

Rewriting in a more suitable form gives

$$\Delta G_{f, \text{CH}_4}^{\circ} - 2\Delta G_{f, \text{H}_2}^{\circ} = -RT_e \ln[(y_{\text{CH}_4} P)/(y_{\text{H}_2} P)^2]$$

But the change in Gibbs free energy for the reaction is given by

$$\Delta G = \Delta G_{f, \text{CH}_4}^{\circ} - 2\Delta G_{f, \text{H}_2}^{\circ}$$

and the definition of K_p is given by

$$\ln K_p = -\Delta G/RT_e$$

and so we get

$$K_p = \frac{(y_{\text{CH}_4} P)}{(y_{\text{H}_2} P)^2}$$

which is precisely the expression for K_p given by Equation (3.2-14). If all the λ 's were eliminated in Equations (3.2-16) to 3.2-24) and the definition of K_p were used, we would get the conventional equilibrium equations of the form of Equations (3.2-14). Clearly the two methods are completely equivalent.

As we have discussed earlier, the effective enthalpy of the coal is obtained by using the Dulong approximation to give the coal composition in terms of fixed carbon (C), hydrogen (H_2), water vapor (H_2O), nitrogen (N_2), and sulfur (S_2). The weight fraction of liquid water and ash in the coal remains unchanged. Let ω_{df} be the weight fraction of species i

in the coal after application of the Dulong approximation, where i takes on values 1 to 7 as shown in Table 3.2-5. Similarly, let v_{di} be the molecular weight of species i , where i again is defined by Table 3.2-5.

Table 3.2-5
Meaning of the Subscripts Applied to Coal after
Application of Dulong Approximation

Subscript (d_i)	Species
d1	C
d2	H ₂
d3	H ₂ O(g)
d4	N ₂
d5	S ₂
d6	H ₂ O(l)
d7	Ash

The first law of thermodynamics may now be written for the gasifier:

$$h_{afc}(T_c, P_c) + c_{p_{ash}} \omega_{d7}(T_c - T_{ref}) + w_a \bar{h}_a(T_a, P_a) / v_a + Q_{gas} + w_s h_s \\ = N_g \bar{h}_g(T_g, P_g) + c_{p_{ash}} \omega_{d7}(T_{ash} - T_{ref}) \quad (3.2-25)$$

where the subscripts are defined as follows: 'afc' denotes ash-free coal, 'a' air, 'c' coal with ash, and 'g' gasifier outlet gas. The enthalpy of the ash-free coal (based on a unit mass of coal with ash) at temperature T_c and pressure P_c is denoted by $h_{afc}(T_c, P_c)$, and the heat added to the gasification process per unit mass of coal is Q_{gas} , while $\bar{h}_a(T_a, P_a)$ and $\bar{h}_g(T_g, P_g)$ are the enthalpy per mole (or molar enthalpy) of air and product gas, respectively, at the indicated temperatures (T) and pressures (P). Finally $c_{p_{ash}}$ is the specific heat of the ash (assumed to be constant), T_{ash} is the ash discharge

temperature, and T_{ref} is an arbitrary reference temperature which cancels out of the final form of the energy equation.

The enthalpy of the ash free coal, h_{afc} , per unit mass of coal is given by

$$h_{afc}(T_c, P_c) = \sum_{i=1}^8 (w_{di}/v_{di}) \bar{h}_{di}(T_c, \mu_{di} P_c)$$

where \bar{h}_{di} is the molar enthalpy of species i at a specified temperature T_c and pressure P_c and μ_{di} is the mole fraction of species i based on the Dulong approximation. It is tacitly implied by the nomenclature $\bar{h}_g(T_g, P_g)$ and $\bar{h}_a(T_a, P_a)$ that the composition of the gas indicated by the subscript is an argument of the enthalpy function. For conciseness, we do not write this explicitly. The enthalpy of the air, h_a , per unit mass of air is given by

$$h_a(T_a, P_a) = \sum_{i=1}^4 (w_{ai}/v_{ai}) \bar{h}_{ai}(T_a, \mu_{ai} P_a)$$

where μ_{ai} is the mole fraction of species i for the air. On a basis of a unit mass of coal, the enthalpy of the air is $w_a h_a$, since there are w_a unit masses of air per unit mass of coal. Similarly, the enthalpy of the steam used in the gasification process is simply $w_s h_s(P_s, T_s)$ where h_s is specific enthalpy of steam and w_s is the mass of steam required per unit mass of coal. Clearly, the subscript 's' denotes that the fluid is steam or water. Finally, the enthalpy of the gaseous products per unit mass of coal is given by

$$N_g \bar{h}_g(T_g, P_g) = \sum_{i=1}^{10} n_{gi} \bar{h}_{gi}(T_g, \mu_{gi} P_g)$$

where μ_{gi} is the mole fraction of species i for the power gas. Again note that the enthalpy has an implied mole fraction dependency. It should be noted that when a summation occurs, one should use the appropriate table to get the correspondence between subscripts c_i , a_i , g_i , and d_i and the corresponding species. Before substituting all these expressions into Equation 3.2-25, let us divide it first by N_g since again we prefer to work with mole fractions instead of mole numbers. The final form of the energy equation for the gasifier then becomes:

$$\left\{ \begin{aligned} & \sum_{i=1}^6 (w_{di}/v_{di}) \bar{h}_{di}(T_c, \mu_{di} P_c) + c_{p_{ash}} w_{d7} (T_c - T_{ash}) + w_s h_s(T_s, P_s) \\ & + w_a \sum_{i=1}^4 (w_{ai}/v_{ai}) \bar{h}_{ai}(T_a, \mu_{ai} P_a) \\ & + Q_{gas} \end{aligned} \right\} \left[(w_{c1}/v_{c1}) (y_{g2} + y_{g3} + y_{g5} + y_{g9}) \right] \quad (3.2-26) \\
 = \sum_{i=1}^{10} y_{gi} \bar{h}_{gi}(T_g, y_{gi} P_g)$$

In this equation, the y_{gi} are unknown along with w_a and w_s . All other parameters are either specified in the input to this model or are calculated directly from the input.

We have thus identified sixteen equations which we may use to solve for the sixteen unknowns. We complete the model by noting that the mass flow of the product gas w_g per unit mass flow of coal is given by

$$w_g = 1 + w_a + w_s - w_{c7}$$

and it is a trivial matter to get the corresponding mole flows. Finally, the higher and lower heating values of the power gas can be computed since

we know the gas composition, after we solve for the y_{gi} 's. We get conservatively low estimates for the heating values by assuming only H_2 , CO , and CH_4 contribute to the heating values of the power gas.

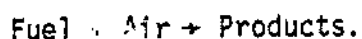
In summarizing, we have identified sixteen unknown parameters: the ten mole fractions, the four Lagrange multipliers (which have no obvious physical significance), the steam flow, and the air flow. Fortunately sixteen equations in these same variables have also been identified: six mass balances, nine equilibrium equations, and the energy equation. The method of solution is presented in Section 3.2.2

Now we can readily see why the endothermic gasifier model is a special case of the one above. We have already agreed that for endothermic gasification, we want to gasify the coal with steam only; that is, the air flow, w_a , is zero. Setting w_a equal to zero in the six mass balance equations and nine equilibrium equations and solving the resulting system of fifteen equations gives values to the fifteen unknowns. The energy equation is then solved for the amount of heat, Q_{gas} , needed to allow gasification of coal without any air. Again the method of solution given in Section 3.2.2 easily accommodates this mode of gasifier operation.

Before leaving this model, a subtle point should be made with regard to the temperature T_e used in the nine equilibrium equations and the temperature T_g used in the energy equation. While these should be equal to be consistent with our assumption of thermodynamic equilibrium, the provision has been made to allow for them to be different. This was done to allow for the possibility of "freezing" the reactions at a certain temperature which is sometimes done or implied in the literature.

3.2.1.1 Combustor Model

In the combustor model, we must have provisions for two different modes of operation. One mode allows the combustor outlet temperature to be specified and the other allows the excess air to be specified. These parameters will become apparent in the development of the combustor model. The method of solution for each of these modes is presented in Section 3.2.2. The basic reaction for the combustor is



We normalize the calculation by assuming a mole of gaseous fuel, not a unit mass of fuel as was the case in the gasifier model.

Let us assume that the composition of the gaseous fuel by mole fraction μ_{ff} is specified along with its pressure P_f and temperature T_f . Again Table 3.2-3 must be used to correlate the subscript f with a particular chemical species. Let us further assume that the air composition by weight fraction w_{ai} is specified, where Table 3.2-2 provides the meaning of the subscript ai . This composition by weight fraction can easily be converted to one by mole fraction μ_{ai} where again Table 3.2-2 is applicable. Let us also assume the pressure P_a and temperature T_a of the air entering the combustor are specified. Denoting the number of moles of stoichiometric air per mole of fuel as β and the excess air fraction as ξ , the number of moles of air per mole of fuel becomes $\beta(1+\xi)$. Finally, let n_{pi} be the number of moles of species i in the product gas per mole of fuel, where species i is identified in Table 3.2-6. From this table, we see that the following species are assumed to be present in the product gas: carbon dioxide (CO_2), water vapor (H_2O), nitrogen (N_2), oxygen (O_2), argon (Ar),

nitric oxide (NO), carbon monoxide (CO), monatomic hydrogen (H), monatomic oxygen (O), hydroxyl (OH), hydrogen (H₂), nitrogen dioxide (NO₂), sulfur monoxide (SO), sulfur dioxide (SO₂), and sulfur trioxide (SO₃).

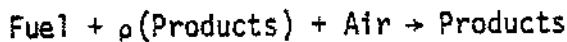
Table 3.2-6
Meaning of Subscripts Applied to Products
of Combustion

Subscript (p _i)	Species in Gas
p1	CO ₂
p2	H ₂ O(g)
p3	N ₂
p4	O ₂
p5	Ar
p6	NO
p7	CO
p8	H
p9	O
p10	OH
p11	H ₂
p12	NO ₂
p13	SO
p14	SO ₂
p15	SO ₃

Let the pressure of the product gas be P_p , which is presumably specified, and the temperature be T_p , which may be either an unknown or is assumed to be specified. We will eventually get an expression for β which will depend on known parameters, and ϵ is either an unknown (T_p must be specified) or is specified (T_p is then one of the unknowns).

Because it is shown in Section 5.5, that a nitric oxide (NO) emission problem exists for the waste heat combined cycle configurations, flue gas recirculation is used as a means to reduce the amount of NO which goes up the stack and into the atmosphere. In other words, a

certain fraction, ρ , of the flue gas at near atmospheric pressure is compressed, cooled to a specific temperature, T_r , and fed into the combustor at pressure P_r . The combustor model then must include a provision for flue gas recirculation. With this modification, the basic reaction in the combustor becomes



and we are now in a position to develop the mass balance equations.

First, we do a mass balance on carbon (C). By referring to Table 3.2-2 for the species in the air, Table 3.2-3 for the species in the fuel, and Table 3.2-6 for the species in the product gas, the first mass balance on carbon becomes

$$\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9} + \rho n_{p_1} + \rho n_{p_7} = n_{p_1} + n_{p_7}$$

or

$$\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9} = (1-\rho)(n_{p_1} + n_{p_7}) \quad (3.2-27)$$

Similarly, a mass balance on H, O, N, S, and Ar gives the following five relationships

$$2\mu_{f_1} + 4\mu_{f_3} + 2\mu_{f_4} + 2\mu_{f_8} + 3\mu_{f_{10}} + 2\beta(1+\epsilon)\mu_{a_4} = (1-\rho)(2n_{p_2} + n_{p_8} + n_{p_{10}} + 2n_{p_{11}}), \quad (3.2-28)$$

$$\begin{aligned} \mu_{f_2} + \mu_{f_4} + 2\mu_{f_5} + \mu_{f_9} + (2\mu_{a_2} + \mu_{a_4})(1+\epsilon)\beta = \\ = (1-\rho)(2n_{p_1} + n_{p_2} + 2n_{p_4} + n_{p_6} + n_{p_7} + n_{p_9} \\ + n_{p_{10}} + 2n_{p_{12}} + n_{p_{13}} + 2n_{p_{14}} + 3n_{p_{15}}), \end{aligned} \quad (3.2-29)$$

$$2\mu_{f_6} + \mu_{f_{10}} + 2\beta(1+\xi)\mu_{a_1} = (1-\rho)(2n_{p_3} + n_{p_6} + n_{p_{12}}), \quad (3.2-30)$$

$$\mu_{f_8} + \mu_{f_9} = (1-\rho)(n_{p_{13}} + n_{p_{14}} + n_{p_{15}}), \quad (3.2-31)$$

and

$$\mu_{f_7} + \beta(1+\xi)\mu_{a_3} = (1-\rho)(n_{p_5}), \quad (3.2-32)$$

respectively.

Again we prefer to work with mole fractions, y_{pi} , instead of mole numbers, n_{pi} . Dividing Equation (3.2-27) by N_c , where

$$N_c = \sum_{i=1}^{15} n_{pi},$$

and solving the resulting equation for N_c gives

$$N_c = \frac{\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9}}{(1-\rho)(y_{p_1} + y_{p_7})} \quad (3.2-33)$$

where $y_{pi} = n_{pi}/N_c$ has been used. Now dividing each of the remaining mass balance equations (3.2-28 to 3.2-32) by N_c and using $y_{pi} = n_{pi}/N_c$ gives the following relations where the factor $(1-\rho)$ has been divided from both sides and, therefore, no longer appears in the mass balances

$$\begin{aligned} & \left[2\mu_{f_1} + 4\mu_{f_3} + 2\mu_{f_4} + 2\mu_{f_8} + 3\mu_{f_{10}} + 2\beta(1+\xi)\mu_{a_4} \right] \left\{ \frac{y_{p_1} + y_{p_7}}{\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9}} \right\} \\ & = 2y_{p_2} + y_{p_3} + y_{p_{10}} + 2y_{p_{11}} \end{aligned} \quad (3.2-34)$$

$$\begin{aligned} & \left[\mu_{f_2} + \mu_{f_4} + 2\mu_{f_5} + \mu_{f_9} + (2\mu_{a_2} + \mu_{a_4})(1+\xi)\beta \right] \left\{ \frac{y_{p_1} + y_{p_7}}{\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9}} \right\} \\ & = 2y_{p_1} + y_{p_2} + 2y_{p_4} + y_{p_6} + y_{p_7} + y_{p_9} \\ & \quad + y_{p_{10}} + 2y_{p_{12}} + y_{p_{13}} + 2y_{p_{14}} + 3y_{p_{15}} \end{aligned} \quad (3.2-35)$$

$$\left[2\mu_{f_6} + \mu_{f_{10}} + 2\beta(1+\xi)\mu_{a_1} \right] \left\{ \frac{y_{p_1} + y_{p_7}}{\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9}} \right\} = 2y_{p_3} + y_{p_6} + y_{p_{12}} \quad (3.2-36)$$

$$\left[\mu_{f_8} + \mu_{f_9} \right] \left\{ \frac{y_{p_1} + y_{p_7}}{\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9}} \right\} = y_{p_{13}} + y_{p_{14}} + y_{p_{15}} \quad (3.2-37)$$

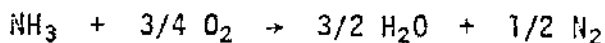
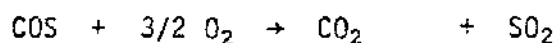
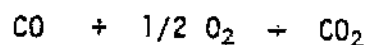
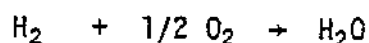
$$\left[\mu_{f_7} + \beta(1+\xi)\mu_{a_3} \right] \left\{ \frac{y_{p_1} + y_{p_7}}{\mu_{f_2} + \mu_{f_3} + \mu_{f_5} + \mu_{f_9}} \right\} = y_{p_5} \quad (3.2-38)$$

Like the gasifier model, the sixth equation is provided by the fact that the sum of the mole fractions must be unity:

$$\sum_{i=1}^{15} y_{p_i} = 1 \quad (3.2-39)$$

It is important to remember that it is the y_{p_i} and possibly ξ that are the unknowns in the last six equations. An expression for β , the number of moles of stoichiometric air per mole of fuel, may now be developed.

The following species, present in the gaseous fuel, are capable of combustion with the oxygen in the air: hydrogen (H_2), carbon monoxide (CO), methane (CH_4), hydrogen sulfide (H_2S), carbonyl sulfide (COS), and ammonia (NH_3). The number of moles of oxygen (O_2) required for complete combustion of each of the above constituents is easily determined from the following balanced chemical equations:

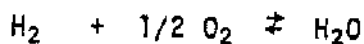
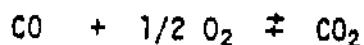


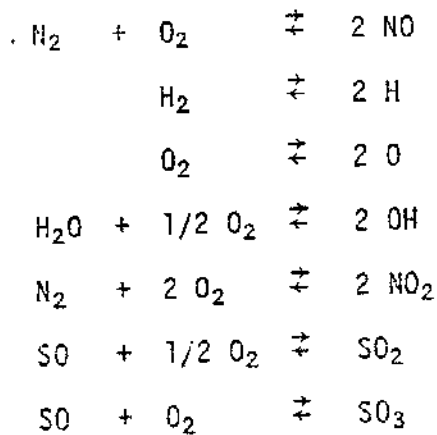
From the first reaction, we see that $1/2$ mole of O_2 is required for each mole of H_2 , but there are μ_{f_1} moles of H_2 per mole of fuel, so there are $1/2 \mu_{f_1}$ moles of O_2 required per mole of fuel due to the H_2 only. A similar line of reasoning results in the following O_2 requirements in moles of O_2 per mole of fuel: $1/2\mu_{f_2}$ due to the CO, $2\mu_{f_3}$ due to the CH_4 , $3/2\mu_{f_8}$ due to the H_2S , $3/2\mu_{f_9}$ due to the COS, and $3/4\mu_{f_{10}}$ due to the NH_3 . The total oxygen requirement is clearly the sum of these. But there are μ_{a_2} moles of O_2 per mole of air, so

$$\beta = \frac{1/2\mu_{f_1} + 1/2\mu_{f_2} + 2\mu_{f_3} + 3/2\mu_{f_8} + 3/2\mu_{f_9} + 3/4\mu_{f_{10}}}{\mu_{a_2}} \quad (3.2-40)$$

which is the theoretical air requirement in moles of air per mole of fuel. Clearly, the number of moles of air per mole of fuel actually used depends on the excess air fraction ξ and is equal to $\beta(1+\xi)$. This fact has been used in the derivation of the mass balance equations. Note that in Equation (3.2-40) since all the parameters on the right-hand side are known, β can be readily calculated.

Before writing the equilibrium equations, nine independent reactions among the gaseous species may be identified. One should clearly understand, however, that identification of these reactions is *not* necessary to the Lagrange multiplier approach. One possible set of reactions is as follows:





Now the equilibrium equations may be written using Equation (3.2-15) applied to the combustor product gas (after changing T_e to T_p and dividing by RT_p). The a_{ik} matrix is given in Table 3.2-7. The subscript i on the

Table 3.2-7
Assignment of Values to the a_{ik}
for the Combustor Model

Species	i	Element (k)				
		C(1)	H(2)	O(3)	N(4)	S(5)
CO ₂	1	1	0	2	0	0
H ₂ O	2	0	2	1	0	0
N ₂	3	0	0	0	2	0
O ₂	4	0	0	2	0	0
Ar	5	0	0	0	0	0
NO	6	0	0	1	1	0
CO	7	1	0	1	0	0
H	8	0	1	0	0	0
O	9	0	0	1	0	0
OH	10	0	1	1	0	0
H ₂	11	0	2	0	0	0
NO ₂	12	0	0	2	1	0
SO	13	0	0	1	0	1
SO ₂	14	0	0	2	0	1
SO ₃	15	0	0	3	0	1

y_{pi} now correspond, of course, to those in Tables 3.2-6 or 3.2-7. The following equilibrium equations are to be satisfied:

$$\Delta G_{f_{CO_2}^o}^o(T_p)/RT_p + \ln(y_{p1} \hat{\phi}_{p1} P_p) + \lambda_C/RT_p + 2\lambda_O/RT_p = 0 \quad (3.2-41)$$

$$\Delta G_{f_{H_2O}^o}^o(T_p)/RT_p + \ln(y_{p2} \hat{\phi}_{p2} P_p) + 2\lambda_H/RT_p + \lambda_O/RT_p = 0 \quad (3.2-42)$$

$$\Delta G_{f_{N_2}^o}^o(T_p)/RT_p + \ln(y_{p3} \hat{\phi}_{p3} P_p) + 2\lambda_N/RT_p = 0 \quad (3.2-43)$$

$$\Delta G_{f_{O_2}^o}^o(T_p)/RT_p + \ln(y_{p4} \hat{\phi}_{p4} P_p) + 2\lambda_O/RT_p = 0 \quad (3.2-44)$$

$$\Delta G_{f_{NO}^o}^o(T_p)/RT_p + \ln(y_{p6} \hat{\phi}_{p6} P_p) + \lambda_O/RT_p + \lambda_N/RT_p = 0 \quad (3.2-45)$$

$$\Delta G_{f_{CO}^o}^o(T_p)/RT_p + \ln(y_{p7} \hat{\phi}_{p7} P_p) + \lambda_C/RT_p + \lambda_O/RT_p = 0 \quad (3.2-46)$$

$$\Delta G_{f_H}^o(T_p)/RT_p + \ln(y_{p8} \hat{\phi}_{p8} P_p) + \lambda_H/RT_p = 0 \quad (3.2-47)$$

$$\Delta G_{f_O}^o(T_p)/RT_p + \ln(y_{p9} \hat{\phi}_{p9} P_p) + \lambda_O/RT_p = 0 \quad (3.2-48)$$

$$\Delta G_{f_{OH}^o}^o(T_p)/RT_p + \ln(y_{p10} \hat{\phi}_{p10} P_p) + \lambda_H/RT_p + \lambda_O/RT_p = 0 \quad (3.2-49)$$

$$\Delta G_{f_{H_2}^o}^o(T_p)/RT_p + \ln(y_{p11} \hat{\phi}_{p11} P_p) + 2\lambda_H/RT_p = 0 \quad (3.2-50)$$

$$\Delta G_{f_{NO_2}^o}^o(T_p)/RT_p + \ln(y_{p12} \hat{\phi}_{p12} P_p) + 2\lambda_O/RT_p + \lambda_N/RT_p = 0 \quad (3.2-51)$$

$$\Delta G_{f_{SO}^o}^o(T_p)/RT_p + \ln(y_{p13} \hat{\phi}_{p13} P_p) + \lambda_O/RT_p + \lambda_S/RT_p = 0 \quad (3.2-52)$$

$$\Delta G_{f_{SO_2}^o}^o(T_p)/RT_p + \ln(y_{p14} \hat{\phi}_{p14} P_p) + 2\lambda_O/RT_p + \lambda_S/RT_p = 0 \quad (3.2-53)$$

$$\Delta G_{f,SO_3}^{\circ}(T_p)/RT_p + \ln(y_{P15} \hat{\phi}_{P15} P/P) + 3\lambda_0/RT_p + \lambda_5/RT_p = 0 \quad (3.2-54)$$

Note that for the combustor model, λ_c is not necessarily zero and that, as was the case with the gasifier model, no equilibrium equation is written for argon, since it is inert.

The total number of equations for the combustor model is now twenty: six mass balances and fourteen equilibrium equations. But there are now twenty-one unknowns: the fifteen mole fractions, the five Lagrange multipliers, and either the excess air fraction ξ or the combustor outlet temperature T_p . Again, the energy equation provides the final necessary relationship to completely define the model.

The first law of thermodynamics for the combustor may be written as

$$\bar{h}_f(T_f, P_f) + \beta(1+\xi)\bar{h}_a(T_a, P_a) + \rho N_c \bar{h}_p(T_r, P_r) + Q_{cmb} = N_c \bar{h}_p(T_p, P_p) \quad (3.2-55)$$

where the subscript "f" corresponds to the fuel, "a" to the air, "r" to the flue gas recirculation inlet flow, and "p" to the products of combustion. The variable $\bar{h}(T,P)$ has the same meaning as in Section 3.2.1.1, and Q_{cmb} is heat added to the combustion process per mole of fuel (if heat is removed, Q_{cmb} is negative). All other variables have previously been defined. Again it is tacitly implied by the nomenclature, $\bar{h}(T,P)$, that the composition of the gas is also part of the argument since the partial pressure is really the pressure for which \bar{h} is to be evaluated and the partial pressure of species i in a gaseous mixture is given by $\mu_i P$.

Since the composition of the fuel is specified by the mole fractions, μ_{fi} , the enthalpy of the fuel per mole of fuel is simply

$$\bar{h}_f(T_f, P_f) = \sum_{i=1}^{10} \mu_{fi} \bar{h}_{fi}(T_f, \mu_{fi} P_f) \quad (3.2-56)$$

where i denotes the particular species shown in Table 3.2-3 with f_i replacing g_i . The enthalpy of the incoming air is similarly written

$$\beta(1+\xi) \bar{h}_a(T_a, P_a) = \beta(1+\xi) \sum_{i=1}^4 \mu_{ai} \bar{h}_{ai}(T_a, \mu_{ai} P_a). \quad (3.2-57)$$

For the product gas at T_r and P_r ,

$$\bar{h}_p(T_r, P_r) = \sum_{i=1}^{15} y_{pi} \bar{h}_{pi}(T_r, y_{pi} P_r) \quad (3.2-58)$$

and at T_p and P_p ,

$$\bar{h}_p(T_p, P_p) = \sum_{i=1}^{15} y_{pi} \bar{h}_{pi}(T_p, y_{pi} P_p). \quad (3.2-59)$$

It is to be understood that the partial pressure arguments above are to be deleted for those species which are assumed to be ideal gases (all but H_2O , CH_4 , and CO_2). Using the expression for N_c from Equation (3.2-33), and Equations (3.2-56) to (3.2-59), Equation (3.2-55) becomes

$$\left\{ \frac{(1-p)(y_{p1} + y_{p7})}{(\mu_{f2} + \mu_{f3} + \mu_{f5} + \mu_{f9})} \right\} \left\{ \sum_{i=1}^{10} \mu_{fi} \bar{h}_{fi}(T_f, \mu_{fi} P_f) + \beta(1+\xi) \sum_{i=1}^4 \mu_{ai} \bar{h}_{ai}(T_a, \mu_{ai} P_a) + Q_{cmb} \right\} = \sum_{i=1}^{15} y_{pi} \bar{h}_{pi}(T_p, y_{pi} P_p) - p \sum_{i=1}^{15} y_{pi} \bar{h}_{pi}(T_r, y_{pi} P_r) \quad (3.2-60)$$

This is the final form of the energy equation for the combustor. In this model, unlike the gasifier model, the temperature used in the equilibrium equations is the same as that of the product gas leaving the combustor. "Freezing" of the NO producing reaction is handled in a simpler way and is explained in Section 4.6. Equation (3.2-60) provides the twenty-first equation thus enabling a unique solution for the twenty-one unknowns.

Three important points should be made with respect to the flue gas recirculation. The first is that the flue gas recirculation parameter p appears only in the energy equation, since we elected to work in terms of mole fractions instead of mole numbers. Secondly, when no recirculation is assumed, Equation (3.2-60) reduces to the correct form of the first law of thermodynamics for a combustor without recirculation; that is, the enthalpy of the fuel, plus that of the air, plus the heat added must equal the enthalpy of the product gas. Finally, if the temperature of the recirculation gas T_r equals the combustor exit temperature T_p (and $P_r = P_p$), then a factor of $(1-p)$ may be divided from both sides of Equation (3.2-60) and the benefit associated with flue gas recirculation in reducing NO effluents is lost. We shall see in Chapter 5 how this affects the power plant efficiency.

We have identified twenty-one equations which we may use to solve for the twenty-one unknowns. We complete the model by noting that the mass flow of air w_a into the combustor (per unit mass of coal into the gasifier) is given by

$$w_a = \beta(1+\xi)v_a w_f / v_f$$

where v_a and v_f are the molecular weights of the air and fuel respectively and w_f is mass flow of fuel (per unit mass of coal). A mass balance on the entire combustor gives

$$w_f + w_a + \rho w_p = w_p$$

where w_p is the mass flow of product gas from the combustor (per unit mass of coal). The last equation may be solved for w_p as

$$w_p = \frac{w_f + w_a}{1 - \rho} .$$

This completes the combustor model. In the next section, we shall see how a solution to these systems of non-linear equations for the gasifier and combustor model can be obtained.

3.2.2 Method of Solution

As we have seen, a system of non-linear algebraic equations results when the steady-state thermodynamic models for the gasifier and combustor are developed. One method of solution is brute force. Osterle, Impink, and Lipner¹⁷ have succeeded in reducing the gasifier equations to two equations in two unknowns (with no COS or NH₃ assumed to be present in the power gas). The resulting equations, although complicated, are solved using a search routine. The chief disadvantage of this approach arises when one wants to add more species to the model or otherwise change the model, since the algebraic exercise must be repeated. An approach which can easily accommodate changes in the model was sought.

A multi-dimensional Newton-Raphson iterative method of solution provides such a solution. The system of equations can be "stored" in a computer subroutine practically in the form in which we wrote them. Changing the model means changing the affected equations and not redoing the algebra. Also, as we shall see, it is a trivial matter to accommodate the two gasifier modes and the two combustor modes. The general method will be developed with its application to the two mathematical models then indicated.

Consider a system of n general non-linear algebraic equations of the form

$$f_1(x_1, x_2, \dots, x_n) = 0$$

$$f_2(x_1, x_2, \dots, x_n) = 0$$

$$f_n(x_1, x_2, \dots, x_n) = 0$$

where the x_j are the unknowns and the usual functional notation is employed. This may be represented more concisely as

$$\vec{f}(\vec{x}) = \vec{0} \tag{3.2-61}$$

where vector notation is now indicated by the overscript ($\vec{}$). A more general form of Taylor's Theorem may be applied to the left-hand side of Equation (3.2-61) to give

$$\vec{f}(\vec{x} + \Delta\vec{x}) = \vec{f}(\vec{x}) + [\nabla\vec{f}(\vec{x})]\Delta\vec{x} \tag{3.2-62}$$

where the gradient of the vector $\vec{f}(\vec{x})$ is indicated by $\nabla\vec{f}(\vec{x})$ and $\Delta\vec{x}$ is an incremental change in the vector \vec{x} . Now let us associate the k -th set

of values for the vector \vec{x} by \vec{x}_k ; that is, the k-th iteration. For this particular iteration, $\Delta\vec{x}_k = \vec{x}_{k+1} - \vec{x}_k$ and Equation (3.2-62) becomes

$$\vec{f}(\vec{x}_{k+1}) = \vec{f}(\vec{x}_k) + [\nabla\vec{f}(\vec{x}_k)](\vec{x}_{k+1} - \vec{x}_k). \quad (3.2-63)$$

But we would like the k+1-th set of values for \vec{x} to be close to the solution if convergence is to take place or $\vec{f}(\vec{x}_{k+1}) = \vec{0}$. Indeed let us force $\vec{f}(\vec{x}_{k+1})$ to be zero and see if the resulting condition is capable of converging to the solution. So, solving Equation (3.2-63) for \vec{x}_{k+1} after setting $\vec{f}(\vec{x}_{k+1})$ equal to zero gives

$$\vec{x}_{k+1} = \vec{x}_k - [\nabla\vec{f}(\vec{x}_k)]^{-1} \vec{f}(\vec{x}_k) \quad (3.2-64)$$

where the inverse of the gradient matrix is indicated. Note that if $\vec{f}(\vec{x}_k) = \vec{0}$ (that is, the \vec{x}_k are a solution), then $\vec{x}_{k+1} = \vec{x}_k$ as it should. We see that the correction vector $\Delta\vec{x}_k$ to the previous iteration (\vec{x}_k) is

$$\Delta\vec{x}_k = -[\nabla\vec{f}(\vec{x}_k)]^{-1} \vec{f}(\vec{x}_k). \quad (3.2-65)$$

The meaning of $\nabla\vec{f}(\vec{x}_k)$ is evident from the following matrix representation

$$\nabla\vec{f}(\vec{x}_k) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & & & \frac{\partial f_2}{\partial x_n} \\ \cdot & & & \\ \cdot & & & \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & & \frac{\partial f_n}{\partial x_n} \end{pmatrix}$$

where each entry is to be evaluated for values of \vec{x} at the k-th iteration. However, since the computer will be used to get a solution, this gradient

matrix may be approximated to a high degree of accuracy by using a central difference approximation to each partial derivative indicated. This eliminates the need to provide the computer with these partial derivatives. In fact, it is impossible to generate explicit formulas for some of the derivatives anyway; for example, the mole fraction of water vapor appears as an argument in the enthalpy function.

One more point should be made regarding Equations (3.2-64) and (3.2-65) before we apply this method to our two mathematical models. During the implementation of this scheme, it often happened that the next value for a particular unknown would become negative. This is disastrous if the unknown happens to be a mole fraction, since we must take the natural logarithm in the equilibrium equation for that species. This problem must be avoided if we are to use this method. The following slight modification happens to solve the problem. Let us concentrate on only one of the unknowns x (x could be x_1 , x_2 , or x_n and may represent a mole fraction). Let the correction to x be given by δ [provided by Equation (3.2-65)], and let x^1 be the value of x at the next iteration. Then

$$x^1 = x + \delta$$

and dividing by x gives

$$\frac{x^1}{x} = 1 + \frac{\delta}{x}$$

Now assuming that $|\delta/x| \ll 1$, and using the fact that $\ln(1 + \delta/x) = \delta/x$, we can take the natural logarithm of both sides of the last equation to give

$$\ln(x^1/x) = \delta/x$$

or

$$x^1 = x e^{\delta/x} \quad (3.2-66)$$

Note if we are at the solution ($\delta=0$), then $x^1=x$ as it should. Whenever a particular variable (unknown) must remain positive, Equation (3.2-66) is used in the iteration to get the next value for the unknown. Otherwise, Equation (3.2-64) is used directly.

Now we apply this solution method to the mathematical models of the gasifier and combustor. The adiabatic gasifier will be discussed first. The first ten unknowns are taken to be the mole fractions of the ten species indicated in Table 3.2-3, where the reason for numbering the species is now apparent. The next four unknowns are λ_H/RT_e , λ_O/RT_e , λ_N/RT_e , and λ_S/RT_e respectively. The fifteenth unknown is the steam flow and the sixteenth one is the air flow. By including RT_e in the terms containing the Lagrange multipliers, we get a much better conditioned gradient matrix which ensures a well-behaved matrix inversion. This scaling was crucial to the success of this method of solution. Without this simple modification, the iteration would not converge properly. A typical case takes seven iterations to get five significant figures on each mole fraction.

As mentioned during the development of the gasifier model, the endothermic gasifier is a special case of the adiabatic gasifier. By setting the sixteenth unknown, w_a , equal to zero (zero air flow) and solving the first fifteen equations, a unique solution is obtained.

Then the energy equation is used to calculate the amount of heat, Q_{gas} , which is required. Note that f_1 to f_6 are the mass balance equations, f_7 to f_{15} are the equilibrium equations, and f_{16} is the energy equation. Thus, the two gasifier modes are easily accommodated.

A very similar approach is taken to obtain a solution to the combustor equations. Now the first fifteen unknowns are taken to be the mole fractions of the fifteen species indicated in Table 3.2-6. The next five unknowns are λ_{C}/RT_p , λ_{H}/RT_p , λ_{O}/RT_p , λ_{N}/RT_p , and λ_{S}/RT_p . The twenty-first and final unknown is either the excess air fraction ξ (with T_p specified) or the product gas exit temperature T_p (with ξ specified). When the endothermic gasifier mode is needed in a cycle, the heat which must be supplied to the gasifier comes from the combustor so $Q_{\text{cmb}} = -Q_{\text{gas}}/N_{\text{cel}}$ where N_{cel} represents the number of moles of clean power gas produced per pound of coal (after the desulfurization process). Note now that f_1 to f_6 are the mass balance equations, f_7 to f_{20} are the equilibrium equations, and f_{21} is the energy equation. Convergence to five significant figures on the mole fractions usually occurs within eight iterations.

3.3 Waste Heat Boiler

The waste heat boiler is composed of three sections: an economizer (EC), an evaporator (EV), and a superheater (SH). The economizer section acts essentially as an additional stage of feedwater heating where the relatively hot combustion gases provide the necessary heat instead of steam extraction from the steam turbine. Without the

economizer, more energy would be lost through the stack as sensible heat. The evaporator section is self-descriptive. The slightly subcooled water which enters the boiler is evaporated to dry saturated steam by the heat provided by the hot combustion gases. Finally, the superheater section superheats the steam. A schematic representation of the waste heat boiler is shown in Figure 3.3-1.

It is instructive to construct a T-Q or temperature-heat flow diagram. This is shown in Figure 3.3-2 not necessarily to any scale. The upper unbroken line represents the flow of the hot product gases from the entrance to gas-side of the boiler, through the superheater, evaporator, and economizer sections respectively, and finally to the stack. The lower broken line represents the flow on the water side of the boiler. Feedwater enters the water-side of the economizer section in a counterflow arrangement, boils in the evaporator section, and finally is superheated in the superheater section again in a counterflow arrangement.

The temperature nomenclature at key points in the boiler for both the steam- and gas-sides is indicated on Figure 3.3-2. The same subscripts will be used for the other properties (enthalpy and pressure) for these points. The pressure is denoted by the symbol P , while the molar enthalpy is represented by \bar{h} and specific enthalpy by h . Furthermore, let m_G represent the number of moles of product gas and w_S the mass flow of steam generated in the waste heat boiler. Let us further define the pinch point temperature difference ΔT_{pp} to be the minimum temperature difference between the gas-side and water-side of the

boiler. We do not know a priori if this is $T_{G1} - T_{S4}$, $T_{G3} - T_{S3g}$, or $T_{G4} - T_{S1}$. The determination of where the actual pinch point occurs makes this model somewhat interesting.

Before explaining how the pinch point is found, it is appropriate now to mention the variables which we assume to have known values. As in all the models, the pressures at each point are specified: P_{G1} , P_{G2} , P_{G3} , P_{G4} , P_{S1} , P_{S2} , P_{S3f} , and P_{S4} . Both the number of moles of gas, m_G , and the composition of this gas are presumably known (from prior component calculations). While the composition dependency on enthalpy for the gas is not explicitly written, it is implied; for example, h_{G3} is written with the understanding that the pressure P_{G3} , the temperature T_{G3} , and the mole fractions are all implied arguments. The temperatures T_{G1} and T_{S4} are assumed to be known. However, we shall see very shortly that it may become necessary to lower T_{S4} . Finally, the pinch point temperature difference ΔT_{pp} and the degrees of subcooling of the inlet fluid to the evaporator section ΔT_{sc} are also presumably specified. All other temperatures, enthalpies, mass flows, and heat flows are calculated. One more restriction, however, must be imposed: the stack gas temperature T_{G4} must be above the dew point temperature. This ensures that the water vapor in the gas does not condense, thus avoiding possible corrosion problems in a real plant.

Now the solution strategy can be discussed. First, the possible pinch point between T_{G1} and T_{S4} must be checked to ensure that the difference $T_{G1} - T_{S4}$ is greater than or equal to ΔT_{pp} . If it is not, the input value of T_{S4} is modified according to

$$T_{S4} = T_{G1} - \Delta T_{pp} \quad (3.3-1)$$

Otherwise, T_{S4} is unchanged. In any event, the next step is to assume a location for the actual pinch point. From Figure 3.3-2, this can be either between T_{G3} and T_{S3g} or between T_{G4} and T_{S1} . The latter is assumed first and all calculations proceed on this basis. This assumption is checked by calculating $T_{G3} - T_{S3g}$ and verifying that this difference is larger than ΔT_{pp} . If it is not, then the pinch point is assumed to be between T_{G3} and T_{S3g} with the calculations proceeding on this basis. (A redundant check is provided by checking to see if $T_{G4} - T_{S1}$ is greater than ΔT_{pp} ; at this point, it must be or there is no solution.) After the pinch point has been located, the remaining unknown parameters can be calculated.

No matter where the pinch point occurs, T_{S3f} is immediately known since P_{S3f} is specified and the water is in the saturation state. Also, $T_{S3g} = T_{S3f}$, since we further assume no pressure drop in the saturation portion of the evaporator section; that is, $P_{S3g} = P_{S3f}$. Then T_{S2} is also easily calculated from

$$T_{S2} = T_{S3f} - \Delta T_{sc} \quad (3.3-2)$$

As mentioned above, T_{S4} either is a specified input or is modified according to Equation (3.3-1).

3.3.1 Pinch Point between T_{G4} and T_{S1}

By assumption

$$T_{G4} = T_{S1} + \Delta T_{pp}$$

and since P_{G1} , T_{G1} and P_{G4} , T_{G4} (and the gas composition) all have known values, \bar{h}_{G1} and \bar{h}_{G4} , respectively, are obtained via the property relations. Similarly, h_{S1} and h_{S4} are also easily determined from the steam tables since P_{S1} , T_{S1} and P_{S4} , T_{S4} , respectively, are known. An energy balance on the entire waste heat boiler gives

$$w_S(h_{S4} - h_{S1}) = m_G(\bar{h}_{G1} - \bar{h}_{G4})$$

which may be solved for the steam flow,

$$w_S = m_G \left(\frac{\bar{h}_{G1} - \bar{h}_{G4}}{h_{S4} - h_{S1}} \right) \quad (3.3-3)$$

Because T_{S2} , P_{S2} are known, h_{S2} is known and an energy balance on the superheater and evaporator sections taken together gives

$$w_S(h_{S4} - h_{S2}) = m_G(\bar{h}_{G1} - \bar{h}_{G3})$$

which may be solved for \bar{h}_{G3} as

$$\bar{h}_{G3} = \bar{h}_{G1} - \frac{w_S}{m_G}(h_{S4} - h_{S2}) \quad (3.3-4)$$

Now since P_{G3} and \bar{h}_{G3} (and the gas composition) are known, T_{G3} is found from the property relations. If $T_{G3} - T_{S3g}$ is greater than or equal

to ΔT_{pp} , then the correct pinch point has been assumed. Otherwise, the pinch point must be between T_{G3} and T_{S3g} .

3.3.2 Pinch Point between T_{G3} and T_{S3g}

By assumption, P_{G3} is known and

$$T_{G3} = T_{S3g} + \Delta T_{pp}$$

from which \bar{h}_{G3} may be found from the property relations. Now an energy balance on the superheater and evaporator sections taken together gives

$$w_S(h_{S4} - h_{S2}) = m_G(\bar{h}_{G1} - \bar{h}_{G3})$$

which may be solved for the corrected steam flow, or

$$w_S = m_G \left(\frac{\bar{h}_{G1} - \bar{h}_{G3}}{h_{S4} - h_{S2}} \right) \quad (3.3-5)$$

Now an energy balance on the entire boiler gives

$$w_S(h_{S4} - h_{S1}) = m_G(\bar{h}_{G1} - \bar{h}_{G4})$$

from which \bar{h}_{G4} may be obtained,

$$\bar{h}_{G4} = \bar{h}_{G1} - \frac{w_S}{m_G}(h_{S4} - h_{S1}) \quad (3.3-6)$$

where w_S is provided by Equation (3.3-5). Since \bar{h}_{G4} and P_{G4} are known, T_{G4} is obtained via the property relations and $T_{G4} - T_{S1}$ must be greater than ΔT_{pp} or else no solution is possible. This fact is used to provide a check, since physically a solution must exist.

3.3.3 Check of Dew Point Temperature

Let the mole fraction of water vapor in the gas be denoted by μ_{H_2O} . Then the partial pressure of the water vapor P_{H_2O} in the stack is given by

$$P_{H_2O} = \mu_{H_2O} P_{G4}$$

From the steam tables, we can obtain the saturation temperature corresponding to P_{H_2O} which is, by definition, the dew point temperature, T_{DP} . If T_{G4} is not greater than T_{DP} , the analyst is alerted (by an appropriate message in the corresponding computer subroutine). However, the calculations described in Section 3.3.4 still proceed.

3.3.4 Calculation of Remaining Unknown Parameters

Since P_{S3g} and T_{S3g} are known, h_{S3g} is readily determined from the gas tables, and an energy balance on the superheater gives

$$w_S(h_{S4} - h_{S3g}) = m_G(\bar{h}_{G1} - \bar{h}_{G2})$$

which may be solved for \bar{h}_{G2} as

$$\bar{h}_{G2} = \bar{h}_{G1} - \frac{w_S}{m_G}(h_{S4} - h_{S3g}). \quad (3.3-7)$$

Since P_{G2} is also known, T_{G2} may be obtained from the property relations.

It should be noted that the proper relation for w_S must be used in Equation (3.3-7) depending on the location of the pinch point. Let the amount of heat transferred in the economizer, evaporator, and

superheater sections be Q_{EC} , Q_{EV} , and Q_{SH} , respectively. It immediately follows that

$$Q_{EC} = w_S(h_{S2} - h_{S1}),$$

$$Q_{EV} = w_S(h_{S3g} - h_{S2}),$$

and

$$Q_{SH} = w_S(h_{S4} - h_{S3g}).$$

For completeness, h_{S3f} is easily obtained from the steam tables since T_{S3f} is known.

This completes the derivation of the mathematical model for the waste heat boiler.

3.4 Supercharged Boiler

Like the waste heat boiler, the supercharged boiler is composed of three sections: an economizer (EC), and evaporator (EV), and a superheater (SH). These serve the same purpose as in the waste heat boiler and the discussion at the beginning of Section 3.3 will not be repeated here. A schematic representation of the supercharged boiler is shown in Figure 3.4-1. Note that we shall include the gas turbine as part of the model. The reason for doing this will become apparent when we develop the governing equations.

As mentioned in Section 2.1, the path of the gases in the supercharged boiler is different than that in the waste heat boiler. In the latter, the gas which is exhausted from the gas turbine enters the

superheater, evaporator, and economizer sections in that order before exiting the system through the stack. In the former, the hot gas directly from the combustor first enters the evaporator and then the superheater. The exhaust gas from the superheater enters the gas turbine where useful work is obtained from the fluid. The exhaust gas from the turbine then enters the economizer before exiting the system through the stack.

Once again it is useful to construct a T-Q or temperature-heat flow diagram, which is shown in Figure 3.4-2, again not necessarily to any scale. The upper line represents the flow of the hot gas as it is cooled in the boiler. The drop in temperature of the gas between the superheater and economizer sections is due to the presence of the gas turbine at this point. The lower broken, dashed line represents the flow on the water side of the boiler. Feedwater enters the water-side of the economizer in a counterflow arrangement, boils in the evaporator section, and finally is superheated in the superheater section again in a counterflow arrangement.

The temperature nomenclature at key points in the boiler for both the steam- and gas-sides is indicated in Figure 3.4-2. Again, these same subscripts will be used for the other properties (pressure and enthalpy) for these points. The pressure is once again denoted by P , the molar enthalpy by \bar{h} , and the specific enthalpy by h . Once more, let m_G represent the number of moles of product gas and w_S the mass flow of steam generated in the supercharged boiler. Again we define the pinch point temperature difference ΔT_{pp} as in Section 3.3, but now we do know where this will occur in the boiler. Because of the magnitudes of the temperatures at each of these points (see Chapter 5),

the pinch point will invariably occur at the exit of the stack. However, for this model, we shall see that T_{S2} is not simply calculated as it was for the waste heat boiler but rather has a value which depends on the energy balances as shown below.

The following variables are assumed to have known values. As in all the models, the pressures at each point are specified: P_{G1} , P_{G2} , P_{G3} , P_{G4} , P_{G5} , P_{S1} , P_{S2} , P_{S3f} , and P_{S4} . Again both m_G and the gas composition are presumably known, as well as the temperatures T_{G1} , T_{G3} , T_{S1} , and T_{S4} . The minimum pinch point temperature difference ΔT_{pp} and the minimum number of degrees of subcooling of the inlet fluid to the evaporator section ΔT_{min} are also assumed to be specified. Because the gas turbine is included in the model, we assume also that the gas turbine efficiency is specified. (See Section 3.10). If the dewpoint temperature T_{DP} of the stack gas is reached, then the stack gas temperature is raised appropriately, increasing the effective pinch point temperature difference. We shall see shortly that the effective ΔT_{pp} at the stack may be increased for another reason.

Now we are in a position to discuss the solution strategy. First, the dew point temperature T_{DP} must be found to ensure that T_{G5} is greater than T_{DP} . Let μ_{H_2O} be the mole fraction of water vapor in the stack gas. The partial pressure of the water vapor p_{H_2O} in the stack gas is then given by

$$p_{H_2O} = \mu_{H_2O} P_{G5} \quad (3.4-1)$$

Now from the steam tables, we can obtain the saturation temperature corresponding to p_{H_2O} which is, by definition, the dew point temperature

T_{DP} . If $T_{DP} - T_{S1}$ is greater than ΔT_{pp} , then T_{G5} is taken to be equal to T_{DP} . Otherwise, T_{G5} is taken to be equal to $T_{S1} + \Delta T_{pp}$. Next, since the gas turbine efficiency is specified, along with P_{G3} , T_{G3} , P_{G4} , and the gas composition, the gas turbine model described in Section 3.10 gives values for T_{G4} , \bar{h}_{G3} , and \bar{h}_{G4} (as well as the work done per unit mass of fluid). Because P_{S4} , T_{S4} and P_{S1} , T_{S1} are known, h_{S4} and h_{S1} are determined from the steam tables. Similarly, P_{G1} and T_{G1} (and the gas composition) uniquely determines \bar{h}_{G1} from the gas table property relations. It is assumed that $P_{S3g} = P_{S3f}$ and so it follows that $T_{S3g} = T_{S3f}$ where T_{S3f} is the saturation temperature corresponding to P_{S3f} from the steam tables. Similarly we get h_{S3f} and h_{S3g} .

Using the value for T_{G5} as described above with that for P_{G5} , we can get h_{G5} from the gas tables. By defining ψ to be the following ratio

$$\psi = \frac{\bar{h}_{G4} - \bar{h}_{G5}}{\bar{h}_{G1} - \bar{h}_{G3}} \quad (3.4-2)$$

where all the \bar{h} 's now have known values, we can show that \bar{h}_{S2} is then given by

$$h_{S2} = \frac{h_{S1} + \psi h_{S4}}{1 + \psi} \quad (3.4-3)$$

Note that all the parameters on the right-hand side are known. Then P_{S2} and h_{S2} may be used to get T_{S2} from the steam tables. If the difference between T_{S3f} and T_{S2} is not greater than ΔT_{min} , then T_{G5} is increased by 10 degree Fahrenheit increments and the calculation beginning with Equation (3.4-2) is repeated until $T_{S3f} - T_{S2}$ is greater than

ΔT_{\min} . In any event, once h_{S2} is known, the steam flow w_S may be found by the following energy balance on the economizer

$$w_S(h_{S2} - h_{S1}) = m_G(\bar{h}_{G4} - \bar{h}_{G5}) \quad (3.4-4)$$

which may be solved for w_S as

$$w_S = m_G \left(\frac{\bar{h}_{G4} - \bar{h}_{G5}}{h_{S2} - h_{S1}} \right) \quad (3.4-5)$$

An energy balance on the superheater gives

$$w_S(h_{S4} - h_{S3g}) = m_G(\bar{h}_{G2} - \bar{h}_{G3})$$

which may be solved for \bar{h}_{G2} as

$$\bar{h}_{G2} = \bar{h}_{G3} + \frac{w_S}{m_G}(h_{S4} - h_{S3g}). \quad (3.4-6)$$

This result and the known value for P_{G2} determines T_{G2} . Finally, the amount of heat transferred in the economizer, evaporator, and superheater sections are

$$Q_{EC} = w_S(h_{S2} - h_{S1}) \quad (3.4-7)$$

$$Q_{EV} = w_S(h_{S3g} - h_{S2}), \quad (3.4-8)$$

and

$$Q_{SH} = w_S(h_{S4} - h_{S3g}),$$

respectively.

Equation (3.4-3) will now be justified. An energy balance on the evaporator and superheater taken together gives

$$w_S(h_{S4} - h_{S2}) = m_G(\bar{h}_{G1} - \bar{h}_{G3})$$

which when considered with Equation (3.4-4), may be solved for h_{S2} as

$$h_{S2} = \frac{h_{S1} + \left(\frac{\bar{h}_{G4} - \bar{h}_{G5}}{\bar{h}_{G1} - \bar{h}_{G3}} \right) h_{S4}}{1 + \left(\frac{\bar{h}_{G4} - \bar{h}_{G5}}{\bar{h}_{G1} - \bar{h}_{G3}} \right)} \quad (3.4-3a)$$

which is Equation (3.4-3) with the term in the parentheses being ψ defined by Equation (3.4-2). In retrospect, it probably would have been better to specify T_{S2} (or ΔT_{sc} instead of ΔT_{min} with $T_{S2} = T_{S3f} - \Delta T_{sc}$) which along with P_{S2} would establish h_{S2} . Then Equation (3.4-3a) could have been solved for \bar{h}_{G5} which with P_{G5} would establish T_{G5} . The pinch point temperature difference ΔT_{pp} would then only be used as a check to ensure that this minimum difference is not violated. This alternate approach would yield a value for T_{G5} within 10 degrees Fahrenheit of that from the original formulation. This difference is not significant and, furthermore, the amount of subcooling is somewhat arbitrary anyway.

This completes the derivation of the mathematical model for the supercharged boiler.

3.5 Air and Gas Compressor

Consider the adiabatic compression of a mole of a gaseous fluid (air or another gaseous mixture) from pressure P_1 to pressure P_2 in a steady-flow process for which the kinetic and potential energy changes are negligible. A schematic representation of such a device

is shown in Figure 3.5-1. Because there are irreversibilities associated with the compression process, the molar entropy \bar{s} must increase since we already assumed the process to be adiabatic. The irreversible process is shown in Figure 3.5-2 in temperature-entropy coordinates as a dashed line since the path is not really known. The isentropic compression from P_1 to P_2 is shown as a solid line on the same figure.

For this type of process, we use the usual definition for the efficiency η_c which is defined to be the ratio of the isentropic work required \bar{W}_{isen} to the actual work required \bar{W}_{act} both defined here on a mole basis,

$$\eta_c = \frac{\bar{W}_{isen}}{\bar{W}_{act}} \quad (3.5-1)$$

Denoting the properties at the end of the isentropic process by the prime (') and those at the end of the actual process without the prime, we may write from the first law.

$$\bar{W}_{isen} = \bar{h}_2' - \bar{h}_1$$

and

$$\bar{W}_{act} = \bar{h}_2 - \bar{h}_1 \quad (3.5-2)$$

where the h_1 , h_2 , and h_2' are molar enthalpies. Therefore, the definition of compressor efficiency then becomes

$$\eta_c = \frac{\bar{h}_2' - \bar{h}_1}{\bar{h}_2 - \bar{h}_1} \quad (3.5-3)$$

The following parameters are assumed to be known: the gas or air composition, the pressure P_1 and P_2 , the temperature T_1 , and the efficiency

n_c . The state at the end of the actual process is to be determined as well as the amount of work required during the process.

Since P_1 , T_1 , and the gas or air composition are known, the state at the beginning of the process is completely specified. From the gas tables we may get both \bar{h}_1 and \bar{s}_1 where \bar{s} denotes the molar entropy. But by definition $\bar{s}_2' = \bar{s}_1$ which considered with P_2 completely specifies the state at the end of the isentropic process. Therefore, \bar{h}_2' is determined. Now Equation (3.5-3) may be solved for \bar{h}_2 as

$$\bar{h}_2 = \bar{h}_1 + \frac{\bar{h}_2' - \bar{h}_1}{n_c} \quad (3.5-4)$$

The actual work required W_{act} per unit mass is then given by

$$W_{act} = (\bar{h}_2 - \bar{h}_1)/v$$

where v is the molecular weight of either the air or gas under consideration. We have, therefore, determined the work done during the process and the state of the fluid at the end of the irreversible process.

3.6 Condenser

Let us consider the condensation of wet steam to a saturated liquid condition on the shell-side of a condenser by the transfer of the latent heat to a secondary water stream on the tube-side. To be more general we allow for a second inlet stream on the steam-side to the hotwell, since we anticipate that the condensate from the feedwater heater closest to the condenser will be flashed through a throttle valve and finally through a return line into the hotwell. A schematic representation of the condenser is shown in Figure 3.6-1.

It is convenient to assume that the following parameters are specified: the temperature T_{W1} and pressure P_{W1} of the cooling water inlet; the pressure P_{W2} of the cooling water outlet; the temperature rise of the cooling water ΔT_W ; the pressure P_{S1} , the quality x_{S1} , and the mass flow of steam-water mixture w_{S1} into the condenser (from the steam turbine); the pressure P_{S2} of the saturated liquid condensate; and, finally, the pressure P_R , the quality x_R , and the mass flow w_R for the return line.

In practice, P_R is generally equal to P_{S1} since a throttle valve is used in the return line to make these pressures compatible. Also, since no pressure drop is assumed on the shell-side, then P_{S2} is equal to P_{S1} . Furthermore, the fluid at the shell-side outlet is assumed to be saturated liquid water. The temperature-heat flow diagram is shown in Figure 3.6-2. The condensing steam line in this figure is horizontal since the saturation temperature is constant for a constant pressure.

The same subscript designation will also be applied to the specific enthalpies, thus defining h_{S1} , h_{S2} , h_R , h_{W1} , and h_{W2} . From the steam tables we immediately can determine values for h_{S1} , h_R , and h_{W1} since the corresponding states are completely specified. Clearly,

$$T_{W2} = T_{W1} + \Delta T_W \quad (3.6-1)$$

by definition, which with P_{W2} , completely specifies the state of the cooling water at the exit; therefore, h_{W2} is determined from the steam tables. Because the condensate leaving the hotwell is assumed to be in a saturated liquid condition and the pressure at this state is known, we determine T_{S2} from the steam tables as the saturation temperature

corresponding to P_{S2} and h_{S2} is also easily determined. From continuity of mass, we must have

$$w_{S2} = w_{S1} + w_R \quad (3.6-2)$$

for the shell-side of the condenser. Now an energy balance on the entire condenser gives

$$w_W(h_{W2} - h_{W1}) = w_{S1}h_{S1} + w_R h_R - w_{S2}h_{S2}$$

which we may solve for the cooling water flow w_W as

$$w_W = \frac{w_{S1}h_{S1} + w_R h_R - w_{S2}h_{S2}}{h_{W2} - h_{W1}} \quad (3.6-3)$$

The amount of heat rejected Q_W is then obviously

$$Q_W = w_W(h_{W2} - h_{W1}). \quad (3.6-4)$$

For completeness, T_R is also determined since P_R is known and the fluid is a saturated steam-water mixture.

3.7 Deaerator

Many times a deaerator is referred to as an open feedwater heater. These two terms can be used interchangeably. In order to avoid corrosion problems in the heat transfer devices, it is necessary to remove the entrapped air in the feedwater. This is most commonly done by using an open feedwater heater. For our purposes, we do not have to actually model the air ejection, since this is not relevant to our problem. Therefore, we shall treat the deaerator as a simple open feedwater heater.

A schematic representation is shown in Figure 3.7-1. Again we include the possibility of a return line for a reason similar to that cited in the development of the condenser model in Section 3.6.

We assume the following parameters are specified: the pressure P_{L1} and temperature T_{L1} of the feedwater into the deaerator; the outlet pressure P_{L2} and the outlet flow w_{L2} ; the pressure P_R , the quality x_R , and the mass flow w_R of the saturated steam-water mixture in the return line; the pressure P_S and either the quality x_S (if saturated) or the temperature T_S (if superheated) of the extraction fluid. By definition of an open feedwater heater, the mass flows into the heater intimately mix, producing one outlet flow stream in a saturated liquid condition.

As is the usual case, the same subscript designations will be applied to the specific enthalpies, thus defining h_S , h_R , h_{L1} , and h_{L2} . From the steam tables, we can immediately determine values for h_S , h_R , and h_{L1} since the corresponding states are completely defined. If the extraction fluid is saturated, then specifying P_S fixes T_S as the saturation temperature corresponding to P_S ; if superheated, x_S is no longer meaningful. The temperature T_{L2} at the feedwater outlet is also easily obtained from the steam tables as the saturation temperature corresponding to pressure P_{L2} , and h_{L2} is simply the saturated liquid enthalpy of the outlet fluid. Because the return flow fluid is saturated, T_R is the saturation temperature corresponding to P_R .

Now with all the appropriate enthalpies at each state point specified, an energy balance on the deaerator will give an expression for the extraction flow w_S as follows. The energy balance yields

$$w_{L1}h_{L1} + w_S h_S + w_R h_R = w_{L2} h_{L2} \quad (3.7-1)$$

which when the mass balance equation

$$w_{L2} = w_{L1} + w_S + w_R \quad (3.7-2)$$

is considered to eliminate the unknown mass flow w_{L1} between Equations (3.7-1) and (3.7-2) we may solve for w_S as

$$w_S = \frac{w_{L2}(h_{L2} - h_{L1}) + w_R(h_{L1} - h_R)}{h_S - h_{L1}} \quad (3.7-3)$$

Now with w_S known, Equation (3.7-2) may be solved for the unknown feedwater inlet flow as

$$w_{L1} = w_{L2} - w_S - w_R \quad (3.7-4)$$

Thus, the states and mass flows of the four flow streams are completely specified.

One may ask why w_{L2} is considered to be a known while w_{L1} is unknown. This is most simply answered by referring to Figures 2.3-1, 2.3-2, 2.3-3, or 2.3-4. When we add feedwater heaters later the last component in the feedwater train will be a deaerator. Since the steam flow to the steam turbine is presumed to be known at this point in the cycle calculation, it is easily seen in these figures that w_{L2} is precisely equal to steam turbine inlet flow which is known from a prior component calculation, namely the waste heat or supercharged boiler calculations discussed in Sections 3.3 and 3.4, respectively. This kind of reasoning is used throughout the model development and has resulted in simplifying the

complexity of the model input and output considerably. In rare cases where an assumed input parameter is not really known, an iterative procedure using the model as developed could be easily implemented.

3.8 Closed Feedwater Heater

A closed feedwater heater is a heat exchanger in which steam extracted from a steam turbine provides the heat necessary to raise the temperature of the feedwater. A schematic representation is shown in Figure 3.8-1. As we have done in the condenser and deaerator models, we shall allow for more flexibility by including a return line from a downstream feedwater heater to the shell side of the feedwater heater under consideration.

Now it is convenient to assume the following parameters are specified from the outset: the pressure P_{L1} , the temperature T_{L1} , and the mass flow w_{L1} of the feedwater into the heater; the pressure P_{S1} and either the quality x_{S1} or temperature T_{S1} of the steam extraction fluid; the pressure P_R , the quality x_R , and the mass flow w_R of the fluid entering the shell-side through the return line; the pressure P_{L2} of the feedwater outlet flow; and, finally, the terminal temperature difference ΔT_{TTD} between the shell-side temperature T_{S1} (or T_{S2} or T_R) and the temperature T_{L2} of the feedwater outlet.

As in the condenser model, the return line pressure P_R is in general equal to P_{S1} . Also, since no pressure drop is assumed on the shell-side, then P_{S2} is equal to P_{S1} . Furthermore, the fluid at the shell-side outlet is assumed to be saturated liquid water. The temperature-heat flow diagram is shown in Figure 3.8-2, where the terminal temperature difference ΔT_{TTD} is indicated. The condensing steam line in this figure is

horizontal since the saturation temperature is constant for a constant pressure.

We note that the model allows for specification of the state of the steam extraction fluid by either P_{S1} , x_{S1} if saturated or P_{S1} , T_{S1} if superheated. It is a simple matter to then determine T_{S1} in the former as the saturation temperature corresponding to P_{S1} . If the fluid is superheated steam, then x_{S1} is not meaningful. In any event, the specific enthalpy h_{S1} is also easily obtained from the steam tables. Figure 3.8-2 is valid only if the steam extraction fluid is in a saturated state, which is the usual case in practice.

The steam tables once again provide us with the enthalpies of the states which are completely specified by the variables assumed to be known. First, P_{L1} , T_{L1} determine h_{L1} . Since we assume the shell-side outlet fluid to be saturated water, then T_{S2} is the saturation temperature corresponding to the pressure P_{S2} which is taken to be equal to P_{S1} . Clearly, this also fixes h_{S2} . Then from the definition of the terminal temperature difference,

$$T_{L2} = T_{S2} - \Delta T_{TTD} \quad (3.8-1)$$

This with P_{L2} fixes h_{L2} , since we have a subcooled liquid state. Finally, P_R and x_R completely fix h_R . Now with all the enthalpies known, the energy balance equation for the entire heater is

$$w_{L2}h_{L2} - w_{L1}h_{L1} = w_{S1}h_{S1} + w_Rh_R - w_{S2}h_{S2} \quad (3.8-2)$$

But by continuity of mass on the tube-side, we have

$$w_{L2} = w_{L1}, \quad (3.8-3)$$

and on the shell side,

$$w_{S2} = w_{S1} + w_R. \quad (3.8-4)$$

Using Equations (3.8-4) and (3.8-3) in Equation (3.8-2) and solving for w_{S1} , we get

$$w_{S1} = \frac{w_{L1}(h_{L2} - h_{L1}) - w_R(h_R - h_{S2})}{h_{S1} - h_{S2}} \quad (3.8-5)$$

With the steam extraction flow w_{S1} , fixed by Equation (3.8-5), the shell-side outlet flow is given by Equation (3.8-4). We have thus determined all the remaining unknown parameters.

3.9 Gas Cooler

This model is especially simple since the main purpose is to calculate the amount of heat which is discarded. Because the rejected heat is not used, this represents a heat loss from the cycle in which such a component is used but does not necessarily lower cycle performance. This particular component may be part of an intercooled compressor as mentioned in Section 3.1 or, as we shall see later, it may be used to cool the gas before the sulfur removal process.

It is convenient to assume the following parameters are known in the model: the gas composition, the pressure P_1 and temperature T_1 at the

inlet, the pressure P_2 and temperature T_2 at the outlet, and the number of moles, m , of gas passing through the intercooler. Figure 3.9-1 shows the schematic representation of a gas cooler, which may at times be referred to as an intercooler. The heat removed Q from the gas is then simply

$$Q = m(\bar{h}_1 - \bar{h}_2)$$

where T_1 is assumed to be greater than T_2 , and \bar{h}_1 and \bar{h}_2 are the molar enthalpies of the inlet and outlet fluids respectively.

3.10 Gas Turbine

Now we consider the reverse of the process described in the air and gas compressor models. We want to model the adiabatic expansion of a mole of a mixture of gases from a pressure P_1 to a pressure P_2 in a steady-flow process. Again we neglect the changes the kinetic and potential energy and heat losses. A schematic representation of the gas turbine is shown in Figure 3.10-1. Like the compression process we have irreversibilities associated with the expansion process. Thus the molar entropy \bar{s} must increase during the process. We show the irreversible process in Figure 3.10-2 on temperature-entropy coordinates as a dashed line since the path is not really known. The isentropic expansion from P_1 to P_2 is shown as a solid line on the same figure.

Now we define the efficiency of the gas turbine η_T to be the ratio of the actual work produced W_{act} to the isentropic work produced W_{isen} , both defined here on a mole basis, or

$$\eta_T = \frac{\bar{W}_{act}}{\bar{W}_{isen}} \quad (3.10-1)$$

Following our convention of denoting the state at the end of an isentropic process by a prime ($'$), we can write from the first law that

$$\bar{W}_{isen} = \bar{h}_1 - \bar{h}_2' \quad (3.10-2)$$

and

$$\bar{W}_{act} = \bar{h}_1 - \bar{h}_2 \quad (3.10-3)$$

where the \bar{h} 's are all molar enthalpies at the states indicated by the subscripts. So the efficiency becomes

$$\eta_T = \frac{\bar{h}_1 - \bar{h}_2}{\bar{h}_1 - \bar{h}_2'} \quad (3.10-4)$$

For convenience, we assume the following parameters are known: the gas composition, the pressures P_1 and P_2 , and temperature T_1 , and the efficiency η_T . We want to determine the state of the gas mixture at the end of the expansion and the actual amount of work produced on a mass basis, W_{act} .

Since the gas composition, P_1 , and T_1 are known, the state at the beginning of the process is completely determined. We get both \bar{h}_1 and \bar{s}_1

from the gas table properties. Then by definition, $\bar{s}_2' = \bar{s}_1$, and with P_2 fixed, we have established \bar{h}_2' . Solving Equation (3.10-4) for \bar{h}_2 gives

$$\bar{h}_2 = \bar{h}_1 - \eta_T(\bar{h}_1 - \bar{h}_2'). \quad (3.10-5)$$

If we denote the molecular weight of the gaseous mixture as v , then the actual work produced on a pound basis is given by

$$w_{\text{act}} = (\bar{h}_1 - \bar{h}_2)/v \quad (3.10-6)$$

With \bar{h}_2 and P_2 fixed, we can easily get the temperature T_2 of the fluid at the end of the actual expansion, as well as any other property.

3.11 Gas-to-Gas Counterflow Heat Exchanger

The concept of heat exchanger effectiveness may be used to advantage in a thermodynamic analysis of any power cycle in which heat exchangers may be required. Earlier we have recognized the fact that we are limiting this modeling effort to the thermodynamics of the processes only. We agreed that for our purposes it is not necessary to know how large a particular component would have to be. But the very concept of a heat exchanger entails considering such factors as heat transfer coefficients, heat transfer areas, and so forth, which all depend on the geometry of the device. We shall see below how our using the effectiveness ϵ , defined to be the ratio of the actual heat transfer to the maximum possible, sufficiently characterizes the heat exchanger to enable us to retain our thermodynamic approach. We further limit this model to gas-to-gas heat

exchange in a counterflow arrangement because in Chapter 5 we shall see that this particular component will improve the cycle performance significantly.

A schematic representation of the gas-to-gas counterflow heat exchanger is shown in Figure 3.11-1. Because we shall use this device to regenerate heat from one fluid to another, we may also refer to this component as a regenerator. Let us assume the following parameters are specified from the outset: the effectiveness ϵ ; the molar flows of the hot and cold fluids, m_h and m_c , respectively; the pressures at inlet to and outlet from the hot side or P_{h1} and P_{h2} , respectively, and at the inlet to and outlet from the cold side or P_{c1} and P_{c2} respectively; the temperatures at the inlet to both the hot and cold sides or T_{h1} and T_{c1} , respectively; and finally, the composition of the gases on both sides.

Depending on the relative heat capacities which is the product of the molar flows and molar specific heats, we may get two different temperature-heat flow diagrams as shown in Figure 3.11-2. In Figure 3.11-2(a), the hotter fluid is assumed to have the smaller heat capacity or $m_h \bar{c}_{ph}$ is less than $m_c \bar{c}_{pc}$ where \bar{c}_{ph} and \bar{c}_{pc} are the molar specific heats of the hot and cold fluids, respectively. In Figure 3.11-2(b), we assume $m_c \bar{c}_{pc}$ is less than $m_h \bar{c}_{ph}$. These devices are usually well insulated and so it is reasonable to assume no heat loss. An energy balance on entire regenerator then gives

$$m_c \bar{c}_{pc} (T_{c2} - T_{c1}) = m_h \bar{c}_{ph} (T_{h1} - T_{h2}) \quad (3.11-1)$$

From this equation, we see that the difference between T_{h1} and T_{h2} must be larger than that between T_{c2} and T_{c1} when $m_h \bar{c}_{ph}$ is less than $m_c \bar{c}_{pc}$.

and vice versa. Based on our definition of effectiveness, we can get two different expressions depending on which fluid has the minimum heat capacity. If the hot fluid is assumed, then

$$\epsilon = \frac{T_{h1} - T_{h2}}{T_{h1} - T_{c1}} \quad (3.11-2a)$$

but if the cold fluid is assumed, then

$$\epsilon = \frac{T_{c2} - T_{c1}}{T_{h1} - T_{c1}} \quad (3.11-2b)$$

We must be careful, therefore, in choosing the correct defining equation for the effectiveness.

Because we prefer to work with enthalpies rather than specific heats, an alternate equivalent approach will be taken. We shall first assume the hot fluid has the minimum heat capacity and use Equation (3.11-2a) to solve for T_{h2} . Then an energy balance will give T_{c2} . The amount of heat transfer is then readily calculated. Then, we shall assume the cold fluid has the minimum heat capacity and use Equation (3.11-2b) to solve for T_{c2} . Now the energy balance will give T_{h2} and again the amount of heat transfer may be calculated. The minimum fluid must be the one which, when assumed as above, results in the smaller amount of heat transfer, since the heat transfer Q is given by²⁰

$$Q = \epsilon(m\bar{c}_p)_{\min}(T_{h1} - T_{c1})$$

where $(m\bar{c}_p)_{\min}$ is the smaller of $m_c\bar{c}_{pc}$ and $m_h\bar{c}_{ph}$.

First, we assume that the hot fluid is the minimum one. Then Equation (3.11-2a) is solved for T_{h2} as

$$T_{h2} = T_{h1} - \varepsilon(T_{h1} - T_{c1}) \quad (3.11-3)$$

With T_{h2} fixed by Equation (3.11-3) and with P_{h2} known (the gas composition is also known), we can get h_{h2} from the property tables. Similarly P_{c1} , T_{c1} and P_{h1} , T_{h1} fix \bar{h}_{c1} and \bar{h}_{h1} . The energy balance in terms of the enthalpies becomes

$$m_h(\bar{h}_{h1} - \bar{h}_{h2}) = m_c(\bar{h}_{c2} - \bar{h}_{c1}) \quad (3.11-4)$$

which may be solved for \bar{h}_{c2} as

$$\bar{h}_{c2} = \bar{h}_{c1} + \frac{m_h}{m_c} (\bar{h}_{h1} - \bar{h}_{h2}). \quad (3.11-5)$$

Since P_{c2} (along with the gas composition) is known and \bar{h}_{c2} is fixed by Equation (3.11-5), we can obtain T_{c2} from the property tables. The heat transfer Q_H , if the hot fluid is the minimum one, may then be given as

$$Q_H = m_h(\bar{h}_{h1} - \bar{h}_{h2}) \quad (3.11-6)$$

Next, we follow a similar procedure by now assuming the cold fluid is the minimum one. Now Equation (3.11-2b) is solved for T_{c2} as

$$T_{c2} = T_{c1} + \varepsilon(T_{h1} - T_{c1}). \quad (3.11-7)$$

We then get \bar{h}_{c2} from the gas tables, which we use in Equation (3.11-4) which we solve for \bar{h}_{h2} to get

$$\bar{h}_{h2} = \bar{h}_{h1} - \frac{m_c}{m_h} (\bar{h}_{c2} - \bar{h}_{c1}) \quad (3.11-8)$$

This fixes T_{h2} . Now the heat transfer Q_C may be taken as

$$Q_C = m_h (\bar{h}_{h1} - \bar{h}_{h2}). \quad (3.11-9)$$

If Q_H is greater than Q_C , then the cold fluid has the minimum heat capacity and we use Equations (3.11-7) to (3.11-9) to describe the heat exchanger.

If Q_C is greater than Q_H , then Equations (3.11-3) to (3.11-6) are used.

3.12 Steam Generator

The steam generator provides the steam needed by the coal gasifier by utilizing the sensible heat in the gasifier power gas. A schematic representation is shown in Figure 3.12-1. The model for the steam generator appears on the surface to be identical to that of the waste heat boiler. However, they are quite different since the parameters which are known are different. For example, in the waste heat boiler model we had to determine the steam flow using the fact that the minimum pinch point temperature difference was to be respected. Here, the steam flow is known (fixed by the gasifier model) with the pinch point temperature difference being used only to determine if, in fact, it is even possible to raise the required amount of steam. Fortunately, in every case of practical interest, we are able to do this.

It is convenient to assume the following parameters are initially known: the pressure P_L and temperature T_L of the water flowing into the steam generator; the pressure P_S and temperature T_S of the superheated steam; the mass flow of steam w_S ; the pressure P_{G1} and temperature T_{G1}

of the power gas flowing into the gas-side; the molar flow of power gas m_G and the gas composition (which, as usual, is needed to determine the enthalpies); the pressure P_{G3} of the gas flowing out of the gas-side; the pressure P_{G2} of the gas at the internal pinch point shown in Figure 3.12-2; and, finally, the minimum pinch point temperature difference ΔT_{pp} .

The temperature-heat flow diagram is shown in Figure 3.12-2 for the steam generator. From the steam tables we may immediately obtain the specific enthalpies h_S and h_L . The required amount of heat is then given by

$$Q_{SG} = w_S(h_S - h_L). \quad (3.12-1)$$

Since we assume no heat losses, this also must be equal to

$$Q_{SG} = m_G(\bar{h}_{G1} - \bar{h}_{G3}) \quad (3.12-2)$$

where \bar{h}_{G1} is the molar enthalpy from the gas tables since the corresponding state is specified. Equating the right-hand sides of Equations (3.12-1) and (3.12-2), we may then solve for \bar{h}_{G3} as

$$\bar{h}_{G3} = \bar{h}_{G1} - \frac{w_S}{m_G}(h_S - h_L) \quad (3.12-3)$$

which, with P_{G3} , fixes T_{G3} . An energy balance on the section in the steam generator between T_{G2} and T_{G3} gives an expression which may be solved for \bar{h}_{G2} as

$$\bar{h}_{G2} = \bar{h}_{G3} + \frac{w_S}{m_G}(h_{LS} - h_L) \quad (3.12-4)$$

where h_{LS} is the saturated liquid enthalpy for water at pressure P_{LS} which is taken to be equal to P_L . From the steam tables we also get T_{LS} which is the saturation temperature corresponding to P_{LS} . With \bar{h}_{G2} fixed by Equation (3.12-4) and P_{G2} known, we get T_{G2} from the gas table properties.

We complete the model by checking to make sure that $T_{G1} - T_S$, $T_{G2} - T_{LS}$, and $T_{G3} - T_L$ are all greater than ΔT_{pp} . If this were not the case, then it would be impossible to raise the required amount of steam by this method and an alternative method would have to be found. Fortunately, this is not the case as we shall see in Chapter 5.

3.13 Steam Turbine

The steam turbine model is very similar to the gas turbine model. There are two key differences, however. The first is the fact that the inlet fluid to the turbine may be superheated steam or a saturated steam-water mixture, making the model more complicated. The second, which simplifies the model, is that we have only one species to consider, namely H_2O .

We find it convenient to assume the following parameters are initially known: the pressures P_1 and P_2 at the inlet and outlet of the steam turbine; the efficiency η_T defined similarly to that in Section 3.10 for the gas turbine; and finally either the temperature T_1 or quality x_1 of the inlet fluid. A schematic representation of the steam turbine is shown in Figure 3.13-1.

To get a multi-stage steam turbine with steam extraction for feedwater heating we simply connect as many of these single-stage models in series as are required. This approach allows much flexibility in the use of this single model. If we were to try to actually model a multi-stage steam turbine with extraction, we would see that the feedwater heater models are coupled to the steam turbine model through the extraction flows. We avoid this complication by obeying our general rule to model each process via a single component model where possible.

The solution procedure is similar to that of the gas turbine model. First, we construct the temperature-entropy diagrams shown in Figure 3.13-2. In Figure 3.13-2(a), the fluid is assumed to be initially in a superheated state and in Figure 3.13-2(b) a steam-water saturated state. The final state is shown in the saturation region but we shall allow in our model for the final state to be either superheated steam or wet steam. For the case shown in Figure 3.13-2(a), we define the initial state by P_1 and T_1 since these properties are independent. For that shown in Figure 3.13-2(b), the initial state is defined by P_1 and x_1 , where x is used to denote steam quality. In any event, we can easily obtain the specific enthalpy h_1 and specific entropy s_1 from the steam tables. Again we denote the states at the end of the isentropic process by the prime ($'$), so by definition $s_2' = s_1$. But P_2 is known so, h_2' may be found from the steam tables. But η_T is defined by

$$\eta_T = \frac{h_1 - h_2'}{h_1 - h_2} \quad (3.13-1)$$

which we may solve for h_2 as

$$h_2 = h_1 - \eta_T(h_1 - h_2^*). \quad (3.13-2)$$

The work done by the fluid on a unit mass basis W_{act} is then

$$W_{act} = h_1 - h_2 \quad (3.13-3)$$

If the state at the end of the expansion process turns out to be in saturated region, the quality x_2 can be easily calculated. The temperature T_2 is also now fixed since P_2, h_2 specify the state at the end of the actual expansion process.

3.14 Gas Cleanup System

The purpose of the gas cleanup system is to remove a significant amount of the undesirable species in the power gas produced in the coal gasifier. For example, as we shall see in Chapter 5, most of the sulfur in the coal combines with some of hydrogen present to form hydrogen sulfide, H_2S , with a smaller amount combining with carbon and oxygen to form carbonyl sulfide, CO_2S . Fortunately, as we saw in Chapter 2, there are many well-known processes which are designed to remove H_2S from a gas to just about any desired purity. In fact, as we have discussed in Section 2.2, this is one of the motivating reasons for gasifying the coal in the first place. A schematic representation is shown in Figure 3.14-1.

It is convenient to assume that the following parameters are known: the composition of the power gas into the gas cleanup system

on a mole fraction basis $\mu_{i,1}$; the pressure P_{G1} and temperature T_{G1} of the dirty power gas; the pressure P_{G2} of the clean power gas; the mass flow w_{G1} of the dirty power gas; and finally the removal efficiencies of the hydrogen sulfide, carbonyl sulfide, carbon dioxide, and ammonia vapor or η_{H_2S} , η_{COS} , η_{CO_2} , and η_{NH_3} , respectively.

Given the gas composition into the system on a mole fraction basis $\mu_{i,1}$ it is simple to convert it to a composition on a weight fraction basis $\omega_{i,1}$. Having done this, we can get the mass flow of the waste product stream w_{WPS} from

$$w_{WPS} = w_{G1} [\eta_{H_2S} \omega_{H_2S,1} + \eta_{COS} \omega_{COS,1} + \eta_{CO_2} \omega_{CO_2,1} + \eta_{NH_3} \omega_{NH_3,1}] \quad (3.14-1)$$

where, as above, the removal efficiencies η_i are defined to be the ratio of the mass of species i removed per unit mass present. The weight fractions $\omega_{i,2}$ of the gas leaving the system may now be adjusted by defining Ω as

$$\Omega = \sum_{i=1}^{10} (1-\eta_i) \omega_{i,1} \quad (3.14-2)$$

where the η_i are zero for those species which are not H_2S , COS , CO_2 , or NH_3 . Table 3.2-3 defines the species associated with each subscript i . Now we get the composition of the gas $\omega_{i,2}$ on a weight fraction basis leaving the cleanup system as

$$\omega_{i,2} = \omega_{i,1} / \Omega \quad (3.14-3a)$$

for all species but H₂S, COS, CO₂, and NH₃ and as

$$\omega_{i,2} = (1-n_i)\omega_{i,1}/\Omega \quad (3.14-3b)$$

for these species. The molecular weight of the gas v_{G2} out of the system is given by

$$v_{G2} = \sum_{i=1}^{10} \frac{\omega_{i,2}}{v_i} \quad (3.14-4)$$

where the v_i are the molecular weights of the individual species. The outlet gas composition $\mu_{i,2}$ on a mole fraction basis becomes

$$\mu_{i,2} = v_{G2} \frac{\omega_{i,2}}{v_i} \quad (3.14-5)$$

for each of the ten species in Table 3.2-3. The mole flow of gas m_{G2} out of the system becomes

$$m_{G2} = (w_{G1} - w_{WPS})/v_{G2} \quad (3.14-6)$$

At this point, we restrict our model to those sulfur removal processes which use water as the solvent. The gas leaving the cleanup system is then assumed to be saturated with water vapor. We further assume that T_{G2} is equal to T_{G1} . So the mole fraction of water vapor in the clean gas μ_{REQ} is given by

$$\mu_{REQ} = \frac{P_{sat}}{P_{G2}} \quad (3.14-7)$$

where P_{sat} is the saturation pressure corresponding to temperature T_{G2} .
 The number of moles of H_2O , m_{H_2O} , required to saturate the gas can be shown to be given by

$$m_{H_2O} = \frac{m_{G2}(\mu_{REQ} - \mu_{H_2O,2})}{1 - \mu_{REQ}} \quad (3.14-8)$$

and so the mass of water w_{H_2O} which is required is

$$w_{H_2O} = m_{H_2O} v_{H_2O} \quad (3.14-9)$$

The actual mass flow of clean saturated gas $w_{G2_{sat}}$ out of the system is

$$w_{G2_{sat}} = w_{G1} - w_{WPS} + w_{H_2O} \quad (3.14-10)$$

The mole fractions of the saturated gas $\mu_{i,2_{sat}}$ must be adjusted by

$$\mu_{i,2_{sat}} = \frac{m_{G2} \mu_{i,2}}{m_{G2} + m_{H_2O}} \quad (3.14-11)$$

Finally, the mole flow of clean saturated gas $m_{G2_{sat}}$ is given by

$$m_{G2_{sat}} = \frac{w_{G2_{sat}}}{v_{G2}} \quad (3.14-12)$$

It is then a simple matter to get the corresponding composition of the clean saturated gas on a mass fraction basis.

3.15 Throttle Valve

The throttle valve is a very simple component which is used to reduce the pressure of the incoming fluid. A schematic representation is shown in Figure 3.15-1. By neglecting changes in kinetic and potential energy and heat losses, we see that the first law of thermodynamics for this steady-flow process reduces to

$$h_1 = h_2 \quad (3.15-1)$$

where the specific enthalpies are denoted by h and the subscripts, 1 and 2, correspond to the incoming fluid at pressure P_1 and pressure P_2 , respectively.

Rather than combining the two possible fluids that we need to consider into one model, we shall develop one model for gas and one for steam. As one might expect, however, the calculations involved are very simple.

3.15.1 Throttle Valve for Mixture of Gases

In this model, we assume that the pressure P_1 and temperature T_1 of the incoming fluid are known, as well as the downstream pressure P_2 and the gas composition. From this information, the molar enthalpy \bar{h}_1 for the incoming gas is easily obtained from the gas tables. Equation (3.15-1) may be written in terms of molar enthalpies \bar{h} as

$$\bar{h}_1 = \bar{h}_2 \quad (3.15-2)$$

So the final state is completely specified by P_2 , \bar{h}_2 , and the gas composition. The temperature T_2 of the gas at the end of the throttling

process may then be obtained from the gas tables. It is this temperature T_2 that we need to know, since it inevitably will provide an input to another component model in our cycle.

3.15.2 Throttle Valve for Steam

We now assume that the pressure P_1 and the temperature T_1 (if superheated or subcooled) or steam quality x_1 (if saturated) for the incoming fluid are known, as well as the downstream fluid pressure P_2 . If the state of the incoming fluid is superheated or subcooled, we use P_1 and T_1 to determine h_1 . However, if the incoming fluid is saturated, we use P_1 and x_1 to determine h_1 . In any event, by Equation (3.15-1), we take h_2 to be equal to h_1 . Then with P_2 and h_2 fixed, we can with the help of the steam tables determine T_2 . Again, it is important to know the value of T_2 , since this temperature is inevitably an input (along with P_2) to another component model in the cycle.

3.16 Water Pump

The primary purpose of a water pump is to raise the pressure of the subcooled water by doing work on the fluid. If we assume the changes in kinetic and potential energy during the process and the heat loss from the fluid are negligible, then the first law for this steady-flow process reduces to

$$W_{\text{act}} = h_2 - h_1 \quad (3.16-1)$$

where h_1 and h_2 are the specific enthalpy of the fluid into and out of the pump, respectively, and W_{act} is the work required per unit mass of water. A schematic representation is shown in Figure 3.16-1

Again we denote the end of the isentropic process shown in Figure 3.16-2 by the prime ($'$) and using a definition of efficiency η_p similar to that of the air or gas compressor, we write

$$\eta_p = \frac{h_2' - h_1}{h_2 - h_1} \quad (3.16-2)$$

We find it convenient now to assume the following parameters are known: the pressure P_1 and temperature T_1 of the subcooled inlet to the pump, the outlet pressure P_2 , and the pump efficiency η_p .

Since we have a single species fluid, we may write

$$dh = v dP + T ds \quad (3.16-3)$$

from elementary thermodynamics, where v is the specific volume and T is the temperature of the fluid and dh , dP , and ds are infinitesimal changes in specific enthalpy, pressure, and specific entropy, respectively. But for an isentropic process,

$$ds = 0$$

and so

$$dh' = v dP \quad (3.16-4)$$

which may be integrated between the two states to give

$$h_2 - h_1 = \int_{P_1}^{P_2} v \, dP. \quad (3.16-5)$$

So Equation (3.16-1) becomes with the help of Equation (3.16-2) and the last equation

$$W_{\text{act}} = \frac{1}{\eta_p} \int_{P_1}^{P_2} v \, dP \quad (3.16-6)$$

Furthermore, since subcooled water is practically incompressible, we may approximate Equation (3.16-6) by taking the specific volume v in the integrand to be v_1 , a constant, and get

$$W_{\text{act}} = \frac{v_1}{\eta_p} (P_2 - P_1) \quad (3.16-7)$$

We then get h_2 from Equation (3.16-1) or

$$h_2 = h_1 + W_{\text{act}} \quad (3.16-8)$$

The solution procedure is obvious by now. We get v_1 and h_1 from the steam tables using P_1 and T_1 to define the state. We compute W_{act} according to Equation (3.16-7) and then h_2 from Equation (3.16-8). Then T_2 may be determined from the steam tables since P_2 and h_2 define this state. The appropriate conversion factors, of course, must be used to make the units consistent.

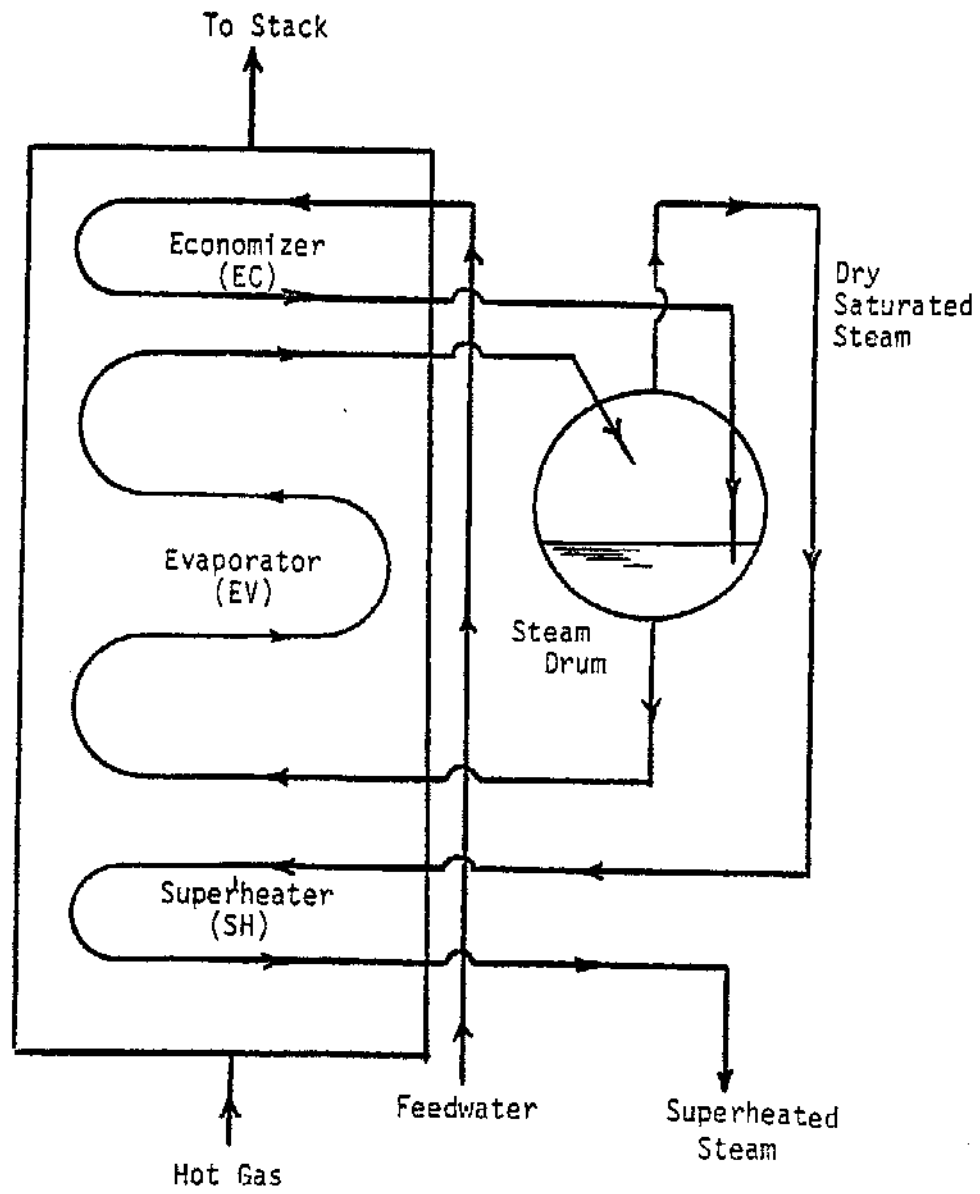


Figure 3.3-1 Schematic of Waste Heat Boiler

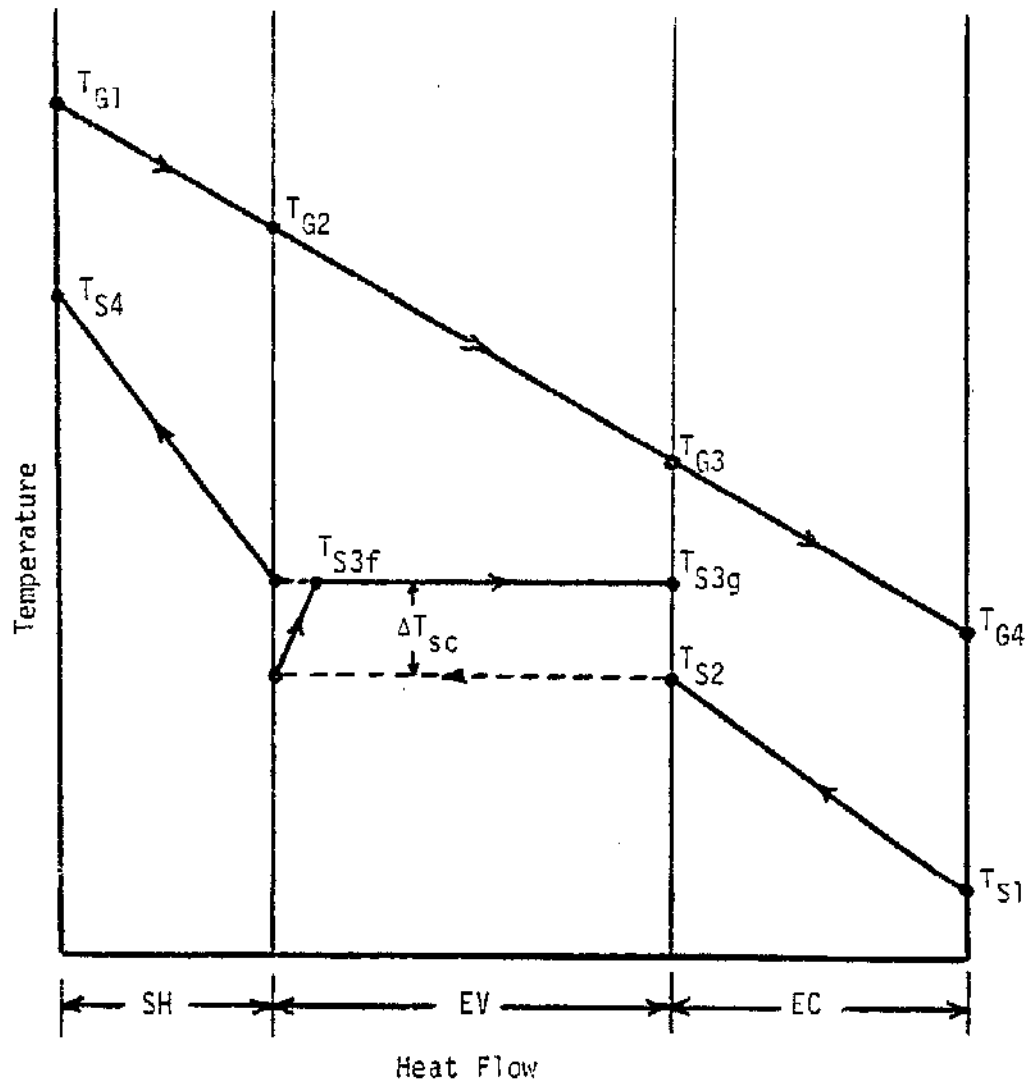


Figure 3.3-2 Temperature-Heat Flow Diagram for Waste Heat Boiler

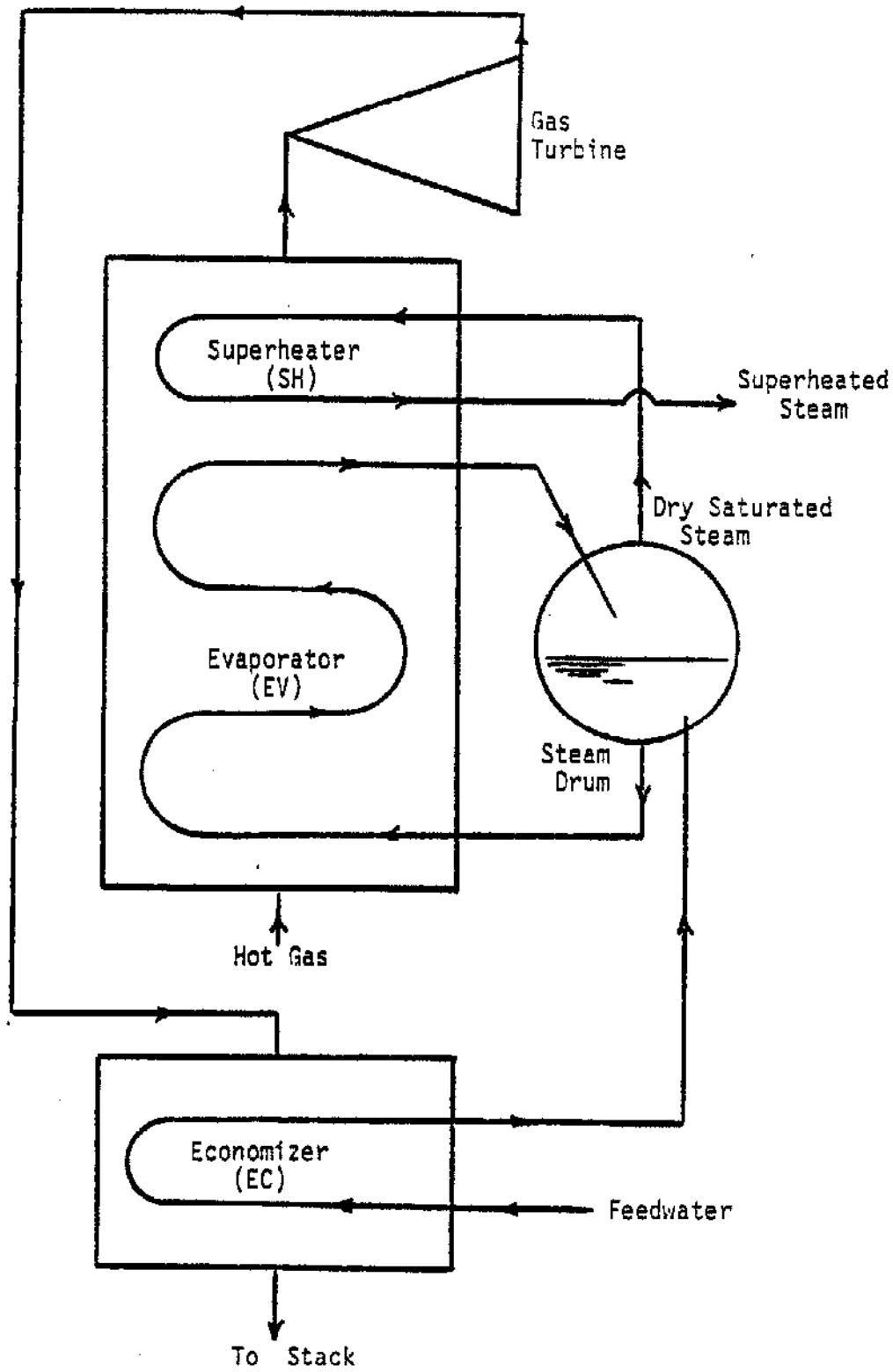


Figure 3.4-1 Schematic of Supercharged Boiler with Gas Turbine

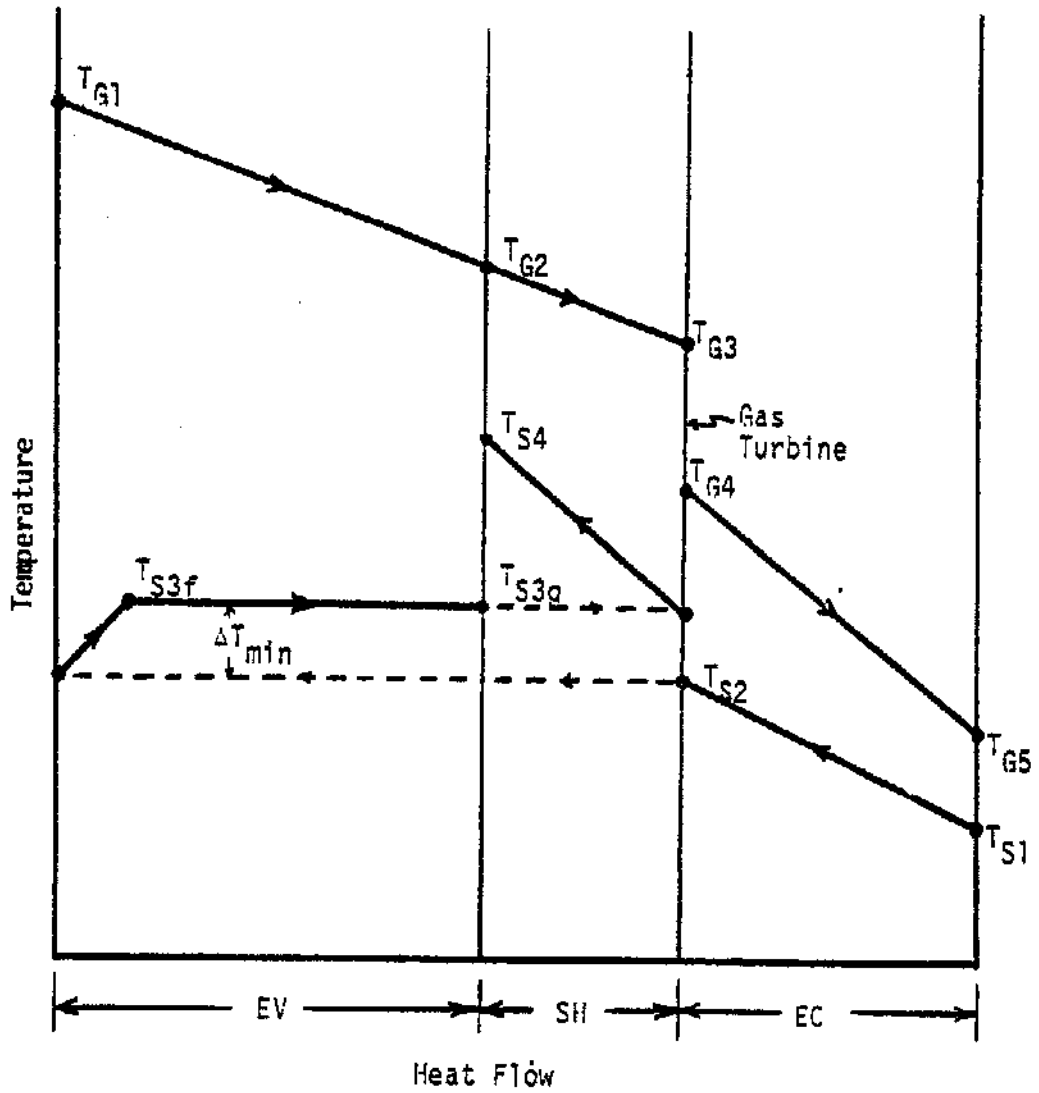


Figure 3.4-2 Temperature-Heat Flow Diagram for Supercharged Boiler

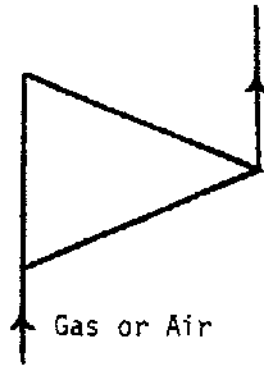


Figure 3.5-1 Schematic of Air and Gas Compressor

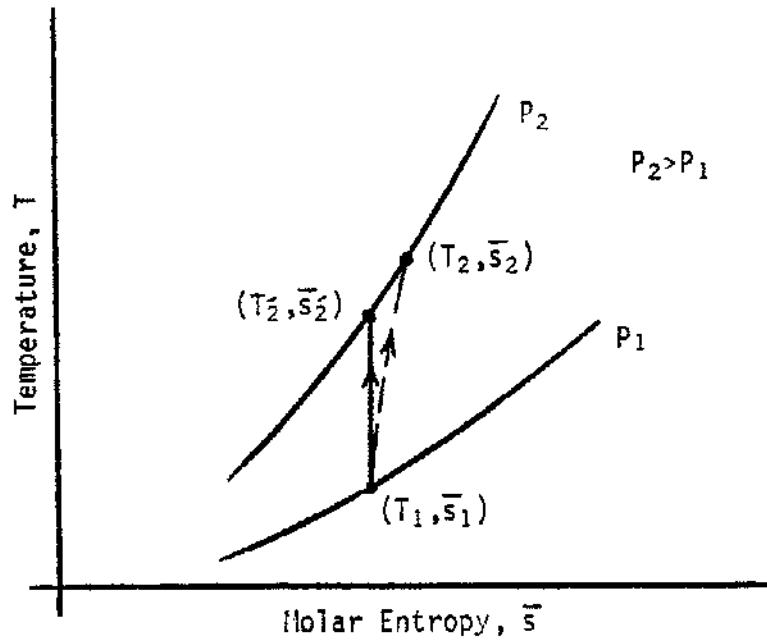


Figure 3.5-2 Temperature-Entropy Diagram for Compression of a Gaseous Fluid