

Figure 3.6-1 Schematic of Condenser

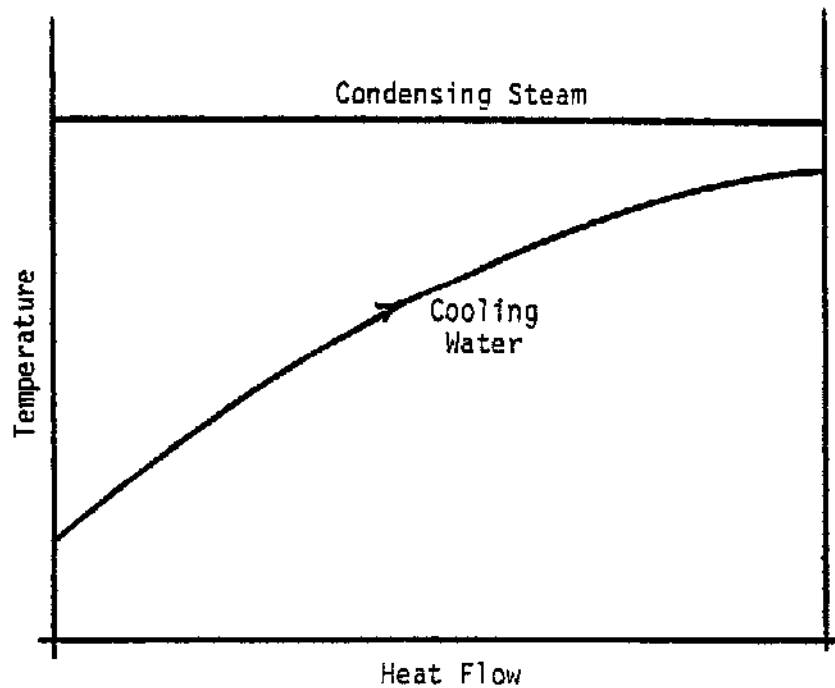


Figure 3.6-2 Temperature-Heat Flow Diagram for Condenser

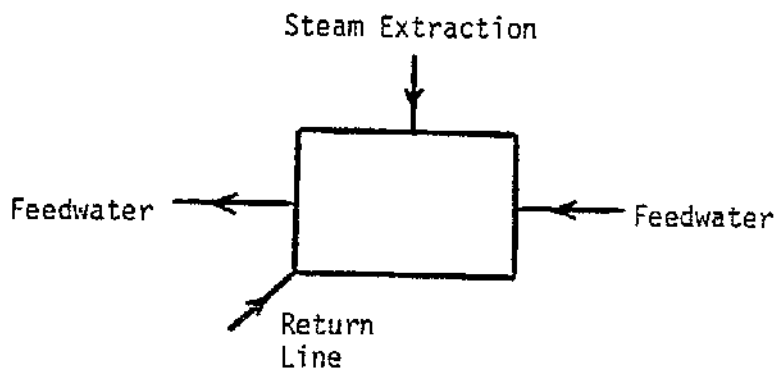


Figure 3.7-1 Schematic of Deaerator

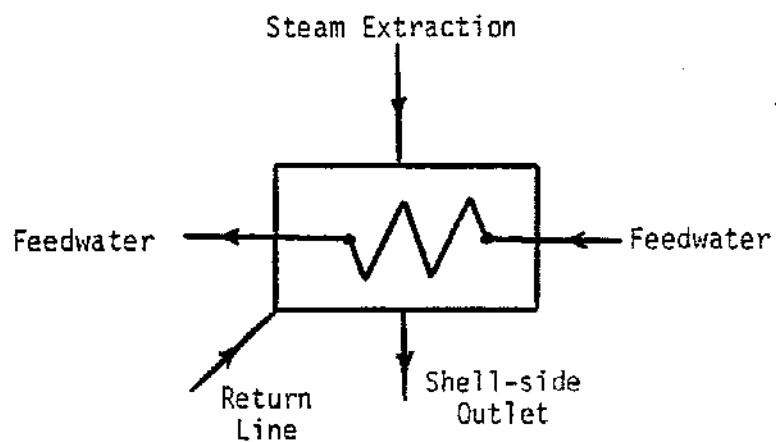


Figure 3.8-1 Schematic of Closed Feedwater Heater

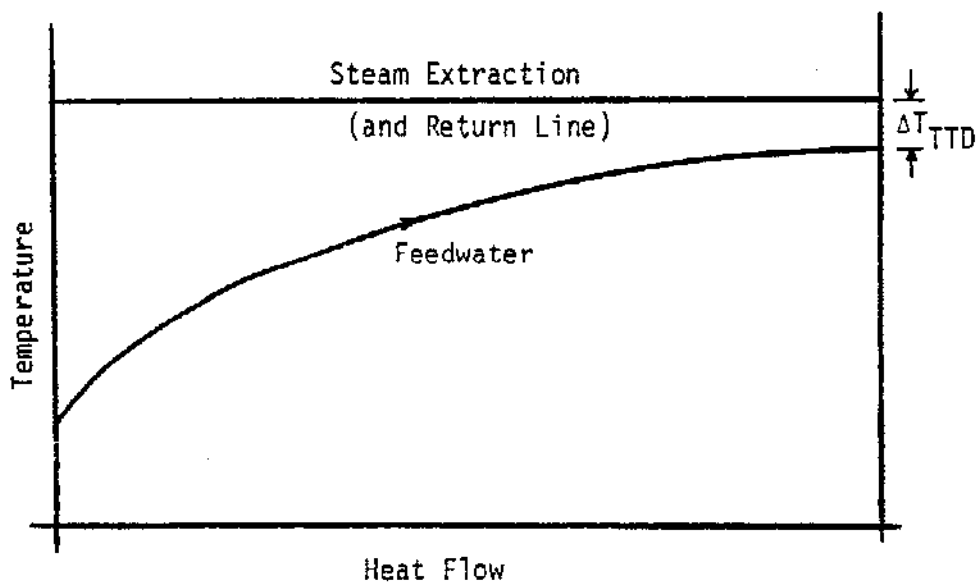


Figure 3.8-2 Temperature-Heat Flow Diagram for Closed Feedwater Heater

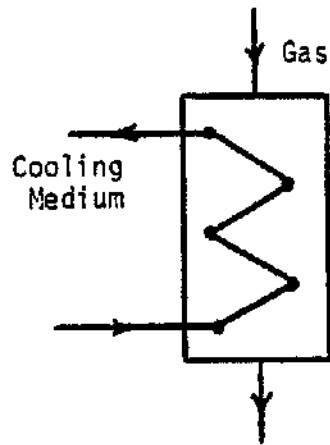


Figure 3.9-1 Schematic of Gas Cooler

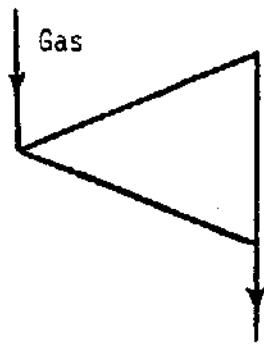


Figure 3.10-1 Schematic of Gas Turbine

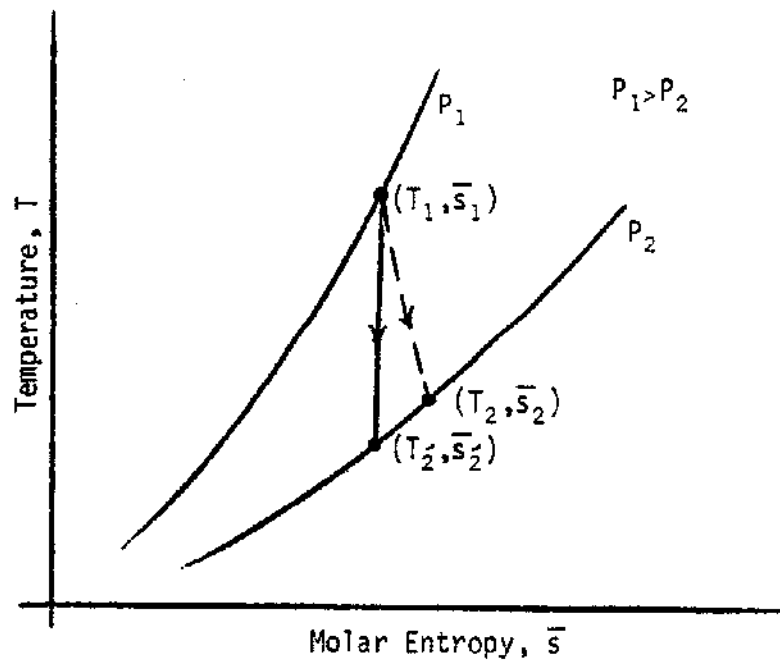


Figure 3.10-2 Temperature-Entropy Diagram for Expansion of a Gaseous Fluid

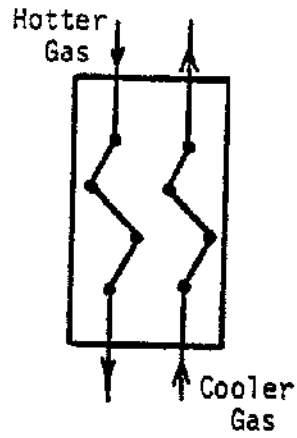


Figure 3.11-1 Schematic of Gas-to-Gas Counterflow Heat Exchanger

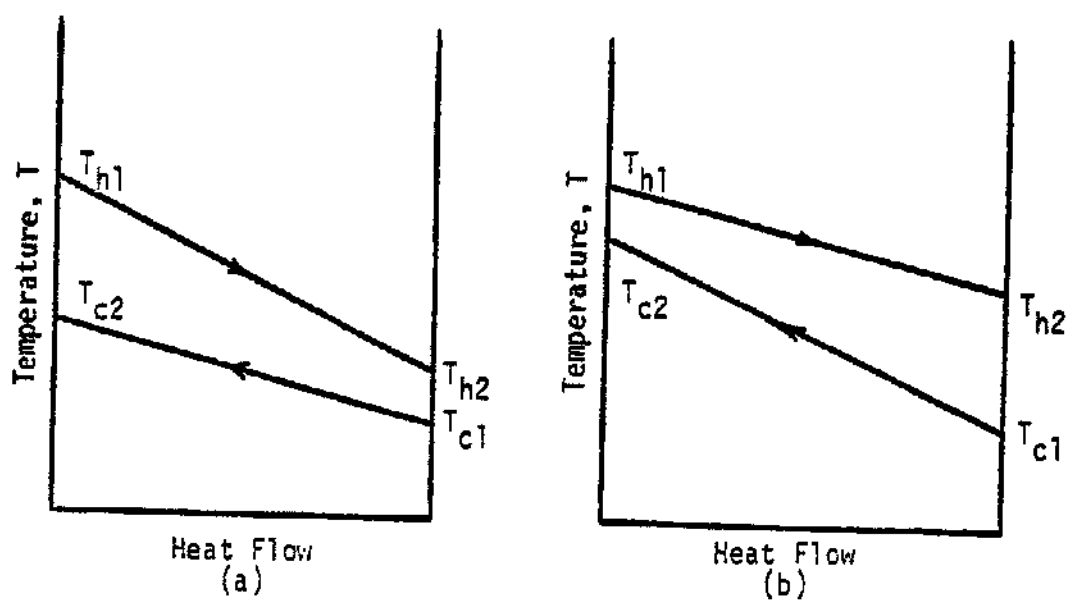


Figure 3.11-2 Temperature-Heat Flow Diagram Assuming Minimum Heat Capacity Associated with (a) Hotter and (b) Cooler Fluid

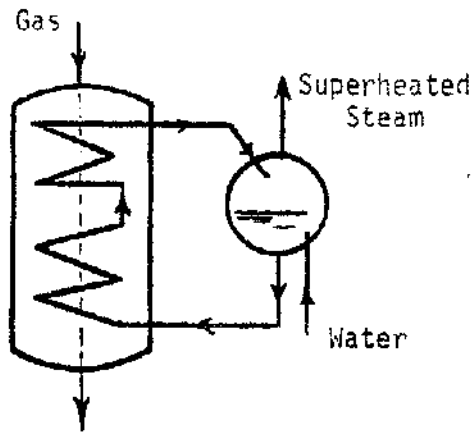


Figure 3.12-1 Schematic of Steam Generator

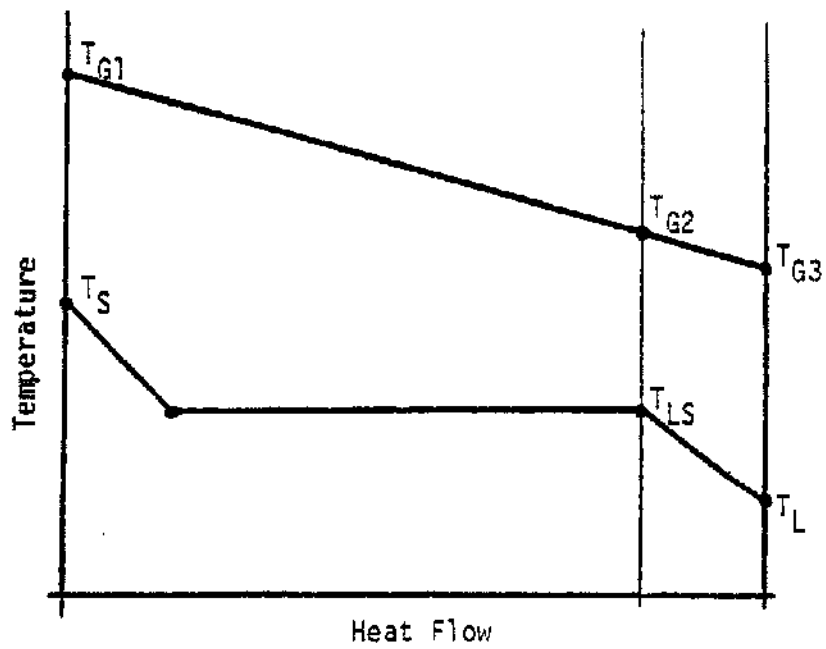


Figure 3.12-2 Temperature-Heat Flow Diagram for Steam Generator

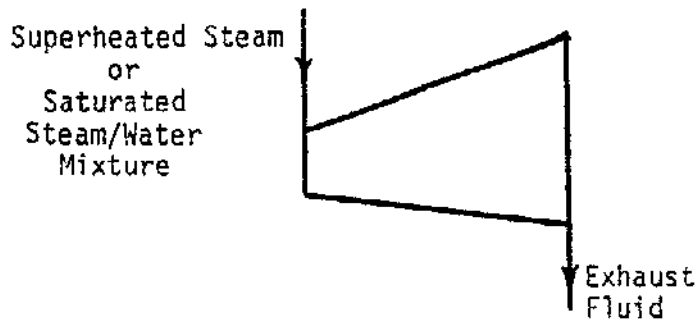


Figure 3.13-1 Schematic of Steam Turbine

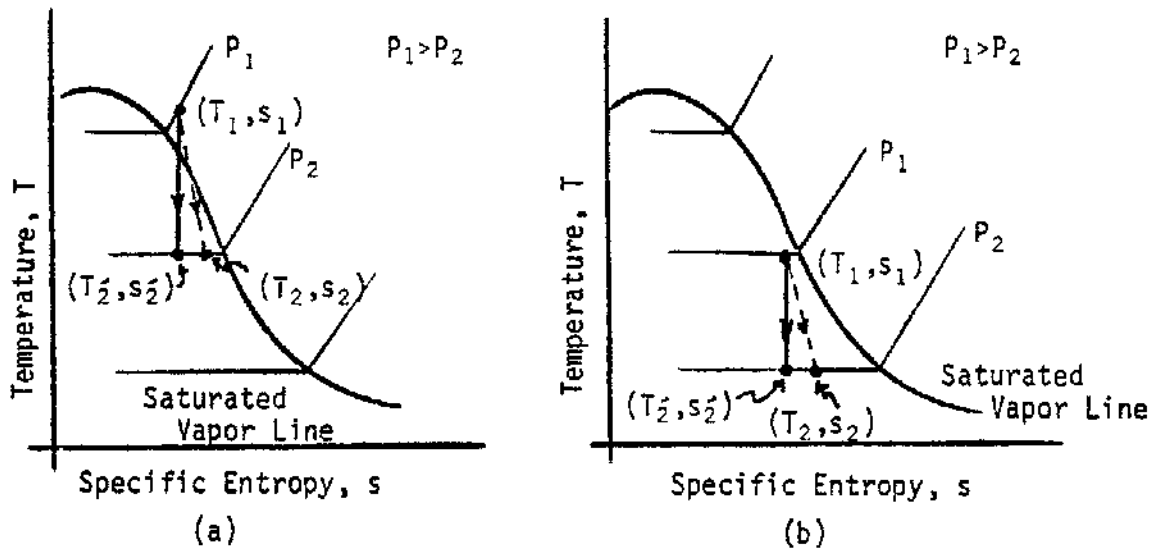


Figure 3.13-2 Temperature-Entropy Diagram for Expansion of (a) Superheated Steam or (b) Saturated Steam-Water Mixture into Saturated Region

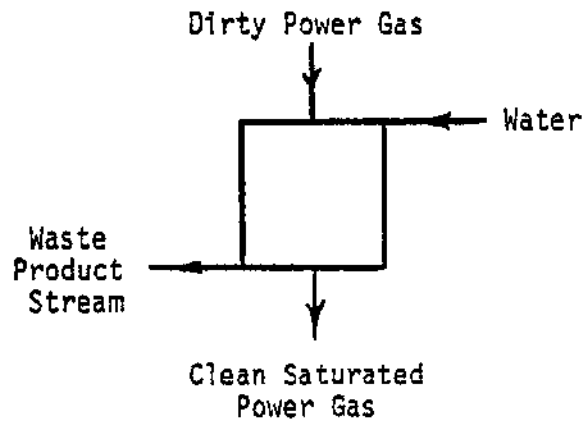


Figure 3.14-1 Schematic of Gas Clean-up System

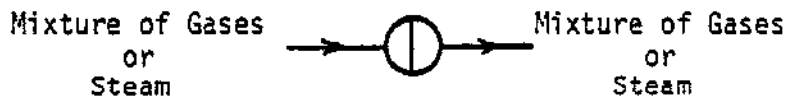


Figure 3.15-1 Schematic of Throttle Valve



Figure 3.16-1 Schematic of Water Pump

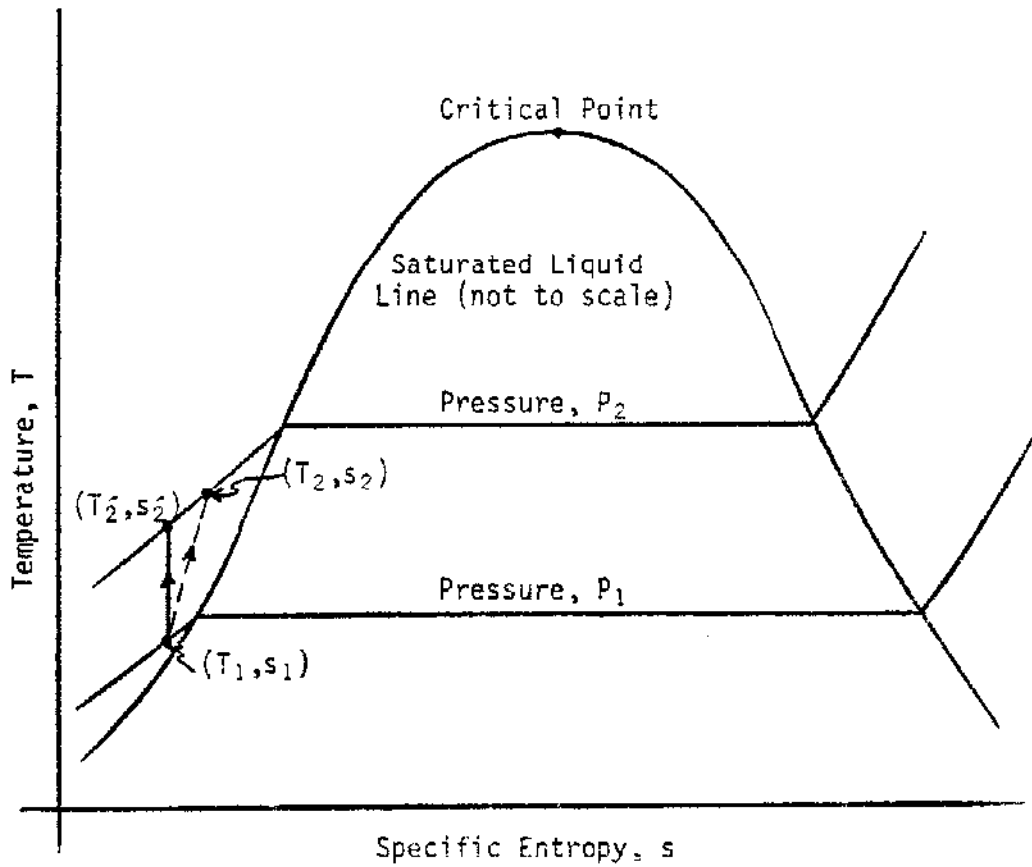


Figure 3.16-2 Temperature-Entropy Diagram for Pumping Process (Not to any scale)

CHAPTER 4

THE COMPUTER PROGRAM AND SUPPORTIVE CALCULATIONS

4.1 Introduction

In this chapter, we shall indicate how the four cycle configurations which we discussed in Chapter 2 are actually assembled in a FORTRAN computer program. The program structure has been designed to be modular. The main program CGACC, which stands for Coal Gasification and Combined Cycles, calls only the four configuration subprograms CNFG1, CNFG2, CNFG3, and CNFG4, depending on the configuration that the analyst wishes to study. In these subprograms, all the component subroutines, whose mathematical models were developed in Chapter 3, are connected together in a way which models the configuration of interest. Also special duty subroutines, which contain the default values (Subroutine DINTi), initialize the cycle point pressures (Subroutine PRIi) and print the results (Subroutine PRINI) and which are unique to CNFGi, are used. As we saw in Chapter 3, the steam table and gas table properties were used extensively in all the component models. The need for casting these properties into subroutines or functions for use on the computer is obvious. Finally, for completeness we shall also list all auxiliary subroutines and functions which facilitated the programming effort.

The input and output to CGACC are described in Appendices B and C respectively. However, several comments should be made at this point. The basic data packet (only batch input is available) consists of three items. The first is a title card, which if blank terminates execution of the program. It is convenient to describe the case under consideration on this card. The second item is the namelist \$MASTER, which is

always read no matter what configuration is being analyzed. It is through \$MASTER that the user tells the computer which configuration he wishes to study via the variable CONFIG. Based on this value (CONFIG=i, where i may be 1, 2, 3, or 4), the third item in the data packet, namelist \$CONFi, is read. The namelist is unique to Configuration i. Each variable in all of these namelists has a built-in default value which the computer uses if the user does not redefine its value. Appendix B defines all the input parameters as well as the default values and units for each of the five namelists.

It should be noted that "canned" programs are available to do much of the same type of calculations that we require here. In one such program, it is claimed that any cycle can be modeled by appropriate input of FORMAT data cards. While this is an excellent approach on the part of the programmer, it is a "black box" approach on the part of a user who has not written the program. The user cannot easily modify the program and must accept results on blind faith. Also, the advantages of the quick, easy input are lost since bulky input decks using FORMAT must be prepared. Aside from the cost consideration, the disadvantages of using these programs are significant enough to warrant development of a personalized computer program.

The program hierarchy is summarized in Figure 4.1-1. The main program will be discussed further in Section 4.2, the configuration subroutines in Section 4.3, the component subroutines in Section 4.4, the property subprograms in Section 4.5, and finally the auxiliary subprograms in Section 4.6.

4.2 Main Program

The primary purpose of the main program CGACC is to allow access to the appropriate configuration which we wish to analyze. A flow chart of the main program is shown in Figure 4.2-1. From this flow chart, we see that the first task to be done by CGACC is to read a title card, which we may use to document the case since this is printed near the top of every output page (see Appendix C). If this card is blank, execution is terminated. Otherwise, the computer will then read the namelist \$MASTER, which among other parameters contains the variable CONFIG. The user is able to analyze configuration *i* by specifying CONFIG=*i* in this namelist. Another variable in \$MASTER, called LISTIN, enables the user to list the current values of all the variables in \$MASTER by setting LISTIN to an integer different than zero. In other words, if LISTIN equals zero, then the current values of variables in \$MASTER are not printed in the output. Finally, based on the value of the variable CONFIG, the appropriate configuration subroutine is called. When the calculations in CNFG*i* are finished, control is transferred back to the main program and a new title card, indicating a new case, is read. If the title card is blank, execution is terminated; otherwise, the above is repeated.

Appendix B.2 should be consulted for a complete list of variables in namelist \$MASTER and their associated definitions and default values.

4.3 Configuration Subroutines

As we have mentioned before, the configuration subroutines are actually the subprograms in which we assemble the component models to

model the cycle configuration of interest. Let us remain general in our discussion by discussing configuration subroutine CNFGi. A simplified flow chart is shown in Figure 4.3-1. It is simplified in the sense that all the CALL statements for the component subroutines are lumped together in the area within the dashed box in the figure.

Subroutine CNFGi first initializes all the input parameters in namelist \$CONFi if the variable DINT read in namelist \$MASTER is not equal to zero, or if this case is the first one of Configuration i to be analyzed in the data deck. This data initialization is accomplished by calling subroutine DINTi. The default values of the input parameters are given in Appendix B.3 along with their meanings and units. Next, the second and final namelist \$CONFi for this case is read which enables the user to change the built-in values for the various parameters for Configuration i. If the variable LISTIN is different than zero (defined in namelist \$MASTER), then each variable in \$CONFi is printed in the output with its current value for the case under consideration. Then, all cycle point pressures are calculated in subroutine PRIi using the pressure drop data which are input (or the default values used). All the component subroutines are then called with the output from one providing the input to the next. By referring to the listing of the configuration subroutines in Appendix A, we may see that very little additional programming is done. Finally, all the various efficiencies are calculated in subroutine EFFICY, the gaseous air pollution effluents in subroutine POLUTE, and the results printed by subroutine PRINi. Refer to Appendix C for a brief description of the output. The various

efficiencies which are calculated in EFFICY are defined in Section 4.6, which also describes how the pollution information is generated, since these are considered to be auxiliary calculations.

By way of summary, we list in Table 4.3-1 the cycle configuration description associated with each of the four configuration subroutines. In Chapter 5, we shall see how the configurations presented in Chapter 2 may be improved by the addition of certain components. At that time, we shall expound on the details of each configuration after it has been modified to improve cycle performance and to meet the air pollution criteria set by the federal government. The basic computer program structure, however, remains unchanged from the description given in the present chapter.

Table 4.3-1
Summary of Configuration Subroutines

<u>Configuration Number</u>	<u>Subroutine</u>	<u>Description of Cycle</u>	<u>Subroutines which are Uniquely Called</u>
1	CNFG1	Adiabatic gasifier integrated with waste heat boiler combined cycle.	DINT1 PRI1 PRIN1
2	CNFG2	Adiabatic gasifier integrated with super-charged boiler combined cycle.	DINT2 PRI2 PRIN2
3	CNFG3	Endothermic gasifier integrated with waste heat boiler combined cycle.	DINT3 PRI3 PRIN3
4	CNFG4	Endothermic gasifier integrated with super-charged boiler combined cycle.	DINT4 PRI4 PRIN4

4.4 Component Subroutines

Each of the component models described in Chapter 3 has been cast into the form of easy-to-use subroutines. We can distinguish at a glance which variables are input, which are output, and which may be input or output. This is done by interpreting the parameter list after the subroutine name as described below.

To be specific, let us consider the subroutine FWHTR, which models the closed feedwater heater according to Section 3.8. By referring to the listing of subroutine FWHTR in Appendix A, we see that the subroutine declaration statement is

```
      SUBROUTINE FWHTR(PLIN,TLIN,WLIN,PSIN,PLOUT,TTD,PRIN,  
X      QRIN,WRIN,  
Y      QSIN,TSIN,  
Z      HLIN,WSIN,HSIN,WLOUT,HLOUT,TLOUT,TRIN,HRIN,TSOUT,  
Z      HSOUT,WSOUT,QSOUT)
```

where the following input/output convention is adopted. The parameters which are always input to the subroutine are those on the first line or those on a line on which an "X" appears in the card continuation column (column 6). The parameters which are sometimes input and/or sometimes output are those which appear on cards with a "Y" in the card continuation column. Finally, the parameters which are always output are located on cards with a "Z" in the continuation column. This convention greatly facilitates the use of these subroutines.

The gasifier and combustor component subroutines have been subdivided to make them more manageable since the models were quite lengthy. In particular, the system of equations for each model are contained in the

auxiliary subroutine called SYSTEM with the equations practically in the same form in which we wrote them in Section 3.2. The multi-dimensional Newton-Raphson iteration procedure described in Section 3.2.2 to obtain a solution to these non-linear algebraic governing equations is programmed in auxiliary subroutine NEWTON. These two subroutines along with all the other auxiliary subroutines are discussed in Section 4.6.

The component subroutines are summarized in Table 4.4-1. The component subroutine listings in Appendix A should be consulted to determine the input and output parameters. Also for convenience, comment cards after the subroutine statement in the listing indicate what the subroutine calculates. The correlation between the Fortran variables and those in the model developments in Chapter 3 should be made rather easily.

Table 4.4-1
Summary of Component Subroutines

<u>Component Model</u>	<u>Subroutine Name</u>	<u>For Model Description Refer to Section</u>
Gasifier	GSFR	3.2.1.1
Combustor	CMBSTR	3.2.1.2
Waste Heat Boiler	WHBOIL	3.3
Supercharged Boiler	SCBOIL	3.4
Air Compressor	AIRCOM	3.5
Gas Compressor	GASCOM	3.5
Condenser	CNDSR	3.6
Deaerator	DATOR	3.7
Closed Feedwater Heater	FWHTR	3.8
Gas Cooler	GASCLR	3.9
Gas Turbine	GASTUR	3.10
Gas-to-Gas Counterflow Heat Exchanger	HXCGG	3.11
Steam Generator	STMGEN	3.12
Steam Turbine	STURB	3.13
Gas Cleanup	SULREM	3.14
Gas Throttle Valve	THRGAS	3.15.1
Steam Throttle Valve	THRSTM	3.15.2
Water Pump	PUMPW	3.16

4.5 Property Subprograms

The property subprograms take the form of Fortran functions. Furthermore, we may divide the property routines into two broad classes: those associated with the gas tables and those with the steam tables. Most of the gas table property subprograms were developed by Osterle and Impink¹⁷ for use in their work for the Pennsylvania Science and Engineering Foundation (see Section 2.4). They elected to curve fit the properties using a least squares method. When the need arose in the present work for additional properties (like the Gibbs free energy of formation) or the same properties for new species (like the enthalpy and entropy for CO₂, NH₃, and so forth), it was decided to use a table form for the property routines with linear interpolation. This approach saved a significant amount of time in programming the new properties. Arbitrary accuracy may be achieved by including more data in the tables.

In this section, we shall include only those routines which are the basic property subprograms. For example, it was convenient to write some auxiliary subroutines like TGASS which calculates the temperature of the gas using the gas composition, pressure, and molar entropy to define the state. Somewhat arbitrarily, we shall refer to this type of subroutine as an auxiliary subprogram, to be discussed in Section 4.6.

4.5.1 Gas Table Property Subprograms

By referring to Tables 3.2-2, 3.2-3, 3.2-5, and 3.2-6, we see that we need to consider the thermodynamic properties of twenty gaseous species and, although not a gas, the enthalpy of solid carbon. We need the standard Gibbs free energy change of formation, the molar enthalpy, and

the molar entropy for each of these gaseous species. Some of the properties like the Gibbs free energy of formations may, in fact, be zero. In addition, we shall need the equilibrium constant K_p for the reaction $1/2 N_2 + 1/2 O_2 \rightleftharpoons NO$ for reasons which will become apparent in Section 4.6.

All of the enthalpies are assumed to be functions of the gas temperature only, consistent with the ideal gas assumption, except for carbon dioxide (CO_2), methane (CH_4), and water vapor (H_2O) for which the pressure effect is included. The entropy, of course, is a function of both the temperature and pressure, even for an ideal gas. The enthalpy of a species in reaction may be considered to be composed of three terms: the enthalpy of formation at some reference temperature minus the sensible enthalpy at the same reference temperature plus the sensible enthalpy at the temperature of interest. The reference temperature is taken to be absolute zero. Each of the above terms may be taken directly from the JANAF²¹ tables, which uses the usual convention for enthalpy of formation; namely, the enthalpy of formation for an elemental gaseous compound (H_2 , O_2 , and so forth) is zero. The entropy and standard Gibbs free energies of formation are also taken directly from the JANAF tables. The pressure correction on entropy amounts to subtracting the product of the universal gas constant and the natural logarithm of the partial pressure (psia) of the species under consideration, which implies an arbitrary reference pressure of 1 psia. The gas table property subprograms are also listed in Appendix A.

The JANAF²¹ tables have been used for all the properties except for the enthalpy of the CO_2 , CH_4 , and H_2O vapor, mentioned above. For these species, the steam tables and various thermodynamic charts have been used

in order to include the pressure effect. Before listing the purpose, the calling sequence, and the limitations for each routine, let us establish the following notation:

<u>Symbol</u>	<u>FORTRAN Symbol</u>	<u>Meaning (Units)</u>
ΔG_f°	DG	Standard Gibbs free energy of formation (Btu/lbmole)
\bar{h}	H	Molar enthalpy (Btu/lbmole)
\bar{s}	S	Molar entropy (Btu/lbmole-°R)
P	P	Pressure (psia)
P_i	Pi	Partial pressure (psia) of species i
T	T	Temperature (°F)
$K_{p,NO}$	KPNO	Equilibrium constant of NO formation reaction

4.5.1.1 Hydrogen (H₂)

Function HH2

Purpose: Computes the enthalpy of hydrogen as a function of temperature; $\bar{h} = f(T)$

Form: $H = HH2(T)$

Restrictions: Ideal gas

Function SH2

Purpose: Computes the entropy of hydrogen as a function of temperature and pressure; $\bar{s} = f(T, P_{H_2})$

Form: $S = SH2(T, PH_2)$

Restrictions: Ideal gas
 $P_{H_2} > 0$

4.5.1.2 Methane (CH₄)

Function HCH4

Purpose: Computes the enthalpy of methane as a function of temperature and pressure; $\bar{h} = f(T, p_{\text{CH}_4})$

Form: $H = \text{HCH4}(T, P_{\text{CH4}})$

Restrictions: Limited to vapor region

Function SCH4

Purpose: Computes the entropy of methane as a function of temperature and pressure; $\bar{s} = f(T, p_{\text{CH}_4})$

Form: $S = \text{SCH4}(T, P_{\text{CH4}})$

Restrictions: Limited to vapor region
 $p_{\text{CH}_4} > 0$

Function DGCH4

Purpose: Computes the standard Gibbs free energy change of formation for methane as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = \text{DGCH4}(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.3 Water Vapor (H₂O)

Function HH2O

Purpose: Computes the enthalpy of water vapor as a function of temperature and pressure; $\bar{h} = f(T, p_{\text{H}_2\text{O}})$

Form: $H = \text{HH2O}(T, P_{\text{H2O}})$

Restrictions: Limited to vapor region

Function SH20

Purpose: Computes the entropy of water vapor as a function of temperature and pressure; $\bar{s} = f(T, p_{H_2O})$

Form: $S = SH20(T, PH20)$

Restrictions: Limited to vapor region
 $p_{H_2O} > 0$

Function DGH20

Purpose: Computes the standard Gibbs free energy change of formation for water vapor as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGH20(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.4 Carbon Monoxide (CO)

Function HCO

Purpose: Computes the enthalpy of carbon monoxide as a function of temperature; $\bar{h} = f(T)$

Form: $H = HCO(T)$

Restrictions: Ideal gas

Function SCO

Purpose: Computes the entropy of carbon monoxide as a function of temperature and pressure; $\bar{s} = f(T, p_{CO})$

Form: $S = SCO(T, PCO)$

Restrictions: Ideal gas
 $p_{CO} > 0$

Function DGCO

Purpose: Computes the standard Gibbs free energy change of formation for carbon monoxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGCO(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.5 Nitrogen (N_2)

Function HN2

Purpose: Computes the enthalpy of nitrogen as a function of temperature; $\bar{h} = f(T)$

Form: $H = HN2(T)$

Restrictions: Ideal gas

Function SN2

Purpose: Computes the entropy of nitrogen as a function of temperature and pressure; $\bar{s} = f(T, p_{N_2})$

Form: $S = SN2(T, p_{N_2})$

Restrictions: Ideal gas
 $p_{N_2} > 0$

4.5.1.6 Oxygen (O_2)

Function H02

Purpose: Computes the enthalpy of oxygen as a function of temperature; $\bar{h} = f(T)$

Form: $H = H02(T)$

Restrictions: Ideal gas

Function S02

Purpose: Computes the entropy of oxygen as a function of temperature and pressure; $\bar{s} = f(T, p_{O_2})$

Form: $S = S02(T)$

Restrictions: Ideal gas
 $p_{O_2} > 0$

4.5.1.7 Argon (Ar)

Function HAR

Purpose: Computes the enthalpy of argon as a function of temperature; $\bar{h} = f(T)$

Form: $H = HAR(T)$

Restrictions: Ideal gas

Function SAR

Purpose: Computes the entropy of argon as a function of temperature and pressure; $\bar{s} = f(T, p_{Ar})$

Form: $S = SAR(T, p_{Ar})$

Restrictions: Ideal gas
 $p_{Ar} > 0$

4.5.1.8 Carbon Dioxide (CO₂)

Function HCO2

Purpose: Computes the enthalpy of carbon dioxide as a function of temperature and pressure;
 $\bar{h} = f(T, p_{CO_2})$

Form: $H = HCO2(T, p_{CO_2})$

Restrictions: Limited to vapor region

Function SC02

Purpose: Computes the entropy of carbon dioxide as a function of temperature and pressure;
 $\bar{S} = f(T, P_{CO_2})$

Form: $S = SC02(T, PCO2)$

Restrictions: Limited to vapor region
 $P_{CO_2} > 0$

Function DGC02

Purpose: Computes the standard Gibbs free energy change of formation of carbon dioxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGC02(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.9 Hydrogen Sulfide (H₂S)

Function HH2S

Purpose: Computes the enthalpy of hydrogen sulfide as a function of temperature; $\bar{h} = f(T)$

Form: $H = HH2S(T)$

Restrictions: Ideal gas

Function SH2S

Purpose: Computes the entropy of hydrogen sulfide as a function of temperature and pressure;
 $\bar{S} = f(T, P_{H_2S})$

Form: $S = SH2S(T, PH2S)$

Restrictions: Ideal gas
 $P_{H_2S} > 0$

Function DGH2S

Purpose: Computes the standard Gibbs free energy changes of formation for hydrogen sulfide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGH2S(T)$

Restrictions: Ideal Gas
 $80 < T < 5300$

4.5.1.10 Carbonyl Sulfide (COS)

Function H COS

Purpose: Computes the enthalpy of carbonyl sulfide as a function of temperature; $\bar{h} = f(T)$

Form: $H = H COS(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

Function S COS

Purpose: Computes the entropy of carbonyl sulfide as a function of temperature and pressure; $\bar{s} = f(T, p_{COS})$

Form: $S = S COS(T, p_{COS})$

Restrictions: Ideal gas
 $80 < T < 5300$; $p_{COS} > 0$

Function DGCOS

Purpose: Computes the standard Gibbs free energy change of formation for carbonyl sulfide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGCOS(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.11 Nitric Oxide (NO)

Function HNO

Purpose: Computes the enthalpy of nitric oxide as a function of temperature; $h = f(T)$

Form: $H = HNO(T)$

Restrictions: Ideal gas

Function SNO

Purpose: Computes the entropy of nitric oxide as a function of temperature and pressure; $\bar{s} = f(T, P_{NO})$

Form: $S = SNO(T, PNO)$

Restrictions: Ideal gas
 $P_{NO} > 0$

Function DGNO

Purpose: Computes the standard Gibbs free energy change of formation for nitric oxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGNO(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

Function AKPNO

Purpose: Computes the equilibrium constant of the NO formation reaction $1/2 N_2 + 1/2 O_2 \rightarrow NO$ as a function of temperature; $K_{p_{NO}} = f(T)$

Form: $KPNO = AKPNO(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$

4.5.1.12 Hydroxyl (OH)

Function HOH

Purpose: Computes the enthalpy of hydroxyl as a function of temperature; $\bar{h} = f(T)$

Form: $H = HOH(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$

Function SOH

Purpose: Computes the entropy of hydroxyl as a function of temperature and pressure; $\bar{s} = f(T, p_{OH})$

Form: $S = SOH(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$; $p_{CH} > 0$

Function DGOH

Purpose: Computes the standard Gibbs free energy change of formation for hydroxyl as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGOH(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.13 Monatomic Hydrogen (H)

Function HH

Purpose: Computes the enthalpy of monatomic hydrogen as a function of temperature; $\bar{h} = f(T)$

Form: $H = HH(T)$

Restrictions: Ideal gas
 $-200 < T < 5300$

Function SH

- Purpose: Computes the entropy of monatomic hydrogen as a function of temperature and pressure; $\bar{s} = f(T, p_H)$
- Form: $S = SH(T, p_H)$
- Restrictions: Ideal gas
 $-280 < T < 5300$; $p_H > 0$

Function DGH

- Purpose: Computes the standard Gibbs free energy change of formation for monatomic hydrogen as a function of temperature; $\Delta G_f^\circ = f(T)$
- Form: $DG = DGH(T)$
- Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.14 Monatomic Oxygen (O)

Function HO

- Purpose: Computes the enthalpy of monatomic oxygen as a function of temperature; $\bar{h} = f(T)$
- Form: $H = HO(T)$
- Restrictions: Ideal gas
 $-280 < T < 5300$

Function SO

- Purpose: Computes the entropy of monatomic oxygen as a function of temperature and pressure; $\bar{s} = f(T, p_O)$
- Form: $S = SO(T, p_O)$
- Restrictions: Ideal gas
 $-280 < T < 5300$; $p_O > 0$

Function DGO

Purpose: Computes the standard Gibbs free energy change of formation for monatomic oxygen as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGO(T)$

Restrictions: Ideal gas
 $80 < T < 5300$

4.5.1.15 Ammonia (NH_3)

Function HNH3

Purpose: Computes the enthalpy of ammonia as a function of temperature; $h = f(T)$

Form: $H = \text{HNH3}(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$

Function SNH3

Purpose: Computes the entropy of ammonia as a function of temperature and pressure; $\bar{s} = f(T, p_{\text{NH}_3})$

Form: $S = \text{SNH3}(T, p_{\text{NH}_3})$

Restrictions: Ideal gas
 $-280 < T < 5300; p_{\text{NH}_3} > 0$

Function DGNH3

Purpose: Computes the standard Gibbs free energy change of formation for ammonia as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = \text{DGNH3}(T)$

Restrictions: Ideal gas
 $-280 < T < 5300; p_{\text{NH}_3} > 0$

4.5.1.16 Nitrogen Dioxide (NO₂)

Function HNO2

Purpose: Computes the enthalpy of nitrogen dioxide as a function of temperature; $\bar{h} = f(T)$

Form: $H = HNO2(T)$

Restrictions: Ideal gas

Function SNO2

Purpose: Computes the entropy of nitrogen dioxide as a function of temperature and pressure;
 $\bar{s} = f(T, P_{NO_2})$

Form: $S = SNO2(T, PNO2)$

Restrictions: Ideal gas
 $P_{NO_2} > 0$

Function DGN02

Purpose: Computes the standard Gibbs free energy change of formation for nitrogen dioxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGN02(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$

4.5.1.17 Sulfur Monoxide (SO)

Function HSO

Purpose: Computes the enthalpy of sulfur monoxide as a function of temperature; $\bar{h} = f(T)$

Form: $H = HSO(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$

Function SS0

Purpose: Computes the entropy of sulfur monoxide as a function of temperature and pressure;

$$\bar{s} = f(T, p_{SO})$$

Form: $S = SS0(T, p_{SO})$

Restrictions: Ideal gas
 $-280 < T < 5300; p_{SO} > 0$

Function DGS0

Purpose: Computes the standard Gibbs free energy change of formation for sulfur monoxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGS0(T)$

Restrictions: Ideal gas
 $-280 < T < 5300; p_{SO} > 0$

4.5.1.18 Sulfur Dioxide (SO_2)

Function HS02

Purpose: Computes the enthalpy of sulfur dioxide as a function of temperature; $\bar{h} = f(T)$

Form: $H = HS02(T)$

Restrictions: Ideal gas

Function SS02

Purpose: Computes the entropy of sulfur dioxide as a function of temperature and pressure;

$$\bar{s} = f(T, p_{SO_2})$$

Form: $S = SS02(T, p_{SO_2})$

Restrictions: Ideal gas
 $p_{SO_2} > 0$

Function DGS02

Purpose: Computes the standard Gibbs free energy change of formation for sulfur dioxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGS02(T)$

Restrictions: Ideal gas
 $-280 < T < 5300$

4.5.1.19 Sulfur Trioxide (SO_3)

Function HS03

Purpose: Computes the enthalpy of sulfur trioxide as a function of temperature; $\bar{h} = f(T)$

Form: $H = HS03(T)$

Restrictions: Ideal gas

Function SS03

Purpose: Computes the entropy of sulfur trioxide as a function of temperature and pressure;
 $\bar{s} = f(T, P_{SO_3})$

Form: $S = SS03(T)$

Restrictions: Ideal gas
 $P_{SO_3} > 0$

Function DGS03

Purpose: Computes the standard Gibbs free energy change of formation for sulfur trioxide as a function of temperature; $\Delta G_f^\circ = f(T)$

Form: $DG = DGS03(T)$

Restrictions: Ideal gas
 $-280 < T < 5300; P_{SO_3} > 0$

4.5.1.20 Sulfur (S_2)

Function HS2

Purpose: Computes the enthalpy of gaseous sulfur as a function of temperature; $\bar{h} = f(T)$

Form: $H = HS2(T)$

Restrictions: Ideal gas

4.5.1.21 Carbon (C)

Function HC

Purpose: Computes the enthalpy of pure solid carbon as a function of temperature; $\bar{h} = f(T)$

Form: $H = HC(T)$

Restrictions: Solid carbon

4.5.2 Steam Table Subprograms

We saw in Chapter 3 that many of the components utilize subcooled water, saturated steam-water mixtures, or superheated steam as the working fluid. We also saw that we need the capability to obtain just about all the thermodynamic properties in each of these three fluid regions. For this purpose, a proprietary set of steam tables has been used which is called by a master steam table subroutine FINDER. This subroutine returns all the other thermodynamic properties given the pressure and one other property as input. The subroutine has the following calling sequence

```
CALL FINDER(P,K,T,H,Q,S,V,IPH)
```

where P is pressure (psia); T, temperature ($^{\circ}$ F); H, specific enthalpy (Btu/lbm); Q, quality (fraction); S, specific entropy (Btu/lbm $^{\circ}$ R); V, specific volume (ft 3 /lbm); and IPH, the phase of the fluid according to the convention established in Table 4.5-1. As we have already mentioned, the pressure P is always one input. The second input depends on the integer value for K, according to Table 4.5-2. All other properties are

Table 4.5-1
Correlation between IPH and Fluid Condition

IPH	Fluid Condition
1	Subcooled Water
2	Saturation Region
3	Superheated Steam
4	Supercritical Fluid

Table 4.5-2
Correlation between K and Input Parameters

K	Input Parameters
+1	P, T
-1	P, H
-2	P, Q
0	P, S

subsequently returned. Obviously, when $K = +1$, the fluid state must be superheated, subcooled, or supercritical, and when $K = -2$, the fluid must be saturated.

Zero specific enthalpy and zero specific entropy are assigned to the saturated liquid states at the freezing point of water (32.02° F). Note that this reference state is different from that used in the gas table

property routines where we used zero absolute temperature as the base. The enthalpies with respect to the two bases are related by

$$\bar{h} = 18.016 h - 118256.07 \quad (4.5-1)$$

where h is the specific enthalpy (Btu/lbm) from the steam tables using subroutine FINDER and \bar{h} is the molar enthalpy (Btu/lbmole) from the gas tables using function HH20. The entropies are similarly related by

$$\bar{s} = 18.016(s + 0.5443) \quad (4.5-2)$$

where s is the specific entropy (Btu/lbm^oR) from the steam tables using subroutine FINDER and \bar{s} is the molar entropy (Btu/lbmole^oR) from the gas tables using the function SH20. When using FINDER and HH20 or SH20 in the same calculation, we must use Equations (4.5-1) and/or (4.5-2) to ensure consistency in our calculations.

4.6 Auxiliary Subprograms

The auxiliary subprograms perform a wide range of duties. These particular subprograms do not fit into the other four main categories of subprograms which we have discussed thus far. Again each subprogram is listed in Appendix A.

4.6.1 Subroutine ATERP

This subroutine performs a modified linear interpolation based on the equation for a straight line

$$y = mz + b \quad (4.6-1)$$

where z is the abscissa, m the slope, b the y -intercept, and y the ordinate. The real dependent variable, however, is x which related to z by

$$x = \frac{1}{z}. \quad (4.6-2)$$

This type of interpolation is appropriate when one tries to determine the equilibrium constant K_p for a temperature T between two temperatures in a table, since a plot of $\ln K_p$ versus $1/T$ is linear over a wide range of temperatures. The calling sequence is

```
CALL ATERP(X,Y,M,XX,YY)
```

where X is the array of abscissa values,
 Y is the corresponding array of ordinate values,
 M is the number of (X,Y) pairs ($M \leq 50$),
 XX is the abscissa of interest, and
 YY is the interpolated ordinate corresponding to XX .

If XX is less than $X(1)$ or if XX is greater than $X(M)$, appropriate error messages are printed out.

4.6.2 Block Data BLDATA

This non-executable subprogram provides a convenient location for storing data which are transferred to other subprograms via COMMON blocks. The primary types of data which are stored here are default values for variables in namelist \$MASTER, molecular weights of various species in the coal and in various gaseous mixtures, higher and lower heating values of combustible species in the coal and power gas, and other constants.

We shall summarize the numerical values used for some of these parameters by way of Table 4.6-1 to Table 4.6-8. For the default values of the variables in namelist \$MASTER, Appendix B.2 should be consulted, where the meaning of each variable is also given.

From Chapter 3, it became apparent that the molecular weights of the various species in the coal (before and after application of the Dulong approximation) and in the various gaseous mixtures (air, power gas, and products of combustion) must be specified. The variables WTC(I), where I=1 to 6, are the molecular weights of the C, H, O, N, S, and H₂O (liquid) in the coal. The numerical values used are summarized in Table 4.6-1. Note that the need for the molecular weight of the ash

Table 4.6-1
Molecular Weights of Species in Coal
(Before Dulong Approximation)

I	Species	Molecular Weight WTC(I)
1	C(s)	12.011
2	H	1.008
3	O	16.000
4	N	14.006
5	S	32.064
6	H ₂ O(l)	18.016

in the coal never arose and, fortunately, no value for this needs to be specified. After application of the Dulong approximation, the species become C, H₂, H₂O (vapor), N₂, S₂, and H₂O (liquid), for which the molecular weights are assigned the values shown in Table 4.6-2 in the array WTCO(I), for i=1 to 6. Again, the molecular weight of the ash

is not needed. The molecular weights of the species in the air which we assumed to be composed of N_2 , O_2 , Ar, and $H_2O(g)$, are assigned to the variable $WTA(I)$, for $I=1$ to 4, and are shown in Table 4.6-3. For completeness, we assign the molecular weight of steam to WTS , where $WTS = 18.016$, since we also have steam entering the gasifier.

Table 4.6-2
Molecular Weights of Species in Coal
(After DuLong Approximation)

I	Species	Molecular Weight $WTCD(I)$
1	C(s)	12.011
2	H_2	2.016
3	$H_2O(g)$	18.016
4	N_2	28.013
5	S_2	64.128
6	$H_2O(l)$	18.016

Table 4.6-3
Molecular Weights of Species in Air

I	Species	Molecular Weight $WTA(I)$
1	N_2	28.013
2	O_2	32.000
3	Ar	39.948
4	$H_2O(g)$	18.016

In the gasifier model in Chapter 3, we assumed the presence of ten gaseous species in the power gas which was formed. The molecular weight of each of these species is summarized in Table 4.6-4, where the variable

name WTGF(I), I=1 to 10, is used. Similarly in the combustor model we assumed the presence of fifteen species, whose molecular weights which

Table 4.6-4
Molecular Weights of Species in Power Gas

I	Species	Molecular Weights WTGF(I)
1	H ₂	2.016
2	CO	28.010
3	CH ₄	16.042
4	H ₂ O(g)	18.016
5	CO ₂	44.010
6	N ₂	28.016
7	Ar	39.950
8	H ₂ S	34.080
9	COS	60.075
10	NH ₃	17.031

we denote by WTCM(I), I=1 to 15, are summarized in Table 4.6-5. Finally it is convenient to combine the nineteen species in Tables 4.6-4 and 4.6-5

Table 4.6-5
Molecular Weights of Species in Combustor Product Gas

I	Species	Molecular Weights WTCM(I)
1	CO ₂	44.010
2	H ₂ O(g)	18.016
3	N ₂	28.016
4	O ₂	32.000
5	Ar	39.950
6	NO	30.008
7	CO	28.010
8	H	1.008
9	O	16.000
10	OH	17.008
11	H ₂	2.016
12	NO ₂	46.008
13	SO	48.066
14	SO ₂	64.066
15	SO ₃	80.066

into one array, with the molecular weights assigned to array WTGMIX(I), I=1 to 19, as shown in Table 4.6-6. The subscript-species correlation shown in Table 4.6-6 is used in all subprograms in which a gaseous mixture is present except the gasifier (GSFR) and combustor (CMBSTR) subroutines and their associated auxiliary subroutines (SYSTEM and NEWTON).

Table 4.6-6
Molecular Weights of Species in the
Generalized Gaseous Mixture

I	Species	Molecular Weight WTGMIX(I)
1	H ₂	2.016
2	CH ₄	16.042
3	H ₂ O(g)	18.016
4	CO	28.010
5	N ₂	28.016
6	O ₂	32.000
7	Ar	39.950
8	CO ₂	44.010
9	H ₂ S	34.080
10	COS	60.075
11	NO	30.008
12	OH	17.008
13	H	1.008
14	O	16.000
15	NH ₃	17.031
16	NO ₂	46.008
17	SO	48.066
18	SO ₂	64.066
19	SO ₃	80.066

The species for which we take credit for contributing to the heating value of the power gas are H₂, CO, and CH₄, and in the coal C(s), H₂, and S₂. We use the values shown in Tables 4.6-7 and 4.6-8 to compute effective heating values for the power gas and coal, respectively. Note the

Table 4.6-7
Heating Values of Combustible Species in Power Gas

I	Species	Higher Heating Values HHVG(I) (Btu/lbmole)	Lower Heating Value LHVG(I) (Btu/lbmole)
1	H ₂	122,971	104,040
2	CO	121,750	121,750
3	CH ₄	383,027	345,170

Table 4.6-8
Heating Values of Combustible Species in Coal

I	Species	Higher Heating Value HHVC(I) (Btu/lbm)	Lower Heating Value LHVC(I) (Btu/lbm)
1	C(s)	14,095	14,095
2	H ₂	60,997	51,605
3	S ₂	4,848.4	4,848.4

difference in units. The resulting effective heating values for the power gas and coal are used only in the efficiency calculations which are described in Section 4.6.6 and in the pollution calculation described in Section 4.6.16. The actual calculation of the heating values for the power gas takes place in subroutine GSFR and for the coal in subroutine DULONG, which is described in Section 4.6.3.

We complete the description of the data stored in BLOCK DATA by assigning the universal gas constant the value 1.987 Btu/lbmole^oR, the difference between the Rankine and Fahrenheit temperatures the value 460 (°R), and atmospheric pressure the value 14.696 psia. The data sorted in BLOCK DATA is used throughout the computer program.

4.6.3 Subroutine DULONG

The purpose of subroutine DULONG is two-fold: to obtain the coal composition for the purpose of enthalpy determination using the Dulong approximation described in Section 3.2 and to then compute the higher and lower heating values of the coal based on this approximation. Using the assumptions and nomenclature of Section 3.2.1, the relevant equations for the weight fractions of C(s), H₂, H₂O(g), N₂, S₂, H₂O(l), and ash in the coal are the following.

$$\omega_{d1} = \omega_{c1} \quad (4.6-1)$$

$$\omega_{d2} = \omega_{c2} - \frac{v_{d2}}{v_{c3}} \omega_{c3} \quad (4.6-2)$$

$$\omega_{d3} = \omega_{c3} + \frac{v_{d2}}{v_{c3}} \omega_{c3} \quad (4.6-3)$$

$$\omega_{d4} = \omega_{c4} \quad (4.6-4)$$

$$\omega_{d5} = \omega_{c5} \quad (4.6-5)$$

$$\omega_{d6} = \omega_{c6} \quad (4.6-6)$$

$$\omega_{d7} = \omega_{c7} \quad (4.6-7)$$

Using these adjusted weight fraction compositions, the higher and lower heating values are easily calculated with the help of the values in Table 4.6-8. For completeness, the effective molecular weight v_{afc} of the ash free coal is also calculated here using

$$v_{afc} = \frac{1}{\sum_{i=1}^6 \frac{\omega_{ci}}{v_{ci}(1-\omega_{c7})}} \quad (4.6-8)$$

The calling sequence is

```

!!
!!
!!CALL DULONG(WFC,
!!  WFCO, LVCOAL, HVCOAL, WTAFC)
!!
!!

```

where WFC(I) corresponds to ω_{ci} above, WFCO(I) to ω_{oi} , and WTAFC to v_{afc} . LVCOAL and HVCOAL are the calculated lower and higher heating values (But/lbm of coal) of the coal, respectively.

4.6.4 Subroutine DUMCMB

Subroutine DUMCMB is a dummy subroutine which simply takes the values of the parameters in the argument list of subroutine CMBSTR and puts them into a common block (labeled CMBST1) for use in subroutine SYSTEM. The reason for this rather strange maneuver is to facilitate the use of the component subroutines by using parameter lists to transfer data between two subprograms. However, in SYSTEM it is more convenient to use labeled common. It is not permissible in FORTRAN to have the same variable in both a parameter list and common block in the same subroutine.

4.6.5 Subroutine DUMGAS

Like subroutine DUMCMB, subroutine DUMGAS is also a dummy subroutine. The values in the argument list of subroutine GSFR are put into common

blocks (labeled GASFY1 and GASFY2). The reason for doing this is similar to that given for subroutine DUMCMB.

4.6.6 Subroutine EFFICY

It is appropriate here to define the four kinds of efficiencies which we shall use to assess the cycle performance in Chapter 5. The first efficiency which we define is the gasification efficiency. As the name suggests, we define this to be the ratio of the heating value of the power gas to the sum of the heating value of the coal and the heat added to the gasifier, all in consistent units, of course. The steam cycle efficiency is defined as the ratio of the net work output from the steam cycle to the heat input to the steam cycle. This is the only efficiency which does not depend on whether the higher or lower heating values are used. We define the combined cycle efficiency as the ratio of the net work output for the entire system to the heating value of the power gas. Finally, we define the coal-pile-to-bus-bar or station efficiency as the product of the combined cycle and gasification efficiencies reduced by a specified percentage because of station requirements for power, such as lighting, heating, and so forth. With the exception of steam cycle efficiency, the use of higher or lower heating values gives different results. As we shall see in Chapter 5, we shall consistently and somewhat arbitrarily use the station efficiency based on lower heating values to assess the performance of each cycle.

4.6.7 Subroutine HGAS2

This simple subroutine calculates the molar enthalpy of a gas specified to have a certain pressure (psia), temperature ($^{\circ}\text{F}$), and composition (mole fraction). The species assumed to be present (with corresponding subscripts) are those shown in Table 4.6-6. The mole fraction composition $\text{MFG}(I)$ for $I=1$ to 19, of the gaseous mixture along with the pressure P and temperature T are used in the call statement

```
CALL HGAS2(P,T,MFG,HG)
```

to obtain the molar enthalpy $\text{HG}(\text{Btu}/\text{lbmole})$ of the gaseous mixture. As mentioned before, pressure effects on enthalpy are included only for CH_4 , H_2O , and CO_2 . All remaining species are assumed to behave like ideal gases, for which the enthalpy is a function of temperature only. The molar enthalpy of each individual species, of course, is provided by the appropriate property subprograms described in Section 4.5.

4.6.8 Subroutine SGAS2

Like HGAS2, subroutine SGAS2 calculates another important property of a gaseous mixture given its pressure (psia), temperature ($^{\circ}\text{F}$), and composition (mole fraction). This property is the molar entropy ($\text{Btu}/\text{lbmole}^{\circ}\text{R}$) which we represent by SG . The calling sequence becomes

```
CALL SGAS2(P,T,MFG,SG)
```

where P , T , and MFG have the same meaning as in subroutine HGAS2. It should be recalled that the entropy, even for an ideal gas, is a function

of pressure. The molar entropy of each individual species is provided by the appropriate property subprograms described in Section 4.5.

4.6.9 Subroutine INVDET

Subroutine INVDET²² provides the matrix inversion required by the multi-dimensional Newton-Raphson iteration to obtain a solution to the gasifier and combustor models. Numerical round-off error is reduced by maximizing the pivotal elements in the algorithm.

4.6.10 Subroutine MAIR

Subroutine MAIR takes the air composition on a four-component weight fraction basis and converts it to a composition on a four-component mole fraction basis, and compositions on nineteen-component mole and weight fraction bases. In addition, the molecular weight of the air is calculated. This enables the air to be treated as a special gas for which we may use the other auxiliary subprograms like HGAS2 which facilitate the calculations. Table 3.2-2 and Table 4.6-6 must be used to establish the correlation between species and subscript designations for the four- and nineteen-component compositions respectively.

4.6.11 Subroutine MGAS1

Subroutine MGAS1 takes the gasifier power gas composition on the ten-component mole fraction basis as defined by Table 3.2-3 and converts it to mole and weight fraction compositions on the nineteen-component basis defined in Table 4.6-6. In addition, the molecular weight of the power gas is calculated.

4.6.12 Subroutine MGAS2

Subroutine MGAS2 takes the fifteen-component combustor product gas composition as defined by Table 3.2-6 and converts it to the nineteen-component composition as defined by Table 4.6-6 by mole and weight fractions. The molecular weight of the product gas is also calculated.

4.6.13 Subroutine MGAS3

Subroutine MGAS3 simply converts the gas composition by mole fraction on the nineteen-component basis as defined by Table 4.6-6 to one by weight fraction on the same basis. The molecular weight of the gas is also calculated.

4.6.14 Subroutine NEWTON

Subroutine NEWTON performs the multi-dimensional Newton-Raphson iterations on the two systems of equations which describe the gasifier and combustor. The initial guess for the solution vector was chosen to minimize the number of iterations required to obtain a solution and is, in fact, the solution to a representative case. The mathematics of this iteration scheme are described in Section 3.2.2 and is not repeated here. The implementation of this scheme on the computer is rather tedious but straightforward. Mole fractions are generally calculated to fifth-place accuracy.

4.6.15 Subroutine SYSTEM

Subroutine SYSTEM contains the equations which we developed in Sections 3.2.1.1 and 3.2.1.2 for the gasifier and combustor models,

respectively. Each of the governing equations in these sections was written so that zero appeared on one side and all the other terms on the other. Except for this trivial modification, the equations which are stored in SYSTEM are practically identical in form to the ones written in Sections 3.2.1.1 and 3.2.1.2.

4.6.16 Subroutine POLUTE

In subroutine POLUTE, we compute the amount of nitric oxides NO_x and sulfur oxides SO_x that go up the power plant stack and into the atmosphere. The subroutine requires as input the composition of the stack gas (by mole fraction μ_i and weight fraction ω_i), the mass flow w_{dg} of the stack gas (per lbm of coal), the higher heating value of the coal H_{HVC} and the "freeze temperature" T_F for the NO producing reaction. We shall calculate the amount of pollutants in units of pounds of NO_x (or SO_x) per million Btu of heat input. The higher heating value of the fuel is used for the heat input based on federal regulations.

The NO producing reaction $1/2 \text{N}_2 + 1/2 \text{O}_2 \rightleftharpoons \text{NO}$ appears to slow down significantly in the reverse direction when the temperature is below about 2400°F .²³ Consequently, we shall calculate two values for the amount of NO_x pollution: NO_{Equil} assuming equilibrium at the combustor outlet temperature and $\text{NO}_{\text{Freeze}}$ assuming the NO producing reaction "freezes" at T_F . Rather than doing a full-blown equilibrium calculation for temperature T_F , we assume that the mole fractions of N_2 (μ_{N_2}) and O_2 (μ_{O_2}) will not change significantly for the two temperatures and calculate the mole fraction of NO ($\mu_{\text{NO}_{\text{Freeze}}}$) from

$$\mu_{\text{NO}_{\text{Freeze}}} \cong K_p \sqrt{\mu_{\text{N}_2} \mu_{\text{O}_2}}$$

which is the equilibrium equation for $1/2 \text{N}_2 + 1/2 \text{O}_2 \rightleftharpoons \text{NO}$ with equilibrium constant K_p , to be evaluated at temperature T_F . Function AKPNO , of course, is used to get K_p at T_F . We shall see in Chapter 5 that the mole fraction of $\text{NO}(\mu_{\text{NO}})$ is practically numerically equal to the weight fraction of $\text{NO}(\omega_{\text{NO}})$, so it is reasonable to assume that

$$\omega_{\text{NO}_{\text{Freeze}}} \cong \mu_{\text{NO}_{\text{Freeze}}}$$

We have two weight fractions for NO : ω_{NO} from the original stack gas composition and $\omega_{\text{NO}_{\text{Freeze}}}$ from the NO producing reaction frozen at T_F . The expression for NO_{Equil} is given by

$$\text{NO}_{\text{Equil}} = 10^6 \frac{(\omega_{\text{NO}} + \omega_{\text{NO}_2})w_{\Delta g}}{H_{\text{HVC}}}$$

For $\text{NO}_{\text{Freeze}}$, we neglect the contribution by NO_2 , since it turns out to be much smaller than that due to NO , and get

$$\text{NO}_{\text{Freeze}} = 10^6 \frac{\mu_{\text{NO}_{\text{Freeze}}} w_{\Delta g}}{H_{\text{HVC}}}$$

The amount of SO_x produced, SO_{Equil} , is similarly calculated by

$$\text{SO}_{\text{Equil}} = \frac{10^6 (\omega_{\text{SO}} + \omega_{\text{SO}_2} + \omega_{\text{SO}_3}) w_{\Delta g}}{H_{\text{HVC}}}$$

Freezing of the SO_x producing reactions apparently does not occur physically and, therefore, is not modeled.

4.6.17 Subroutine TERP

This subroutine performs a linear interpolation based on the equation for a straight line

$$y = mx + b$$

where x is the abscissa, m the slope, b the y -intercept, and y the ordinate.

The calling sequence is

```
CALL TERP(X,Y,M,XX,YY)
```

where X is the array of abscissa values,
 Y is the corresponding array of ordinates,
 M is the number of (X,Y) pairs ($M < 50$),
 XX is the abscissa of interest, and
 YY is the interpolated ordinate corresponding to XX .

As in ATERP, appropriate error messages are printed out if interpolation is attempted outside the domain of X values.

4.6.18 Subroutine TGASH

Subroutine TGASH performs the inverse function of subroutine HGAS2. It was frequently necessary in the component models to determine the gas temperature $TG(^{\circ}F)$ given its pressure P (psia), molar enthalpy H (Btu/lbmole), and gas composition $MFG(I)$ on the nineteen component mole fraction basis. Subroutine HGAS2 is used in a simple one-dimensional

Newton-Raphson iteration to accomplish this task. If convergence to a relative error of 10^{-5} does not occur in 15 iterations, an appropriate error message is printed. The calling sequence is

```
CALL TGASH(P,H,MFG,TG)
```

where P, H, and MFG are inputs and the gas temperature TG is the output.

4.6.19 Subroutine TGASS

Subroutine TGASS is completely analogous to subroutine TGASH. Now the gas temperature TG($^{\circ}$ F) is to be found given the gas pressure P (psia), molar entropy S (Btu/lbm $^{\circ}$ R), and gas composition MFG(I) on the nineteen-component mole fraction basis. Again a simple Newton-Raphson iteration is used and an appropriate error message is printed if convergence does not occur in 15 iterations. The calling sequence is

```
CALL TGASS(P,S,MFG,TG)
```

where P, S, and MFG are the inputs and the gas temperature TG is the output.

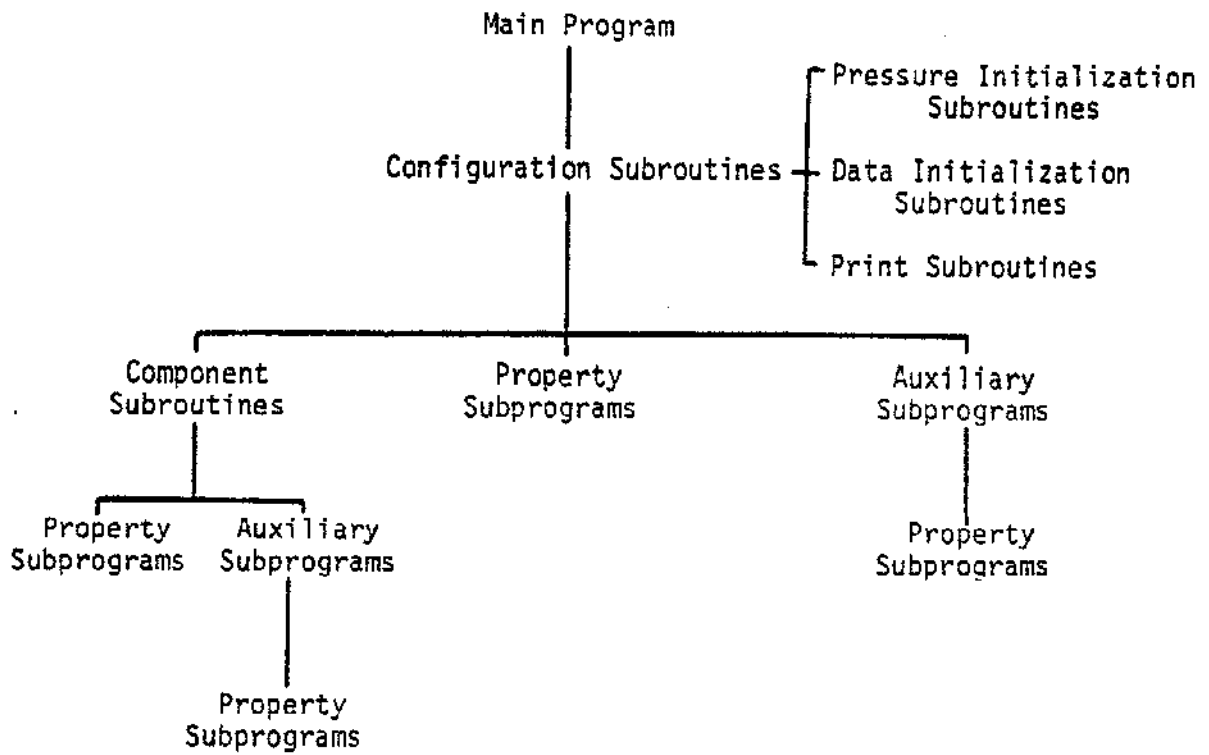


Figure 4.1-1 Program Hierarchy

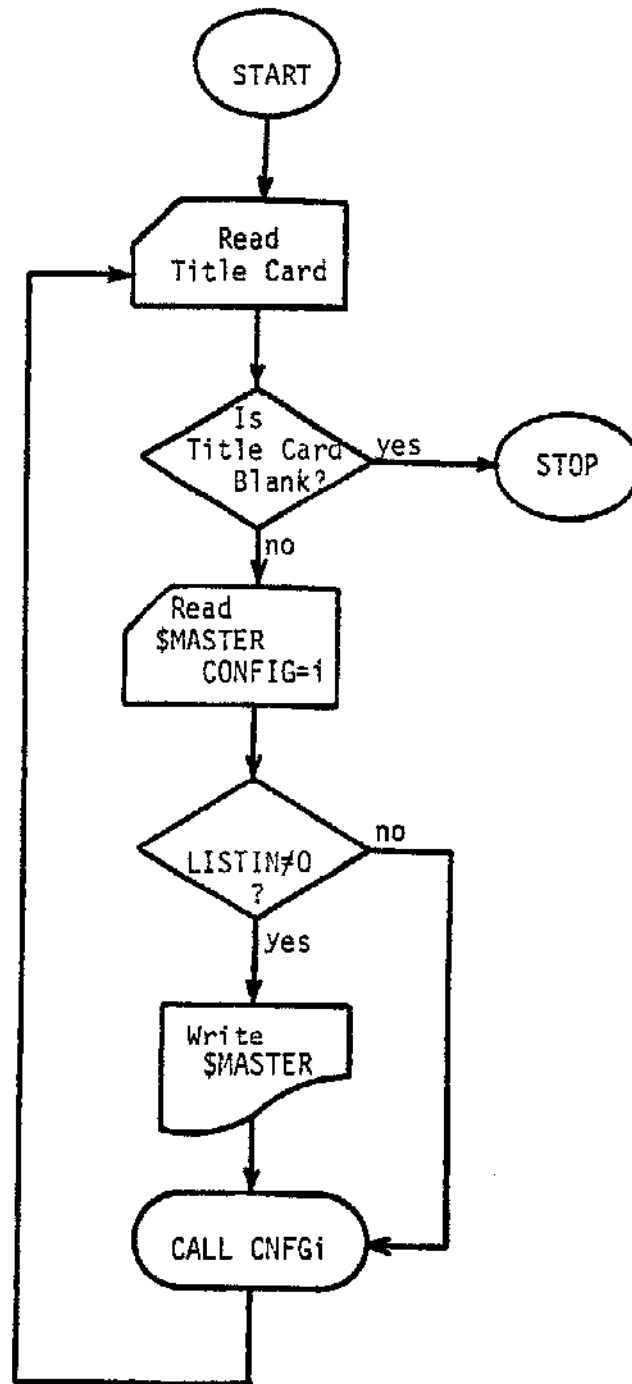


Figure 4.2-1 Flow Chart of Main Program CGACC

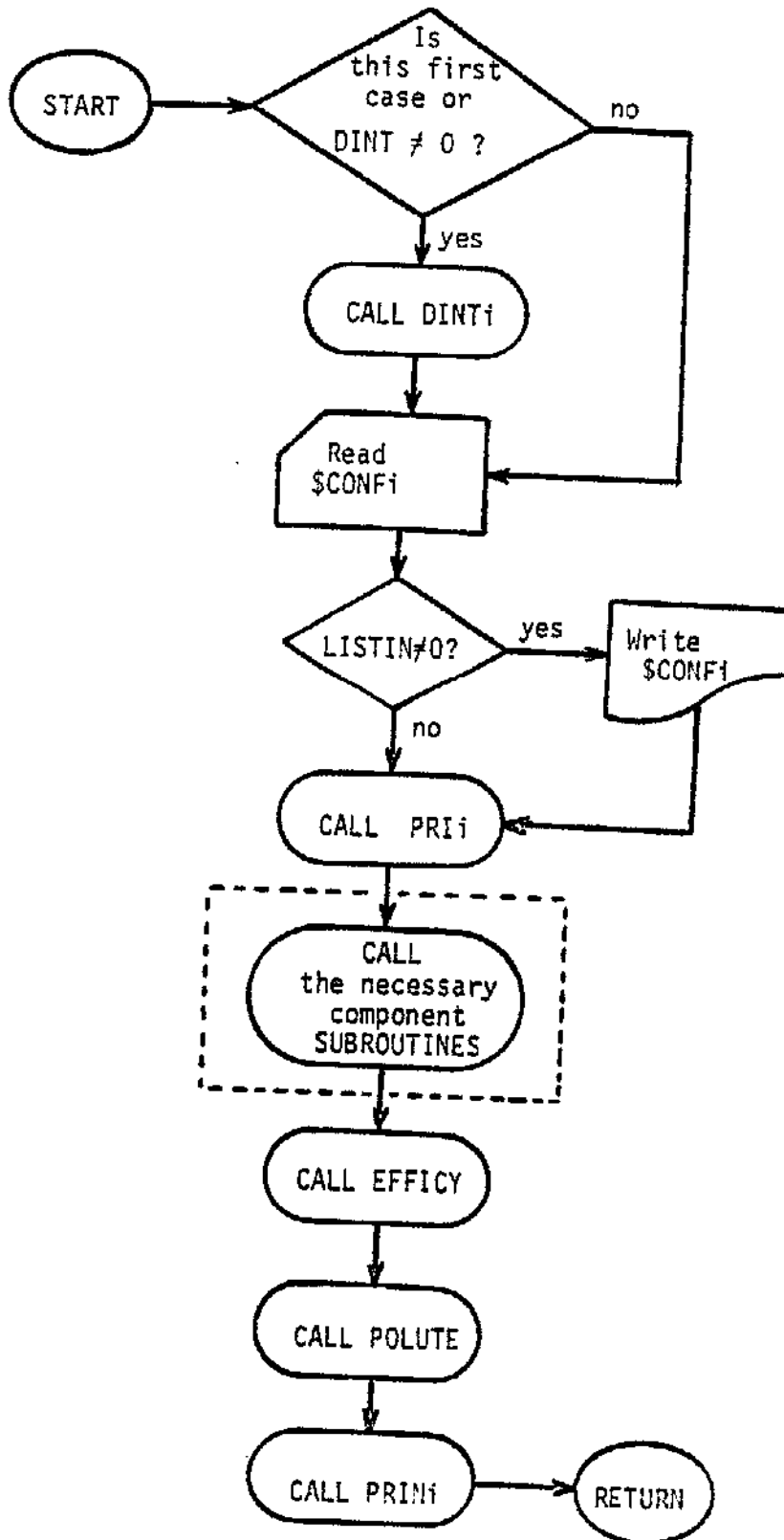


Figure 4.3-1 Simplified Flow Chart of Configuration Subroutines--CNFGi

CHAPTER 5

RESULTS

5.1 Introduction

In this chapter the computer program described in Chapter 4 is used to obtain the results which are needed to improve each basic configuration as well as to perform some parametric studies. It should be emphasized that the primary objective is to improve the performance of each integrated combined cycle within certain constraints. For example, the designs must meet federal gaseous emission criteria on SO_x and NO_x . Water and heat rejection requirements will be inherently determined from these analyses.

In Section 5.2, reasonable values are assigned to all specifiable cycle point parameters for the systems shown in Figures 2.3-1 to 2.3-4 followed by the calculation of the resulting station efficiency for each of these four base cases. The computer program, of course, provides this result as well as all other results to follow. Then in Section 5.3, the effect on station efficiency of adding regenerative feedwater heaters, gas-to-gas regenerators, and intercooled compressors to each configuration will be examined. As each effect is determined, a judgement will be made as to whether that particular addition remains in each cycle or not. Each configuration will subsequently be optimized in Section 5.4 by varying certain key cycle point parameters without consideration of the pollution criteria. Then in Section 5.5 each configuration will be reviewed to determine if the designs meet the criteria on gaseous effluents. Any of the configurations which will require modifications will be re-optimized. Following this, each optimized configuration will be summarized in Section 5.6 by way of presenting new cycle schematics and discussing the resulting

water and heat rejection requirements. Then in Section 5.7, a limited number of parametric studies will be presented. Finally in Section 5.8, some of the assumptions that have been made during the course of these analyses will be discussed.

It is important to note that the computer program was not written to provide an automatic optimization. The purpose of the program is to perform all the tedious calculations which are necessary to obtain the kind of results to be presented in this chapter. We shall soon see that a careful examination of the results printed in the computer output will enable us to make certain observations that may otherwise be overlooked. This approach is also helpful in trying to explain some of the sometimes surprising results to be presented shortly. For obvious reasons it is not possible to include the computer printout for every case which is analyzed; rather, only results which are germane to the discussion at hand or possibly a subsequent discussion will be presented, usually in tabular form.

5.2 Specification of Parameters and Calculation of Base Case Station Efficiencies

In Section 2.3 cycle component layouts for each of the four configurations were developed, with the resulting cycle schematics shown in Figures 2.3-1 to 2.3-4. In this section it is now necessary to assign values to each of the specifiable parameters for these cycles. While this may seem somewhat arbitrary, it is justified since many of these assigned values will be varied later during either the optimization or the parametric studies. The goal for now is simply to obtain four bases cases, one for each configuration, from which this study may begin. Let us first restrict our attention to

Configuration 1, the case of an adiabatic gasifier integrated with a waste heat combined cycle. For the other configurations, it will be necessary only to indicate the pertinent changes from the input to Configuration 1.

First, let us fix the coal and air compositions and the specific heat of the ash. Table 5.2-1 gives the ultimate analysis of the coal, which is

Table 5.2-1
Ultimate Analysis of Coal
(Weight Fraction)

Carbon	0.7304
Hydrogen	0.0528
Oxygen	0.0616
Nitrogen	0.0088
Sulfur	0.0264
Moisture	0.0300
Ash	0.0900

assumed to be Pennsylvania high volatile bituminous¹⁷, the composition of which has been adjusted for 3 percent moisture and 9 percent ash. Note that the weight fraction of *liquid* water is included in the ultimate analysis and recall that the Dulong approximation assumed that all the oxygen combines with the necessary hydrogen to form water *vapor*; this distinction is necessary when the enthalpy of the coal is later determined in the gasifier model. It should be noted that the ash will leave the gasifier at an elevated temperature representing a sensible heat loss and that most of the sulfur will be converted to hydrogen sulfide of which most is removed representing a chemical energy loss. The air composition is given in Table 5.2-2. Note that dry air is assumed for these and all remaining calculations. Raznjevic²⁴ gives the specific heat of ash as 0.19 Btu/lbm-°F, and in the interest of being slightly conservative

Let us use 0.20 Btu/lbm-°F. The effect of coal composition on the cycle performance of only Configuration 1 will be examined in Section 5.7 by using three other types of coal.

Table 5.2-2
Composition of Air
(Weight Fraction)

N ₂	0.7546
O ₂	0.2319
Ar	0.0135
H ₂ O(g)	0.0000

Next, it is convenient to specify all the pressure-related data including any assumed pressure drops. The gasifier is assumed to be operated at 11 atm, the combustor at 10 atm, the steam-side of the boiler at 1600 psia, and the condenser at 1.75 psia (or approximately 3.5 inches of mercury). Ambient pressure is taken to be 14.7 psia. The following pressure drops are assumed in the gas cycle portion: none through the gasifier and combustor, a 10 psi drop through the steam-side of the steam generator with a total of 0.7 psi through the gas-side, a 0.1 psi drop through the gas cooler, and a 0.1 psi drop through the gas cleanup system. Note that there is an implied pressure drop of more than 10 psi through the gas throttle valve, representing additional conservatism in the analysis. In the steam-cycle portion the following pressure drops are assumed: 0.0362, 0.2569, and 0.3974 psi through the gas-side of the superheater, evaporator, and economizer sections of the boiler, respectively (see Appendix B), and 10, 0, and 0.1 psi through the same sections on the steam-side; a 400 psi drop through the steam throttle valve; and none in the condenser.

Now the temperature-related input is specified. Ambient conditions are assumed for each air, coal, and water inlet to the system, with

ambient temperature taken to be 77°F. The gasifier is assumed to operate at 2000°F with the same ash discharge temperature. Superheated steam is assumed to enter the gasifier at 620°F. The gas is assumed to be cooled to 200°F by the gas cooler. The combustor is assumed to operate at 2000°F, the practical limit for a conventional land-based gas turbine. Superheated steam at a temperature of 960°F is generated in the boiler with 7°F of subcooling assumed at the evaporator inlet. The cooling water to the condenser is at 70°F and is assumed to undergo a 5°F temperature rise. Finally, the pinch point temperature differences within the steam generator and boiler is specified to be greater than or equal to 40°F.

The various efficiencies may now be assigned representative values. The following component efficiencies are assumed: 0.90 for the air compressors, 0.75 for the pump serving the steam generator, 0.85 for the gas turbine, 0.90 for the steam turbine, and 0.85 for the feedwater pump. According to Section 3.14, the capability exists to remove H₂S, COS, CO₂, and NH₃ from the power gas. It is conservatively assumed that only 90 percent by weight of the H₂S is removed; all the remaining gas is eventually burned in the combustor, since this would result in economical operation of the gas cleanup system. This completes the input specifications for Configuration 1.

In the other three configurations, the cycle point input is chosen deliberately to be identical to that of Configuration 1 where possible. This will enable us to make a more straightforward comparison of the results for the four base cases. In Configurations 2 and 4, the combustor exit temperature is no longer assumed to be 2000°F; instead combustion

with 10 percent excess air is required, since these configurations use a supercharged boiler. It is also assumed for these two configurations that the water which enters the evaporator section of the boiler is at least 7°F subcooled. Refer to Section 3.4 for a description of the subtle distinction between the models for the two different types of boilers. In Configurations 3 and 4, there is no air compressor serving the gasifier, and so the corresponding input conditions are no longer relevant. All other input for these configurations remains the same. One other point should be made. In Configuration 3, the heat source for the endothermic gasifier is the combustor, and both of these components operate at 2000°F which implies heat transfer through a zero temperature difference and an infinite heat transfer area. For now, let us accept this and reexamine this issue after the optimization is completed.

Recall that in Section 4.6, for the description of subroutine EFFICY, four different efficiencies were defined: the station, the combined cycle, the steam cycle, and the gasification efficiencies. In all of these, low heating values will be used consistently. Furthermore, let us agree to use the station efficiency to assess cycle performance. Included in this will be an assumed 10 percent station load, which includes station auxiliaries, lighting, generation losses, and so forth. Table 5.2-3 summarizes the resulting efficiencies for each configuration.

Table 5.2-3
Summary of Efficiencies for Base Cases

	Efficiency (%) of Configuration			
	1	2	3	4
Station	34.57	29.87	38.63	32.72
Combined Cycle	44.36	38.34	45.48	38.52
Steam Cycle	35.02	35.02	35.02	35.02
Gasification	86.58	86.58	94.38	94.38

By examining the station efficiencies, we note that the waste heat configurations perform better than those using a supercharged boiler, and that the configurations incorporating an endothermic gasifier perform better than those with an adiabatic gasifier. To help explain these trends, let us summarize from the computer output the flow, heat, and work quantities for each configuration as well as other pertinent miscellaneous information as shown in Table 5.2-4. It should be noted at this point that all flows, heat, and work quantities are always given with respect to a pound of coal. Furthermore, the lower heating value of the coal described earlier is 12747 Btu (per pound of coal). This provides a convenient reference value to which all work and heat quantities may be compared. For example, we see that approximately 20 percent of the heating value of the coal is thrown away in the gas cooler for Configurations 1 and 2, but only 5 percent for Configurations 3 and 4. For completeness, the lower heating values of the power gas are also given in this table. These values are qualitatively consistent with those obtained in Section 2.2, where coal gasification is first discussed.

Table 5.2-4
Summary of Miscellaneous Results for Base Cases

	Configuration			
	1	2	3	4
Flows (lbm)				
Gasifier				
Coal	1.000	1.000	1.000	1.000
Steam	0.022	0.022	0.997	0.997
Air	3.783	3.783	--	--
Dirty Gas	4.715	4.715	1.907	1.907
Ash	0.090	0.090	0.090	0.090

Table 5.2-4 (Continued)

	Configuration			
	1	2	3	4
Flows (lbm) (continued)				
Gas Cleanup				
Dirty Gas	4.715	4.715	1.907	1.907
Water	0.285	0.285	0.179	0.179
Clean Gas				
Waste	4.977	4.977	2.061	2.061
	0.023	0.023	0.025	0.025
Combustor				
Fuel	4.977	4.977	2.061	2.061
Air	19.845	6.732	23.764	10.887
Products	24.822	11.709	25.825	12.948
Boiler				
Gas-side	24.822	11.709	25.825	12.948
Steam-side	3.920	5.649	4.258	5.568
Net Work (Btu)				
Gas Cycle	3018	1525	3432	1967
Steam Cycle	1878	2706	2039	2667
Total	4896	4231	5471	4634
Low Heating Values				
Coal (Btu/lbm)	12747	12747	12747	12747
Gas (Btu/SCF)	135	135	288	288
Heat Transfer (Btu)				
To Gasifier from Combustor	0	0	5041	5041
To Steam Cycle	5362	7727	5823	7615
Gas Cycle Loss	4367	3495	3492	3165
From Steam Cycle	3484	5021	3784	4948
Excess Air to Combustor (%)	224	10	140	10
Combustor Exit Temp. (°F)	2000	3250	2000	3057
Stack Gas Temp. (°F)	324	263	319	423
Gas Cooler Heat Loss (Btu)	2606	2606	623	623
Minimum Temp. Differences (°F)				
Steam Generator	1380	1380	733	733
Boiler	40	140	40	300

Let us first restrict our attention to Configurations 1 and 2. From the flows given in Table 5.2-4 it may be seen that these two configurations basically differ in the amount of gas flow through the boilers. The reason for this, of course, is that the fuel is burned by design with a large amount of excess air for Configuration 1 compared to the specified 10 percent for Configuration 2. The net effect of this and the larger amount of heat transfer to the steam cycle for the supercharged boiler cases is to de-emphasize the gas cycle. Recall from Section 2.1 that an alternate expression for the combined cycle efficiency was given as

$$\eta_{cc} = 1 - \left(\frac{Q_L + Q_2}{Q_1} \right) + \frac{Q_2}{Q_1} \eta_2 \quad (2.1-10)$$

Actually calling η_{cc} the combined cycle efficiency is a misnomer here since it is convenient to interpret Q_1 as the heating value of the coal, not of the gas, actually resulting in an effective station efficiency without the usual 10 percent station load included. Note further that η_2 represents the steam cycle efficiency and Q_2 the amount of heat transferred to the steam cycle from the gas cycle. The sum of Q_L and Q_2 must be less than Q_1 in order to have work produced by the first cycle. Table 5.2-4 clearly shows that the sum of Q_L and Q_2 is higher for Configuration 2 compared to Configuration 1, while η_2 is identical. Note that Q_L is lower for Configuration 2 but Q_2 is much higher, resulting in lower performance for Configuration 2. The same line of reasoning applies to the comparison between Configurations 3 and 4. When Configuration 3 is compared to Configuration 1, it is seen that the former is superior primarily because of the much lower gas cycle heat loss which more than makes up for the higher heat transfer to the steam cycle. In Configuration 4, both the

heat loss and heat transfer to the steam cycle are lower than in Configuration 2 with both having the same steam cycle efficiency. Equation (2.1-10) clearly shows that the efficiency of Configuration 4 should be greater than that of Configuration 2. When all the above considerations are taken into account, Configuration 3 should be expected to have the best performance and does.

Let us briefly discuss some of the other efficiencies shown in Table 5.2-3. Note that the gasification efficiencies for the same gasifier type are identical, and that those for the endothermic configurations are higher than those for the adiabatic. We must be cautious, however, and not read too much into this. If the latent heat of vaporization of the steam required by the gasification process were included in the denominator of the definition of the gasification efficiency, then all such efficiencies would have practically the same value. This is of no real concern since the station efficiency is independent of the definition of gasification efficiency. Note that the combined cycle efficiencies, as they have been defined, are significantly higher than the station efficiencies, since the later include gasification system losses and the assumed 10 percent station load. Also, as has been already noted, the steam cycle efficiency is identical for all four configurations, since the steam cycle operating conditions are identical. For completeness, let us define gas cycle efficiency as the ratio of the net work produced by the gas cycle including the gasification system to the heating value of the gaseous fuel, in consistent units of course. For Configurations 1 to 4 respectively, these are 27.35, 13.83, 28.52, and 16.35 percent. It is seen that the

gas cycle in the configurations employing a supercharged boiler is definitely de-emphasized. The result, as we have seen, has been poorer performance for these configurations. Clearly by increasing the work produced in the gas cycle compared to that of the steam cycle, better performance can be expected.

Let us verify that the minimum temperature differences within the steam generator and boilers are equal to or greater than the specified minimum of 40°F. Table 5.2-4 shows that this condition is easily met in the steam generator for each configuration. This clearly shows that there is sufficient sensible heat in the power gas to raise the required amount of steam needed for the gasification process. Since endothermic gasification requires more steam, the minimum temperature difference is lower for Configurations 3 and 4 compared to Configurations 1 and 2. The minimum temperature difference within the waste heat boilers of Configurations 1 and 3 is seen to be exactly 40°F, but must be greater than this in the supercharged boilers to ensure the presence of subcooled water in the economizer section. In Figures 5.2-1 and 5.2-2, the T-Q diagrams are shown for the boilers of Configurations 1 and 2, respectively. These temperatures are representative of each type of boiler. Note that the heat transfer within each boiler section is also given on each figure. Note also the locations of the pinch points. In Chapter 3 it was claimed that the pinch point for the supercharged boiler must occur between the economizer and stack. This is indeed the case here. Finally note the much larger temperature clearance throughout the supercharged boiler compared to the waste heat boiler; this results in greater irreversibilities