', E15.6  )
92    FORMAT ( '  F',8E15.6 )
C
      END
```

ORIGINAL DEVO SUBROUTINE

```
      SUBROUTINE DEVO ( WMI, T, CMET, DCO, DCO2, DH2, DCH4, DH2O, DN2,
     + DH2S, DTAR, TAR )
C
      LOGICAL OK, DEB, MON, TPLOT, FPLOT
      DIMENSION TAR(3)
      COMMON / D1 / RMOIST, VM, FIXC, ASH
      COMMON / D2 / FC, FH, FO, FN, FS, FASH
      COMMON / D3 / COAL, STEAM, AIR, OAIR, TCOAL, TSTEAM, TAIR
      COMMON / FF / F(8)
      COMMON / RD / C, CCOM, AC
      COMMON / DEB / OK, DEB, MON, FPLOT, TPLOT, METHOD
      IMPLICIT REAL*8 (A-H,O-Z)
C
      TO = TCOAL
      TT = T
      IF ( FPLOT .OR. TPLOT ) THEN
          WRITE(6,*) '  CALLING DEVOLP '
          CALL DEVOLP ( WMI, T, TO, DTAR, DGAS )
        ELSE
          WRITE(6,*) '  CALLING DEVOL '
          CALL DEVOL ( WMI, T, TO, DTAR, DGAS )
      ENDIF

C       DTAR=0.2
C       DGAS=0.5
      T = TT
      AMF = ( VM + FIXC ) / 100.0
      DGAS = DGAS * AMF * COAL
      DTAR = DTAR * AMF * COAL
      TOTAL = DGAS + DTAR
C
      CDEVOL = TOTAL - ( FH + FO + FN + FS ) * COAL
      CMET = ( 1.0 - AC ) * FC * COAL - CDEVOL
      IF ( CMET .GE. 0.0 ) GO TO 100
      DGAS = ( TOTAL + CMET ) * DGAS / TOTAL
      DTAR = ( TOTAL + CMET ) * DTAR / TOTAL
      TOTAL = TOTAL + CMET
      CMET = 0.0
      GO TO 200
C
100   CMET = CMET / 12.0
      F(7) = F(7) + CMET
      F(6) = F(6) - CMET * 2.0
```

```
C
200   GAN = FN * COAL
C
      TOTAL = DTAR / ( FC + FH + FO )
      TAR(1) = FC * TOTAL
      TAR(2) = FH * TOTAL
      TAR(3) = FO * TOTAL
C
      DN2 = GAN / 28.0
      DH2S = FS * COAL / 32.0
C
      GH = FH * COAL - TAR(2) - 2.0 * DH2S
      GOXY = FO * COAL - TAR(3)
      GC = DGAS - GOXY - GH - DN2 * 28.0 - DH2S * 34.0
C
      R = GC / ( F(3) + F(4) + F(7) )
      R = R / 12.0
      DCO = F(3) * R
      DCO2 = F(4) * R
      DCH4 = F(7) * R
      DH2O = GOXY / 16.0 - DCO - DCO2 * 2.0
      DH2 = ( GH - 2.0 * DH2O - 4.0 * DCH4 ) / 2.0
C
      RETURN
      END
```

D) Coal Gasifier Devolatilization Subroutines

MODIFIED DEVO SUBROUTINE

```
      SUBROUTINE DEVO1 ( WMI, T, CMET, DCO, DCO2, DH2, DCH4, DH2O, DN2,
     + DH2S, DTAR, TAR, COUNT )
C
      DIMENSION TAR(3), X(2), DIFF(2)
      IMPLICIT REAL*8 (A-H,O-Z)
      LOGICAL  OK, DEB, MON, FPLOT, TPLOT
      COMMON / D1 / RMOIST, VM, FIXC, ASH
      COMMON / D2 / FC, FH, FO, FN, FS, FASH
      COMMON / D3 / COAL, STEAM, AIR, OAIR, TCOAL, TSTEAM, TAIR
      COMMON / FF / F(8), AREA
      COMMON / RD / C, CCOM, AC, YNUMBER
      COMMON / ROLL / NDX
      COMMON / DEB / OK, DEB, MON, FPLOT, TPLOT, METHOD
      COMMON / DV / DDGAS,HFTARV,HFTARL,HFGAS,CPTAR,CPGAS,DVTIME,HOV
C
      NDX= 10
      TO = TCOAL
      TT = T
      ADEVOL = (1.0D0 - AC)*FC*COAL
      X(1) = 1.3D0*VM/(VM+FC)+.025D0
      X(2) = .95D0*X(1)
      COUNT = 0.0D0
    5 COUNT = COUNT + 1.0D0
C
      CALL DEVOL1 ( WMI, T, TO, DTAR, DGAS, X(I) )
C
      T = TT
      AMF = ( VM + FIXC ) / 100.0
      DGAS = DGAS * AMF * COAL
      DDGAS = DDGAS * AMF * COAL
      DTAR = DTAR * AMF * COAL
      TOTAL = DGAS + DTAR
      CDEVOL = TOTAL - ( FH + FO + FN + FS ) * COAL
C
   10 DIFF(I) = CDEVOL - ADEVOL
      X(2)=(X(2)*DIFF(1)-X(1)*DIFF(2))/(DIFF(1)-DIFF(2))
      X(1)=.98D0*X(2)
      IF(COUNT.GT.10)GO TO 20
      TEST=DABS(DIFF(2))/ADEVOL
      IF(TEST.GT.1D-4)GO TO 5
C
  200 GAN = FN * COAL
C
```

```
      TOTAL = DTAR / ( FC + FH + FO )
      TAR(1) = FC * TOTAL
      TAR(2) = FH * TOTAL
      TAR(3) = FO * TOTAL
C
      DN2 = GAN / 28.0
      DH2S = FS * COAL / 32.0
C
      GH = FH * COAL - TAR(2) - 2.0 * DH2S
      GOXY = FO * COAL - TAR(3)
      GC = DGAS - GOXY - GH - DN2 * 28.0 - DH2S * 34.0
C
      R = GC / ( F(3) + F(4) + F(7) )
      R = R / 12.0
      DCO = F(3) * R
      DCO2 = F(4) * R
      DCH4 = F(7) * R
      DH2O = GOXY / 16.0 - DCO - DCO2 * 2.0
      DH2 = ( GH - 2.0 * DH2O - 4.0 * DCH4 ) / 2.0
C
      GO TO 30
 20   WRITE(6,300)
 30   RETURN
 300  FORMAT(3X,'UNABLE TO FIND SUITABLE X1 IN SUBROUTINE DEVO')
      END
```

MODIFIED DEVOL SUBROUTINE

```
      SUBROUTINE DEVOL(WMI,TEMF,TEMO,TTWLV,TTWLG,X1)
      LOGICAL DEB, OK, MON, FPLOT, TPLOT
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 YY(1),TWLVVV1(20),TWLVVV2(20),TIME(20),B2(11),B3(11)
      REAL*8 K1(11),K2(11),K3(11),K4(11),A(11),B1(11),KG
      REAL*8 C(11),D1(11),D2(11),D3(11),R(11),R1(11),R2(11),R3(11)
      REAL*8 Y1(11),Y2(11),Y3(11),Y4(11),Y5(11),Y6(11)
      REAL*8 QRTP(11),QYP(7,11),TWLVVV3(20),TWLVVV4(20),CCOAL(11)
      REAL*8 K5(11),Y7(11),A4(11),B4(11),C4(11),D4(11),CK1(11)
      REAL*8 CK2(11),CK3(11),K6(11),K7(11),K8(11),K9(11),K10(11)
      COMMON / D1 / RMOIST, VM1, FIXC, ASH
      COMMON / D4 / JND, ITYPE
      COMMON / D5 / HVCOAL, P, DIA, DP1, VMD, PA
      COMMON / DE / THK, FR, DH, DENSO, CP, DENW, CPW, HOVW
      COMMON / CC / DP
      COMMON / DEB / OK, DEB, MON, FPLOT, TPLOT, METHOD
      COMMON / ROLL / NDX
      COMMON / DV / DDGAS,HFTARV,HFTARL,HFGAS,CPTAR,CPGAS,DVTIME,HOV
C
C   CONSTANTS FOR TEMPERATURE PROFILE
C
      HFGAS= -940.46
      HFTARV = -1429.1
      HFTARL = -1497.9
      HFINERT = -85.41
      CPTAR = 0.98D0
      CPGAS = 0.98D0
      CPINERT = 0.27D0
      COALK=6.2D-4
      DP = DP1
      VM = VM1 / ( VM1 + FIXC )
C
C     INITIALZE CONSTANTS
C
      NDXP=NDX+1
      DO 1 I=1,NDXP
        K1(I)=0.0D0
        K2(I)=0.0D0
        K3(I)=0.0D0
        K4(I)=0.0D0
        K5(I)=0.0D0
        K6(I)=0.0D0
        K7(I)=0.0D0
```

```
         K8(I)=0.0D0
         K9(I)=0.0D0
 1       K10(I)=0.0D0
C
       TEMAV = ( TEMO + TEMF)/2.0D0
       CALL CONV ( TEMAV, DP, HOV )
       STEP = DP/100.0D0/HOV
C
       SIGM=1.355D-12
       DEFF=5.0D-3
       CNSTW=HOVW/CPW/DENW
       COALO=1.0D0
       WGB=0.0D0
       WVB=0.0D0
       WVS=0.0D0
       WGS=0.0D0
       SHN=2.0D0+6.024D0*DP**0.5D0
       DEML=7.2D-2
       KG=DEML*SHN/DP
       DX=DP/2.0D0/FLOAT(NDX)
       WIB=P*WMI/82.06D0/TEMF
       R(1)=DX/2.0D0
       R(NDXP)=DP/2.0D0
       K1(1)=3.0D0*STEP/R(1)**3.0D0
       K2(1)=R(1)**2.0D0
       K5(1)=(R(1)*R(1)*R(1))*STEP/3.0D0
       DO 45 I=2,NDX
 45      R(I)=R(I-1)+DX
       DO 451 I=1,NDXP
 451     QRTP(I)=R(I)
       DO 40 I=2,NDXP
         K1(I)=3.0D0*STEP/(R(I)**3.0D0-R(I-1)**3.0D0)
         K2(I)=R(I)**2.0D0
 40      K5(I)=(R(I)**3.0D0-R(I-1)**3.0D0)*STEP/3.0D0
       DO 41 I=1,NDXP
         CCOAL(I)=COALO
         Y1(I)=0.0D0
         Y2(I)=0.0D0
         Y3(I)=0.0D0
         Y4(I)=0.0D0
         Y5(I)=0.0D0
         Y6(I)=WIB
 41      Y7(I)=TEMO
       TWLV=0.0
       TWLG=0.0
```

```
      TEMWP=0.0
      TEMW=TEMO
      CALL CONSTK1(ITYPE,CK10,CK20,CK30,E1,E2,E3)
      CK20 = 2.9D12
      E2 = 49200.0D0
      CK30 = CK20
      E3 = E2
      DO 3 J=1,1000
       T=STEP*FLOAT(J)
       DO 990 I=1,NDXP
         CK1(I)=CK10*DEXP(-E1/1.987/Y7(I))
         CCOAL(I)=CCOAL(I)*DEXP(-CK1(I)*STEP)
         CK2(I)=CK20*DEXP(-E2/1.987/Y7(I))
 990     CK3(I)=CK30*DEXP(-E3/1.987/Y7(I))
       K3(1)=(Y1(1)+Y2(1)+Y3(1))/(Y4(1)+Y5(1)+Y6(1)+
     &            Y4(2)+Y5(2)+Y6(2))
       K4(1)=0.0D0
       DO 421 I=2,NDX
         K3(I)=(Y1(I)+Y2(I)+Y3(I))/(Y4(I)+Y5(I)+Y6(I)+
     &     Y4(I+1)+Y5(I+1)+Y6(I+1))
         K4(I)=(Y1(I-1)+Y2(I-1)+Y3(I-1))/(Y4(I)+Y5(I)+Y6(I)+
     &     Y4(I-1)+Y5(I-1)+Y6(I-1))
  421  CONTINUE
       K3(NDXP)=(Y1(NDXP)+Y2(NDXP)+Y3(NDXP))/(Y4(NDXP)+Y5(NDXP)+
     &         Y6(NDXP))
       K4(NDXP)=(Y1(NDX)+Y2(NDX)+Y3(NDX))/(Y4(NDXP)+Y5(NDXP)+Y6(NDXP)+
     &          Y4(NDX)+Y5(NDX)+Y6(NDX))
C
       A(1)=0.0D0
       B1(1)=1.0D0+(CK2(1)+CK3(1))*STEP+K1(1)*K2(1)*(DEFF/DX+K3(1))
       C(1)=K1(1)*K2(1)*(-DEFF/DX+K3(1))
       D1(1)=X1*CK1(1)*CCOAL(1)*STEP+Y4(1)
       DO 43 I=2,NDX
         A(I)=-K1(I)*K2(I-1)*(DEFF/DX+K4(I))
         B1(I)=1.0D0+K1(I)*K2(I)*(DEFF/DX+K3(I))-K1(I)*K2(I-1)
     &         *(-DEFF/DX+K4(I))+(CK2(I)+CK3(I))*STEP
         C(I)=K1(I)*K2(I)*(-DEFF/DX+K3(I))
  43     D1(I)=X1*CK1(I)*CCOAL(I)*STEP+Y4(I)
       A(NDXP)=-K1(NDXP)*K2(NDX)*(DEFF/DX+K4(NDXP))
       B1(NDXP)=1.0D0+K1(NDXP)*(KG*K2(NDXP)-K2(NDX)*(-DEFF/DX+K4(NDXP)))
     &         +(CK2(NDXP)+CK3(NDXP))*STEP+K1(NDXP)*K2(NDXP)*K3(NDXP)
       C(NDXP)=0.0D0
       D1(NDXP)=X1*CK1(NDXP)*CCOAL(NDXP)*STEP+Y4(NDXP)+K1(NDXP)
     &         *K2(NDXP)*WVB*KG
C
```

```
        CALL TRINI (A,B1,C,D1,Y4,NDXP)
C
C   RATES FOR TEMPERATURE EQUATIONS
C
       DO 436 I=1,NDXP
        R1(I)=X1*CK1(I)*CCOAL(I)-(CK2(I)+CK3(I))*Y4(I)
        R2(I)=CK2(I)*Y4(I)
 436    R3(I)=0.0D0
C
C
       B2(1)=1.0D0+K1(1)*K2(1)*(DEFF/DX+K3(1))
       B3(1)=B2(1)
       D2(1)=CK2(1)*Y4(1)*STEP+Y5(1)
       D3(1)=Y6(1)
       DO 435 I=2,NDX
         B2(I)=1.0D0+K1(I)*K2(I)*(DEFF/DX+K3(I))-K1(I)*K2(I-1)
     &          *(-DEFF/DX+K4(I))
         B3(I)=B2(I)
         D2(I)=CK2(I)*Y4(I)*STEP+Y5(I)
 435     D3(I)=Y6(I)
       B2(NDXP)=1.0D0+K1(NDXP)*(KG*K2(NDXP)-K2(NDX)*(-DEFF/DX+K4(NDXP)))
     &          +K1(NDXP)*K2(NDXP)*K3(NDXP)
       B3(NDXP)=B2(NDXP)
       D2(NDXP)=CK2(NDXP)*Y4(NDXP)*STEP+Y5(NDXP)+K1(NDXP)*K2(NDXP)*
     &          WGB*KG
       D3(NDXP)=Y6(NDXP)+K1(NDXP)*K2(NDXP)*WIB*KG
C
       CALL TRINI (A,B2,C,D2,Y5,NDXP)
       CALL TRINI (A,B3,C,D3,Y6,NDXP)
C
       DO 44 I=1,NDX
         Y1(I)=-DEFF*(Y4(I+1)-Y4(I))/DX+(Y4(I+1)+Y4(I))*K3(I)
         Y2(I)=-DEFF*(Y5(I+1)-Y5(I))/DX+(Y5(I+1)+Y5(I))*K3(I)
  44     Y3(I)=-DEFF*(Y6(I+1)-Y6(I))/DX+(Y6(I+1)+Y6(I))*K3(I)
       Y1(NDXP)=KG*(Y4(NDXP)-WVB)+Y4(NDXP)*K3(NDXP)
       Y2(NDXP)=KG*(Y5(NDXP)-WGB)+Y5(NDXP)*K3(NDXP)
       Y3(NDXP)=KG*(Y6(NDXP)-WIB)+Y6(NDXP)*K3(NDXP)
C
C    TEMPERATURE
C
       DO 441 I=1,NDXP
         K6(I)=Y1(I)*CPTAR/2.0+Y2(I)*CPGAS/2.0D0+Y3(I)*CPINERT/2.0D0
         K6(I)=K6(I)*K2(I)*STEP
         K7(I)=(R1(I)+R2(I))*CPTAR
         K7(I)=K7(I)*K5(I)
```

```
          K8(I)=Y1(I)*HFTARV+Y2(I)*HFGAS+Y3(I)*HFINERT
          K8(I)=K8(I)*K2(I)*STEP
          K9(I)=(R1(I)+R2(I))*HFTARL
          K9(I)=K9(I)*K5(I)
 441      K10(I)=COALK*K2(I)*STEP/DX
        A4(1)=0.0D0
        B4(1)=CP*K5(1)/STEP+K6(1)+K10(1)-K7(1)
        C4(1)=K6(1)-K10(1)
        D4(1)=CP*K5(1)/STEP*Y7(1)-K8(1)+K9(1)
        DO 442 I=2,NDX
          A4(I)=-K6(I-1)-K10(I-1)
          B4(I)=CP*K5(I)/STEP+K6(I)-K6(I-1)-K7(I)+K10(I)+K10(I-1)
          C4(I)=K6(I)-K10(I)
 442      D4(I)=CP*K5(I)/STEP*Y7(I)-K8(I)+K8(I-1)+K9(I)
        A4(NDXP)=-K6(NDX)-K10(NDX)
        B4(NDXP)=CP*K5(NDXP)/STEP+2.0D0*K6(NDXP)-K6(NDX)-K7(NDXP)+
     &           K10(NDX)+HOV*K2(NDXP)*STEP
        C4(NDXP)=0.0D0
        D4(NDXP)=CP*K5(NDXP)/STEP*Y7(NDXP)-K8(NDXP)+K8(NDX)+K9(NDXP)
     &           +HOV*TEMF*STEP*K2(NDXP)
C
        CALL TRINI(A4,B4,C4,D4,Y7,NDXP)
C
        WLV=R1(1)*(R(1))**3.0D0/(DP**3.0D0/8.0D0)
        WLG=R2(1)*(R(1))**3.0D0/(DP**3.0D0/8.0D0)
        DO 991 I=2,NDXP
          WLVV=R1(I)*(R(I)**3.0D0-R(I-1)**3.0D0)/(DP**3.0D0/8.0D0)
          WLGV=R2(I)*(R(I)**3.0D0-R(I-1)**3.0D0)/(DP**3.0D0/8.0D0)
          WLV=WLV+WLVV
 991      WLG=WLG+WLGV
  37    TWLV=TWLV+WLV
  66    TWLG=TWLG+WLG
        TWL=(TWLG+TWLV)*STEP
        WVS=WLV*DP/6.0*DP/DEML/SHN+WVB
        WGS=WLG*DP/6.0*DP/DEML/SHN+WGB
        WLR=WLV+WLG
        IF(TEMF-Y7(1)-1.0D0)88,88,3
   3  CONTINUE
88      TTWLV=STEP*TWLV
        TTWLG=STEP*TWLG
        DVTIME = T
        IF ( DEB ) WRITE (6,10) T,TTWLV,TTWLG,TWL
        RETURN
10      FORMAT(//,4X,'TIME FOR PYROLYSIS = ',F10.3,  '  SEC',
     */,4X,'WEIGHT LOSS OF TAR = ',F10.4, '  FRACTION OF ORIGINAL WEIGHT
```

```
*OF COAL',
*/,4X,'WEIGHT LOSS OF GAS = ',F10.4,'  FRACTION OF ORIGINAL WEIGHT
*OF COAL',
*/,4X,'TOTAL WEIGHT LOSS OF COAL =',F10.4, '  FRACTION OF ORIGINAL
*WEIGHT OF COAL')
 END
```

TRIDIAGONAL MATRIX SOLVER SUBROUTINE

```
      SUBROUTINE TRINI(A,B,C,D,Y,N)
      SAVE
      REAL*8 A(N),B(N),C(N),D(N),Y(N),BETA(50),GAMA(50)
      BETA(1)=B(1)
      GAMA(1)=D(1)/BETA(1)
      DO 10 I=2,N
        BETA(I)=B(I)-A(I)*C(I-1)/BETA(I-1)
10      GAMA(I)=(D(I)-A(I)*GAMA(I-1))/BETA(I)
      Y(N)=GAMA(N)
      DO 20 I=2,N
        M=N-I+1
20      Y(M)=GAMA(M)-C(M)*Y(M+1)/BETA(M)
      RETURN
      END
```

HEAT TRANSFER COEFFICIENT SUBROUTINE

```
C
C   CONVECTION HEAT TRANSFER COEFFICIENT SUBROUTINE
C
      SUBROUTINE CONV( TEMPC, DP, HC)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON / HE / H(9), CP(9)
      COMMON / FF / F(8), AREA
      DIMENSION XK(9), PR(9), XM(9)
      COMMON / PPP / FN2
      DATA PR / 0.0,0.0,.71,.71,.74,.66,.70,1.0,.7 /
      DATA XM / 0.0,0.0,28.,44.,32.,2.,16.,18.,28. /
      XK(3)=4.3+0.0635*TEMPC
      XK(4)=-19.62+.0934*TEMPC
      XK(5)=5.6+.0636*TEMPC
      XK(6)=51.6+.397*TEMPC
      XK(7)=-21.17+.193*TEMPC
      XK(8)=-7.0+.0828*TEMPC
      XK(9)=6.7+.0575*TEMPC
      XKAV=FN2*XK(9)
      XPRAV=FN2*PR(9)
      SUMG=FN2
      SUMM=FN2*XM(9)
      CPAV=FN2*CP(9)
      DO 10 I=3,8
        SUMG = SUMG + F(I)
        SUMM = SUMM + F(I)*XM(I)
        CPAV = CPAV + F(I)*CP(I)
        XKAV = XKAV + F(I)*XK(I)
 10     PRAV = PRAV + F(I)*PR(I)
      CPAV=CPAV/SUMM
      XKAV=XKAV/SUMG/418680.0D0
      PRAV=PRAV/SUMG
      XMUAV=PRAV*XKAV/CPAV
      RE=SUMM*DP/AREA/XMUAV
      XNU=2.06*RE**(.425)*PRAV**(1/3)/.4
      HC=XNU*XKAV/DP
      RETURN
      END
```

HEAT RECOVERY CYCLE SUBROUTINE

```
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     HEAT RECOVERY SUBROUTINE
C
C     POINT   LOCATION
C        1      SATURATED WATER LEAVING THE CONDENSER
C        2      COMPRESSED WATER LEAVING PUMP #1
C        3      COMPRESSED WATER LEAVING THE FEEDWATER HEATER
C        4      COMPRESSED WATER LEAVING PUMP #2
C        5      SATURATED STEAM LEAVING HP ECONOMIZER
C        6      SUPERHEATED STEAM LEAVING THE SUPERHEATER
C        7      SUPERHEATED STEAM ENTERING TURBINE #1 (PIPE LOSS CORRECT)
C        8      SUPERHEATED STEAM ENTERING TURBINE #2
C        9      SATURATED STEAM LEAVING TURBINE #2
C       10      SATURATED STEAM ENTERING TURBINE #3
C       11      SATURATED STEAM ENTERING TURBINE #4
C       12      SATURATED ENTERING FEEDWATER HEATER
C       13      SATURATED STEAM ENTERING THE CONDENSER
C       14      COMPRESSED WATER LEAVING PUMP #3
C       15      SATURATED STEAM LEAVING LP ECONOMIZER
C       16      SUPERHEATED STEAM MIXING WITH STEAM LEAVING TURBINE #2
C
C     VARIABLES:
C
C       COUNTA2  = COUNTS THE NUMBER OF ITERATIONS FOR CALCULATING TA2
C       COUNTA3  = COUNTS THE NUMBER OF ITERATIONS FOR CALCULATING TA3
C       COUNTA4  = COUNTS THE NUMBER OF ITERATIONS FOR CALCULATING TA4
C       CPAIR    = THE CP FOR THE PRODUCTS ENTERING THE HEATEXCHANGERS
C       CPPROD   = THE CP FOR THE PRODUCTS ENTERING THE HEATEXCHANGERS
C       CPWATER  = THE CP FOR WATER
C       CPWATER1 = THE CP FOR WATER IN THE HIGH PRESSURE ECONIMIZER
C       CPWATER2 = THE CP FOR WATER IN THE LOW PRESSURE ECONIMIZER
C       DIFFA2   = THE DIFFERENCES BETWEEN TO VALUES FOR TA2
C       DTMEAN   = THE LOG MEAN TEMPERATURE DIFFERENCE IN THE SUPERHEAT
C       H#       = THE ENTHALPY AT THE ABOVE APPLICABLE POINTS
C       HF#      = THE LIQUID ENTHALPY AT THE ABOVE APPLICABLE POINTS
C       HG#      = THE GASEOUS ENTHALPY AT THE ABOVE APPLICABLE POINTS
C       MDOTAIR  = THE MASS FLOW RATE OF GAS THROUGH THE HEATEXCHANGER
C       MDOTB1   = THE MASS FLOW RATE OF WATER THROUGH THE HP ECONIMIZER
C       MDOTB2   = THE MASS FLOW RATE OF WATER THROUGH THE LP ECONIMIZER
C       MDOTF    = THE MASS FLOW RATE OF WATER/STEAM TO FEEDWATER HEATER
C       MDOTGAS  = THE MASS FLOW RATE OF STEAM TO THE GASIFIER
```

```
C       NP        = THE EFFICIENCY OF THE PUMPS
C       NT        = THE EFFICIENCY OF THE TURBINES
C       P#        = THE PRESSURE AT EACH OF THE ABOVE POINTS
C       QBD       = HEAT LOSS THROUGH STEAM BLOWDOWN
C       QCONDENSER = HEAT REJECTED OUT OF THE CONDENSER
C       QGAS      = HEAT LOSS WHEN STEAM GOES TO THE GASIFIER
C       QHPBOIL   = HEAT TRANSFERED TO THE WATER IN THE HP ECONIMIZER
C       QIN       = HEAT ADDED TO THE SYSTEM FROM THE PRODUCT GAS
C       QLPBOIL   = HEAT TRANSFERED TO THE WATER IN THE LP ECONIMIZER
C       QPIPELOSS  = HEAT LOSS DO PIPE LOSSES
C       QSUPER    = HEAT TRANSFERED TO THE STEAM IN THE SUPERHEATER
C       RCRIT1    = CRITICAL VALUE USED TO HELP DETERMINE C1
C       RCRIT2    = CRITICAL VALUE USED TO HELP DETERMINE C1
C       RCRIT3    = CRITICAL VALUE USED TO HELP DETERMINE C2
C       RCRIT4    = CRITICAL VALUE USED TO HELP DETERMINE C2
C       RSTAR1    = EITHER RCRIT1 OR RCRIT2 WHICH IS GREATER
C       RSTAR2    = EITHER RCRIT3 OR RCRIT4 WHICH IS GREATER
C       R1        = THE INVERSE OF C1(1)
C       R2        = THE INVERSE OF C1(2)
C       R3        = THE INVERSE OF C2(1)
C       R4        = THE INVERSE OF C2(2)
C       S#        = THE ENTROPHY AT THE ABOVE APPLICABLE POINTS
C       SF#       = THE LIQUID ENTROPHY AT THE ABOVE APPLICABLE POINTS
C       SG#       = THE GASEOUS ENTROPHY AT THE ABOVE APPLICABLE POINTS
C       T#        = THE TEMPERATURE AT EACH OF THE ABOVE POINTS
C       TA1       = THE TEMPERATURE OF THE GAS ENTERING THE SUPERHEATER
C       TA2       = THE TEMPERATURE OF THE GAS ENTERING THE HP BOILER
C       TA2PRIME  = THE TEST VALUE FOR TA2
C       TA3       = THE TEMPERATURE OF THE GAS ENTERING THE LP BOILER
C       TA4       = THE TEMPERATURE OF THE GAS LEAVING THE LP BOILER
C       TESTA2    = THE ACCURACY CHECK FOR TA2
C       TESTA3    = THE ACCURACY CHECK FOR TA3
C       TESTA4    = THE ACCURACY CHECK FOR TA4
C       T12T      = TRIAL VALUE FOR THE TEMPERATURE AT POINT 12
C       T16T      = TRIAL VALUE FOR THE TEMPERATURE AT POINT 16
C       UABOIL1   = THE HEAT TRANSFER COEFICIENT FOR ECONIMIZER #1
C       UABOIL2   = THE HEAT TRANSFER COEFICIENT FOR ECONIMIZER #2
C       UASUPER   = THE HEAT TRANSFER COEFICIENT FOR THE SUPERHEATER
C       UA1       = THE UA FOR ECONIMIZER #1 AT A TRIAL TEMPERATURE
C       UA2       = THE UA FOR ECONIMIZER #2 AT A TRIAL TEMPERATURE
C       V#        = THE VOLUVE AT THE ABOVE APPLICABLE POINTS
C       VF#       = THE LIQUID VOLUME AT THE ABOVE APPLICABLE POINTS
C       VG#       = THE GASEOUS VOLUME AT THE ABOVE APPLICABLE POINTS
C       WNET      = THE NET WORK OF THE HEATRECOVERY SYSTEM
C       WPUMPR1   = THE WORK OF HEATRECOVERY PUMP #1
```

```
C       WPUMPR2  = THE WORK OF HEATRECOVERY PUMP #2
C       WPUMPR3  = THE WORK OF HEATRECOVERY PUMP #3
C       WPUMP1   = THE WORK OF HEATRECOVERY PUMP #1 PER KILOGRAM
C       WPUMP2   = THE WORK OF HEATRECOVERY PUMP #2 PER KILOGRAM
C       WPUMP3   = THE WORK OF HEATRECOVERY PUMP #3 PER KILOGRAM
C       WTURBR1  = THE WORK OF HEATRECOVERY PUMP #1
C       WTURBR2  = THE WORK OF HEATRECOVERY PUMP #2
C       WTURBR3  = THE WORK OF HEATRECOVERY PUMP #3
C       WTURBR4  = THE WORK OF HEATRECOVERY PUMP #4
C       WTURB1   = THE WORK OF HEATRECOVERY PUMP #1 PER KILOGRAM
C       WTURB2   = THE WORK OF HEATRECOVERY PUMP #2 PER KILOGRAM
C       WTURB3   = THE WORK OF HEATRECOVERY PUMP #3 PER KILOGRAM
C       WTURB4   = THE WORK OF HEATRECOVERY PUMP #4 PER KILOGRAM
C       X#       = QUALITY AT THE ABOVE APPLICABLE POINTS
C
C     ARRAYS:
C
C       C1(2)     = CONSTANTS USED TO DETERMINE UA1
C       C2(2)     = CONSTANTS USED TO DETERMINE UA2
C       DIFFA3(2) = DIFFERENCES IN TWO TRIAL VALUES OF TA3
C       DIFFA4(2) = DIFFERENCES IN TWO TRIAL VALUES OF TA4
C       MDOT(60)  = THE MASS FLOW RATES AT EACH POINT OF THE MAIN SYSTEM
C       P(60)     = THE PRESSURES AT EACH POINT OF THE MAIN SYSTEM
C       T(60)     = THE TEMPERATURES AT EACH POINT OF THE MAIN SYSTEM
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
      SUBROUTINE HEATRECOVERY(T,P,MDOT,WNET,WPUMPR1,WPUMPR2,WPUMPR3,
     &   WTURBR1,WTURBR2,WTURBR3,WTURBR4,QSUPER,QHPBOIL,QLPBOIL,
     &   QCONDENSER,QPIPELOSS,CPPROD)
      REAL*8 WNET,TA1,TA2,TA3,TA4,P1,P2,P3,P4,P5,P6,P7,P8,P9,P10,P11,
     &   P12,P13,P14,P15,P16,CPAIR,MDOTAIR,NP,NT,MDOTGAS,CPWATER,
     &   CPWATER1,CPWATER2,UABOIL1,UABOIL2,WTURBR1,UA1,WTURBR2,WTURBR3,
     &   WTURBR4,WTURB,WPUMP,WPUMP1,WPUMP2,WPUMP3,C1,C2,DIFFA3,DIFFA4,
     &   RCRIT1,RCRIT2,RCRIT3,RCRIT4,R1,R2,R3,R4,MDOTB1,MDOTB2,MDOTF,
     &   COUNTA2,COUNTA3,COUNTA4,VF1,VG1,HF1,HG1,SF1,SG1,VF3,VG3,HF3,
     &   HG3,SF3,SG3,VF5,VG5,HF5,HG5,SF5,SG5,UA2,RSTAR1,RSTAR2,V6,H6,S6,
     &   V12,H12,S12,VF12,VG12,HF12,HG12,SF12,SG12,V10,H10,S10,VF10,
     &   VG10,HF10,HG10,SF10,SG10,X10,V16,H16,S16,VF16,VG16,HF16,HG16,
     &   SF16,SG16,H2,H4,V7,H7,S7,T12T,T16T,H8,S8,H9,S9,H11,S11,TESTA2,
     &   TESTA3,TESTA4,DIFFA2,UASUPER,DTMEAN,TA2PRIME,VF15,VG15,HF15,
     &   HG15,SF15,SG15,H13,S13,H14,QIN,T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,
     &   T11,T12,T13,T14,T15,T16,MDOTGASE,QPIPELOSS,MDOT,T,P,QREJ,
     &   CPPROD,QCONDENSER,QSUPER,QHPBOIL,QLPBOIL,WTURB1,WTURB2,WTURB3,
```

```
&    WTURB4,WPUMPR1,WPUMPR2,WPUMPR3,QGAS,QBD
      INTEGER I
      DIMENSION C1(2),DIFFA3(2),C2(2),DIFFA4(2),MDOT(60),T(60),P(60)
      P1=10.0D0
      P2=140.0D0
      P3=140.0D0
      P4=6276.0D0
      P5=P4
      P6=P4
      P14=1207.0D0
      P7=.95D0*P6
      P8=2172.0D0
      P9=P14*.95D0
      P10=P14*.95D0
      P11=140.0D0/.95D0
      P12=140.0D0
      P13=10.0D0
      P15=P14
      P16=P14*.95D0
      TA1=T(19)
      T6=838.70D0
      T7=T6-3.0D0
      NP=.6D0
      NT=.75D0
      UABOIL1=1082.7D0
      UABOIL2=700.0D0
      MDOTAIR=.985D0*MDOT(19)
      MDOTGAS=MDOT(22)
      CPAIR=CPPROD
      CPWATER=4.167D0
      CALL DSAT(T1,P1,VF1,VG1,HF1,HG1,SF1,SG1,2)
      WPUMP1=VF1*(P2-P1)/NP
      T2=WPUMP1/CPWATER+T1
      H2=WPUMP1+HF1
      CALL DSAT(T3,P3,VF3,VG3,HF3,HG3,SF3,SG3,2)
      WPUMP2=VF3*(P4-P3)/NP
      T4=WPUMP2/CPWATER+T3
      H4=WPUMP2+HF3
      WPUMP3=VF3*(P14-P3)/NP
      T14=WPUMP3/CPWATER+T3
      H14=WPUMP3+HF3
      TA2=480.0D0+273.15D0
      CALL DSAT(T5,P5,VF5,VG5,HF5,HG5,SF5,SG5,2)
      CALL DSUPER(T6,P6,V6,H6,S6,1)
      COUNTA2=0.0D0
```

```
10    COUNTA2=COUNTA2+1.0D0
      COUNTA3=0.0D0
      CPWATER1=(HF5-H4)/(T5-T4)
      RCRIT1=(HG5-HF5)/CPWATER1/(TA2-T5)
      RCRIT2=CPWATER1*(TA2-T4)/(HG5-HF5+CPWATER1*(T5-T4))
      IF(RCRIT1.GE.RCRIT2)THEN
        RSTAR1=RCRIT1
       ELSE
        RSTAR1=RCRIT2
      ENDIF
      R1=RSTAR1/(1.D0-DEXP(-UABOIL1/MDOTAIR/CPAIR))
      R2=R1+(UABOIL1/MDOTAIR/CPAIR)*(R1-RSTAR1)
      C1(1)=1/R1
      C1(2)=1/R2
20    COUNTA3=COUNTA3+1.0D0
      DO 30 I=1,2
        UA1=MDOTAIR*CPAIR*(C1(I)/(C1(I)-1.0D0)*DLOG((TA2-T5-C1(I)*(HG5-
     &      HF5)/CPWATER1)/(TA2-T4-C1(I)*((HG5-HF5)/CPWATER1+T5-T4))+
     &      DLOG((TA2-T5)/(TA2-T5-C1(I)*((HG5-HF5)/CPWATER1))))
30      DIFFA3(I)=UA1-UABOIL1
      TESTA3=DABS(DIFFA3(2))
      C1(2)=(C1(2)*DIFFA3(1)-C1(1)*DIFFA3(2))/(DIFFA3(1)-DIFFA3(2))
      C1(1)=.97*C1(2)
      IF(COUNTA3.GT.20.0D0)GO TO 99
      IF(TESTA3-.1)40,40,20
40    MDOTB1=C1(2)*CPAIR/CPWATER1*MDOTAIR
      TA3=TA2-C1(2)*(T5-T4+(HG5-HF5)/CPWATER1)
      TA2PRIME=TA1-.97D0*MDOTB1*(H6-HG5)/CPAIR/MDOTAIR
      DIFFA2=TA2-TA2PRIME
      TESTA2=DABS(DIFFA2)
      TA2=(TA2+TA2PRIME)/2.0D0
      IF(COUNTA2.GT.90.0D0)GO TO 99
      IF(TESTA2-.1D0)50,50,10
50    DTMEAN=(TA1-T6-TA2+T5)/DLOG((TA1-T6)/(TA2-T5))
      UASUPER=MDOTAIR*CPAIR*(TA1-TA2)/DTMEAN
      COUNTA4=0.0D0
      CALL DSAT(T15,P15,VF15,VG15,HF15,HG15,SF15,SG15,2)
      CPWATER2=(HF15-H14)/(T15-T14)
      RCRIT3=(HG15-HF15)/CPWATER2/(TA3-T15)
      RCRIT4=CPWATER2*(TA3-T14)/(HG15-HF15+CPWATER2*(T15-T14))
      IF(RCRIT3.GE.RCRIT4)THEN
        RSTAR2=RCRIT3
       ELSE
        RSTAR2=RCRIT4
      ENDIF
```

```
      R3=RSTAR2/(1.0D0-DEXP(-UABOIL2/CPAIR/MDOTAIR))
      R4=R3+(UABOIL2/MDOTAIR/CPAIR)*(R1-RSTAR2)
      C2(1)=1/R3
      C2(2)=1/R4
60    COUNTA4=COUNTA4+1.0D0
      DO 70 I=1,2
        UA2=MDOTAIR*CPAIR*(C2(I)/(C2(I)-1.0D0)*DLOG((TA3-T15-C2(I)*(HG15
     &      -HF15)/CPWATER2)/(TA3-T14-C2(I)*((HG15-HF15)/CPWATER2+T15-
     &      T14)))+DLOG((TA3-T15)/(TA3-T15-C2(I)*((HG15-HF15)/
     &      CPWATER2))))
70      DIFFA4(I)=UA2-UABOIL2
      TESTA4=DABS(DIFFA4(2))
      C2(2)=(C2(2)*DIFFA4(1)-C2(1)*DIFFA4(2))/(DIFFA4(1)-DIFFA4(2))
      C2(1)=.97D0*C2(2)
      IF(COUNTA4.GT.90.D0)GO TO 98
      IF(TESTA4-.1)80,80,60
80    MDOTB2=C2(2)*CPAIR/CPWATER2*MDOTAIR
      TA4=TA3-C2(2)*(T15-T14+(HG15-HF15)/CPWATER2)
      CALL DSUPER(T7,P7,V7,H7,S7,1)
      CALL DTURBINE(NT,P7,P8,T7,T8,H7,H8,S7,S8,WTURB1)
      CALL DTURBINE(NT,P8,P9,T8,T9,H8,H9,S8,S9,WTURB2)
      CALL DSAT(T16T,P16,VF16,VG16,HF16,HG16,SF16,SG16,2)
      T16=T15-3.0D0
      IF(T16.GT.T16T)THEN
        CALL DSUPER(T16,P16,V16,H16,S16,1)
       ELSE
        CALL DSAT(T16,P16,VF16,VG16,HF16,HG16,SF16,SG16,2)
        H16=HG16
        S16=SG16
      END IF
      H10=((.97D0*MDOTB1-MDOTGAS)*H9+.97D0*MDOTB2*H16)/(.97D0*MDOTB1+
     &   .97D0*MDOTB2-MDOTGAS)
      CALL DSAT(T10,P10,VF10,VG10,HF10,HG10,SF10,SG10,2)
      IF(H10.GT.HG10)THEN
        CALL DSUPER(T10,P10,V10,H10,S10,3)
       ELSE
        X10=(H10-HF10)/(HG10-HF10)
        S10=X10*SG10+(1.0D0-X10)*SF10
      END IF
      CALL DTURBINE(NT,P10,P11,T10,T11,H10,H11,S10,S11,WTURB3)
      CALL DTURBINE(NT,P11,P13,T11,T13,H11,H13,S11,S13,WTURB4)
      CALL DSAT(T12T,P12,VF12,VG12,HF12,HG12,SF12,SG12,2)
      IF(T12.GT.T12T)THEN
        CALL DSUPER(T12,P12,V12,H12,S12,1)
       ELSE
```

```
        H12=HG12
        S12=SG12
        T12=T12T
      END IF
      MDOTF=(MDOTB1+MDOTB2)*(HF3-H2)/(H12-H2)
      WTURB=.97D0*MDOTB1*WTURB1+(.97D0*MDOTB1-MDOTGAS)*WTURB2+(.97D0*
     &  MDOTB1+.97D0*MDOTB2-MDOTGAS)*WTURB3+(.97D0*MDOTB1+.97D0*MDOTB2-
     &  MDOTGAS-MDOTF)*WTURB4
      WPUMP=(MDOTB1+MDOTB2-MDOTF)*WPUMP1+MDOTB1*WPUMP2+MDOTB2*WPUMP3
      WNET=WTURB-WPUMP
      MDOT(39)=MDOTF
      MDOT(24)=MDOT(18)
      MDOT(25)=MDOT(18)
      MDOT(26)=MDOT(18)
      MDOT(27)=.97D0*MDOTB1+.97D0*MDOTB2-MDOTF-MDOTGAS
      MDOT(28)=MDOTB1+MDOTB2-MDOTF
      MDOT(29)=MDOT(28)+MDOT(39)
      MDOT(30)=MDOTB1
      MDOT(31)=MDOTB1
      MDOT(32)=.97D0*MDOTB1
      MDOT(33)=MDOT(32)
      MDOT(34)=MDOT(33)
      MDOT(35)=MDOT(34)-MDOT(21)
      MDOT(36)=MDOT(35)
      MDOT(37)=MDOT(36)+.97D0*MDOTB2
      MDOT(38)=MDOT(37)
      MDOT(40)=MDOT(38)-MDOT(39)
      MDOT(41)=MDOT(40)
      MDOT(42)=.03D0*MDOTB1+.03D0*MDOTB2+MDOTGAS
      MDOT(43)=MDOT(27)+MDOT(42)
      MDOT(44)=MDOTB2
      MDOT(45)=MDOTB2
      MDOT(46)=.97D0*MDOTB2
      MDOT(47)=MDOT(46)
      MDOT(48)=.03D0*MDOTB1
      MDOT(49)=.03D0*MDOTB2
      P(27)=P1
      P(28)=P2
      P(29)=P3
      P(30)=P4
      P(31)=P5
      P(32)=P6
      P(33)=P7
      P(34)=P8
      P(35)=P8
```

```
P(36)=P9
P(37)=P10
P(38)=P11
P(39)=P12
P(40)=P11
P(41)=P13
P(42)=P1
P(43)=P1
P(44)=P14
P(45)=P15
P(46)=P15
P(47)=P16
P(48)=P5
P(49)=P15
P(24)=P(18)
P(25)=P(18)
P(26)=P(18)
T(24)=TA2
T(25)=TA3
T(26)=TA4
T(27)=T1
T(28)=T2
T(29)=T3
T(30)=T4
T(31)=T5
T(32)=T6
T(33)=T7
T(34)=T8
T(35)=T8
T(36)=T9
T(37)=T10
T(38)=T11
T(39)=T12
T(40)=T11
T(41)=T13
T(42)=T1
T(43)=T1
T(44)=T14
T(45)=T15
T(46)=T15
T(47)=T16
T(48)=T5
T(49)=T15
WTURBR1=MDOT(33)*WTURB1
WTURBR2=MDOT(35)*WTURB2
```

```
      WTURBR3=MDOT(37)*WTURB3
      WTURBR4=MDOT(40)*WTURB4
      WPUMPR1=MDOT(28)*WPUMP1
      WPUMPR2=MDOT(30)*WPUMP2
      WPUMPR3=MDOT(44)*WPUMP3
      QREJ=(.97D0*MDOTB1+.97D0*MDOTB2-MDOTF-MDOTGAS)*H13
     &  -(.97D0*MDOTB1+.97D0*MDOTB2-MDOTF-MDOTGAS)*HF1
      QCONDENSER=QREJ
      QBD=.03D0*MDOTB1*(HG5-HF1)+.03D0*MDOTB2*(HG15-HF1)
      QGAS=MDOTGAS*(H8-HF1)-MDOTGAS*(H7-H8)
      QPIPELOSS=.97D0*MDOTB1*(H6-H7)+.97D0*MDOTB2*(HG15-H16)
      QIN=MDOTAIR*CPAIR*(TA1-TA4)
      QSUPER=MDOT(24)*(T(18)-T(24))*CPAIR
      QHPBOIL=MDOT(25)*(T(24)-T(25))*CPAIR
      QLPBOIL=MDOT(26)*(T(25)-T(26))*CPAIR
      RETURN
 98   WRITE(6,*)'THE TA3 IS WRONG FOR SOME REASON'
      WRITE(6,119)TA3
 119  FORMAT(1X,'TEMP OF AIR AT BOILER #2 IS ',6X,F10.3,1X,'K')
      RETURN
 99   WRITE(6,*)'GUESS ANOTHER TA2'
      RETURN
      END
```

J.) STEAM TURBINE SUBROUTINE

```
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     STEAM TURBINE FOR HEAT RECOVERY SYSTEM SUBROUTINE
C       FOR METRIC UNITS AND IN DOUBLE PRECISION
C
C     VARIABLES:
C
C       HENTER   = ENTHALPY OF STEAM ENTERING THE TURBINE
C       HEXIT    = ENTHALPY OF STEAM LEAVING THE TURBINE
C       HFX      = ENTHALPY OF SATURATED STEAM (LIQ) AT EXIT PRESSURE
C       HGX      = ENTHALPY OF SATURATED STEAM (GAS) AT EXIT PRESSURE
C       HIS      = ENTHALPY OF STEAM FOR ISENTROPIC TURBINE
C       NT       = EFFICIENCY OF THE TURBINE
C       PENTER   = PRESSURE OF STEAM ENTERING THE TURBINE
C       PEXIT    = PRESSURE OF STEAM EXITING THE TURBINE
C       SENTER   = ENTROPHY OF STEAM ENTERING THE TURBINE
C       SEXIT    = ENTROPHY OF STEAM EXITING THE TURBINE
C       SFX      = ENTROPHY OF SATURATED STEAM (LIQ) AT EXIT PRESSURE
C       SGX      = ENTROPHY OF SATURATED STEAM (GAS) AT EXIT PRESSURE
C       TENTER   = TEMPERATURE OF STEAM ENTERING THE TURBINE
C       TEXIT    = TEMPERATURE OF STEAM EXITING THE TURBINE
C       TXS      = ISENTROPIC TURBINE EXIT TEMPERATURE
C       VEXIT    = THE SPECIFIC VOLUME OF STEAM EXITING THE TURBINE
C       VFX      = THE SPECIFIC VOLUME OF SATURATED STEAM (LIQ) AT
C                    EXIT PRESSURE
C       VGX      = THE SPECIFIC VOLUME OF SATURATED STEAM (GAS) AT
C                    EXIT PRESSURE
C       WORKTURB = THE TURBINE WORK PER UNIT MASS
C       XR       = THE REAL QUALITY OF STEAM EXITING THE TURBINE
C       XS       = THE ISENTROPIC QUALITY OF STEAM EXITING THE TURBINE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
      SUBROUTINE DTURBINE(NT,PENTER,PEXIT,TENTER,TEXIT,HENTER,HEXIT,
     &SENTER,SEXIT,WORKTURB)
      REAL*8 NT,PENTER,PEXIT,TENTER,TEXIT,HENTER,HEXIT,SENTER,SEXIT,
     &   WORKTURB,XS,XR,VFX,VGX,HFX,HGX,SFX,SGX,TXS,VXS,HXS,VEXIT
      CALL DSAT(TEXIT,PEXIT,VFX,VGX,HFX,HGX,SFX,SGX,2)
      IF(SENTER.GE.SGX)THEN
        CALL DSUPER(TXS,PEXIT,VXS,HXS,SENTER,2)
        WORKTURB=NT*(HENTER-HXS)
```

```
        HEXIT=HENTER-WORKTURB
        CALL DSUPER(TEXIT,PEXIT,VEXIT,HEXIT,SEXIT,3)
       ELSE
        XS=(SENTER-SFX)/(SGX-SFX)
        HXS=XS*HGX+(1.0D0-XS)*HFX
        WORKTURB=NT*(HENTER-HXS)
        HEXIT=HENTER-WORKTURB
        XR=(HEXIT-HFX)/(HGX-HFX)
        SEXIT=XR*SGX+(1.0D0-XR)*SFX
      ENDIF
      RETURN
      END
```

K.) STEAM TABLES SUBROUTINES

```
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE SUPER CALCULATES THE PROPERTIES OF STEAM GIVEN
C       EITHER TEMPERATURE AND PRESSURE OR PRESSURE AND ENTHALPY OR
C       PRESSURE AND ENTROPY.
C
C       N = 1   GIVEN TEMPERATURE AND PRESSURE
C       N = 2   GIVEN PRESSURE AND ENTHALPY
C       N = 3   GIVEN PRESSURE AND ENTROPY
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE SUPER (T,P,V,H,S,N)
      REAL*8 T,P,V,S,H,PROP,X,DIFF,PR,TR,B,C,XI,RHO,RHOZ,TEST
      INTEGER N,COUNT,I
      DIMENSION PROP(5),X(2),DIFF(2)
      PR=P/22089.
      IF(N-2) 10,20,30
 10   TR=T/647.29
      X(1)=RHOZ(TR,PR)
      X(2)=.98*X(1)
      COUNT=0
 15   COUNT=COUNT+1
      DO 16 I=1,2
      CALL SUPERPROP(T,X(I),PROP)
 16   DIFF(I)=PROP(3)-P
      X(2)=(X(2)*DIFF(1)-X(1)*DIFF(2))/(DIFF(1)-DIFF(2))
      X(1)=.98*X(2)
      IF(COUNT.GT.10) GO TO 17
      TEST=ABS(DIFF(2)/P)
      IF(TEST.GT..00001) GO TO 15
      H=PROP(4)
      S=PROP(5)
      GO TO 40
 17   WRITE(6,600) T,P
600   FORMAT("  DID NOT CONVERGE AT T=",E14.7,"  P=",E14.7)
      GO TO 40
 20   B=8.57-S-.4615*ALOG(P/101.35)
      C=-.2652-.4615*PR
      XI=(-B+SQRT(B*B-.8136*C))/.4086
      TR=XI**.33333
      T=TR*647.29
```

```
      RHO=RHOZ(TR,PR)
      V=1./RHO
      CALL LOOK(T,RHO,P,S,3,5,PROP)
      T=PROP(1)
      H=PROP(4)
      GO TO 40
 30   B=3072.3-H
      C=-418.2119*PR-130.2
      XI=(-B+SQRT(B*B-1210.6*C))/605.3
      TR=XI**.4
      T=TR*647.29
      RHO=RHOZ(TR,PR)
      V=1./RHO
      CALL LOOK(T,RHO,P,H,3,4,PROP)
      T=PROP(1)
      S=PROP(5)
 40   V=1./PROP(2)
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE LOOK LOOKS FOR SUPER HEATED PROPERTIES GIVEN
C       THE DENSITY AND THE TEMPERATURE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE LOOK(X1,X2,Y1,Y2,M,N,PROP)
      REAL*4 X1,X2,Y1,Y2,PROP,DX,B1,B2,DX1,TEST,PROPO,DX2,A11,A12,A21,
     &   A22
      INTEGER N,M,COUNT
      DIMENSION PROP(5),PROPO(5)
      COUNT=0
 10   COUNT=COUNT+1
      CALL SUPERPROP(X1,X2,PROPO)
      B1=Y1-PROPO(M)
      B2=Y2-PROPO(N)
      DX=.01D0*X1
      X1=X1+DX
      CALL SUPERPROP(X1,X2,PROP)
      A11=(PROP(M)-PROPO(M))/DX
      A21=(PROP(N)-PROPO(N))/DX
      X1=X1-DX
      DX=.01D0*X2
      X2=X2+DX
```

```
      CALL SUPERPROP(X1,X2,PROP)
      A12=(PROP(M)-PROPO(M))/DX
      A22=(PROP(N)-PROPO(N))/DX
      X2=X2-DX
      DX2=(B2-A21*B1/A11)/(A22-A21*A12/A11)
      DX1=(B1-A12*DX2)/A11
      TEST=ABS(DX2/X2)+ABS(DX1/X1)
      X2=X2+DX2
      X1=X1+DX1
      IF(COUNT.GT.10)GO TO 20
      IF(TEST.GT..00001) GO TO 10
      GO TO 30
 20   WRITE(6,600)X1,X2
 600  FORMAT('  NO CONVERGE, T=',E14.7,'   RHO=',E14.7)
 30   CALL SUPERPROP(X1,X2,PROP)
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     FUNCTION RHOZ
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      FUNCTION RHOZ(TR,PR)
      REAL*4 TR,PR,Z,X,RHOZ
      IF(TR-1.0)20,10,10
 10   X=(PR/TR**3.0)**2.0
      Z=1.0-X*(1.289/TR-.532*TR*X)
      GO TO 30
 20   Z=1.0-.7*(PR/TR)**2.0
 30   RHOZ=73.94*PR/Z/TR
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE SUPERPROP CALCULATES THE SUPERHEATED STEAM PROPERTIES
C       GIVEN THE TEMPERATURE AND DENSITY OF THE STEAM
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE SUPERPROP(T,RHO,PROP)
      REAL*4 T,RHO,PROP,A,RHOA,C,G,CP,H,HI,E,TA,XM,TC,PC,RHOC,TO,R,S,
     &  U,TAU,TAUC,TEMP,P,TE
```

```
      INTEGER I,J
      DIMENSION PROP(5),A(10,7),RHOA(7),C(7),G(6),CP(7),H(7),HI(7)
      DATA(A(I,1),I=1,10)/2.9492937E-2,-1.3213917E-4,2.7464632E-7,
     *-3.6093828E-10,3.4218431E-13,-2.4450042E-16,1.5518535E-19,
     *5.9728487E-24,-.41030848,-4.1605860E-4/
      DATA(A(I,2),I=1,10)/-5.198586E-3,7.7779182E-6,-3.3301902E-8,
     *-1.6254622E-11,-1.7731074E-13,1.2748742E-16,1.3746153E-19,
     *1.5597836E-22,.3373118,-2.0988866E-4/
      DATA(A(I,3),I=1,10)/6.8335354E-3,-2.6149751E-5,6.532639E-8,
     * -2.6181978E-11,0.,0.,0.,0.,-1.3746618E-1,-7.3396848E-4/
      DATA(A(I,4),I=1,10)/-1.5641040E-4,-7.2546108E-7,-9.2734289E-9,
     *4.3125840E-12,0.,0.,0.,0.,6.7874983E-3,1.0401717E-5/
      DATA(A(I,5),I=1,10)/-6.3972405E-3,2.6409282E-5,-4.7740374E-8,
     *5.6323130E-11,0.,0.,0.,0.,.13687317,6.4581880E-4/
      DATA(A(I,6),I=1,10)/-3.9661401E-3,1.5453061E-5,-2.9142470E-8,
     *2.9568796E-11,0.,0.,0.,0.,7.9847970E-2,3.9917570E-4/
      DATA(A(I,7),I=1,10)/-6.9048554E-4,2.7407416E-6,-5.1028070E-9,
     *3.9636085E-12,0.,0.,0.,0.,1.3041253E-2,7.1531353E-5/
      DATA(RHOA(J),J=1,7)/634.,1000.,1000.,1000.,1000.,1000.,1000./
      DATA(G(I),I=1,6)/4.6E4,1.011249E3,.83893,-2.19989E-4,
     *2.46619E-7,-9.7047E-11/
      DATA E,TA,XM,TC,PC,RHOC,T0/.0048,1000.,18.016,647.286,22.089,
     *317.,273.16/
      R=8314.34/XM
      S=6696.5776-G(1)/T+G(2)*ALOG(T/T0)+T*(G(3)+T*(G(4)/2.+T*(G(5)/3.
     *+T*G(6)/4.)))+G(1)/T0-T0*(G(3)+T0*(G(4)/2.+T0*(G(5)/3.+T0*G(6)
     */4.)))
      U=2375020.7+G(1)*ALOG(T/T0)+T*(G(2)+T*(G(3)/2.+T*(G(4)/3.+T*(
     *G(5)/4.+T*G(6)/5.))))-T0*(G(2)+T0*(G(3)/2.+T0*(G(4)/3.+T0*
     *(G(5)/4.+T0*G(6)/5.))))
      TAU=TA/T
      TAUC=TA/TC
      C(1)=R*T
      C(2)=C(1)*(TAU-TAUC)
      CP(1)=R
      TEMP=R*TAU
      CP(2)=C(2)/T-TEMP
      DO 10 I=3,7
      C(I)=C(I-1)*(TAU-2.5)
      CP(I)=C(I)/T-TEMP*(TAU-2.5+(I-2)*(TAU-TAUC))
 10   TEMP=TEMP*(TAU-2.5)
      TE=EXP(-E*RHO)
      DO 40 J=1,7
      TEMP=RHO-RHOA(J)
      H(J)=A(1,J)+A(2,J)*(TEMP+RHO)
```

```
      HI(J)=RHO*(A(1,J)+A(2,J)*TEMP)
      DO 30 I=3,8
      H(J)=H(J)+A(I,J)*TEMP*(RHO-RHOA(J)+(I-1.)*RHO)
      TEMP=TEMP*(RHO-RHOA(J))
 30   HI(J)=HI(J)+A(I,J)*RHO*TEMP
      H(J)=H(J)+(A(9,J)+RHO*(2.*A(10,J)-E*A(9,J)-E*A(10,J)*RHO))*TE
      H(J)=H(J)*RHO*RHO
 40   HI(J)=HI(J)+RHO*(A(9,J)+A(10,J)*RHO)*TE
      P=RHO*R*T
      DO 50 J=1,7
      P=P+C(J)*H(J)
      U=U+(C(J)-T*CP(J))*HI(J)
 50   S=S-CP(J)*HI(J)
      S=S-R*ALOG(RHO)
      PROP(1)=T
      PROP(2)=RHO
      PROP(3)=P/1000.
      PROP(4)=U/1000.+PROP(3)/RHO
      PROP(5)=S/1000.
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE SAT CALCULATES THE SATURATION PROPERTIES FOR STEAM
C       FOR A GIVEN TEMPERATURE AND PRESSURE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE SAT(T,P,VF,VG,HF,HG,SF,SG,N)
      REAL*4 T,P,VF,VG,HF,HG,SF,SG,DPDT,RHOL,PO,ERR,HFG
      INTEGER N,COUNT
      IF(N-1) 10,10,20
 10   CALL SATPROP(T,P,DPDT,RHOL)
      GO TO 30
 20   T=4900./(17.572-ALOG(P))
      COUNT=0
 25   COUNT=COUNT+1
      CALL SATPROP(T,PO,DPDT,RHOL)
      T=T+(P-PO)/DPDT
      ERR=ABS((P-PO)/P)
      IF(COUNT.GT.10) GO TO 26
      IF(ERR.GT..00001) GO TO 25
      GO TO 30
 26   WRITE(6,610) T
```

```
 610  FORMAT("  NO CONVERGE AT TSAT=",E14.7)
 30   VF=1./RHOL
      CALL SUPER(T,P,VG,HG,SG,1)
      HFG=T*(VG-VF)*DPDT
      HF=HG-HFG
      SF=SG-HFG/T
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE SATPROP CALCULATES THE SATURATION PROPERTIES FOR
C       STEAM GIVEN THE TEMPERATURE, PRESSURE, CHANGE IN PRESSURE WITH
C       RESPECT TO TEMPERATURE, AND THE DENSITY
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE SATPROP(T,P,DPDT,RHOL)
      REAL*4 D,F,T,P,DPDT,RHOL,A,TP,TC,PC,RHOC,X,Y,DYDX,X3
      INTEGER I
      DIMENSION D(8),F(8)
      DATA (D(I),I=1,8)/3.6711257,-28.512396,222.6524,-882.43852,
     *2000.276,-2612.2557,1829.7674,-533.5052/
      DATA(F(I),I=1,8)/-7.41924,.29721,-.1155286,8.685635E-3,
     * 1.094098E-3,-4.39993E-3,2.520658E-3,-5.218684E-4/
      DATA A,TP,TC,PC,RHOC/.01,338.15,647.286,22089.,317./
      X=A*(T-TP)
      Y=F(1)+X*(F(2)+X*(F(3)+X*(F(4)+X*(F(5)+X*(F(6)+X*(F(7)+
     *X*F(8)))))))
      DYDX=F(2)+X*(2.*F(3)+X*(3.*F(4)+X*(4.*F(5)+X*(5.*F(6)+
     *X*(6.*F(7)+X*7.*F(8))))))
      P=PC*EXP((TC/T-1.)*Y)
      DPDT=P*(-Y*TC/T/T+(TC/T-1.)*DYDX*A)
      X=(1.-T/TC)**(1./3.)
      X3=X*X*X
      RHOL=RHOC*(1.+X*(D(1)+X3*(D(4)+D(7)*X3)+X*(D(2)+X3*(D(5)+
     *D(8)*X3)+X*(D(3)+D(6)*X3))))
      RETURN
      END
```

END

DATE
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3/25/92