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ANALYSIS OF THE COED PROCESS AND OPTIMIZATION OF FLUE GAS HEAT RECOVERY FROM A SECOND LAW PERSPECTIVE

by

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CHAPTER 1

INTRODUCTION

The United States depends extensively on fossil fuel imports for energy and chemicals. To reduce this foreign dependency and become energy self-sufficient we must convert alternate energy resources to liquid fuels and chemical feedstocks. Many forecasters predict that coal, oil shale, and tar sands among other nonrenewable energy resources can supply this country's energy needs for several hundred years once the technology is realized and the economics become attractive. Ultimately future energy resources will have to be renewable. A major renewable energy resource, biomass, results from the utilization of plant material, an accumulation of solar energy. In addition to these alternate energy resources the United States must proceed with a program of technological improvements in energy conservation since it is quite clear that energy will never again be as cheap and abundant as in the past.

With the rapidly rising cost of energy one area of conservation that has been receiving increased attention is improved waste heat recovery. The recovery of heat destined to be dissipated into the environment yields many benefits including a reduction in fuel consumption and reductions in air and water pollution because of the reduced heater and cooling tower loads. Thermodynamic analysis should play an important role in the development of energy conservation programs such as this one to correct current wasteful energy practices and in the development of alternate energy resources to help fend off foreign dependency.

Currently the Chemical Manufacturing Association as reported by Fallwell and Greek (1) is claiming to have reached their first goal of a 15% reduction in energy use through rather simple straightforward conservation techniques.

They have now set an energy conservation goal of yet another 15% by 1985. To achieve this additional savings more sophisticated conservation techniques must be employed that require full-scale plant-by-plant energy audits. These audits would determine which segments of the processes are the most inefficient, and they would show where capital can best be spent in order to realize a large energy savings. Second law analysis can be used most effectively to locate the process segment inefficiencies and determine which are the most inefficient. It can also be used to compare different design alternatives that correct these inefficiencies.

A thermodynamic analysis of a process can be based upon either the first or the second law of thermodynamics. The first law is an energy conservation principle whereas the second law assigns a quality or worth to energy. Each energy source has a certain potential to perform work related to the second law, i.e. a work equivalent. This is a function of temperature, pressure, chemical composition, and the environment in which it exists. For example, a million kcal of thermal energy in a waste flue gas stream at 500°F is most certainly worth more than the same amount of thermal energy in a wastewater stream at 150°F. In comparing the relative worths of energy sources the work equivalent is the best basis for comparison.

This idea may be extended to form a second law analysis thereby providing a common basis in which different process schemes can be compared and their inefficiencies identified. Although second law analyses have not been widely used, recently, several existing processes or industries have been examined in this manner (2, 3, 4, 5, 6). The second law analysis can be used throughout the development of a new process to determine which approaches utilize energy most efficiently and to identify areas of improvement. For example, currently the subject of Gasohol is attracting much attention and so are the two processes for manufacturing the required ethanol: the farming-fermentation process and the ethylene hydration process. Second law analyses (7) have shown that the farming fermentation route is roughly twice as energy efficient as the other route and that it has a greater potential for improvement than the other route to ethanol production. In this thesis the Char Oil Energy Development (COED) process (8) which has been researched extensively was chosen to illustrate the procedures and necessary considerations in order to apply the thermodynamic principles of this second law analysis to one alternate energy technology.

Second law analysis may also be used to carry out an optimization of a process design from the standpoint of an overall efficiency. The concepts of work equivalents or availabilities which are similar have recently been incorporated into heat exchange synthesis (9) and distillation system synthesis (10). These system syntheses, however, examine the heat exchange network in a general manner from an ultimately economic point of view. Here the optimization of a process design will be considered in detail from a totally thermodynamic point of view wherein the process will be designed for a maximum in the overall second law efficiency. That efficiency as will be discussed shortly is distinguished from the second law efficiency by the additional energy inputs and inefficiencies included therein. In this thesis a flue gas heat recovery process was chosen to illustrate this thermodynamic optimization of one energy conservation technology.

Specifically, the investigation herein will deal with the thermodynamic principles involved with the analysis and optimization of processes with the appropriate considerations needed to proceed with both. The fundamental principles involved with earlier and more recent thermodynamic analysis will be presented in the remainder of Part I while the second law analysis and thermodynamic optimization applications will be presented in Parts II and III respectively. This investigation will show that two different efficiencies may be used in a second law analysis and that each one has distinct advantages and disadvantages. Also the concept of an overall second law efficiency will be dealt with. This involves consideration of energy inputs and inefficiencies not normally included in an efficiency analysis or thermodynamic optimization. One such additional energy input is the energy associated with the fabrication of plant equipment and with the construction of a plant. This factor has not previously been included in efficiency analyses or thermodynamic optimizations. It will be discussed extensively in Chapter 8 with specific reference to its application to the COED plant. Additional inefficiencies that must be considered in an overall second law efficiency are those associated with raw materials processing and electrical generation. Finally an overall second law efficiency will be presented for the COED process and two thermodynamic optimums will be given for two corresponding definitions of the flue gas heat recovery system. The COED second law efficiency will be compared with the first law efficiency of that process, and one of the thermodynamic optimums of the flue gas heat recovery system will be compared with a corresponding economic optimum for that system.

CHAPTER 2

FIRST LAW ANALYSIS OF CHEMICAL PROCESSES

2.1 Derivation of the first law efficiency

This chapter deals with the first law approach in finding an efficiency for a chemical process. Until recently this has been the primary approach given in the literature for evaluating the energy efficiency of any process. Because most previous applications have lacked rigor it will be advantageous to examine the thermodynamic principles and to provide the basis for a general first law efficiency.

Specifically, the first law efficiency may be derived from the statement of the first law for an open steady-state system in which potential and kinetic energies have been ignored:

$$\Delta H = Q + W \tag{2.1}$$

where

ΔH = total change in enthalpy

Q = net heat flow across system boundaries with heat flow in being a positive quantity and heat flow out being a negative quantity

W = net shaft work between system and surroundings with the convention that work done on the system is positive and work done by the system is negative

The total enthalpy change may then be expressed in terms of the standard heat of reaction and the appropriate reactant and product heat effects:

$$\Delta H = \Delta H^o_{298} + \Delta H^o_P - \Delta H^o_R \tag{2.2}$$

where

ΔH^o_{298} = the standard heat of reaction at 298K and 1 atm

ΔH^o_P = enthalpy change as the products in their standard states are taken from 298K and 1 atm to their actual temperatures

ΔH^o_R = analogous enthalpy change for reactants

These terms can be expanded to represent the total enthalpy change of a general chemical process involving any number of chemical reactions as shown in Figure 1. This process has n reactant streams with molar flow rates r_1, r_2, ... r_i, ... r_n and m product streams with molar flow rates p_1, p_2, ... p_j, ... p_m with the sum of all heat flows equal to Q and the sum of all work exchanges equal to W. The components of ΔH may now be expressed in the following manner:

$$\Delta H^o_{298} = \sum_{j=1}^{m} p_j \; \Delta H_j^f - \sum_{i=1}^{n} r_i \; \Delta H_i^f \tag{2.3}$$

$$\Delta H^o_P = \sum_{j=1}^{m} p_j \; Cp_j \; (T_j - T_o) \tag{2.4}$$

$$\Delta H^o_R = \sum_{i=1}^{n} r_i \; Cp_i \; (T_i - T_o) \tag{2.5}$$

where

ΔH_a^f = standard heat of formation for component a (a = i or j)

Cp_a = constant pressure heat capacity for component a (a = i or j) with units consistent with those of ΔH^o

T_o = reference temperature of 298K

Next, the total standard heat of combustion is formed for the reactants and products in terms of standard heats of formation. The chemical species are taken to be composed of the elements C, H, O, N, and S and the combustion equation for an arbitrary species i is

$$C_{\alpha_i} H_{\beta_i} O_{\gamma_i} N_{\delta_i} S_{\lambda_i} + (\alpha_i + \frac{\beta_i}{4} - \frac{\gamma_i}{2} + \lambda_i) O_2$$

$$= \alpha_i CO_2 + \frac{\beta_i}{2} H_2O + \frac{\delta_i}{2} N_2 + \lambda_i \; SO_2 \tag{2.6}$$

In this equation N_2 was taken as the oxidation product instead of NO_x because of the unfavorable equilibrium of the latter for all but very high temperatures. The H_2O is either liquid or vapor depending upon the method

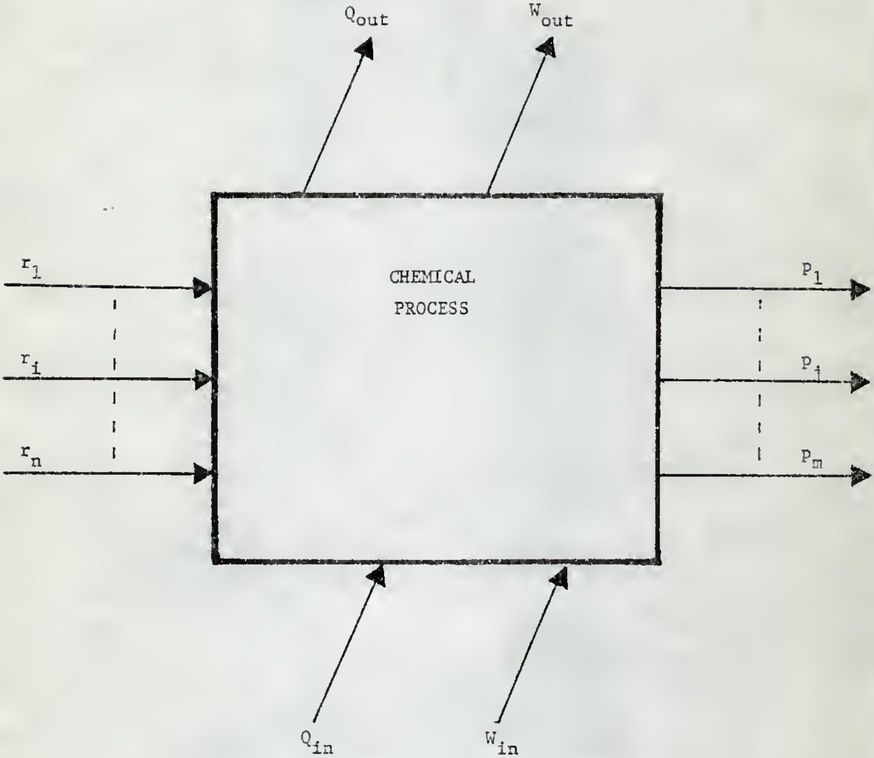


Figure 1. A General Chemical Process

of calculating ΔH which will be considered in section 2.2. The standard heat of combustion for compound i is

$$\Delta H_i^c = \alpha_i \Delta H_{CO_2}^f + \frac{\beta_i}{2} \Delta H_{H_2O}^f + \lambda_i \Delta H_{SO_2}^f - \Delta H_i^f \tag{2.7}$$

Using this equation, the total standard heat of combustion for reactants, ΔH_R^c, and for products, ΔH_P^c, is found:

$$\Delta H_R^c = \Delta H_{CO_2}^f \sum_{i=1}^{n} r_i \alpha_i + \Delta H_{H_2O}^f \sum_{i=1}^{n} r_i \frac{\beta_i}{2} + \Delta H_{SO_2}^f \sum_{i=1}^{n} r_i \lambda_i - \sum_{i=1}^{n} r_i \Delta H_i^f \tag{2.8}$$

$$\Delta H_P^c = \Delta H_{CO_2}^f \sum_{j=1}^{m} p_j \alpha_j + \Delta H_{H_2O}^f \sum_{j=1}^{m} p_j \frac{\beta_j}{2} + \Delta H_{SO_2}^f \sum_{j=1}^{m} p_j \lambda_j - \sum_{j=1}^{m} p_j \Delta H_j^f \tag{2.9}$$

Elemental balances show that ΔH_{298}^o can be expressed as a combination of ΔH_R^c and ΔH_P^c. The elemental balances are

$$\sum_{i=1}^{n} r_i \alpha_i = \sum_{j=1}^{m} p_j \alpha_j \tag{2.10}$$

$$\sum_{i=1}^{n} r_i \frac{\beta_i}{2} = \sum_{j=1}^{m} p_j \frac{\beta_j}{2} \tag{2.11}$$

$$\sum_{i=1}^{n} r_i \lambda_i = \sum_{j=1}^{m} p_j \lambda_j \tag{2.12}$$

Conceptually these are seen to be true because the amount of a combustion product such as CO_2 produced from the combustion of the reactants equals the amount likewise obtained from the products. Using these equalities Eq. (2.9) is subtracted from Eq. (2.8) giving

$$\Delta H_R^c - \Delta H_P^c = \sum_{j=1}^{m} p_j \Delta H_j^f - \sum_{i=1}^{n} r_i \Delta H_i^f \tag{2.13}$$

Comparison with Eq. (2.3) reveals that

$$\Delta H^o_{298} = \Delta H^c_R - \Delta H^c_P \tag{2.14}$$

Eq. (2.2) then becomes

$$\Delta H = \Delta H^c_R - \Delta H^c_P + \Delta H^o_P - \Delta H^o_R \tag{2.15}$$

Now, this result is combined with the first law statement to obtain a basic equality for the energy out terms with the energy in terms. First, Eq. (2.15) is substituted into Eq. (2.1). Second, Q and W are replaced by Q_{in}, Q_{out}, W_{in}, and W_{out} where for convenience these quantities are taken to be positive. These actions result in

$$\Delta H^c_R - \Delta H^c_P + \Delta H^o_P - \Delta H^o_R = Q_{in} - Q_{out} + W_{in} - W_{out} \tag{2.16}$$

Rearranging yields

$$\Delta H^c_P - \Delta H^o_P - W_{out} - Q_{out} = \Delta H^c_R - \Delta H^o_R - W_{in} - Q_{in} \tag{2.17}$$

The equation is now multiplied through by -1 to give

$$-\Delta H^c_P + \Delta H^o_P + W_{out} + Q_{out} = -\Delta H^c_R + \Delta H^o_R + W_{in} + Q_{in} \tag{2.18}$$

Because all heats of combustion are always negative $-\Delta H^c$ will be written as an absolute value, $|\Delta H^c|$. Also, because most processes occur with $T_i > 298$ and $T_j > 298$ it should be noted that ΔH^o_P and ΔH^o_R will almost always be positive. This results in the following general first law statement:

$$|\Delta H^c_P| + \Delta H^o_P + W_{out} + Q_{out} = |\Delta H^c_R| + \Delta H^o_R + W_{in} + Q_{in} \tag{2.19}$$

Again, it should be remembered that when using this equation all Q and W terms are taken as positive. Thus, each term in Eq. (2.19) is expected to be positive making each side of the equation equal to the sum of all types of energy associated with inputs or outputs.

This equality should serve well as a basis for defining the first law efficiency. This efficiency can be expressed as all of the utilized energy out divided by all of the energy in. The situation when all forms of energy are realized to their full potential will be termed the unity case because for that situation the first law efficiency, η_{1st}, equals unity. It should be noted, however, that if all possible inputs are considered it is not possible to have a first law efficiency greater than unity. If any form of energy resulting from the process is not realized to its full potential η_{1st} is less than unity. For example, some conditions that would cause η_{1st} to be less than unity are

1. incomplete combustion resulting in a product such as CO in the stack gas
2. nonrecovery of the sensible heat, $\Delta H^o_{P_j}$, of a product
3. mechanical inefficiencies resulting in a heat flow to the surroundings
4. heat loss to the surroundings

2.2 Calcualtion of ΔH

Bailie and Douer (11) have defined a first law efficiency whose numerical value depends upon the type of thermochemical data used to evaluate ΔH. Even though their formalization was not precise their definition is essentially the same as the one given in the previous section wherein the first law efficiency equals utilized energy out divided by total energy in. They considered heat of formation, higher heating value, and lower heating value data in the calculation of a first law efficiency. They pointed out that the higher heating value data are primarily used in combustion processes and that for most other types of chemical processes the heat of formation data are used. They analyzed a simple conversion system utilizing the reaction $CH_4 = C + 2H_2$. In this example the carbon product was considered waste. The first law efficiencies they calculated were 0, 0.64, and 0.60 corresponding to the use of heat of formation, higher heating value, and lower heating value data respectively.

Using these methods of calculating ΔH three different efficiencies are obtained, however, only two of these are realistic. First, consider calculation of ΔH from heat of formation data. It is possible to show through manipulation of Eqs. (2.1), (2.2), and (2.3) that

$$\Delta H_P^f + \Delta H_P^o + Q_{out} + W_{out} = \Delta H_R^f + \Delta H_R^o + Q_{in} + W_{in} \qquad (2.20)$$

Hence it is thermodynamically legitimate to use the above as the basis of an efficiency, however, it is not physically significant to refer the enthalpy of species to their elements when the energy possessed by any species is realized through an oxidation process. Thus it seems more realistic to refer specie enthalpies to oxidation products by using heats of combustion. In this way ridiculous and meaningless results such as those obtained by Bailie and Doner will be avoided. Next, consider the calculation of ΔH from heat of combustion data for two general chemical process cases. In the first case the chemical process does not involve water in the reactant or product streams. As pointed out by Bailie and Doner in their example the higher and lower heating value data yielded two different first law efficiencies. This is seen to be justifiable because as long as the $\Delta H_{H_2O}^f$ and ΔH_i^f terms in Eqs. (2.7), (2.8), and (2.9) are handled consistently (both referring to same H_2O standard state) either heat of combustion method can correctly be used to calculate ΔH. In the second case the chemical process does involve water in the reactant and/or product streams. Here in order to correctly apply both methods of calculating ΔH, the higher and lower heating value methods, the $\Delta H_{H_2O}^f$ and ΔH_i^f

terms in Eqs. (2.7), (2.8), and (2.9) must again be handled consistently with respect to water's reference state, but also the latent heat of vaporization of water must be either added to or subtracted from Eqs. (2.4) and (2.5) when appropriate. This again will lead to two different first law efficiencies, however, in both of the cases considered the higher heat of combustion method is perhaps preferred because it uses the maximum energy obtainable from any stream in the efficiency calculations. It should be noted, however, that the difference between these two first law efficiencies is expected to be small.

CHAPTER 3

THEORETICAL APPROACH TO SECOND LAW ANALYSIS

3.1 Previous work

This chapter deals with the second law approach in determining an efficiency for a chemical process. Two approaches to this thermodynamic efficiency analysis based on the second law have been given in the literature.

Denbigh (5) delineated the first approach and applied it in his analysis of an ammonia oxidation process. He used the concept of availability to calculate the actual and the ideal work associated with the process. With this information Denbigh found what he termed the thermodynamic efficiency for the ammonia oxidation process. Specifically, he obtained an efficiency of 0.06 for that process. Denbigh recognized that for all practical purposes large scale industrial reactions could not be carried out reversibly so under that limitation an efficiency of unity was not possible. He therefore propcsed the concept of a "prescribed degree of irreversibility" in which chemical reactions and the mixing of reagents are allowed to proceed irreversibly. The reactions' heat effects, however, are realized in a reversible manner and all other physical or mechanical operations are assumed reversible. Using this concept Denbigh calculated a new efficiency, the practical efficiency. He found that efficiency to be 0.11 for the ammonia oxidation process.

The other approach was given by Gyftopolous, Lazaridis, and Widmer (4) who used the concept of available useful work to evaluate the potential for more effective use of fuel. They evaluated the second law efficiency of several basic industries. Riekert (6) formalized this approach and its environmental datum. He employed the available useful work, which he called the work equivalent, to calculate the "efficiency of energy utilization." Riekert calculated that efficiency for an ammonia oxidation process similar to Denbigh's and found an efficiency of 0.16. He explained the discrepancy with Denbigh in the differences in their approaches even though he assumed slightly different operating conditions. Specifically, Riekert counted the work equivalent of the product as an output whereas Denbigh gave the product no value. Riekert's approach will be considered in this chapter.

He defined the work equivalent as the maximum work obtainable when a substance is moved reversibly into equilibrium with a specified environment. The work equivalent may be developed from the statement of the first law for an open steady-state system in which potential and kinetic energies have been ignored, Eq. (2.1). Since the processes taking place are reversible

$$Q = \int TdS \tag{3.1}$$

where

T = heat transfer temperature

dS = differential entropy

Substitution into the first law statement, Eq. (2.1), yields an equation for the maximum shaft work done by the system which after multiplication by -1 is

$$W_{max} = \Delta H - \int TdS \tag{3.2}$$

For the case where the only transfer of heat takes place reversibly at constant temperature, T_o, Eq. (3.2) becomes

$$W_{max} = \Delta H - T_o\Delta S \tag{3.3}$$

If a reference state with properties (T_o, H_o, S_o) exists from which no work can be obtained through interaction with the environment, then the work equivalent, ε, may be defined as

$$\varepsilon = H - H_o - T_o (S - S_o) \tag{3.4}$$

For a homogeneous mixture containing n_i moles of species i a partial molar work equivalent can be defined

$$\varepsilon = \sum_i n_i \varepsilon_i = H - H_o - T_o (S - S_o) \tag{3.5}$$

where

$$\varepsilon_i = H_i - H_{oi} - T_o (S_i - S_{oi}) \tag{3.6}$$

is the partial molar work equivalent of species i in the mixture with respect to the environment.

Riekert considered the environment to be fixed with respect to temperature, T_o, pressure, p_o, and datum level components. These datum level components are assumed to be available from the environment in "unlimited" supply without any expenditure of work. This is analogous to an infinite heat reservoir of temperature T_o. The properties of the datum level components imply that no work can be obtained from them at T_o and p_o, i.e. $\varepsilon = 0$. This would prohibit spontaneous chemical reactions between these components at T_o and p_o. In addition the work equivalent ε_i of any compound i in equilibrium at T_o and p_o with the datum level components is zero. It may be noted that the datum level of a specific element is the state of that element as it exists in "unlimited" supply in the environment. Another property of the datum level components is that they provide the set of reference properties (H_{oi}, S_{oi}) in Eq. (3.6). These reference properties are determined from the manner in which substance i is in equilibrium with the environment, i.e. by itself or as part of a mixture.

3.2 Two efficiency definitions

Work equivalents may be calculated for all the process streams and utilities associated with a given process. In order to do this and then determine an efficiency a large amount of information must be gathered - temperature, pressure, composition, and flow rates of all streams entering or leaving the process, the work inputs and outputs, and the heat inputs and outputs with their temperature levels. Once this is accomplished either one of the two following efficiencies may be found.

The first of these, the second law efficiency or efficiency of energy utilization according to Riekert, is defined on a unit time basis as the total work equivalent output in all the useful outgoing streams divided by the total work equivalent input or

$$\eta = \frac{\varepsilon_{out} + W_{out}}{\varepsilon_{in} + W_{in}} \tag{3.7}$$

The W_{in} and W_{out} refer to the total in and out work equivalents of utilities such as shaft work, steam, condensate, and fuel gas. In this efficiency definition the work equivalent of any stream is zero when it is unutilized and it disappears into the environment. If all possible inputs are considered it is not possible for the second law efficiency to be greater than unity. This efficiency is seen to be analogous to the first law efficiency defined in Chapter 2 where energy has been replaced by the work equivalent.

The other efficiency, Denbigh's thermodynamic efficiency, is referred to here as the incremental efficiency. It is defined on a unit time basis as a ratio of the ideal work involved with the process streams' transformations to the actual work equivalent that brought about these changes. For a work-requiring process the incremental efficiency is

$$\eta_I = \frac{\varepsilon_{out} - \varepsilon_{in}}{W_{net}} \tag{3.8}$$

For a work producing process the inverse of Eq. (3.8) equals η_I. As with the first and second law efficiencies the incremental efficiency cannot be greater than unity if all possible inputs are considered. However, in contrast with these two prior efficiencies the incremental efficiency can be less than zero. Negative values can occur when many of the product streams are unutilized in a work requiring process.

While the second law or absolute efficiency measures the effectiveness of the entire process, often the large work equivalents associated with high energy chemical streams can overshadow the physical work terms which are more often identified with fuel utilization. In this regard Gyftopolous et al. (4) have shown that the absolute efficiency for petroleum refining is 0.91, but the incremental efficiency, which measures fuel utilization, is only 0.09. This difference between the two efficiencies will further be examined in Chapter 6 in light of a specific process evaluation.

CHAPTER 4

WORK EQUIVALENT CALCULATIONS

4.1 Datum level components

In this chapter the method of calculating work equivalents in a specific environment will be detailed. As discussed in the previous chapter the environment must be specified with respect to temperature, pressure, and datum level components. The environment considered here is fixed with respect to these properties:

(a) $T_o = 298K$

(b) $p_o = 1.0$ atm

(c) Datum level components:

$N_{2(g)}$: $x_{N_2} = 0.79$

$O_{2(g)}$: $x_{O_2} = 0.21$

$CO_{2(g)}$: $x_{CO_2} = 0.000314$

$H_2O_{(\ell)}$: $x_{H_2O} = 1.0$

$CaSO_4 \cdot 2H_2O_{(s)}$: $x_{CaSO_4 \cdot 2H_2O} = 1.0$

$CaCO_3(s)$: $x_{CaCO_3} = 1.0$

Riekert (6) considered stack gases to be part of his environment so he used 0.17 as the CO_2 mole fraction. So as to be more general the environment considered here does not include stack gases thus the value used above is the mole fraction of CO_2 in air. The last two components listed above, gypsum ($CaSO_4 \cdot 2H_2O$) and limestone ($CaCO_3$), provide for the calculation of a work equivalent for sulfur. The $CaSO_4 \cdot 2H_2O$ was used as a sulfur source because of its reactive stability, i.e., a very low Gibbs free energy of formation, ΔG_f^o, and because it exists in plentiful supply. Likewise $CaCO_3$ was chosen as a calcium source for similar reasons. In general a datum level component should be abundant in the environment and should not react with other datum level components; this implies a low ΔG_f^o. The state of aggregation of datum level components should also be considered. If it is a liquid or gas the mole fraction is important. If it is a solid then its interaction with water can be important. For example, a solid can become hydrated or it can dissolve. If the latter occurs the component's datum level state must be aqueous so that solution affects can be accounted for.

4.2 Standard state work equivalents

For the environmental properties described in the previous section the work equivalents of the elements N_2, O_2, H_2, C, and S in their pure forms at T_o and p_o, the standard state, can be calculated. These standard state work equivalents, ε_i^o's of pure N_2, O_2, and CO_2 are equal to their standard free energies of unmixing from the environment. For example, $\varepsilon_{O_2}^o$ is calculated from

$$\varepsilon_{O_2}^o = -RT_o \ln x_{O_2} \tag{4.1}$$

Using these air derived values, H_2 and C can be calculated from the H_2O and CO_2 formation reactions. The change in the standard state work equivalent for these reactions equals the standard free energy of formation.

$$\cancelto{0}{\varepsilon_{H_2O}^o} - \varepsilon_{H_2}^o - \frac{1}{2}\varepsilon_{O_2}^o = \Delta G_{f\ H_2O}^o \tag{4.2}$$

$$\varepsilon_{CO_2}^o - \varepsilon_C^o - \varepsilon_{O_2}^o = \Delta G_{f\ CO_2}^o \tag{4.3}$$

The work equivalent for water in Eq. (4.2) is set equal to zero because liquid water is a datum level component.

To calculate ε_s^o the compound $CaSO_4 \cdot 2H_2O$ is taken to be the stable configuration of sulfur. Sulfur is put into this compound from $CaCO_3$, the stable source of Ca. The reaction to bring sulfur or a sulfur compound into equilibrium with the environment is

$$SO_3 + CaCO_3 + 2H_2O = CaSO_4 \cdot 2H_2O + CO_2 \qquad (4.4)$$

It is noted that ε_i^o's are available for all of these components except for SO_3, thus $\varepsilon_{SO_3}^o$ may be calculated from Eq. (4.5) after the standard free energy of reaction, ΔG^o, is determined.

$$\varepsilon_{CO_2}^o + \cancelto{0}{\varepsilon_{CaSO_4 \cdot 2H_2O}^o} - \varepsilon_{SO_3}^o - \cancelto{0}{\varepsilon_{CaCO_3}^o} - 2\,\cancelto{0}{\varepsilon_{H_2O}^o} = \Delta G^o \qquad (4.5)$$

Next, ε_s^o is calculated from the formation reaction of SO_3

$$\varepsilon_{SO_3}^o - \varepsilon_s^o - \frac{3}{2}\,\varepsilon_{O_2}^o = \Delta G_{f\ SO_3}^o \qquad (4.6)$$

The standard state work equivalent of any substance containing C, H, O, N, and S can be calculated using the previous results if standard free energy of formation data are known. This is achieved through

$$\varepsilon_{C_\alpha H_\beta O_\gamma N_\delta S_\lambda}^o = \alpha\varepsilon_c^o + \frac{1}{2}\,\beta\varepsilon_{H_2}^o + \frac{1}{2}\,\gamma\varepsilon_{O_2}^o + \frac{1}{2}\,\delta\varepsilon_{N_2}^o + \lambda\varepsilon_s^o + \Delta G_{f\ C_\alpha H_\beta O_\gamma N_\delta S_\lambda}^o \qquad (4.7)$$

The standard state work equivalents for N_2, O_2, H_2, C, and S are given in Table 1. It may be noted that with the proper selection of datum level components and with the above procedure a consistent set of ε_i^o's for all the elements should be obtainable.

4.3 Heat of combustion approximations

For complex hydrocarbons such as coal and coal-derived oils the method for finding standard state work equivalents cannot be applied because of the absence of ΔG_f^o data. Therefore the approximation that ε_i^o is equal to the standard heat of combustion, ΔH_{298}^c $(H_2O_{(\ell)})$, must be considered. Table 2 compares these two values calculated for several groups of hydrocarbons, including coal tar constituents (12), for which ΔG_f^o data could be found. This table shows that for hydrocarbons the ratio $-\varepsilon_i^o/\Delta H_{298}^c$ increases as the

TABLE 1. Standard State Work Equivalents for Basic Substances

Substance	State	ε_i^{o}(298K, 1 atm) kcal/kmol
N_2	g	143
O_2	g	932
H_2	g	65224
C	c, graphite	98112
S	c, rhombic	139660

Table 2. A Comparison of ε_i^o and ΔH_{298}^c for Various Compounds*

Compound	ε_i^o kcal/kmol	$-\Delta H_{298}^c$ kcal/kmol	$-\varepsilon_i^o/\Delta H_{298}^c \times 100$
Normal Alkane -			
CH_4	198420.	212820.	93.23
C_2H_6	357040.	372810.	95.77
n-C_4H_{10}	669820.	687640.	97.41
n-C_8H_{18}	1294830.	1317440.	98.28
n-$C_{20}H_{42}$	3170980.	3206750.	98.88
Cyclic Alkane -			
C_6H_{12}	933600.	944780.	98.82
trans - $C_{10}H_{18}$	1504690.	1511790.	99.53
**Benzoid Aromatic- Monocylic:			
C_6H_6	788340.	789080.	99.91
C_7H_8	939840.	943580.	99.60
p-xylene C_8H_{10}	1094970.	1098280.	99.70
Bicyclic:			
tetralin $C_{10}H_{12}$	1358360.	1357010.	100.10
napththalene $C_{10}H_8$	1259460.	1249860.	100.77
α-methylnaphthalene $C_{11}H_{10}$	1412390.	1404080.	100.59
biphenyl $C_{12}H_{10}$	1525400.	1513720.	100.77
Tricylic:			
anthracene $C_{14}H_{10}$	1733930.	1713270.	101.21
phenanthrene $C_{14}H_{10}$	1728290.	1707780.	101.20
Oxygenated			
phenol C_6H_6O	749490.	746230.	100.44
p-cresol C_7H_8O	904300.	901660.	100.29
**Heterocyclic Aromatic-			
pyridine	676650.	674550.	100.31

Table 2 - Continued

Compound	ε_i^o kcal/kmol	$-\Delta H_{298}^c$ kcal/kmol	$-\varepsilon_i^o/\Delta H_{298}^c \times 100$
Biochemicals -			
Amino Acids:			
L-Alanine $C_2H_5O_2N$	403340	387210	104.17
L-Aspartic Acid $C_4H_7O_4N$	415730	372720	108.62
L-Cysteine $C_3H_7O_2NS$	549300	532200	103.21(118.3)***
Glycine $C_2H_5O_2N$	248870	232600	106.99
L-Glutamic Acid $C_5H_9O_4N$	540700	537450	106.19
L-Leucine $C_6H_{13}O_2N$	871380	856090	101.79
L-Tyrosine $C_9H_{11}O_3N$	1096070	1058450	103.55
L-Tryptophan $C_{12}H_{13}O_2N_2$	1515340	1472870	102.88
Monosaccharides:			
D-Glucose $C_6H_{12}O_6$	711210	669950	106.16
Galactose $C_6H_{12}O_6$	711210	669950	106.16
Disaccharides:			
β-Lactose $C_{12}H_{22}O_{11}$	1426410	1346000	105.97
Maltose $C_{12}H_{22}O_{11}$	1388330	1349300	102.89
Sucrose $C_{12}H_{22}O_{11}$	1431750	1348200	106.20

* 298K, 1 atm, ideal gas

** aromatic constituents of coal tar (12)

*** ΔH_{298}^c calculated from ΔH^f = -127880 kcal/kmol with products of N_2, $H_2O_{(\ell)}$, CO_2, and SO_2

Thermodynamic data - (13), (14), (15), and (16) carbon to hydrogen ratio increases and in most cases as the molecular weight increases. These results will be taken as empirical and no explanation will be offered. Therefore, in the light of these results the assumption that ε_i^o equals $-\Delta H_{298}^c$ will be used in the case of highly aromatic coal products. This application to coal seems reasonable since Whitehurst (17) has suggested that bituminous coals have an aromaticity of approximately 60% and contain significant amounts of polycylic aliphatic rings.

Another class of compounds of interest are the biochemicals. They, in the form of biomass, may be important in alternate energy conversion technologies therefore second law analysis is appropriate and consequently standard state work equivalents will be needed. Since ΔG_f^o data, and for that matter ΔH_{298}^c data, are seldom available several approximations are needed. First, the heat of combustion approximation will be considered. The latter part of Table 2 deals with applying this approximation to some biomass related compounds for which thermodynamic data are available. The work equivalent - heat of combustion comparison ratios, $-\varepsilon_i^o/\Delta H_{298}^c$'s, for the biochemical compounds are seen to be slightly larger than those for the hydrocarbon compounds. Also, these data suggest that in actual biochemical calculations it may be desirable to let ε_i^o equal 1.05 ΔH_{298}^c rather than equating them one to one. It should be pointed out that this work equivalent - heat of combustion approximation has been established for compounds containing C, H, O, and N. The assumption may not be valid for other types of compounds. For instance, look at this assumption as it applies for carbon and sulfur. The combustion reactions and heats of combustion for these elements are

$$C + O_2 = CO_2 \qquad -\Delta H_{298}^c = 94051 \text{ kcal/kg}$$

$$S + O_2 = SO_2 \qquad -\Delta H_{298}^c = 70960 \text{ kcal/kg}$$

For comparison the standard state work equivalents for carbon and sulfur are 98112 and 139660 kcal/kg respectively. Thus for carbon the comparison ratio is about one but for sulfur it is about two. Clearly, the work equivalent - heat of combustion approximation is invalid for sulfur. This may be explained in that sulfur's combustion product, SO_2, is a datum heat of combustion product, zero energy value, but it is not a work equivalent datum component. Therefore, the addition of sulfur increases the heat of combustion a specific amount, but it increases the work equivalent by more than that amount since a significant amount of work can be obtained from SO_2 as it is moved reversibly into equilibrium with the environment. It may be noted that for this reason the comparison ratio for sulfur-containing L-cysteine is somewhat higher than that for other amino acids when ΔH^c_{298} calculated from ΔH^f data with standard combustion products is used instead of the literature value of the heat of combustion.

The second approximation concerns estimating the heat of combustion. To discuss this it is instructive to consider the problem of estimating the heat of combustion for wheat. Minkevich, Eroshin, and coworkers (18) found that based on the following reaction

$$CH_pO_nN_q + \frac{\gamma_b}{4} O_2 = CO_2 + \frac{1}{2} (p - 3q)H_2O + qNH_3 \tag{4.8}$$

the heat of combustion of a wide variety of organic material is

$$\Delta H^c_{298} = 27\gamma_b \text{ kcal/g mole C} \tag{4.9}$$

where

$$\gamma_b = 4 + p - 3q - 2n$$

Thus, if the elemental composition of wheat is known ΔH^c_{298} can be estimated. However, in the likely event that the composition of wheat is unknown further approximations must be made. Minkevich et al. also found that for most biomass γ_b is about 4.29 and that the weight fraction of carbon is about 0.462. This weight fraction corresponds to 0.0385 g mole C per g biomass and results in $\Delta\hat{H}^c_{298}$ = 2025 kcal/lb (4460 cal/g) for biomass. Therefore, this $\Delta\hat{H}^c_{298}$ value estimates the heat of combustion for dry wheat. For comparison Merrill and Watt (19) report a value of 4.03 kcal/g or 1828 kcal/lb for wheat containing 10.8% moisture. If the heat of combustion estimate for dry wheat is corrected for 10.8% moisture then this estimate becomes 1806 kcal/lb which is very close to the reported value. It would appear that the approximation of $\Delta\hat{H}^c_{298}$ = 2025 kcal/lb (4460 cal/g) for biomass is reasonable; in the absence of other data this combined with the empirically established equality of ε_i^o and ΔH^c_{298} at best allows ε_i^o to be estimated for biomass.

4.4 Total work equivalent

To arrive at the total work equivalent for a substance both the standard state work equivalent, ε_i^o, and the change in work equivalent, $\Delta\varepsilon_i$, to another state (T, p, x_i) must be calculated. Using the molar work equivalent as an approximation for the partial molar work equivalent in Eq. (3.6), $\Delta\varepsilon_i$'s follow from that equation's partial derivatives. In the following derivations the ideal gas and the ideal solution assumptions are used. First, take the partial derivative of Eq. (3.6) with respect to temperature to obtain

$$\frac{\partial\varepsilon_i}{\partial T} = \frac{\partial H_i}{\partial T} - T_o \frac{\partial S_i}{\partial T} \qquad \text{(constant p and } x_i) \qquad (4.10)$$

Next, apply the constant pressure heat capacity relations to arrive at

$$\frac{\partial\varepsilon_i}{\partial T} = (1 - \frac{T_o}{T})\ Cp_i \qquad \text{(constant p and } x_i) \qquad (4.11)$$

This equation may be integrated with a two parameter heat capacity equation, $Cp_i = a_i + b_i T$, from T_o to T to give

$$\Delta\varepsilon_{i_T} = (a_i - b_i T_o)(T - T_o) + \frac{1}{2} b_i (T^2 - T_o^2) - a_i T_o \ln T/T_o \quad (4.12)$$

For constant heat capacity Eq. (4.11) becomes

$$\Delta\varepsilon_{i_T} = Cp_i (T - T_o - T_o \ln T/T_o) \quad (4.13)$$

Now, take the partial derivative of Eq. (3.6) with respect to pressure to find

$$\frac{\partial\varepsilon_i}{\partial p} = \frac{\partial H_i}{\partial p} - T_o \frac{\partial S_i}{\partial p} \qquad \text{(constant T and } x_i) \quad (4.14)$$

Then apply the proper thermodynamic identities to obtain these results

$$\left(\frac{\partial\varepsilon_i}{\partial p}\right)_{T,x_i} = V_i - T\left(\frac{\partial V_i}{\partial T}\right)_{p,x_i} + T_o \left(\frac{\partial V_i}{\partial T}\right)_{p,x_i} \quad (4.15)$$

$$\left(\frac{\partial\varepsilon_i}{\partial p}\right) = V_i - (T - T_o) \left(\frac{\partial V_i}{\partial T}\right)_{p,x_i} \quad (4.16)$$

This equation may be integrated from p_o to p at T_o to give for an ideal gas

$$\Delta\varepsilon_{i_p} = R\, T_o \ln p/p_o \quad (4.17)$$

Finally, consider the change of work equivalent at constant T and p due to a change of mole fraction. For simplification let this change only take place at T_o and p_o then $\Delta\varepsilon_i$ equals the change in free energy or in the case of an ideal solution

$$\Delta\varepsilon_{i_x} = R\, T_o \ln x_i \quad (4.18)$$

Since the work equivalent is a state function, its calculation based on the datum can be performed in the following manner:

$$\begin{array}{ccccccc} \text{State 3} & & \text{State 2} & & \text{State 1} & & \text{State 0} \\ \boxed{\begin{array}{cc} T & p \\ x_i & \varepsilon_i^3 \end{array}} & \xrightarrow[\substack{\text{constant} \\ p \\ x_i}]{\substack{\text{adjust} \\ T \rightarrow T_0}} & \boxed{\begin{array}{cc} T_0 & p \\ x_i & \varepsilon_i^2 \end{array}} & \xrightarrow[\substack{\text{constant} \\ T_0 \\ x_i}]{\substack{\text{adjust} \\ p \rightarrow p_0}} & \boxed{\begin{array}{cc} T_0 & p_0 \\ x_i & \varepsilon_i^1 \end{array}} & \xrightarrow[\substack{\text{constant} \\ T_0 \\ p_0}]{\substack{\text{unmix} \\ x_i \rightarrow 1}} & \boxed{\begin{array}{cc} T_0 & p_0 \\ x_i = 1 & \varepsilon_i^o \end{array}} \\ & \longleftarrow \Delta\varepsilon_{i_T} \longrightarrow & & \longleftarrow \Delta\varepsilon_{i_p} \longrightarrow & & \longleftarrow \Delta\varepsilon_{i_x} \longrightarrow & \end{array}$$

$$\Delta\varepsilon_i = \Delta\varepsilon_{i_T} + \Delta\varepsilon_{i_p} + \Delta\varepsilon_{i_x} \tag{4.19}$$

In evaluating a process stream of materials the total work equivalent can be divided into a chemical work equivalent, ε_{chem}, and a physical work equivalent, ε_{phys}. The chemical work equivalent can be defined as

$$\varepsilon_{chem} = \sum_i n_i \varepsilon_i^o \tag{4.20}$$

where n_i equals the moles of species i in a stream on a unit time basis. In other words, ε_{chem} represents that part of the total work equivalent, ε, which is due to chemical energy at T_o and p_o. The physical work equivalent can be defined as

$$\varepsilon_{phys} = \sum_i n_i \left(\Delta\varepsilon_{i_T} + \Delta\varepsilon_{i_p} + \Delta\varepsilon_{i_x}\right) \tag{4.21}$$

i.e. ε_{phys} is the part of ε resulting from a state different than the datum.

In evaluating the process utilities the work equivalents for steam, condensate, and fuel gas can be calculated in the same way.

PART II

THE ENERGETICS OF THE COED PROCESS FROM A SECOND LAW PERSPECTIVE

CHAPTER 5

COED PROCESS DESCRIPTION

Part II is an application of the thermodynamic analysis presented in Part I. Specifically, the Char Oil Energy Development process of FMC Corp. (8) developed under the sponsorship of the United States Energy Research and Development Administration will be analyzed from a second law perspective with the first law approach used as a comparison. Both the second law and the incremental efficiency will be used to show that each has distinct advantages and disadvantages. Also the concept of an overall second law efficiency which includes an energy debit for plant equipment will be dealt with. This factor has not previously been included in efficiency analyses. The energy associated with manufacturing plant equipment and with plant construction will be discussed and specifically calculated for the COED plant. Also the inclusion of outside inefficiencies involved with raw materials processing and electricity generation will be discussed.

However, the process must first be described before the analysis may proceed. The COED process fits into the general category of liquefaction via pyrolysis. Figure 2 is a schematic diagram illustrating the commercial plant design for processing 25,000 tons (22,680 metric tons) of Illinois No. 6 - seam coal per day. Following coal preparation, the coal is dried in a fluidized-bed dryer at 350°F (450K) using the first stage pyrolysis off-gases. The dried coal is then fed through four stages of pyrolysis, each at succeedingly higher temperatures; 550°F (561K), 850°F (728K), 1050°F (839K), and 1550°F (1116K). The fourth stage pyrolysis is affected by injection of steam and oxygen. The char leaving the fourth stage passes directly to the air blown, Winkler type fluidized-bed gasifiers. Gas produced there consists mainly of N_2, CO, and H_2. This gasifier gas then

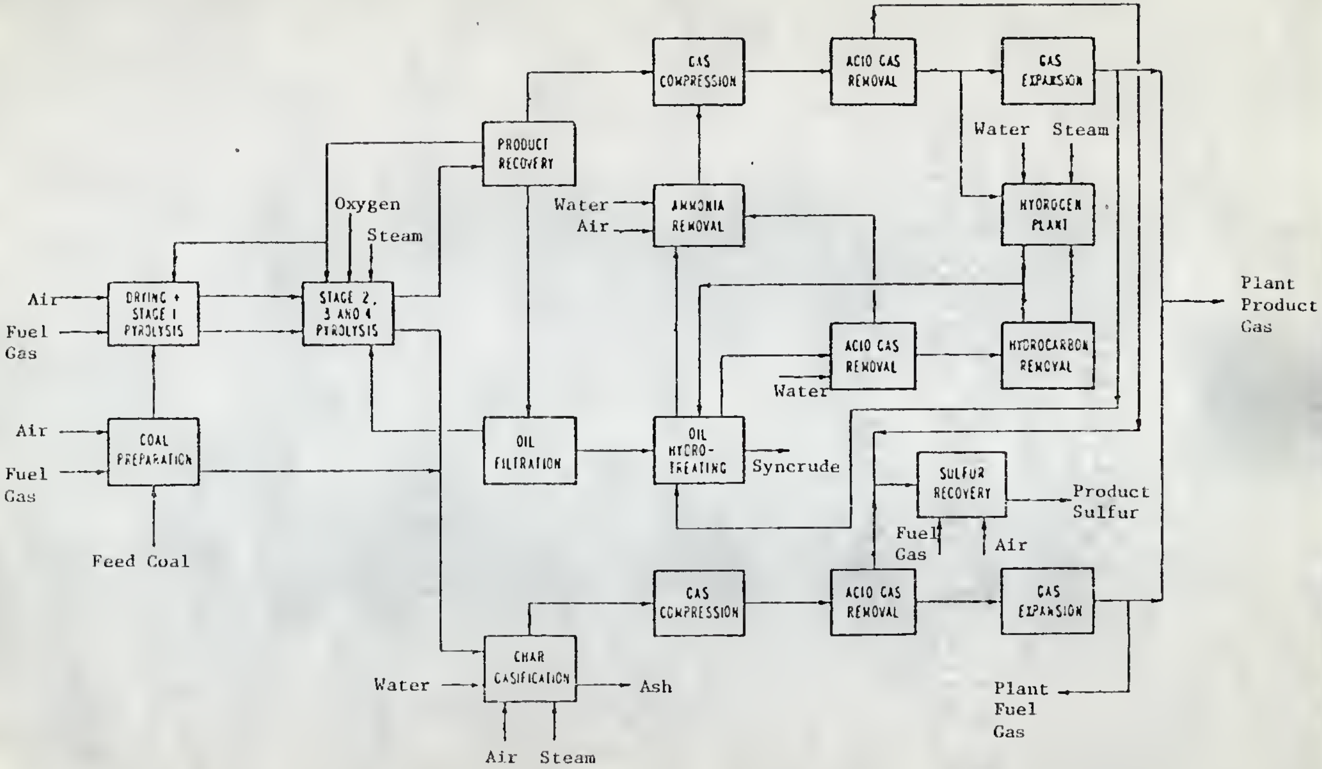


Figure 2. COED Commercial Process Block Diagram with Main Input and Ouput Streams

goes through the acid gas removal scrubber and becomes a high energy product. The pyrolysis gas consists mainly of H_2O, CO_2, CO, H_2, and hydrocarbons. It goes through a recovery section in which the pyrolysis oil is condensed and separated from the product gas. Following oil filtration, the oil is upgraded to a synthetic crude oil, syncrude, by hydrotreating. The hydrogen to do this is produced by gas reforming a portion of the deacidized pyrolysis product gas followed by shift conversion and methanation. In the gas clean-up sections, sulfur is recovered, via a Claus process, as a byproduct.

The COED commercial plant design also contains various systems to satisfy the utility requirements. Included are the cooling, boiler, and process waste water systems. Waste heat boilers produce a net excess of steam primarily from the compression, hydrotreating, and gasification units. The fuel gas needed mainly by the pyrolysis and hydrogen units is taken from the product gas. The net inputs and outputs of quantities used in this COED process are given later in Figure 5.

This COED commercial design was based upon pilot plant studies for only the pyrolysis, filtration, product recovery, and hydrotreating sections. The designs for other sections, most of which are well-known, were obtained from various companies. A very simplified approach was taken in process water treatment that may not represent an actual design.

CHAPTER 6

SECOND LAW ANALYSIS OF THE COED PROCESS

6.1 Computational scheme

In this chapter the COED process will be analyzed with respect to the second law of thermodynamics. A specific unit of this process, the char gasification unit, will serve to illustrate the detailed computational approach. However, first the general computational scheme will be outlined along with several specific assumptions.

The bulk of this analysis of the COED process was accomplished through the use of a FORTRAN computer program developed to analyze a general coal conversion process. With only minor modifications any chemical process may be analyzed through its use as long as thermodynamic data are available for calculating standard state work equivalents for all components and as long as the process is fully described with respect to stream analysis, temperature levels, pressures, and utilities. The computer program checks the material balance for each unit, calculates enthalpies and work equivalents for each stream and utility, checks the energy balance for each unit and calculates first and second law efficiencies for each unit and the overall process. The first law efficiencies are calculated using higher heating value data since, as mentioned in section 2.2, this represents the maximum energy obtainable from a stream. The second law efficiencies are calculated after Eq. (4.7) and Table 1 are used to construct a table of standard state work equivalents for compounds present in the COED process. These are presented in Table 3. A flowchart of this computer program is presented in Figure 3. Appendix A lists the program and a final output, and also contains a detailed block diagram of the COED commercial process with all interconnecting streams.

Table 3. ε_i^o for Compounds in the COED Process

Compound	ε_i^o (kcal/kmol)
H_2	56224
O_2	932
N_2	143
CO_2	4776
CO	65770
CH_4	198420
C_2H_4	308672
C_2H_6	357036
C_3H_6	448018
C_3H_8	513618
n-C_4H_{10}	669814
H_2S	187992
NH_3	59657
S	139660
*Coal	6667
*Char	6167
*Syncrude	10611

*estimated as equal to the standard heat of combustion, value in kcal/kg

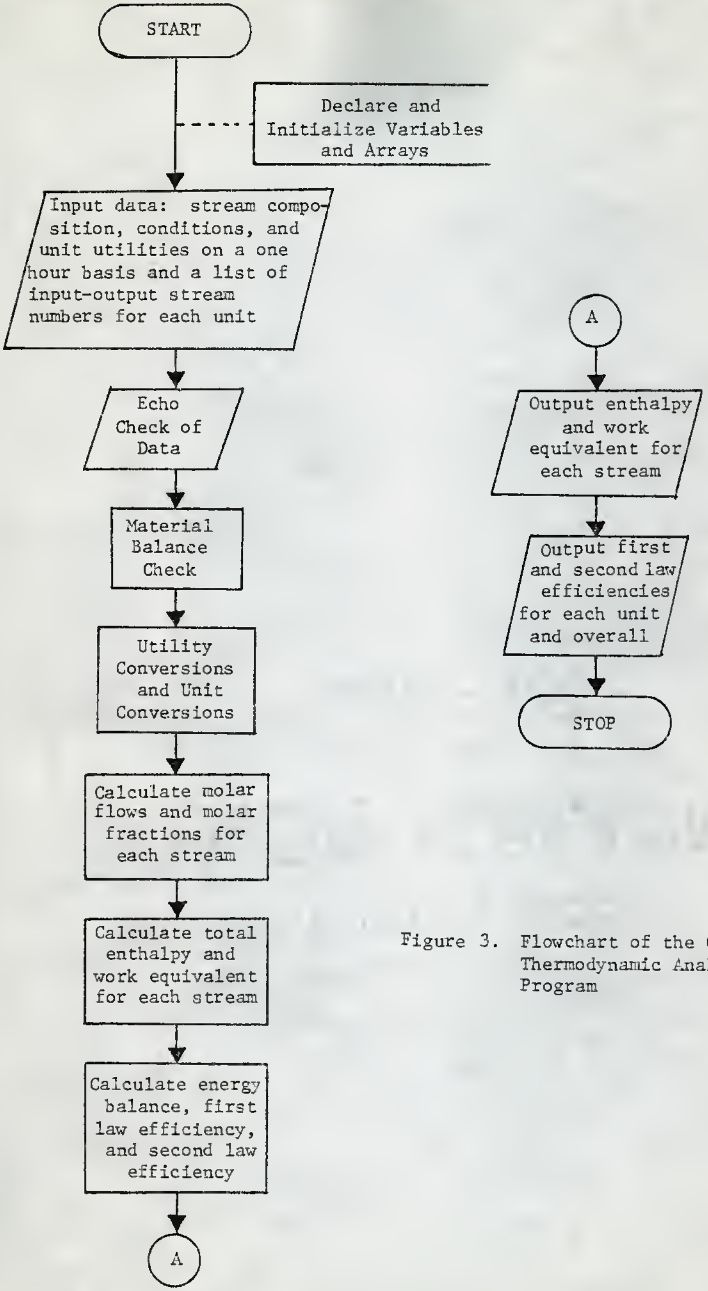


Figure 3. Flowchart of the COED Thermodynamic Analysis Program

Several assumptions were made enroute to the final analysis. First, to be consistent all of the stream and utility data were used as given. However, one additional stream was created as an output from the hydrogen plant unit to account for a discrepency in the material balance. An elemental balance dictated that this stream contain primarily carbon dioxide and water, thus it was considered a waste gas stream. Second, an average saturated condition was assumed for all utility steam used and produced. Third, the physical properties of the derived coal liquids were approximated by those of anthracene oil (13). Finally, the heating values for char and unhydrotreated oil which were not given in the commercial process description were determined from the range of values listed in a COED pilot plant report (20) and from energy balance results of the units involved. These values, of course, do not enter into the analysis of the overall COED process. These and other less important assumptions are detailed in the computer program comments in Appendix A.

6.2 Char gasification unit example

The char gasification unit is one of the major units of the COED process. Figure 4 gives a diagram of the input and output process streams with utilities for this process unit. The essential data are presented in Tables 4 and 5. Each stream's chemical and physical work equivalent is calculated from Eq. (4.20) and Eq. (4.21) respectively. The results of these calculations are given in Table 6. The negative value of ε_{phys} for stream 6 occurs because the stream is a mixture and therefore the ability to perform work according to Eq. (4.18) was lost when pure gases were mixed irreversibly. Application of the second law efficiency definition, Eq. (3.7), produces

$$\eta = \frac{\varepsilon_6 + \varepsilon_{steam}}{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + \varepsilon_5 + \varepsilon_w} = 0.81$$

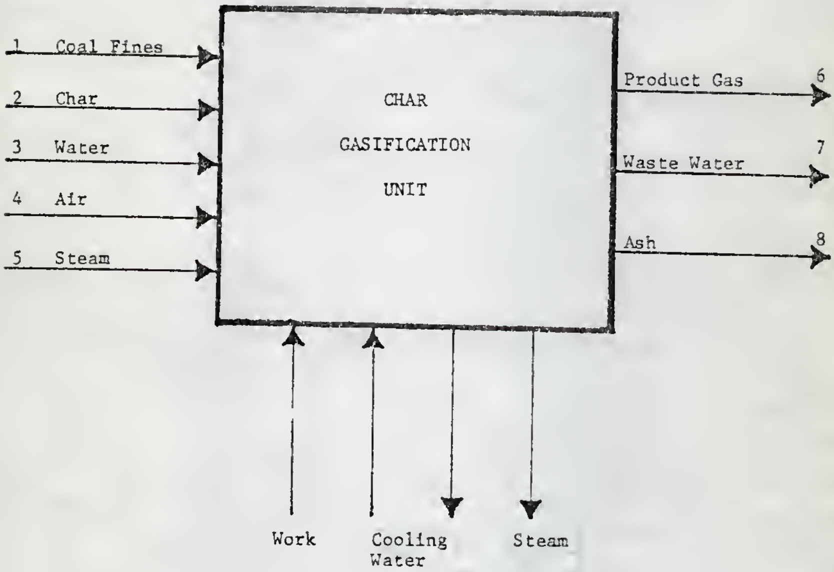


Figure 4. Char Gasification Diagram

Table 4. Process Streams in Char Gasification - 1 Hour Basis

Mat'l kmol \ Stream No.	1	2	3	4	5	6	7	8
*COAL	31.0							
OIL								
AIR				40242.18				
N_2						35125.73		
H_2O	100.71		14650.36		11803.68	5047.79	10852.94	
CO_2						1211.69		
CO						27275.23		
H_2						11884.84		
CH_4						308.75		
H_2S						467.45		
*ASH		1.32						136.87
*CHAR		539.82						
TOTAL (kmol)	100.71		14650.36	40242.18	11803.68	81321.38	10852.94	
STATE	s, ℓ	s	ℓ	g	g	g	ℓ	s
PRESS (atm)	1.0	1.0	1.0	1.90	1.90	1.36	1.0	1.0
TEMP (K)	310.93	1116.48	310.93	366.48	408.15	316.48	319.26	449.82

*Component in tons

Table 5. Char Gasification Utilities

Utility	Value (kcal)
Work	2.533×10^7
**Cooling Water	2.838×10^7
***Steam	4.758×10^8

** $\Delta T = 16.7°C$

*** avg. conditions 138°C, 3.4 atm

Table 6. Work Equivalents for Char Gasification

Stream No.	Component	ε_{chem} (kcal)	ε_{phys} (kcal)	ε (kcal)
1	Coal	1.875×10^8	2.160×10^3	1.875×10^8
2	Char	3.020×10^9	4.670×10^7	3.067×10^9
3	Water	—	7.021×10^4	7.021×10^4
4	Air	—	1.727×10^7	1.727×10^7
5	Steam	—	3.032×10^7	3.032×10^7
6	Product Gas	2.622×10^9	-3.690×10^8	2.585×10^9
7	Waste Water	—	1.395×10^5	1.395×10^5
8	Ash	—	8.081×10^5	8.081×10^5
	Work	—	—	3.167×10^7
	Cooling Water	—	7.651×10^5	7.651×10^5
	Steam	—	1.213×10^8	1.213×10^8

In this efficiency streams 3, 7, and 8 plus the cooling water do not represent useful work equivalents. Stream 4, air, is included because expansion work is possible. The incremental efficiency, Eq. (3.8), is calculated for a work producing process (remember the convention that work out is negative) as

$$\eta_I = \frac{\varepsilon_w - \varepsilon_{cw} - \varepsilon_{steam}}{[\varepsilon_6 + \varepsilon_7 + \varepsilon_8 - (\varepsilon_1 + \varepsilon_2 + \varepsilon_4 + \varepsilon_5)]} = 0.13$$

These two efficiencies are comparable to values given by Gaggioli (21) (22) for a Koppers-Totzek gasifier with coal preparation. He found similar second law and incremental efficiencies to be 0.78 and 0.15 respectively. For comparison a first law efficiency is calculated as 0.94 for the gasification unit.

This char gasification example may also be used to illustrate Denbigh's concept of a "prescribed degree of irreversibility" discussed in section 3.1. In utilizing this concept the criteria for comparison are: chemical reactions are allowed to proceed irreversibly with the heat of reaction recovered as mechanical work in a Carnot type heat engine, and all other parts of the process, except mixing, are carried out reversibly. For the char gasification example the gasification reactions proceed irreversibly at approximately 1500°F (1090K) with the heat of reaction partially recovered as low temperature steam and the rest of it lost to the atmosphere and cooling water. The pumps and compressors are 80% efficient in converting electricity to shaft work. To apply Denbigh's concept the heat of reaction becomes totally recoverable as saturated steam at 1500°F and the mechanical equipment is considered reversible, 100% efficient. Thus a new work equivalent is obtained for the steam, 2.15×10^8 kcal, and a new shaft work value is found, 2.533×10^7 kcal. Using these work equivalents the two maximum efficiencies obtainable under the prescribed conditions are 0.842 and 0.265 for the second law and incremental efficiencies respectively. It should be noted that in calculating the latter efficiency the work equivalent of the cooling water is zero because all of the heat of reaction was recovered as high temperature steam. Since these are maximum efficiencies it may be helpful to compare these with the actual efficiencies by defining a practical efficiency whereby it equals the actual efficiency divided by the maximum efficiency under the prescribed conditions. Thus the practical second law and incremental efficiencies are 0.96 and 0.49 respectively. The large practical second law efficiency is the result of the large chemical work equivalents of the char and gas overshadowing the smaller utility work equivalents.

6.3 Overall COED Results

An overall flow diagram of the COED process is given in Figure 5, and the corresponding stream and utility work equivalents are presented in Table 7. The second law efficiency of the overall process is

$$\eta = \frac{\varepsilon_5 + \varepsilon_6 + \varepsilon_7 + \varepsilon_{steam}}{(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_w + \varepsilon_{condensate})} = 0.75$$

This value is slightly higher than the 0.68 given by Gaggioli for Koppers-Totzek coal gasification. The first law efficiency of the overall process calculated here is 0.80 while the COED designers' calculated value was 0.75. However, in their calculation they considered electrical work to be a negative output term rather than a positive input term which was used here in order to remain consistent with the first law efficiency development in Chapter 2. Table 8 gives the first and second law efficiencies plus the energy balance closure for each unit. It is observed that for the overall process and for the units second law and first law efficiencies are quite

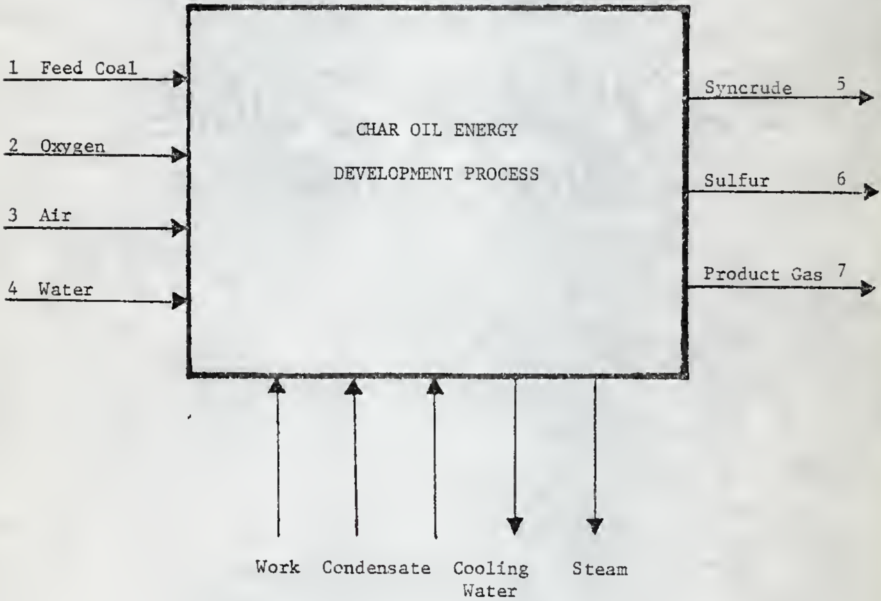


Figure 5. Overall COED Process Diagram

Table 7. Work Equivalents for Overall COED Process

Stream No.	Component	ε (kcal)
1	Coal	6.24×10^9
2	Oxygen	6.06×10^6
3	Air	2.27×10^7
4	Water	—
5	Syncrude	1.69×10^9
6	Sulfur	1.34×10^8
7	Product Gas	3.03×10^9
	Cooling Water	—
	Steam	3.22×10^7
	Work	2.57×10^8
	Condensate	3.95×10^5

Table 8. THERMODYNAMIC EFFICIENCIES AND ENERGY BALANCE CLOSURE FOR THE COED PROCESS

UNIT NAME	FIRST LAW EFFICIENCY	SECOND LAW EFFICIENCY	ENERGY BALANCE CLOSURE (%)
COAL PREPARATION	0.989	0.989	99.9
DRYING & STAGE 1 PYROLYSIS	0.963	0.960	98.5
STAGE 2, 3, AND 4 PYROLYSIS	0.984	0.962	98.4
PRODUCT RECOVERY	0.908	0.966	99.6
PYROLYSIS GAS COMPRESSION	0.993	0.992	99.9
PYROLYSIS ACID GAS REMOVAL	0.880	0.959	91.8
PYROLYSIS GAS EXPANSION	1.007	0.998	100.3
OIL FILTRATION	0.999	0.999	100.1
OIL HYDROTREATING	1.001	0.997	100.4
PURGE ACID GAS REMOVAL	0.997	0.997	99.8
HYDROCARBON REMOVAL	0.998	0.997	99.8
AMMONIA REMOVAL	0.996	0.969	100.8
HYDROGEN PLANT	0.792	0.755	91.0
CHAR GASIFICATION	0.953	0.812	96.6
GASIFIER GAS COMPRESSION	0.979	0.985	99.1
GASIFIER ACID GAS REMOVAL	0.987	0.995	99.2
GASIFIER GAS EXPANSION	1.020	0.996	100.5
SULFUR RECOVERY	0.716	0.598	86.7
OVEFALL COED PROCESS	0.797	0.749	94.2

close. The reason for this is that the dominant terms in the efficiency calculation are those which represent chemical energy and, as has been shown, the heat of combustion and the work equivalent are practically equal.

In Table 8 the second law efficiency is less than the first law efficiency for most units and overall, as would normally be expected. However, for four units, three of which primarily involve separations, the reverse is true. This occurs for the three units involved with separations because the second law analysis takes into account the work of separation. For example, the removal of CO_2 and H_2S in the gasifier acid gas removal unit increases the mole fractions of the other components thereby increasing the work equivalent of the output product gas stream. The large difference between the first and second law efficiencies in the pyrolysis acid gas removal unit is in part explained by the previous discussion, but is perhaps primarily caused by a non closing energy balance. The balance accounted for only 0.91 of the energy input to that unit. The reason for this speculation is that if the lost energy was recovered for example in the form of steam the first law efficiency would gain as additional output one kcal for every kcal of recovered energy whereas the second law efficiency would gain as additional output only about 0.2 kcal of work equivalent per kcal of recovered energy. Therefore the first law efficiency would increase more noticeably than would the second law efficiency. The other unit in which the second law efficiency is greater than the first law efficiency is gasifier gas compression. This occurs in part because of the condensation of water from the gasifier gas, a separation effect, but it occurs primarily because the second law analysis places value on the expansion work that may be obtained from a stream not at the standard pressure and the defined first law efficiency does not. Without the separation and pressure affects the second law efficiency becomes 0.95 in contrast with the first law efficiency of 0.98.

The lower efficiencies generally associated in the literature with physical processes, such as separations and compressions, result from using an incremental efficiency. For example, incremental efficiencies for purge acid gas removal and oil filtration are 0.025 and 0.31 respectively. In addition, these efficiencies for gasifier gas compression and expansion are 0.68 and 0.81 respectively. The corresponding second law efficiencies are much higher. In a process such as fuel gas compression the work equivalent of the gas is much larger than the amount of work lost. In other words, the difference between the ideal and the actual work input is very small relative to the total work equivalent of the fuel gas. For a gas with a very low work equivalent, such as air, the second law efficiency for compression approaches the corresponding incremental efficiency. Consider for instance that the chemical work equivalents of the fuel gas being compressed in the gasifier gas compression unit are equal to zero. The second law efficiency for this compression process then becomes 0.69 which is very close to the incremental value of 0.68 given above. This example tends to show that for physical processes involving low chemical energy streams the second law efficiency approaches the incremental efficiency.

The second law efficiency as applied up to this point charges the overall COED process with only those inefficiencies directly created by the process. However, the process uses items such as oxygen and electricity with which there is an associated inefficiency. Electricity, for example, is generated with an efficiency of approximately 0.38. This value may be included in the work term to give an overall work equivalent for shaft work. An oxygen plant may be added to the overall process to supply the necessary oxygen at an efficiency of about 0.15 (4). With these changes the second law efficiency of the coal conversion endeavor decreases from 0.75 to 0.68.

In the commercial COED design several items were disregarded that may cause the second law efficiency found here to be too high. First, no energy charge was made for new catalyst, regeneration of old catalyst, or general chemicals. The catalyst use amounted to approximately 73 kg/hr (160 lb/hr). An approximate energy charge for the catalyst and chemicals will be given in the next chapter. Second, the energy charge for waste treatment was much less than expected because of a simplified approach to the difficult water treatment problem.

CHAPTER 7

EQUIPMENT AND CONSTRUCTION ENERGY COST

7.1 Introduction

When considering the total energy input to a process, the energy needed to produce the equipment and to construct the plant must be included. The energy input-output matrix as developed by Herendeen (23) allows this additional energy to be estimated. This type of energy evaluation uses Input-Output analysis, a technique borrowed from economics, and takes advantage of the large data base of intersector sales available from the U.S. Department of Commerce. The data were last compiled in 1963 for 367 sectors, each sector being a segment of the economy which produces goods or services, e.g. dairy farm products, machine shop products, and research and development. Also this energy evaluation accounts for all the steps in the complex manufacturer-sales chain. For example, Herendeen gives results which indicate that the auto manufacturer alone uses only 6% of the total energy necessary to produce and to market an automobile.

The primary results of the energy input-output matrix of interest here are the sector energy coefficients. The two most applicable are the energy supplied directly to a sector per dollar of that sector's output, D_c, and the total energy required per dollar of market value, T_c, of which D_c is a part. The T_c and D_c values for pertinent sectors reproduced from Herendeen are listed in Table 9. To correctly use these sector energy coefficients the problem of time variance must be considered. The sector energy coefficients were developed in 1973 using 1963 sales data. Therefore, to use these coefficients they must be taken as time invariant in the sense that only a cost index is needed to change their time basis. However, new manufacturing techniques serve to reduce the sector energy coefficients by

TABLE 9. T_c and D_c Sector Energy Coefficients for Various Sectors*

Sector	T_c 10^3kcal/\$(1963)	D_c 10^3kcal/\$(1963)
(1) fabricated plate work	29.1	2.12
(2) fabricated metal products	23.2	1.00
(3) pumps and compressors	14.7	1.90
(4) fabricated structural steel	31.1	1.27
(5) ready-mixed concrete	36.1	2.49
(6) asbestos products	29.4	3.46
(7) instruments and controls	10.8	0.94
(8) pipe, valves, and pipe fittings	19.5	2.30
(9) new construction, nonresidential buildings	16.7	1.74
(10) new construction, highways	24.8	6.74
(11) electrical equipment	17.9	0.81
(12) clay refractories	40.3	26.94
(13) industrial inorganic and organic chemicals	81.4	45.30

*Taken from reference (23)

reducing energy consumption per product unit. These new manufacturing techniques, however, can be shown to have little affect on T_c with a larger affect on D_c. Remember that D_c is a part of T_c and from Table 9 it is seen that D_c is 5-10% of T_c for most sectors. Also note that D_c can be thought of as the energy it takes per dollar of product to fabricate a product from raw materials whereas the difference $T_c - D_c$ can be considered the energy consumption per dollar of product involved with producing these raw materials, e.g. mining iron ore, transporting iron ore, and processing iron ore into steel. Intuitively the term $T_c - D_c$ will most likely be time invariant with increases in processing efficiencies, less energy per dollar, being negated by an increasing difficulty in mining ore, more energy per dollar. Therefore, T_c will probably be affected little. It should be noted that T_c obscures D_c in the combined energy coefficient calculations which lead directly to the equipment and construction energy cost while D_c will only become important when an energy credit for scrap is determined for the steel sector.

7.2 Computational approach and application to the COED plant

Knowing the fixed capital investment for the COED project, an appropriate breakdown of its components as prescribed by Peters and Timmerhaus (24), and the energy coefficients D_c and T_c, an energy cost may be assigned to all of the equipment and materials needed for the project's construction. An equation will now be briefly derived which will calcualte the total plant energy cost. First, consider an expression for part of the fixed capital investment.

$$C_D = C_1 + C_2 + C_3 + C_4 + C_5 \tag{7.1}$$

where

C_D = total direct plant cost less land

C_1 = purchased equipment cost

C_2 = purchased equipment installation cost

C_3 = instrumentation and controls cost

C_4 = piping cost

C_5 = offsite facilities cost

The individual C_i terms can be expressed as

$$C_i = f_i C_D \qquad i = 1, 2, 3, 4, 5 \tag{7.2}$$

where

f_i = a fractional multiplying factor

The energy associated with each direct cost is determined from

$$E_i = g_i C_i \qquad i = 1, 2, 3, 4, 5 \tag{7.3}$$

where

E_i = energy associated with direct cost i

g_i = combined energy coefficient in kcal/\$ for direct cost i determined from T_c's for appropriate sectors

Combining Eqs. (7.2) and (7.3) yields

$$E_T = C_D \sum_{i=1}^{5} g_i f_i \tag{7.4}$$

where

E_T = total equipment and construction energy cost

Eq. (7.4) is used to calculate the total plant energy cost. The multiplying factors, f_i's, are determined from percentages listed for a solid-liquid-processing plant (24). These percentages were adjusted to fulfill the requirement given in the COED economic analysis (8) that the offsite facilities' cost is 30% of the other direct costs. Table 10 presents these multiplying factors. The combined energy coefficients, g_i's, are determined from a combination of appropriate T_c sector energy coefficients. As an example consider g_1, the combined energy coefficient for purchased equipment. The major components of this include vessels (fluidized beds, tanks,

TABLE 10. Multiplying Factors and Combined Energy Coefficients for the COED Plant

Cost Component	f_i *	g_i ** 10^3kcal/$(1963)
purchased equipment	0.42	22.3
equipment installation	0.16	24.1
instrumentation and controls	0.06	5.4
piping	0.13	11.9
offsite facilities	0.23	19.2

* as given by Peters and Timmerhaus

** calculated from total sector energy coefficients, T_c's, for appropriate sectors and towers), heat exchangers, cyclones, and pumps and compressors. The combined energy coefficient is determined from an average of T_c's in sectors (1), (2), and (3) as listed in Table 9. The other g_i's are similarly found, however, for these the labor cost is significant and must be included as a zero term in the weighting of the appropriate sector energy coefficients. To illustrate this additional point look at the numerical calculation of g_4, the combined energy coefficient for piping. The major nonlabor components in this area with corresponding sectors are pipe, valves and fittings, structural supports, and insulation corresponding to sectors (8), (4), and (6) (asbestos is used as a close approximation to actual insulation). The combined energy coefficient is determined by a weighting of each component: labor - 50%, pipe, valves and fittings - 30%, and structural supports and insulation - 10% each. Therefore g_4 is calculated as

$$g_4 = 0.5\ (0) + 0.3\ (19.5) + 0.1\ (31.1) + 0.1\ (29.4)$$

$$g_4 = 11.9 \times 10^3 \text{ kcal/\$(1963)}$$

The combined energy coefficients are listed in Table 10. Finally the total COED plant energy cost can be determined. The total direct COED plant cost, C_D, was given as 505.7 MM\$(1975). With this information plus the cost index ratio, 1.75\$(1975)/\$(1963), Eq. (7.4) may be used to calculate a total plant energy cost of 5.85×10^{12} kcal. Thus a combined energy coefficient for this plant is 1.14×10^4 kcal/\$(1975). This value can be considered a rough first approximation for a solid-liquid-processing plant. With a service life of 9 years, as assumed by the COED designers (8), and an operation of 330 days/year the energy input assigned to the equipment is found to be 8.21×10^7 kcal/hr. This quantity is approximately 1.2% of the total energy input to the COED plant.

At this point the catalyst and chemical energy charge discussed in section 6.3 may be estimated using total sector energy coefficients, T_c's.

The COED economic analysis gives a combined catalyst and chemical cost of 40.5 MM$(1975). A total sector energy coefficient must now be determined. The catalyst support material is assumed to be the primary source of the catalyst's total energy charge. Sector (12), clay refractories, seems to be the most representative sector corresponding to the support material. The chemicals are assumed to correspond to sector (13), industrial inorganics and organic chemicals. The total sector energy coefficient for catalyst and chemicals, taken to be an average of the two separate coefficients, is 60.8×10^3 kcal/$(1963). After the cost index ratio is applied a final energy charge for catalyst and chemicals is calculated to be 1.40×10^{12} kcal. Applying the operating time conversion the energy input assigned to the catalyst and chemicals is found to be 1.96×10^7 kcal/hr. This non-recoverable energy will be included in the equipment and construction energy input to give a total energy input of 1.02×10^8 kcal/hr or approximately 1.5% of the total energy input to the COED plant.

7.3 Salvage value considerations

At the end of the plant equipment's service life an energy credit from the scrap steel is obtained. Since the actual amount of steel is unknown an approximation method is used to determine this credit. First look at the steel sector and consider what energy is saved by the use of scrap steel over raw ores. This savings may approximately be expressed per dollar of finished steel as

$$E_{sc} = T_{c_{steel}} - (1-h)\, D_{c_{steel}} \tag{7.5}$$

where

E_{sc} = energy credit coefficient of scrap steel

h = fraction of energy saved in the steel sector alone by using scrap instead of ores

In other words, on a dollar of finished steel basis Eq. (7.5) means that the energy value of scrap equals the total energy required to produce steel (energy consumption from mining, transportation, and processing) minus the net energy used only by the steel sector. Gyftopolous (4) gives h as about 0.33 and Herendeen gives $T_{c_{steel}}$ and $D_{c_{steel}}$ as 6.61×10^4 and 4.13×10^4 kcal/\$(1963) respectively. Thus by Eq. (7.5) E_{sc} becomes 3.84×10^4 kcal/\$(1963). Now it is convenient to express the energy savings when scrap is employed as a fraction.

$$f_{sc} = E_{sc}/T_{c_{steel}} \tag{7.6}$$

where

f_{sc} = energy credit fraction for scrap steel

This fraction, f_{sc}, is the fraction of the energy charged to steel which is recovered when salvage is used. Numerically f_{sc} is approximately 0.58 which is larger than h (0.33), the fraction of energy recovered in the steel sector alone when salvage is used, because the use of scrap steel saves all the energy expended to mine and process the ores. Next, this energy credit fraction for scrap steel is used to determine the combined energy credit coefficients, g_{c_i}'s analogous to g_i's. To accomplish this, first a new sector energy coefficient, the total sector energy credit coefficient, T_{cc}, is determined. Here it may be helpful to review the analogy of calculating combined energy credit coefficients so that the equipment energy cost could be found. In that instance the total sector energy coefficients, T_c's, were weighted to find combined energy coefficients, g_i's, which were then used with the proper multiplying factor, f_i, and direct cost, C_D, to ultimately obtain E_T, the total plant energy cost. Returning to the total sector energy credit coefficient, T_{cc} is approximated by assuming that steel is the only raw material and it is calculated from

$$T_{cc} = (T_c - D_c)f_{sc} \tag{7.7}$$

In other words the total sector energy credit coefficient equals the part of the energy consumption per dollar of product involved with producing raw materials that is recovered when salvage is used. Of course this analysis applies only to those sectors having steel to salvage, otherwise T_{cc} equals zero. The combined energy credit coefficients, g_{c_i}'s, are then determined analogous to the combined energy coefficients in the previous section. These are listed in Table 11. Since the f_i terms do not change Eq. (7.4) may be applied after using the cost index ratio to obtain an energy credit for the COED plant of 2.3×10^{12} kcal corresponding to an energy credit flow of 3.2×10^7 kcal/hr or 39% of the total input equipment and construction energy flow. This value can be considered a maximum because factors such as the energy needed to dismantle the plant for scrap and transport the scrap have not been taken into account. Also, not all of the steel may be salvageable. Using this energy credit value the net energy flow into the plant is about 7.0×10^7 kcal/hr or about 1.1% of the total energy input, less equipment, to the plant.

TABLE 11. Combined Energy Credit Coefficients for the COED Plant

Cost Component	g_{c_i} 10^3kcal/$(1963)
purchased equipment	12.2
equipment installation	4.4
instrumentation and controls	0
piping	4.8
offsite facilities	6.9

CHAPTER 8

CONCLUSION

The second law thermodynamic analysis of the Char Oil Energy Development process yielded an efficiency of 0.75 when applied to the immediate process. The scope of the analysis was then broadened to encompass indirect inefficiencies in electrical generation and oxygen production and to include the equipment and construction energy costs. This led to a final overall second law efficiency of 0.67. This shows that the second law efficiency decreases as the scope of the analysis broadens. The analysis can be extended to the point where other energy inputs such as coal mining and ash disposal are included but that was considered to be remote and too detailed for this second law analysis.

The COED units involving physical processes had second law efficiencies that were higher than initially expected. The incremental efficiency was found to give lower, more representative values for the physical process units. However, for units involving chemical transformations the second law efficiency was deemed to be the more useful of the two.

An analysis was developed for determining energy charges for equipment and construction. This charge was found to be only a small part, approximately 1%, of the total energy involved with the COED process. However, this energy may be significant when calculated for a process with few high energy chemical streams. Also the equipment and construction energy charge analysis worked well in the estimation of an energy charge for indirect materials consumed, specifically for catalyst and chemicals for which only an economic cost was available. The other result of this analysis was the approximate 1.14×10^4 kcal/\$(1975) value of the combined energy coefficient which may prove useful for estimating the energy cost for a solid-liquid-processing plant.

PART III

OPTIMIZATION OF FLUE GAS HEAT RECOVERY FROM A SECOND LAW PERSPECTIVE

CHAPTER 9

THERMODYNAMIC AND ECONOMIC OPTIMIZATIONS APPROACHES

9.1 Heat recovery process description

Part III is a further application of the thermodynamic analysis presented in Part I. However, in this case it will be used to optimize the design of a process from the standpoint of an overall efficiency. Specifically, a flue gas heat recovery process design will be optimized from a second law perspective. Included in this thermodynamic optimization will be the concept of an energy debit for equipment and construction as discussed in Chapter 7. The economic optimum design will also be determined for use as a comparison. For both the thermodynamic and the economic optimizations there exist two system definitions that may be employed when the respective objective functions are determined. This will be discussed in section 9.2.

The flue gas heat recovery system which is used here is similar to one given by James and Stokes (25) for the heat recovery from reformer furnace stack gases in ammonia plants. Figure 6 gives a block flow diagram of the flue gas heat recovery system plus furnace. The heat recovery section serves as a combustion air preheater in which heat exchange is accomplished through a number of parallel counter-current shell and tube heat exchangers. The flue gas and air streams were given by James and Stokes to enter the heat recovery section at 500°F (533K) and 100°F (311K) respectively. The pressure drops associated with the flow of these streams through the flue gas heat recovery system are compensated for by forced and induced draft fans.

9.2 Determination of three objective functions

For the previously described flue gas heat recovery system two system definitions may be employed that yield two thermodynamic and two economic

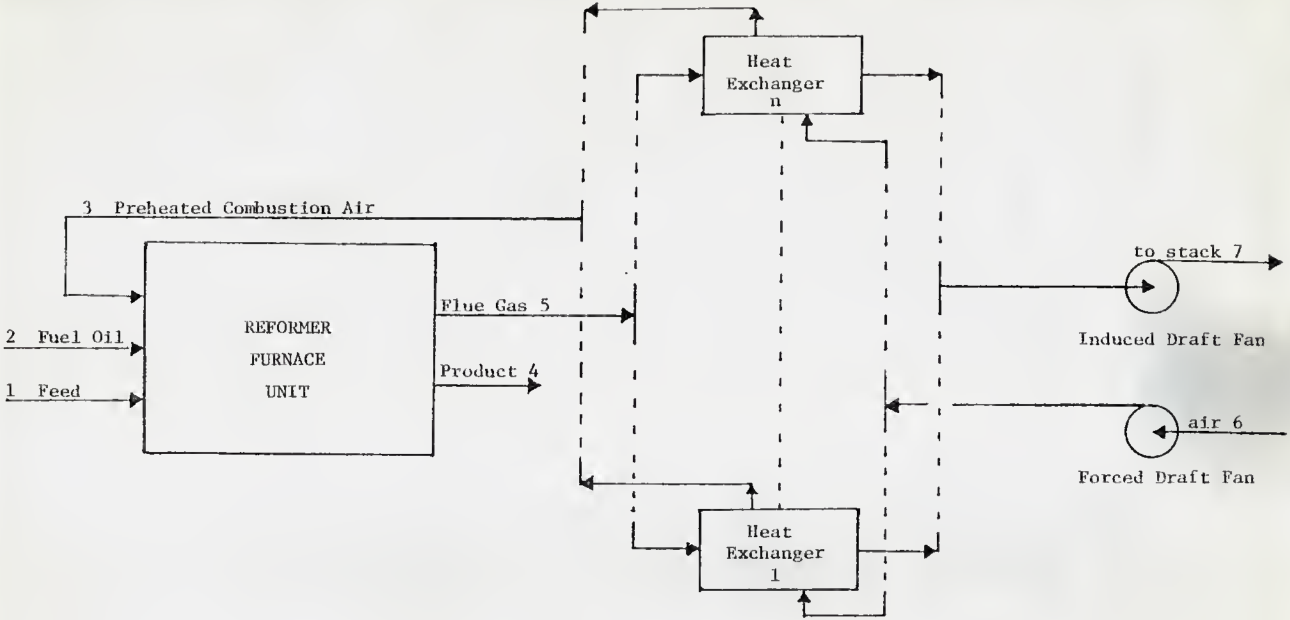


Figure 6. Overall Furnace and Flue Gas Heat Recovery Block Flow Diagram

objective functions each of which may be optimized. The two system definitions differ in that the reformer furnace unit is included in one system definition, the combined heat recovery system, while it is not included in the other system definition, the heat recovery addition system. The thermodynamic and economic objective functions will now be determined for each of these system definitions.

First, consider the combined heat recovery system as shown in Figure 7 with only inputs and outputs. A thermodynamic objective function for this system is ultimately obtained from the application of Eq. (3.7) which yields an overall second law efficiency, η_1.

$$\eta_1 = \frac{\varepsilon_4 + \cancel{\varepsilon_7}^{\,0}}{\varepsilon_1 + \varepsilon_2 + \cancel{\varepsilon_6}^{\,0} + \varepsilon_{equip} + W_{in}} \tag{9.1}$$

Next, let each work equivalent term, ε_n, equal the sum of the work equivalent of the furnace unit before flue gas heat recovery, ε_n', and the work equivalent of the flue gas heat recovery addition, $\Delta\varepsilon_n'$. Therefore Eq. (10.1) becomes

$$\eta_1 = \frac{\varepsilon_4' + 0}{\varepsilon_1' + 0 + \varepsilon_2' + \Delta\varepsilon_2' + \varepsilon_{equip}' + \Delta\varepsilon_{equip}' + W_{in}' + \Delta W_{in}'} \tag{9.2}$$

Since all but the delta quantities are constant this equation may be written as

$$\eta_1 = \frac{C_1}{C_2 + \Delta\varepsilon_2' + \Delta\varepsilon_{equip}' + \Delta W_{in}'} \tag{9.3}$$

where

C_1 = constant 1 (ε_4')

C_2 = constant 2 $(\varepsilon_1' + \varepsilon_2' + \varepsilon_{equip}' + W_{in}')$

Therefore, to maximize the second law efficiency the group of terms $(\Delta\varepsilon_2' + \Delta\varepsilon_{equip}' + \Delta W_{in}')$ must be minimized. Thus that group of terms

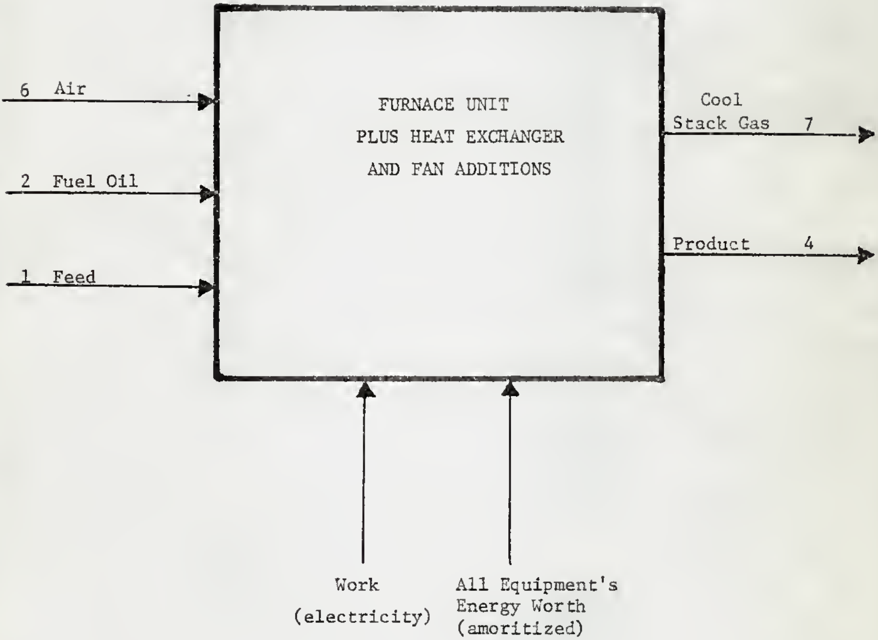


Figure 7. Overall Block Diagram of the Combined Heat Recovery System

comprise the thermodynamic objective function for the combined heat recovery system. The thermodynamic optimum of this system is given in terms of the variable values that minimize $(\Delta\varepsilon_2' + \Delta\varepsilon_{equip}' + \Delta W_{in}')$ instead of the actual overall second law efficiency, η_1, because the constant terms, C_1 and C_2, are unknown. This group of terms may have a negative value because as more heat is exchanged less fuel is used and $\Delta\varepsilon_2$ becomes negative. It may be noted that the work equivalent of the fuel oil in this objective function, $\Delta\varepsilon_2'$, is approximated by its higher heat of combustion as has been shown in section 4.3. The result of this approximation is a thermodynamic analysis that in one respect closely resembles a first law analysis. Every thermal kcal recovered from the stack gas essentially reduces the fuel demand by a corresponding kcal. In other words each kcal of thermal energy recovered from the stack gas stream by the air stream is roughly translated as increasing the work equivalent of the air stream by that same kcal. However, first law efficiencies seldom take into account the electrical generation inefficiency and the energy debit associated with the equipment. Corresponding economic objective functions for this system definition are well known and will not be detailed. For example, James and Stokes (25) present an economic analysis of a similar flue gas heat recovery system in which they give payout periods of their system for two purchased fuel oil costs. The economic objective function used here is the net present value because it gives a means of direct comparison of alternatives while taking into account the time value of money. The net present value is optimized with respect to fuel savings, equipment costs, power costs, and various indirect costs.

Second, consider the other system definition, the heat recovery addition system as given in Figure 8. A thermodynamic objective function for this system is obtained directly from application of the second law efficiency to give

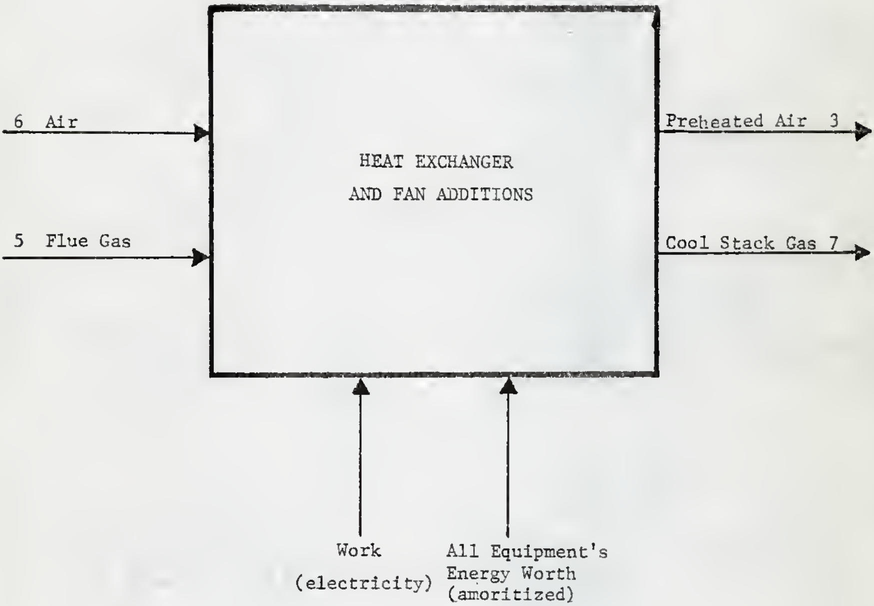


Figure 8. Overall Block Diagram of the Heat Exchanger Addition System

$$\eta_2 = \frac{\varepsilon_3 + \cancelto{0}{\varepsilon_7}}{\varepsilon_5 + \cancelto{0}{\varepsilon_6} + \varepsilon_{equip} + W_{in}} \tag{9.4}$$

For this heat recovery addition system the thermodynamic optimum is determined by the actual maximum overall second law efficiency value corresponding to the optimal variable values. In contrast with the other second law efficiency, η_1, the work equivalent of the preheated air stream, ε_3, does not approximately equal the thermal energy recovered from the stack gas. Thus in this system less emphasis is placed upon the amount of heat recovered since one kcal of thermal energy recovered equals only about one quarter of one kcal of work equivalent. The corresponding economic objective function for this system is similar to the previous one. However, in actual practice this is not as useful since it is not clear as to what credit is given to the recovered heat. Thus the economic objective function for the heat recovery addition system will not be considered further.

CHAPTER 10

THERMODYNAMIC AND ECONOMIC OPTIMAL HEAT RECOVERY DESIGNS

10.1 Computational Scheme

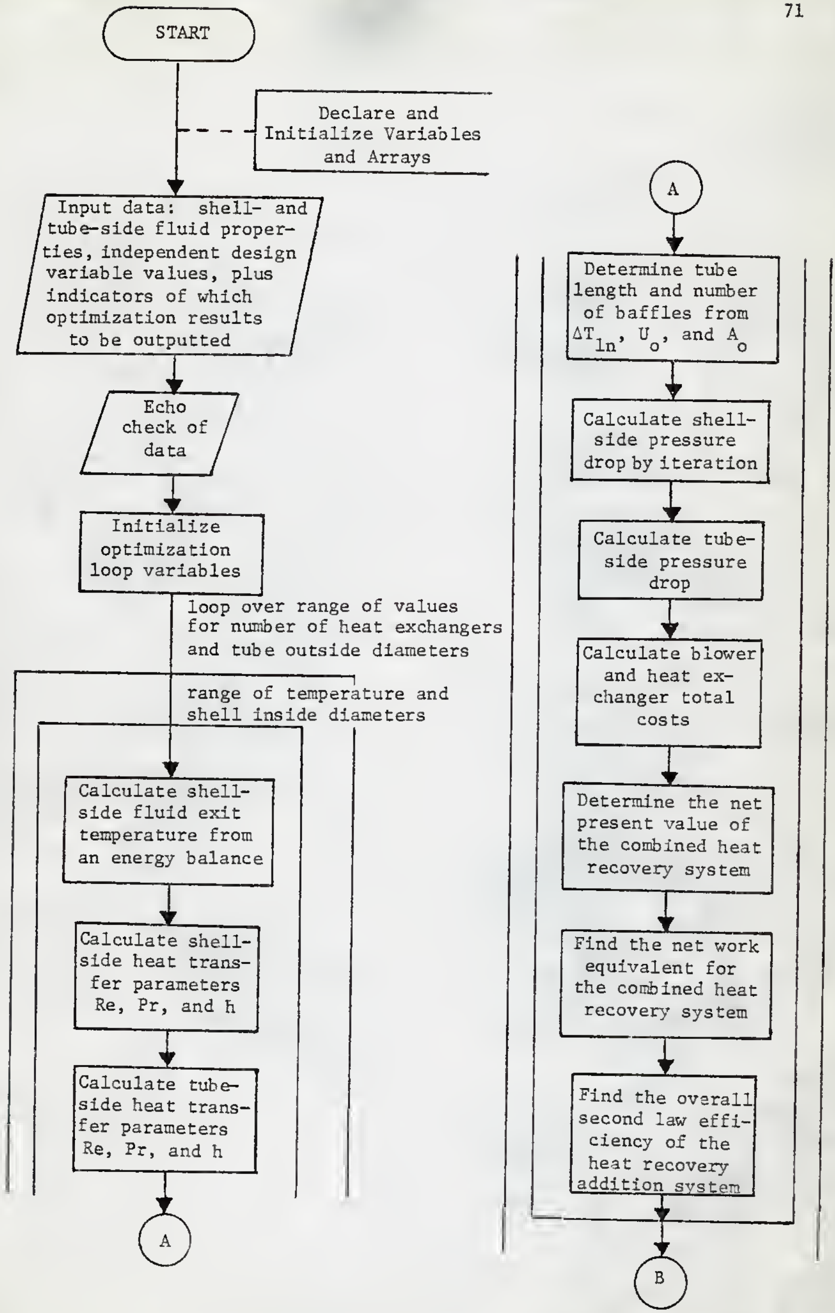
To optimize the thermodynamic and economic objective functions first the physical conditions, constraints, and assumptions must be established. The inlet flue gas and air stream temperatures have been given in section 9.1. The flow rates of these streams are determined from the specific heat recovery situation given by James and Stokes (25) where exit temperatures of 300°F (422K) and 350°F (450K) corresponding to exit flue gas and air streams respectively produce a heat recovery of 40 MM BTU/hr. Using this information plus Perry's (16) empirical formula for sulfurless No. 2 fuel oil, $C_{6.93}H$, a combustion reaction for that fuel with 10% excess air, and constant pressure heat capacities (13) an energy balance is made to determine the flow rates. They are found to be 1.124×10^4 kmol/hr and 1.00×10^4 kmol/hr for the flue gas and air streams respectively. It should be noted that these flow rates are considered constant for this analysis even though more efficient heat recovery will result in the use of less fuel thereby decreasing the air demand. However, calculations show this to be a good assumption: if the heat recovery doubles then the flow rates are only reduced by about 0.5%.

Other physical conditions worth noting involve the heat exchanger placement, the heat exchange fluid flow, and the routing of specific fluids inside the heat exchangers. The heat exchanger system as shown previously in Figure 5 consists of n exchangers connected in parallel. The parallel placement is used instead of a series placement because the large gas flow rates of about 100 m^3/s would create an unreasonable overall pressure drop in the series placement that would cause the power terms to completely overshadow the other terms in the thermodynamic and economic optimizations. Another important physical condition is the heat exchange fluid flow. The heat exchange may take place with either parallel or counter flow of fluids. For a given heat exchange area and set of stream temperatures the loss of work equivalent in a counter-current heat exchanger is smaller than that in a co-current heat exchanger. A co-current heat exchanger is an inherently irreversible process while for counter-current heat exchange the loss of work equivalent can be reduced by increasing heat exchange area. For instance, if a counter-current heat exchanger is balanced, one in which total stream heat capacities are equal, and it has infinite area the result is a reversible heat exchange process. Because of these facts the counter flow design was chosen. It should be noted that work equivalent is lost whenever a temperature difference exists between two streams because a Carnot engine could be operated across that difference. The other important physical conditions is the routing of specific fluids inside the heat exchangers. A choice must be made as to which fluid flows through the shell and which fluid flows through the tubes. Peters and Timmerhaus (24) list several major factors involved in determining the best fluid routing. These factors include fouling, corrosion, pressure drop, and fluid velocities. However, fouling and corrosion are assumed negligible and because of the closeness of the flow rates the pressure drops and fluid velocities will be similar. Since the flue gas contains a condensible vapor, water, it is possibly easier to separate liquid from the gas on the shell side so the flue gas is routed through the shell and the air through the tubes. This fluid routing, though, is still somewhat arbitrary. Further physical details and assumptions concerning the heat exchanger design are found in Appendix B. It should be noted that the most important two remaining physical design limitations are that the tube length cannot exceed 20 ft and that the tube length may also not be less than the shell inside diameter. These will be further discussed in the next section.

An important physical constraint to be considered when heat recovery increases is the existence of a pinchpoint. A pinchpoint occurs when the temperature of the two streams approach each other. When the heating capacities of the fluids are constant the pinchpoint will occur at one end of the heat exchanger, but when the heat capacity of a fluid stream changes it is possible for the pinchpoint to occur inside the heat exchanger. If condensation or vaporization of a component is possible the effective heat capacity of that stream will increase and thus lead to the possibility of an interior pinchpoint. This concept is well illustrated by Tucker and Chen (26) who cite the example of flue gas heating of boiler feed water. In the present study because of the existence of a condensible specie, i.e. water vapor, in the flue gas the possibility of this occurence was examined but was found to be nonexistent.

At the same time that the physical conditions, constraints, and assumptions are being specified the independent design variables must be determined. For this flue gas heat recovery design these variables are the following: number of heat exchangers connected in parallel, tube outside diameter (5/8", 3/4", or 1"), exit temperature of the preheated air, and shell inside diameter. Further details on the ranges of these independent design variables will be given shortly.

Once the physical conditions, constraints, assumptions, and independent design variables are determined a computer program can be written to find the optimum of each objective function given in section 9.2. The bulk of the optimization procedure for the flue gas heat recovery design remains the same irrespective of whether the objective function is economic or thermodynamic. For example, the heat exchanger design section remains unchanged for any of the objective functions. Briefly the computer program written for this optimization problem conducts an iterative search whereby the independent design variables are incremented one at a time over a predetermined search interval. Specifically, the computer program is designed to incrementally search over a range of shell inside diameters and exit preheated air temperatures before the tube outside diameter and the number of heat exchangers is incremented. This results in a table of exit preheated air temperatures versus shell inside diameters for a particular value of tube outside diameter and number of heat exchangers. The basic search ranges for this table are the following: shell inside diameter -- 50-300 cm (19.7 - 118 in) and exit preheated air temperature (stream 3 in Figure 5) -- 330-530K (134.3 - 494.3°F). The program computes values of the objective function for all the design variable combinations and finds the maximum objective function value along with corresponding values of the design variables. A flowchart of this computer program is presented in Figure 9. Appendix B lists the program and sample search results.


START
Declare and Initialize Variables and Arrays
Input data: shell- and tube-side fluid properties, independent design variable values, plus indicators of which optimization results to be outputted
Echo check of data
Initialize optimization loop variables
loop over range of values for number of heat exchangers and tube outside diameters
range of temperature and shell inside diameters
Calculate shell-side fluid exit temperature from an energy balance
Calculate shell-side heat transfer parameters Re, Pr, and h
Calculate tube-side heat transfer parameters Re, Pr, and h
A
A
Determine tube length and number of baffles from ΔT_{ln}, U_o, and A_o
Calculate shell-side pressure drop by iteration
Calculate tube-side pressure drop
Calculate blower and heat exchanger total costs
Determine the net present value of the combined heat recovery system
Find the net work equivalent for the combined heat recovery system
Find the overall second law efficiency of the heat recovery addition system
B

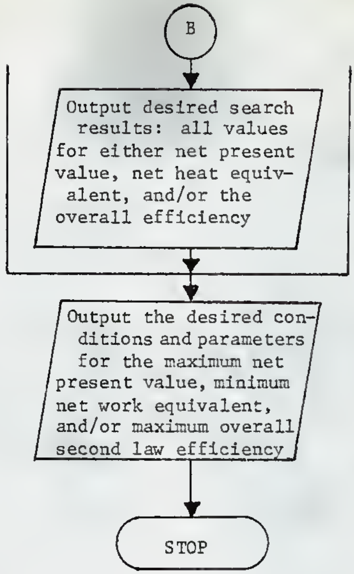


Figure 9. Flowchart of the Flue Gas Heat Recovery Optimization Program

10.2 Optimization results

The results of the optimizations of the economic objective function and the two thermodynamic objective functions determined in section 9.2 are given here. At the outset it will be helpful to explain the basis of comparison for these three objective functions and also to define some of the terminology used in dealing with the optimums of these objective functions. Since four independent design variables are used the number of comparison methods and the detail of each can easily be seen to be large and complex. However, it may be revealed here that only three of these variables can be used for comparison since the tube outside diameter variable is found for all optimums to be one inch, the largest value tested. For simplicity only one independent design variable, the number of heat exchangers, is chosen as the basis of comparison. That variable is chosen over the others because of its inherent unconstrained range of values and its major role in each objective function. For instance, the shell inside diameter is limited to about 118 in. by design constraints and the exit preheated air temperature is limited to the temperature of the inlet flue gas by an end pinchpoint condition. The number of heat exchangers is a major cost factor in the economic objective function and because of its determination of individual exchanger gas flow rates it is a major factor in determining pressure drops. It should be remembered that with the very large flow rates, about 100 m^3/s, associated with this system only a small pressure drop produces both staggering economic and thermodynamic energy costs.

Terminology pertaining to the optimums of the three objective functions is defined next in light of the previous discussion. An objective function optimum at a specified number of heat exchangers will be referred to as a local optimum whereas the objective function optimum found with respect to all the independent design variables including the number of exchangers will be referred to as the global optimum. Economic objective function optimums will be considered as net present value optimums which correspond to the combined heat recovery system (see Figure 6). Optimums of the two thermodynamic objective functions will be considered as exchanger optimums and as exchanger-plus-furnace optimums corresponding to the heat exchanger addition system (see Figure 6) and the combined heat recovery system (Figure 6) respectively.

The simplistic approach mentioned in the early part of this section is well in tune with the major objectives of this heat recovery optimizational study which are to find the conditions at each global optimum and to compare the economic and thermodynamic optimums. As mentioned, because of this simplistic approach it is not considered pertinent to consider the complex functionality that exists between the heat exchanger design criteria and the design variables. The major heat exchanger design criteria of each global optimum are given in Table 12 while Table 13 gives the corresponding objective function value. Table 12 gives outlet flue gas temperatures that indicate the possibility of water vapor condensation. However, no arrangements exist in the computational procedure for condensation because water vapor is only 1.3 mole percent of the total gas corresponding to a very low dew point. In Table 13, the negative value of the thermodynamic objective function for the combined heat recovery system, $(\Delta\varepsilon_2' + \Delta\varepsilon_{equip}' + \Delta W_{in}')$, occurs because as pointed out in section 9.2 fuel is saved which results in a decrease of total fuel work equivalent, i.e. a negative $\Delta\varepsilon_2'$, that in this case is larger in magnitude than the increase in equipment and electrical work equivalents. It is interesting in the light of Part II of this thesis that

Table 12. Heat-Exchanger Design Criteria for the Economic and Thermodynamic Global Optimums

Heat-Exchanger Specification	Optimum Net Present Value*	Optimum Exchanger-Plus-Furnace Value**	Optimum Exchanger Value***	Units
Tube Outside Diameter	1.00	1.00	1.00	in
Shell Inside Diameter	73.62	70.87	94.49	in
Tube Length	18.39	19.95	19.92	ft
Number of Tubes	2990	2761	5043	
Baffle Spacing	73.62	70.87	74.0	in
Number of Baffles	1	2	2	
Number of Heat Exchangers	8	35	27	
Heat Transfer and/or Pressure Drop Quantity				
Shell-Side Reynold's Number	1.70×10^4	4.18×10^3	3.93×10^3	
Shell-Side Prandtl Number	0.748	0.748	0.748	
Shell-Side Heat Transfer Coef.	14.704	5.888	5.774	Btu/hr/ft^2/°F
Tube-Side Reynold's Number	9.25×10^3	2.29×10^3	1.63×10^3	
Tube-Side Prandtl Number	0.723	0.723	0.723	
Tube-Side Heat Transfer Coef.	8.101	2.651	2.015	Btu/hr/ft^2/°F
Overall Heat Transfer Coef.	4.617	1.606	1.301	Btu/hr/ft^2/°F
Total Amount of Heat Transferred	52.82	57.49	62.36	10^6 Btu
Inlet Flue Gas Temperature	500.0	500.0	500.0	°F
Outlet Flue Gas Temperature	235.3	211.7	205.7	°F
Inlet Combustion Air Temp.	100.0	100.0	100.0	°F

Table 12 (Continued)

Heat Transfer and/or Pressure Drop Quantity	Optimum Net Present Value*	Optimum Exchanger-Plus-Furnace Value**	Optimum Exchanger Value***	Units
Exit Preheated Air Temp.	429.5	458.3	465.5	°F
Log Mean Temperature Difference	99.4	71.0	63.6	°F
Outside Tubular Area/ Exchanger	14.4	14.4	26.3	$10^3 ft^2$
Shell-Side Pressure Drop	0.881	0.076	0.087	psi
Tube-Side Pressure Drop	1.936	0.181	0.099	in H_2O

* value of a quantity corresponding to the overall maximum net present value for the combined heat recovery system

** value of a quantity corresponding to the overall minimum of $(\Delta\varepsilon_2' + \Delta\varepsilon_{equip}' + \Delta W_{in}')$ for the combined heat recovery system

*** value of a quantity corresponding to the overall maximum overall second law efficiency, η_2, for the heat exchanger addition system

Table 13. Optimal Values of the Economic and Thermodynamic Objective Functions

Objective Function	Value
Net Present Value*	4.429×10^6 \$(1979)
$(\Delta\varepsilon_2' + \Delta\varepsilon_{equip}' + \Delta W_{in}')$*	-1.376×10^7 kcal/hr
Overall Second Law Efficiency η_2**	0.4704

* for the combined heat recovery system

** for the heat exchanger addition system a first law efficiency corresponding to the heat recovery addition system is calculated without the inclusion of equipment energy or electrical generating inefficiencies to be approximately 0.70. A corresponding incremental efficiency is found to be negative since the work equivalent change between output and input streams is negative and since work is required which by convention is positive. In other words work is required in a process capable of performing work, i.e. a Carnot heat engine could be operated between the stream temperatures.

The other purpose of this study, economic and thermodynamic optimum comparisons, is in part fulfilled by Figure 10. In this figure local optimums normalized with respect to corresponding global optimums are plotted versus the number of heat exchangers. The normalized net present value curve is observed to peak rather sharply at 8 heat exchangers in contrast to the two thermodynamic curves peaking gradually at 27 and 35 heat exchangers corresponding to the normalized exchanger curve and the normalized exchanger-plus-furnace curve respectively. However, these latter two curves reach 0.95, essentially the maximum, at about 12 and 15 heat exchangers respectively. It is observed that the normalized exchanger curve for small numbers of heat exchangers has a lower slope than does the normalized exchanger-plus-furnace curve yet it reaches its global optimum before the normalized exchanger-plus-furnace curve does. The normalized exchanger and exchanger-plus-furnace curves as it should here be remembered correspond to the heat exchanger addition system and the combined heat recovery system respectively. As discussed in section 9.2 in the heat exchanger addition system less emphasis is placed upon the amount of heat recovered than in the combined heat recovery system. The reason for this is that since the furnace is inefficient, because of the combustion of fuel any lessening of the fuel

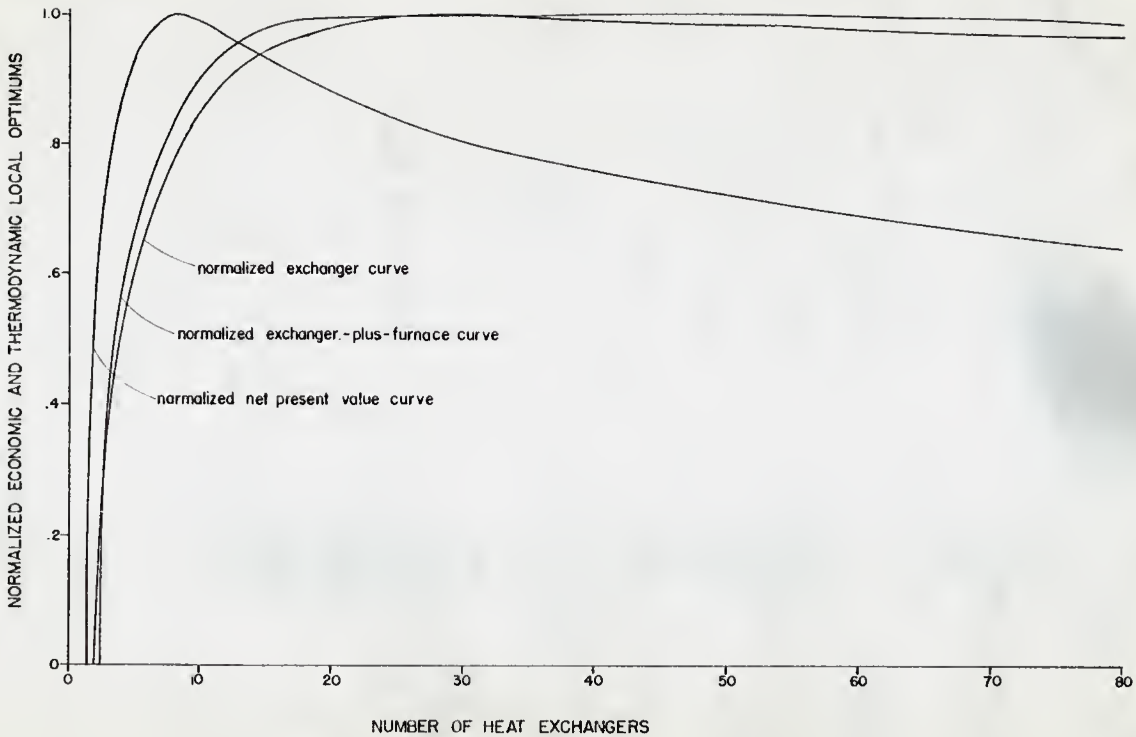


Figure 10. A Comparison of Normalized Economic and Thermodynamic Local Optimums with respect to the Number of Heat Exchangers.

requirement means that the quantity of heat is substituted for a higher grade source. Thus large initial increases in heat recovery have more effect on the combined heat recovery system's objective function resulting in a larger initial slope for the normalized exchanger-plus-furnace curve. The reason that the global optimum of the normalized exchanger curve occurs at a fewer number of heat exchangers than does the global optimum of the normalized exchanger-plus-furnace can be somewhat similarly explained. First, consider what factors actually cause a global thermodynamic optimum to occur with respect to the number of heat exchangers. It is found that as the number of heat exchangers increase the energy debit associated with the equipment (see Chapter 7) finally becomes a large enough fraction of the energy input so that its incremental increase is greater than any incremental decrease in energy cost due to a decreased pressure drop or increased heat recovery. Now, as stated above, recall that the heat exchanger addition system, associated with the normalized exchanger curve, places less value on the heat recovered than does the combined heat recovery system, associated with the normalized exchanger-plus-furnace curve. Thus the equipment energy debit is a larger fraction of the energy input in the exchanger case than in the exchanger-plus-furnace case. Therefore, as the number of heat exchangers increase the global exchanger optimum occurs before the global exchanger-plus-furnace optimum. It may be noted that the equipment energy fraction of the total energy input is 0.045 for the heat exchanger addition system, the exchanger case. A corresponding value for the combined heat recovery system, however, may not be calculated because as seen in section 9.2 the equipment, electrical, feed, product and work equivalents for the furnace system alone are not known. In contrast an equipment cost fraction of the global net present value optimum is 0.48.

The above discussion gives global optimums for the economic and thermodynamic objective functions and shows the functionality of these objective functions with the major independent design variable, the number of heat exchangers. However, that discussion does not provide for a direct comparison between the economic and thermodynamic objective functions. It should be remembered that in Figure 10 these objective functions are only compared on the basis of the same number of heat exchangers and as it happens the same tube outside diameter. The other independent design variables are not fixed. Thus upon further consideration a new comparison approach can be found that yields Figure 11. In this figure the economic and thermodynamic objective functions are directly compared for the combined heat recovery system. Two economic-thermodynamic comparison ratios are plotted versus the number of heat exchangers. One ratio is referred to as $NPV_{\eta_{loc\,opt}}/NPV_{loc\,opt}$ and the other is referred to as $\eta_{NPV_{loc\,opt}}/\eta_{loc\,opt}$. To determine these ratios for a specific number of heat exchangers first the local net present value optimum, $NPV_{loc\,opt}$, and the local exchanger-plus-furnace optimum, $\eta_{loc\,opt}$, are found. Next, the values of the independent design variables corresponding to the local exchanger-plus-furnace optimum are used to calculate a new net present value, $NPV_{\eta_{loc\,opt}}$. Likewise the values of the independent design variables corresponding to the local net present value optimum are used to calculate a new exchanger-plus-furnace value, $\eta_{NPV_{loc\,opt}}$. Finally the new values are divided by the corresponding local optimums to arrive at the two economic-thermodynamic comparison ratios, $NPV_{\eta_{loc\,opt}}/NPV_{loc\,opt}$ and $\eta_{NPV_{loc\,opt}}/\eta_{loc\,opt}$. It should be remembered that local optimums are used here implying that a specific number of heat exchangers are used for each ratio calculation. Therefore, these ratios make possible the direct comparison between the net present value objective

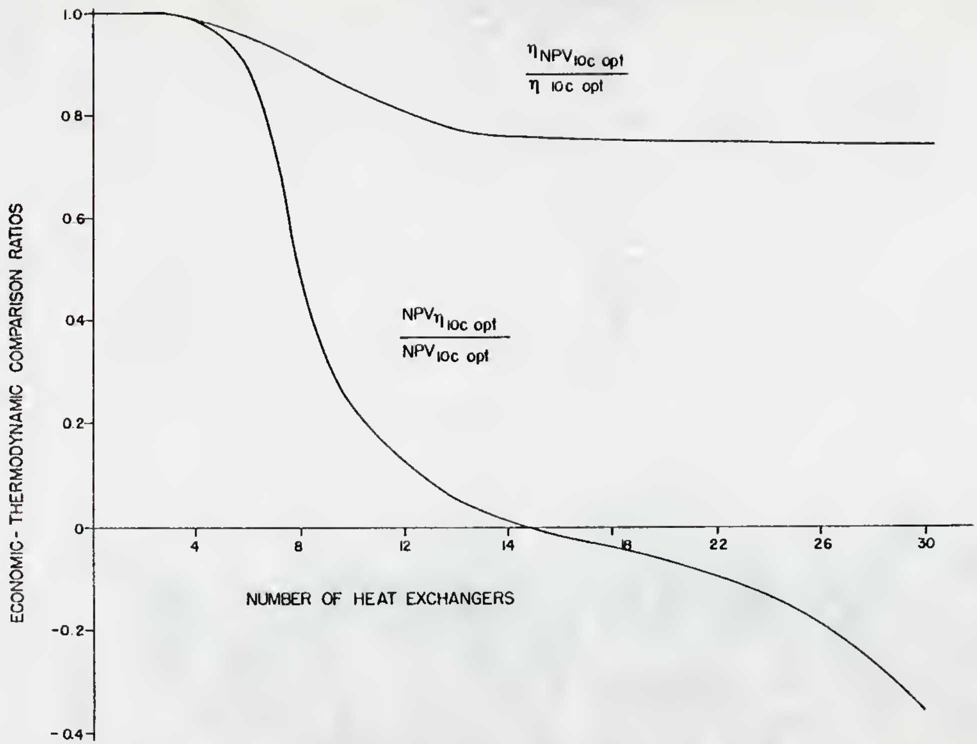


Figure 11. A Direct Comparison of the Net Present Value Objective Function and the Exchanger -- Plus -- Furnace Objective Function with respect to the Number of Heat Exchangers.

function and the exchanger-plus-furnace objective function. Returning to Figure 11 it is first noticed that for one, two, and three heat exchangers both ratios are unity. This implies that both the economic and the thermodynamic optimal designs are identical for these three cases. One explanation for this occurrence is that as had been previously discussed the pressure drop is the dominant factor in both objective functions for this range of heat exchangers thereby producing identical designs that minimize its affect. Another observation is that $\eta_{NPV_{loc\,opt}}/\eta_{loc\,opt}$ gradually decreases asymptotically to 0.74 while $NPV_{\eta_{loc\,opt}}/NPV_{loc\,opt}$ decreases steeply after about 4 exchangers and becomes negative after 15 exchangers. It may be instructive to examine these ratios at the economic and thermodynamic global optimums of 8 heat exchangers and approximately 15 heat exchangers respectively. For 8 heat exchangers $\eta_{NPV_{loc\,opt}}/\eta_{loc\,opt}$ is about 0.9 while $NPV_{\eta_{loc\,opt}}/NPV_{loc\,opt}$ is about 0.5. These values imply that the use of global economic optimum design conditions work well in approximating the actual local thermodynamic optimum but that the reverse of using local thermodynamic optimum design conditions does not satisfactorily approximate the actual global economic optimum. The other case being considered that of 15 heat exchangers gives a similar conclusion since $\eta_{NPV_{loc\,opt}}/\eta_{loc\,opt}$ is 0.76 and $NPV_{\eta_{loc\,opt}}/NPV_{loc\,opt}$ is 0. One additional point may be brought out concerning the global economic optimum case. Since the normalized exchanger-plus-furnace curve in Figure 10 is actually a plot of $\eta_{loc\,opt}/\eta_{global\,opt}$ versus the number of heat exchangers its value at 8 heat exchangers, 0.84, may be multiplied by the $\eta_{NPV_{loc\,opt}}/\eta_{loc\,opt}$ value of 0.91 to give about 0.77 for the new ratio $\eta_{NPV_{global\,opt}}/\eta_{global\,opt}$. This represents the approach of the global economic optimum design to the global thermodynamic optimum design.

CHAPTER 11

CONCLUSION

The thermodynamic optimization of a flue gas heat recovery system using the principles of second law analysis yielded several enlightening conclusions. The thermodynamic optimums produced heat recovery system designs that physically seemed impractical because they required approximately 30 large heat exchangers of about 20,000 ft^2 each. However, specific designs for only 13 heat exchangers were determined to be nearly as optimal as the 30 exchanger cases since those designs gave values of the thermodynamic objective functions within 95% of the optimal values. For comparison a distinct economic optimum occurred at 8 heat exchangers.

In addition, the design conditions of an economic optimum for a predetermined number of heat exchangers was deemed to approximate within at least 20% a corresponding thermodynamic optimum for the same number of heat exchangers as long as that number was less than about 13. The reverse approximation of using thermodynamic optimal conditions to calculate an economic optimum for a preset number of heat exchangers was not satisfactory. This points out that the cost of energy is now becoming high enough so that it is economical to optimize the design of this flue gas heat recovery system within 80% of the actual thermodynamic optimum. However, as this percentage slowly approaches 100% the economics rapidly become less favorable. Thus this additional 20% proves to still be economically quite costly.

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NOMENCLATURE

a_i, bi = constants of a two parameter heat capacity equation for component i used in Eq. (4.12), kcal/(kmol K) and kcal/(kmol K^2), respectively

Cp_a = constant pressure heat capacity for component a (a = i or j), kcal/(kmol K)

C_D = total direct plant cost less land, \$; defined in Eq. (7.1)

C_i = cost component of the total direct cost (i = 1, 2, 3, 4, 5), \$; defined in Eq. (7.1)

C_1, C_2 = constants; defined in Eq.(9.3)

D_C = direct sector energy coefficient, kcal/\$

E_i = energy associated with direct cost i, kcal; defined in Eq. (7.3)

E_{sc} = energy credit coefficient for scrap steel, kcal/\$; defined in Eq. (7.5)

E_T = total equipment and energy construction cost, \$; defined in Eq. (7.4)

f_i = fractional multiplying factor; defined in Eq. (7.2)

f_{sc} = energy credit fraction for scrap steel; defined in Eq. (7.6)

g_{c_i} = combined energy credit coefficient for direct cost i determined from T_{cc}'s for appropriate sectors, kcal/\$

g_i = combined energy coefficient for direct cost i determined from T_c's for appropriate sectors, kcal/\$

ΔG^o = standard free energy of reaction, kcal/kmol

ΔG^o_{fa} = standard free energy of formation for component a, kcal/kmol

h = fraction of energy saved in the steel sector alone by using scrap instead of ores

H = enthalpy of system, kcal

H_i = partial molar enthalpy of component i, kcal/kmol

H_o = enthalpy of system's reference state, kcal

H_{oi} = partial molar reference enthalpy of component i, kcal/kmol

ΔH = total change in enthalpy of system, kcal/hr

ΔH_a^f = standard enthalpy of formation for component a(a = i or j), kcal/kmol

ΔH_{298}^o = standard enthalpy change in reaction, kcal/hr

ΔH_p^o = enthalpy change as products in their standard states are taken from 298K and 1 atm to their actual temperatures, kcal/hr

ΔH_R^o = analogous to ΔH_p^o for reactants instead of products

ΔH_i^c = standard heat of combustion for component i, kcal/kmol

ΔH_{298}^c = standard heat of combustion ($H_2O_{(\ell)}$), kcal/kmol

$\Delta \hat{H}_{298}^c$ = analogous to ΔH_{298}^c except with kcal/lb units

ΔH_p^c, ΔH_R^c = standard heat of combustion for products and reactants, respectively, kcal/kmol

m = number of product streams

n = number of reactant streams

n = stoichiometric coefficient for oxygen in Eq. (4.8)

n_i = molar flowrate of species i, kmol/hr

$NPV_{loc\ opt}$ = local net present value optimum, \$

$NPV_{n_{loc\ opt}}$ = net present value associated with independent design variable values corresponding to the local exchanger-plus-furnace optimum, \$

p = stoichiometric coefficient for hydrogen in Eq. (4.8)

p_j = product stream j

P_o = reference pressure, 1 atm

q = stoichiometric coefficient for nitrogen in Eq. (4.8)

Q = net heat flow across system boundaries with heat flow in being a positive quantity and heat flow out being a negative quantity, kcal/hr

Q_{in},Q_{out} = heat flows into and out of the system, respectively, taken as positive, kcal/hr

R = ideal gas law constant, kcal/(kmol K)

r_i = reactant stream i

S = entropy of system, kcal/K

S_i	=	partial molar entropy of component i, kcal/(kmol K)
S_o	=	entropy of system's reference state, kcal/K
S_{oi}	=	partial molar reference entropy of component i, kcal/(kmol K)
T	=	heat transfer temperature, K
T_a	=	temperature of component a (a = i or j), K
T_c	=	total sector energy coefficient, kcal/$
T_{cc}	=	total sector energy credit coefficient, kcal/$
T_o	=	reference temperature, 298 K
V_i	=	molar volume of species i, ℓ/kmol
W	=	net shaft work between system and surroundings with the convention that work done on the system is positive and work done by the system is negative, kcal/hr
W_{in}, W_{out}	=	shaft work done on the system and by the system, respectively, taken as positive, kcal/hr
W'_{in}	=	shaft work into the furnace unit before flue gas heat recovery, kcal/hr; see Eq. (9.2)
$\Delta W'_{in}$	=	shaft work into the flue gas heat recovery addition, kcal/hr; see Eq. (9.2)
W_{net}	=	actual work equivalent used by a process, kcal/hr; defined in Eq. (3.8)
W_{max}	=	maximum absolute value shaft work done by system under reversible conditions, kcal/hr
x_i	=	mole fraction of species i
α, β, γ	=	stoichiometric coefficients for carbon, hydrogen, and oxygen respectively
γ_b	=	quantity used in estimating the heat of combustion of a variety of organic material; defined in Eq. (4.9)
δ	=	stoichiometric coefficient for nitrogen
ε	=	total work equivalent of a system, kcal
ε_{chem}	=	work equivalent due to chemical energy at T_o and p_o, kcal/hr; defined in Eq. (4.20)

ε_{equip} = work equivalent associated with equipment and construction energy cost, amoritized, kcal/hr; see Eq. (9.1)

ε'_{equip} = analogous to ε_{equip} for the furnace unit before flue gas heat recovery, kcal/hr; defined in Eq. (9.2)

$\Delta\varepsilon'_{equip}$ = analogous to ε_{equip} for the flue gas heat recovery addition, kcal/hr; defined in Eq. (9.2)

ε_i = partial molar work equivalent of species i

$\Delta\varepsilon_i$ = change in work equivalent from pure component i at T_o and p_o to other conditions, kcal/kmol; defined in Eq. (4.19)

$\Delta\varepsilon_{i_p}$ = change in work equivalent due to a change in pressure from p_o at T_o and constant x_i for component i, kcal/kmol; defined in Eq. (4.17)

$\Delta\varepsilon_{i_T}$ = change in work equivalent due to a change in temperature from T_o at constant p and x_i for component i, kcal/kmol; defined in Eq. (4.12) for a two parameter heat capacity and in Eq. (4.13) for a constant heat capacity

$\Delta\varepsilon_{i_x}$ = change in work equivalent due to a change in mole fraction from x_i = 1 at T_o and p_o, kcal/kmol; defined in Eq. (4.18)

ε_i^o = standard state work equivalent for species i, kcal/kmol

ε_{in} = work equivalent input due to process streams, kcal/hr; defined in Eq. (3.7)

ε_n = work equivalent of any stream n (n = 1, 2, ...), kcal/hr

ε'_n = work equivalent of any stream n (n = 1, 2, ...) associated with the furnace unit before flue gas heat recovery, kcal/hr; defined in Eq. (9.2)

$\Delta\varepsilon'_n$ = analogous to ε'_n except associated with the flue gas heat recovery system, kcal/hr; defined in Eq. (10.2)

ε_{out} = work equivalent output due to process streams, kcal/hr; defined in Eq. (3.7)

ε_{phys} = work equivalent due to changes from pure components at T_o and p_o, kcal/hr; defined in Eq. (4.21)

η = second law efficiency; defined in Eq. (3.7)

η_I = incremental efficiency; defined in Eq. (3.8)

$\eta_{loc\,opt}$ = local exchanger-plus-furnace optimum, kcal/hr

$\eta_{NPV_{loc\,opt}}$ = exchanger-plus-furnace value associated with independent design variable values corresponding to the local net present value optimum

η_1	=	overall second law efficiency of the combined heat recovery system; defined in Eq. (9.2)
η_2	=	overall second law efficiency of the heat exchanger addition system; defined in Eq. (9.4)
γ	=	stoichiometric coefficient for sulfur

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APPENDIX A

This appendix refers to the COED process analyzed in Part II. A detailed block flow diagram listing all the stream numbers is given in Figure 12. Corresponding stream descriptions are presented in Table 14. Following that table a listing of the COED thermodynamic computer program with output is given. Throughout the program-listing comments are included that describe the procedures used and give many of the minor assumptions. In reference to the computer output the first table lists the composition and physical conditions of each stream. The next table essentially gives the stream information entailed in Figure 12 plus the utility useage information. After that the material balance check is given which shows a slight discrepancy in the balance that is considered insignificant. Following that table the molar composition, physical conditions, energy values, and work equivalent values are presented for each stream. It may be helpful to define the notation that describe the last two items mentioned above. ACH and ECH refer to the total standard heat of combustion and total standard state chemical work equivalent respectively. APH refers to the total physical enthalpy change from standard state while EPH refers to the total physical work equivalent change from standard state. The E and A represent the total thermal energy and total work equivalent respectively. The next table lists the total input thermal energy and work equivalent for each process unit. Finally the last table gives the final efficiencies and energy balance closure.

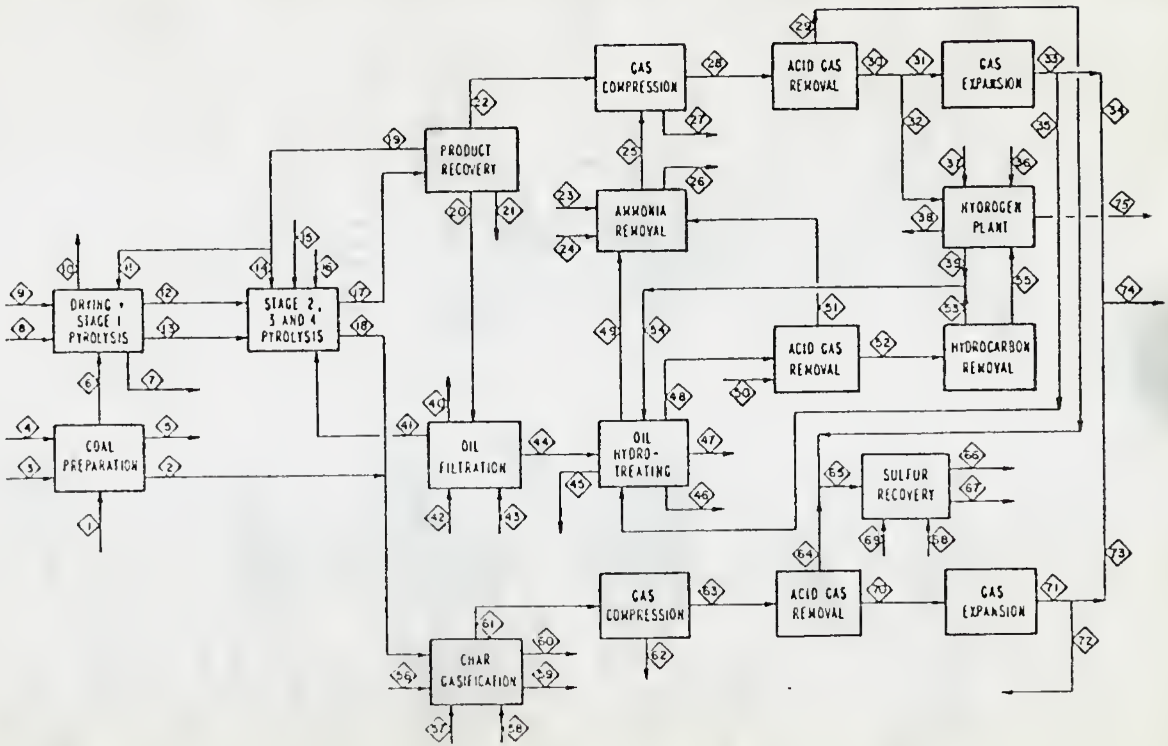

Figure 12. COED Commercial Process Block Diagram with Detailed Streams (from ref. 8)

Table 14. COED Commercial Design Process
Stream Descriptions

Stream Number	Description
1	Feed Goal
2	Goal Fines
3	Fuel Gas
4	Air
5	Stack Gas
6	Crushed Coal
7	Waste Water
8	Fuel Gas
9	Air
10	Stack Gas
11	Second Stage Transport Gas
12	First Stage Char
13	First Stage Waste Liquor
14	Second Stage Transport Gas
15	Oxygen to Stage 4
16	Steam to Stage 4
17	Second Stage Off-Gas
18	Char
19	Second Stage Transport Gas
20	Unfiltered Oil
21	Waste Water
22	Pyrolysis Product Gas
23	Water to Scrubber
24	Water to Stripper
25	Recycled Pyrolysis Gas
26	Stripper Off-Gas
27	Waste Water
28	Pyrolysis Product Gas
29	Acid Gas
30	Clean Pyrolysis Product Gas
31	Clean Pyrolysis Product Gas
32	Glean Pyrolysis Product Gas
33	Clean Pyrolysis Product Gas
34	Clean Pyrolysis Product Gas
35	Clean Pyrolysis Product Gas
36	Steam
37	Water
38	Waste Water
39	Hydrogen
40	Purge Gas
41	Filter Cake
42	Filteraid
43	Hydrogen
44	Filtered Oil
45	Spent Catalyst Plus Coke
46	Waste Water
47	Syncrude
48	Purge Gas
49	Stripper Off-Gas
50	Water to Scrubber
51	Acid Gas
52	Clean Purge Gas
53	Hydrogen
54	Hydrogen
55	Hydrocarbons
56	Water
57	Air
58	Steam
59	Ash
60	Waste Water
61	Gasifier Product Gas
62	Waste Water
63	Gasifier Product Gas
64	Acid Gas
65	Acid Gas
66	Stack Gas
67	Product Sulfur
68	Air
69	Fuel Gas
70	Glean Gasifier Product Gas
71	Glean Gasifier Product Gas
72	Plant Fuel Gas
73	Glean Gasifier Product Gas
74	Plant Product Gas
75	Stack Gas

```
C
C*********************************************************************
C
C SECOND LAW THERMODYNAMIC ANALYSIS OF A GENERAL COMMERCIAL COAL
C CONVERSION PROCESS--APPLIED SPECIFICALLY TO FMC CORP.'S CHAR OIL
C ENERGY DEVELOPMENT PROCESS
C
C WRITTEN BY TERRY L. UNRUH UNDER THE ADVISEMENT OF DR. B. G. KYLE,
C DEPT. OF CHEMICAL ENGINEERING, KANSAS STATE UNIV.
C
C*********************************************************************
C*********************************************************************
C
C                              DATA DESCRIPTION
C
C*********************************************************************
C
C 1. NO. OF PROCESS STREAMS, NO. OF UNITS, AND NO. OF STREAMS IN
C     OVERALL UNIT IF>8
C
C 2. STREAM-COMPONENT ARRAY(1 HR BASIS, ALL AMOUNTS IN TONS)--
C     S(I,J) WHERE I=NO. OF STREAM, AND J=COMPONENT OF PROPERTY
C     S(I,1) -- COAL OR CHAR IF VALUE NEGATIVE
C     S(I,2) -- OIL
C     S(I,3) -- NITROGEN, N2
C     S(I,4) -- OXYGEN, O2
C     S(I,5) -- WATER, H2O
C     S(I,6) -- CARBON DIOXIDE, CO2
C     S(I,7) -- CARBON MONOXIDE, CO
C     S(I,8) -- HYDROGEN,H2
C     S(I,9) -- METHANE, CH4
C     S(I,10)-- ETHYLENE, C2H4
C     S(I,11)-- ETHANE, C2H6
C     S(I,12)-- STATE (1.=GAS, 0.=LIQ. OR SOLID)
C     S(I,13)-- TEMPERATURE, DEGREES F
C     S(I,14)-- PRESSURE, PSIA
C     S(I,15)-- PROPYLENE, C3H6
C     S(I,16)-- PROPANE, C3H8
C     S(I,17)-- NORMAL BUTANE, C4H10
C     S(I,18)-- HYDROGEN SULFIDE, H2S
C     S(I,19)-- AMMONIA, NH3
C     S(I,20)-- SULFUR, S
C     S(I,21)-- ASH
C     S(I,22)-- AIR
C
C 3. PROCESS UNIT ARRAYS (1 HR BASIS)
C     UNAME(I,J) WHERE I=NO. OF UNIT, J=NAME OF UNIT
C     UNIT(I,J) WHERE I=NO. OF UNIT
C     UNIT(I,1-8)-- NO. OF STREAM ENTERING (+) OR LEAVING (-) UNIT I
C                       STREAM NO.<1.--UNUTILIZED STREAM, STREAM NO.>100.
C                       --VALUE ALSO INCLUDED IN UTILITIES
C     UNIT(I,9) -- FUEL GAS, MM BTU
C     UNIT(I,10)-- SHAFT WORK, 1000 HP (IN=+)
C     UNIT(I,11)-- NET STEAM, MM BTU (IN=+)
C     UNIT(I,12)-- NET CONDENSATE, TONS (OUT=+)
C     UNIT(I,13)-- NET COOLING WATER, 1000 GPM (IN=+)
C
C*********************************************************************
```

```
C
C
C     *  DECLARE AND INITIALIZE ARRAYS                                    *
C
      REAL UNAME(20,30)
      REAL UNIT(20,50),PHYS(80),CHEM(80),EFF(20),E(80),S(80,25)
      REAL BHYS(80),CHAM(80),AFF(20),A(80),BFF(20),BNIT(20,13)
      REAL X(80,25),ANIT(20,13),ETOT(20),BTOT(20)
      REAL*8 RWHEAD(23)/'COAL-TON','   OIL  ','   AIR  ',
     *'   N2   ','   O2   ','   H2O  ','   CO2  ','   CO   ',
     *'   H2   ','   CH4  ','  C2H4  ','  C2H6  ','  C3H6  ',
     *'  C4H8  ',
     *'  C4H10 ','   H2S  ','   NH3  ','    S   ','ASH-TONS',
     *'CHAR-TON','TOTAL-KM','PRES-PSI',' TEMP-K '/
      DATA S,PHYS,CHEM,EFF,E,UNIT,UNAME/3860*0./
      DATA BHYS,CHAM,AFF,A,BFF/280*0./
      DATA X/2000*1./
      DATA ANIT,BNIT,ETOT,BTOT/560*0./
C
C     *  READ IN DATA                                                     *
C
      READ(5,100) NSTRM,NUNIT,OVERAL
      READ(5,200) ((S(I,J),J=1,22),I=1,NSTRM)
      READ(5,300) ((UNAME(K,I),I=1,7),(UNIT(K,M),M=1,13),K=1,NUNIT)
      IF(OVERAL.EQ.0.) GO TO 2
      K=NUNIT
      READ(5,400) (UNIT(K,M),M=14,45)
C
C     *  ECHO CHECK DATA                                                  *
C
    2 WRITE(6,1)
      WRITE(6,50)NSTRM,NUNIT
      WRITE(6,164)
      WRITE(6,123)
      DO 153 I=1,NSTRM
      WRITE(6,150)(I,(S(I,J),J=1,22))
      IF(I.NE.42) GO TO 153
      WRITE(6,165)
      WRITE(6,123)
  153 CONTINUE
      WRITE(6,167)
      WRITE(6,165)
      WRITE(6,180)
      WRITE(6,250) ((UNAME(K,I),I=1,7),(UNIT(K,M),M=1,13),K=1,NUNIT)
      IF(OVERAL.EQ.0.) GO TO 70
      K=NUNIT
      WRITE(6,251)(UNIT(K,M),M=14,45)
   70 CONTINUE
      WRITE(6,185)
C
C     ******************************************************************
C
C                           MATERIAL BALANCE CHECK
C
C     ******************************************************************
C
      WRITE(6,174)
      WRITE(6,175)
```

```
C
C     *  MOVE AIR VALUE & REPLACE IT WITH CHAR VALUE IF NECESSARY *
C
      DO 73 I=1,NSTRM
      S(I,24)=S(I,22)
      S(I,22)=0.
      IF(S(I,1).GE.0.) GO TO 73
      S(I,22)=-S(I,1)
      S(I,1)=0.
   73 CONTINUE
      DO 60 K=1,NUNIT
C
C     *  ZERO MATERIAL BALANCE IN & OUT VARIABLES                   *
C
      TIN = 0.
      TOUT = 0.
C
C     *  FIND THE TOTAL MASS ENTERING & LEAVING THE UNIT            *
C
      DO 65 N=1,45
      M=N
C
C     *  SKIP ITEMS 9 - 13                                          *
C
      IF(M.GE.9) M=M+5
      UNT=UNIT(K,M)
      IF(UNT.EQ.0.) GO TO 65
C
C     *  PUT STREAM NO. IN PROPER FORM                              *
C
      IF(ABS(UNIT(K,M)).LT.1.) UNT=UNT*100.
      IF(ABS(UNIT(K,M)).GE.100.) UNT=UNT/10.
      IU=UNT
C
C     *  CORRECT FOR COMPUTER ROUNDOFF ERROR OF DECIMALS            *
C
      AA=ABS(UNT)+.4
      J=AA
      IF(J.LE.NSTRM) GO TO 67
      WRITE(6,299) J
      GO TO 65
   67 CONTINUE
C
C     *  ADD VALUES IN STREAM TO IN OR OUT VARIABLE                 *
C
      DO 68 LL=1,21
      L=LL
C
C     *  SKIP STREAM ITEMS 12 - 14                                  *
C
      IF(L.GE.12) L=L+3
      IF(IU.LT.0) GO TO 69
      TIN=TIN+ABS(S(J,L))
      GO TO 68
   69 TOUT=TOUT+ABS(S(J,L))
   68 CONTINUE
   65 CONTINUE
C
```

```
C     *  SUBTRACT TOTAL OUT VALUE FROM TOTAL IN VALUE                      *
C
      BALCHK=TIN-TOUT
      WRITE(6,176)(UNAME(K,I),I=1,7),BALCHK
   60 CONTINUE
C
C     *******************************************************************
C
C                 UTILITY CALCULATIONS & UNIT CONVERSIONS
C
C     *******************************************************************
C
C          THE ANIT ARRAY IS USED IN THE ENERGY BALANCE CHECK.           *
C     *  THE BNIT ARRAY IS USED IN FIRST LAW IFFICIENCY CALCULA-          *
C     *  TION.  THE UNIT ARRAY BECOMES THE WORK EQUIVALENT FOR            *
C     *  USE IN THE SECOND LAW EFFICIENCY CALCULATIONS.  THE              *
C     *  CORRESPONDING ELEMENTS IN THE FIRST TWC ARRAYS ARE               *
C     *  DEFINED THE SAME AS IN THE UNIT ARRAY.  THE VALUES ARE           *
C     *  CONVERTED TO KCAL.                                               *
C
    7 DO 3 JM=1,NUNIT
      ANIT(JM,9)= UNIT(JM,9)*.252*10.**6
      BNIT(JM,9)=ANIT(JM,9)
C
C     *  ASSUME FUEL GAS PRIMARILY CH4 THUS STANDARD STATE WORK           *
C     *  EQUIVALENT = .93*(HEAT OF COMBUSTION)                            *
C
      UNIT(JM,9)=UNIT(JM,9)*.93*.252*10.**6
      ANIT(JM,10) = UNIT(JM,10)*641.4*1000.
C
C     *  USE AN ELECTRICITY TO WORK CONVERSION EFFICIENCY OF 0.8          *
C
      IF(UNIT(JM,10).GT.0.) BNIT(JM,10)=UNIT(JM,10)*641.4*1000./.8
      IF(UNIT(JM,10).GT.0.) UNIT(JM,10)=UNIT(JM,10)*641.4*1000./.8
      IF(UNIT(JM,10).LT.0.) BNIT(JM,10)=UNIT(JM,10)*641.4*1000.*.8
      IF(UNIT(JM,10).LT.0.) UNIT(JM,10)=UNIT(JM,10)*641.4*1000.*.8
      ANIT(JM,11)=UNIT(JM,11)*.252*10.**6
      BNIT(JM,11)=ANIT(JM,11)
C
C     *  USE 411.5K & 50 PSIA AS THE CONDITIONS FOR STEAM CALCULA-*
C     *  TIONS                                                            *
C
      UNIT(JM,11)=UNIT(JM,11)*22.308*((2054.5+CPI(7.3,2.46,411.5))+
     *1.987*298.2*ALOG(50./14.7))
      ANIT(JM,12)=UNIT(JM,12)*(-68040.)
      UNIT(JM,12)=UNIT(JM,12)*50.357*(-145.8)
      BNIT(JM,12)=ANIT(JM,12)
      ANIT(JM,13)=-3784.*UNIT(JM,13)*1000.
      BNIT(JM,13)=0.
      UNIT(JM,13)=0.
    3 CONTINUE
      DO 27 IT=1,NSTRM
C
C     *  CONVERT FROM DEGREES F TO K                                      *
C
      S(IT,13)=(S(IT,13)-32.)/1.8 +273.15
   27 CONTINUE
C
```

```
C     *  CONVERT THE STREAM COMPONENTS FROM TONS TO KMOLS              *
C
      DO 23 L=1,NSTRM
C
C     *  USE A GIVEN OIL MOLECULAR WEIGHT OF 300 KG/KMOL               *
C
      S(L,2)=S(L,2)*3.024
      S(L,3)=S(L,3)*32.385
      S(L,4)=S(L,4)*28.351
      S(L,5)=S(L,5)*50.357
      S(L,6)=S(L,6)*20.614
      S(L,7)=S(L,7)*32.388
      S(L,8)=S(L,8)*450.013
      S(L,9)=S(L,9)*56.548
      S(L,10)=S(L,10)*32.337
      S(L,11)=S(L,11)*30.169
      S(L,15)=S(L,15)*21.558
      S(L,16)=S(L,16)*20.573
      S(L,17)=S(L,17)*15.608
      S(L,18)=S(L,18)*26.62
      S(L,19)=S(L,19)*53.269
      S(L,20)=S(L,20)*28.293
      S(L,24)=S(L,24)*28.99
   23 CONTINUE
C
C                 TOTAL KMOLS AND CALCULATE MOLE FRACTIONS
C
C     *  THE TOTAL KMOLS OF EACH STREAM ARE PUT INTO                   *
C     *  S(STR. NO.,23) AND THE MOLE FRACTIONS ARE PUT INTO THE        *
C     *  X ARRAY.                                                      *
C
      DO 32 LT=1,NSTRM
      DO 31 LA=2,11
      S(LT,23)=S(LT,23)+ABS(S(LT,LA))
   31 CONTINUE
      DO 30 LA=15,20
      S(LT,23)=S(LT,23)+ABS(S(LT,LA))
   30 CONTINUE
      S(LT,23)=S(LT,23)+S(LT,24)
   32 CONTINUE
      DO 81 J=1,NSTRM
      IF(S(J,23).GT.0.) GO TO 334
      X(J,K)=1.
      GO TO 81
  334 DO 82 K=2,11
      X(J,K)= S(J,K)/S(J,23)
      IF(X(J,K).LE.0.) X(J,K)=1.
   82 CONTINUE
      DO 83 K=15,20
      X(J,K)= S(J,K)/S(J,23)
      IF(X(J,K).LE.0.) X(J,K)=1.
   83 CONTINUE
   81 CONTINUE
C
C     ******************************************************************
C
C           CALCULATE DATA NEEDED TO PERFORM THE ENERGY BALANCE
C             AND TO DETERMINE THE 1ST & 2ND LAW EFFICIENCES
```

```
C
C     ******************************************************************
C
C     *        AFTER SOME PRELIMINARY CONSTANTS ARE ESTABLISHED,        *
C     *  VALUES ARE CALCULATED FOR VARIABLES CORRESPONDING TO           *
C     *  EACH COMPONENT IN THE STREAM--FOUR VARIABLES PER COM-          *
C     *  PONENT:  E| COMPONENT ABBREVIATION |  USED FOR THE CHEM-       *
C     *  ICAL WORK EQUIVALENT, P| COMPONENT ABBREVIATION |  USED        *
C     *  FOR THE PHYSICAL WORK EQUIVALENT, A| COMPONENT ABBREVIA-       *
C     *  TION |  USED FOR THE HEAT OF COMBUSTION AT REFERENCE CON-      *
C     *  DITION, AND B| COMP. ABB. |  USED FOR THE ENTHALPY CHANGE      *
C     *  FROM REFERENCE CONDITION.                                      *
C     *  THE CPI AND CPA FUNCTION SUBPROGRAMS ARE USED TO FIND          *
C     *  VALUES FOR THE P AND B VARIABLES RESPECTIVELY.  CPI AND        *
C     *  CPA CALCULATE THE CHANGE IN WORK EQUIVALENT AND ENTHALPY       *
C     *  RESPECTIVELY AS A COMPONENT IS ADJUSTED TO THE STANDARD        *
C     *  STATE (298.15).                                                *
C
      DO 125 I=1,NSTRM
      T=S(I,13)
      TI=298.15
      RTI= 1.987*TI
      HVCOAL = 12000.
C
C     *  USE THE HEAT OF COMBUSTION-WORK EQUIVALINT APPROXIMATION       *
C     *  WITH THE 12000 BTU/LB VALUE GIVEN FOR COAL                     *
C
      ECOAL=HVCOAL*S(I,1)*504.
C
C     *  TAKE THE AVERAGE HEAT CAPACITY FOR COAL, CHAR, AND ASH         *
C     *  TO BE 0.224 BTU/LB/DEG F AS GIVEN BY PERRY IN THE CHEM-        *
C     *  ICAL ENGINEER'S HANDBOOK.                                      *
C
      PCOAL=S(I,1)*112.90 *(T-TI -TI  *ALOG(T/TI ))*1.8
      ACOAL= S(I,1)*HVCOAL*504.
      BCOAL= S(I,1)*(T-TI)*112.9*1.8
C
C     *  CHECK FOR TYPE OF OIL AND CALCULATE E & A VALUES               *
C     *  ACCORDINGLY.                                                   *
C
      HVOIL = 15300
      IF(S(I,2).GE.0.) GO TO 14
      S(I,2)= -S(I,2)
      EOIL= 19100.*S(I,2)*166.67
      AOIL= 19100.*S(I,2)*166.67
      GO TO 19
C
C     *  USE THE GIVEN SYNCRUDE HIGHER HEATING VALUE OF 19100           *
C     *  BTU/LB ALONG WITH AN APPROXIMATE VALUE OF 14700 BTU/LB         *
C     *  FOR THE RAW OIL.                                               *
C
   14 EOIL=S(I,2)*HVOIL*166.67
      AOIL= S(1,2)*HVOIL*166.7
C
C     *  CHECK OIL FOR LIQUID OR GAS STATE AND CALCULATE P & B          *
C     *  VALUES ACCORDINGLY.                                            *
C     *  ASSUME OIL PHYSICAL PROPERTIES TO BE CLOSE TO THOSE OF         *
C     *  ANTHRACENE:  CP=-14.09+.204*T KCAL/KMOL, HEAT OF VAPORI-       *
```

```
C     *  ZATION=135 KCAL/MOLE, AND VAPOR PRESSURE=.002 MM HG AT    *
C     *  298.15 K.                                                 *
C
   19 POIL=135.*S(I,2)*(T- TI - TI *ALOG(T/ TI ))
      BOIL= S(I,2)*135*(T-TI)
      IF(S(I,12).NE.1.) GO TO 11
      POIL=S(I,2)*(1.987*TI*ALOG(380000.)+CPI(-14.09,204.2,T)+RTI*
     *ALOG(X(I,2)))
      BOIL= S(I,2)*(CPA(-14.09,204.2,T)+137.*166.7)
   11 EN2=S(I,3)*143.
      PN2=S(I,3)*(CPI(6.83,.9,T)+RTI*ALOG(X(I,3)))
      AN2= 0.
      BN2= S(I,3)*CPA(6.83,.9,T)
      EO2=S(I,4)*932.
      PO2=S(I,4)*(CPI(7.16,1.,T)+RTI*ALOG(X(I,4)))
      AO2= 0.
      BO2= S(I,4)*CPA(7.16,1.,T)
C
C     *  CHECK WATER FOR LIQUID OR GAS STATE AND CALCULATE P & B  *
C     *  VALUES ACCORDINGLY.                                       *
C
      IF(S(I,12).EQ.1.) GO TO 10
      EH2O=0.
      AH2O= 0.
      PH2O=S(I,5)*(T-TI-TI*ALOG(T/TI))*18.
      BH2O= S(I,5)*18.*(T-TI)
      GO TO 20
   10 EH2O=0.
      AH2O=0.
      PH2O=S(I,5)*(2054.5+CPI(7.30,2.46,T) +RTI*ALOG(X(I,5)))
      BH2O= S(I,5)*I10519+ ABS(CPA( 7.3,2.46,T)))*(T-TI)/ABS(T-TI)
   20 ECO2=S(I,6)*4776.
      PCO2=S(I,6)*(CPI(10.57,2.10,T)+RTI*ALOG(X(I,6)))
      ACO2= 0.
      BCO2= S(I,6)*CPA(10.57,2.10,T)
      ECO=S(I,7)*65770.
      PCO=S(I,7)*(CPI(6.79,.98,T)+RTI*ALOG(X(I,7)))
      ACO= S(I,7)*67636.
      BCO= S(I,7)*CPA(6.79,.98,T)
      EH2=S(I,8)*56224.
      PH2=S(I,8)*(CPI(6.52,.78,T)+RTI*ALOG(X(I,8)))
      AH2= S(I,8)*68317.
      BH2= S(I,8)*CPAI6.52,.78,T)
      ECH4=S(I,9)*198420.
      PCH4=S(I,9)*(CPI(3.381,18.044,T)+RTI*ALOG(X(I,9)))
      ACH4= S(I,9)*212800.
      BCH4= S(I,9)*CPA(3.381,18.044,T)
      EC2H4=S(I,10)*308672.
      PC2H4=S(I,10)*(CPI(2.83,28.6,T)+RTI*ALOGIX(I,10)))
      AC2H4= S(I,10)*337150.
      BC2H4= S(I,10)*CPA(2.83,28.6,T)
      EC2H6=S(I,11)*357036.
      PC2H6=S(I,11)*(CPI(2.247,38.2,T)+RTI*ALOG(X(I,11)))
      AC2H6= S(I,11)*372820.
      BC2H6= S(I,11)*CPA(2.247,38.2,T)
      EC3H6=S(I,15)*448018.
      PC3H6=S(I,15)*(CPI(3.253,45.12,T)+RTI*ALOG(X(I,15)))
      AC3H6= S(I,15)*491990.
```

```
      BC3H6= S(I,15)*CPA(3.253,45.12,T)
      EC3H8=S(I,16)*513618.
      PC3H8=S(I,16)*(CPI(2.41,57.2,T)+RTI*ALOG(X(I,16)))
      AC3H8= S(I,16)*530600.
      BC3H8= S(I,16)*CPA(2.41,57.2,T)
      EC4H10=S(I,17)*669814.
      PC4H10=S(I,17)*(CPI(3.844,73.35,T)+RTI*ALOG(X(I,17)))
      AC4H10= S(I,17)*687640.
      BC4H10= S(I,17)*CPA(3.844,73.35,T)
      EH2S=S(I,18)*187992.
      PH2S=S(I,18)*(CPI(7.81,2.96,T)+RTI*ALOG(X(I,18)))
      AH2S= S(I,18)*134462.
      BH2S= S(I,18)*CPA(7.81,2.96,T)
      ENH3=S(I,19)*80432.
      PNH3=S(I,19)*(CPI(7.11,6.,T)+RTI*ALOG(X(I,19)))
      ANH3= 0.
      BNH3= S(I,19)*CPA(7.11,6.,T)
      ESLFR=S(I,20)*139660.
      PSLFR=S(I,20)*CPI(3.58,6.24,T)
      ASLFR=S(I,20)*70960.
      BSLFR= S(I,20)*CPA(3.58,6.24,T)
      EASH=0.
      PASH=S(I,21)*112.9*(T -TI-TI*ALOG(T/TI))*1.8
      AASH= 0.
      BASH= S(I,21)*112.9*1.8*(T-TI)
C
C     *  USE TWO DIFFERENT CHAR HEAT OF COMBUSTION VALUES(BTU/LB) *
C     *  DEPENDING UPON STREAM NUMBER.                            *
C
      IF(I.EQ.12) HVCHAR=12000.
      IF(I.EQ.18) HVCHAR=11100.
      ECHAR=S(I,22)*504.*HVCHAR
      PCHAR=S(I,22)*112.9*(T-TI-TI*ALOG(T/TI))*1.8
      ACHAR= S(I,22)*504.*HVCHAR
      BCHAR= S(I,22)*112.9*1.8*(T-TI)
      EAIR=0.
      PAIR=S(I,24)*CPI(6.9,.92,T)
      AAIR= 0.
      BAIR= S(I,24)*CPA(6.9,.92,T)
      PHYS(I)= PCOAL+POIL+PN2+PC2+PH2O+PCO2+PCO+PH2+PCH4+PC2H4+
     * PC2H6+PC3H6+PC3H8+PC4H10+PH2S+PNH3+PSLFR+PASH+PCHAR+PAIR
      CHEM(I)= ECOAL+EOIL+EN2+EC2+EH2O+ECO2+ECO+EH2+ECH4+EC2H4+
     *EC2H6+EC3H6+EC3H8+EC4H10+EH2S+ENH3+ESLFR+EASH+ECHAR
      BHYS(I)= BCOAL+BOIL+BN2+BO2+BH2O+BCO2+BCO+BH2+BCH4+BC2H4+
     *BC2H6+BC3H6+BC3H8+BC4H10+BH2S+BNH3+BSLFR+BASH+BCHAR+BAIR
      CHAM(I)= ACOAL+AOIL+AN2+AC2+AH2O+ACO2+ACO+AH2+ACH4+AC2H4+
     *AC2H6+AC3H6+AC3H8+AC4H10+AH2S+ANH3+ASLFR+AASH+ACHAR
C
C
      IF(S(I,12).NE.1.)GO TO 74
      PHYS(I)=PHYS(I)+S(I,23)*1.987*TI*ALOG(S(I,14)/14.7)
C
C     *  CALCULATE THE TOTAL WORK EQUIVALENTS, E(I), AND THERMAL  *
C     *  ENERGY, A(I), FOR STREAM I.                               *
C
   74 E(I)=PHYS(I)+CHEM(I)
      A(I)=BHYS(I)+CHAM(I)
  125 CONTINUE
```

```
C
C     ********************************************************************
C
C                CALCULATE FIRST AND SECOND LAW EFFICIENCIES
C                       AND ENERGY BALANCE CLOSURES
C
C     ********************************************************************
C
      DO 130 K=1,NUNIT
C
C     *  ZERO THE FIRST AND SECOND LAW EFFICIENCY VARIABLES              *
C
      EIN=0.
      EOUT=0.
      AIN=0.
      BIN=0.
      AOUT=0.
      BOUT=0.
      DO 151 N=1,45
      M=N
C
C     *  SKIP ITEMS 9 - 13                                               *
C
      IF(M.GE.9) M=M+5
      UNT=UNIT(K,M)
      ABSU=ABS(UNT)
C
C     *  PUT STREAM NO. IN PROPER FORM                                   *
C
      IF(ABS(UNIT(K,M)).LT.1.) UNT=UNT*100.
      IF(ABS(UNIT(K,M)).GE.100.) UNT=0.
      IU=UNT
C
C     *  CORRECT FOR COMPUTER ROUND OFF OF DECIMALS                      *
C
      AA=ABS(UNT)+.4
      J=AA
      IF(J.NE.0) GO TO 29
      EUNIT=0.
      AUNIT=0.
      BUNIT=0.
      GO TO 17
   29 EUNIT=E(J)
      BUNIT=A(J)
      AUNIT=A(J)
      IF(IU.LT.0.) GO TO 33
C
C     *  CALCULATE THE TOTAL USEFUL WORK EQUIVALENT, EIN, THE            *
C     *  TOTAL USEFUL THERMAL ENERGY, BIN, AND THE TOTAL THERMAL         *
C     *  ENERGY, AIN, ENTERING THE UNIT AS STREAMS.                      *
C
   17 IF(ABSU.LT.1.) EUNIT=0.
      IF(ABSU.LT.1.) BUNIT=0.
      EIN=EIN+EUNIT
      BIN=BIN+BUNIT
      AIN=AIN+AUNIT
      GO TO 151
C
```

```
C      *  CALCULATE ANALOGOUS QUANTITIES LEAVING THE UNIT AS           *
C      *  STREAMS.                                                     *
C
   33 IF(ABSU.LT.1.) EUNIT=0.
      IF(ABSU.LT.1.) BUNIT=0.
      EOUT=EOUT+EUNIT
      BOUT=BOUT+BUNIT
      AOUT=AOUT+AUNIT
  151 CONTINUE
      W=0.
      Y=0.
      Z=0.
      DO 47 KM=9,13
C
C      *  CALCULATE THE TOTAL WORK EQUIVALENT, W, THERMAL ENERGY,      *
C      *  Y, AND THERMAL ENERGY INCLUDING THE GENERATING EFFICIENCY*
C      *  Z, FOR EACH UNITS UTILITIES.                                 *
C
      IF(UNIT(K,KM).LT.0.) GO TO 46
      W=W+UNIT(K,KM)
      IF(ANIT(K,KM).LT.0.) GO TO 46
      Y= Y+ANIT(K,KM)
      Z=Z+BNIT(K,KM)
      GO TO 47
C
C      *  CALCULATE TOTAL QUANTITIES LEAVING A UNIT.                   *
C
   46 EOUT=EOUT+ABS(UNIT(K,KM))
      AOUT=AOUT+ABS(ANIT(K,KM))
      BOUT=BOUT+ABS(BNIT(K,KM))
   47 CONTINUE
      Q=EIN+W
      IF(Q.NE.0.) GO TO 48
      EFF(K)=0.
      BFF(K)=0.
      GO TO 49
C
C      *  DETERMINE THE SECOND LAW EFFICIENCY, EFF(K), THE ENERGY      *
C      *  BALANCE CLOSURE, AFF(K), AND THE FIRST LAW EFFICIENCY        *
C      *  FOR UNIT K.                                                  *
C
   48 EFF(K)=EOUT/(EIN+W)
      AFF(K)=AOUT/(AIN+Y)*100.
      BFF(K)=BOUT/(BIN+Z)
      BTOT(K) = BIN+Z
      ETOT(K) = EIN+W
   49 EOUT=0.
      AOUT=0.
      BOUT=0.
      EIN=0.
      AIN=0.
      BIN=0.
      W=0.
      Y=0.
      Z=0.
  130 CONTINUE
C
C      *  ADJUST ARRAY ELEMENTS FOR OUTPUT.                            *
```

```
C
      DO 51 K=1,NSTRM
      TS=S(K,13)
      PS=S(K,14)
      DO 52 N=12,20
      S(K,N)=S(K,N+3)
   52 CONTINUE
      S(K,21)=PS
      S(K,22)=TS
      DO 87 M=1,20
      N=24-M
      S(K,N)=S(K,N-1)
   87 CONTINUE
      S(K,3)=S(K,24)
   51 CONTINUE
      NS=0
      M=1
      MF = 10
   88 WRITE(6,310)
      WRITE(6,320) (J,J=M,MF)
      WRITE(6,330)
      WRITE(6,350)(RWHEAD(J),(S(I,J),I=M,MF),J=1,23)
      WRITE(6,551)(CHAM(N),N=M,MF)
      WRITE(6,651)(BHYS(N),N=M,MF)
      WRITE(6,751)(A(JJ),JJ=M,MF)
      WRITE(6,550)(CHEM(N),N=M,MF)
      WRITE(6,650)(PHYS(N),N=M,MF)
      WRITE(6,750)(E(JJ),JJ=M,MF)
      NS = NS+10
      IF(NS.GE.NSTRM) GO TO 89
      M = M+10
      MF = MF+10
      GO TO 88
   89 WRITE(6,423)
      WRITE(6,450)((UNAME(K,I),I=1,7),BTOT(K),ETOT(K),K=1,NUNIT)
      WRITE(6,670)
      WRITE(6,675)
      WRITE(6,680)
      WRITE(6,477)((UNAME(K,I),I=1,7),BFF(K),EFF(K),AFF(K),K=1,NUNIT)
C
C     ******************************************************************
C
C                                   FORMATS
C
C     ******************************************************************
C
    1 FORMAT('1','      ECHO CHECK OF DATA '//)
   50 FORMAT(5X,'NO. STREAMS= ',I2,'  NO. UNITS= ',I2//)
  100 FORMAT(2I10,F10.4)
  123 FORMAT(1X,'NO.',3X,'COAL',2X,'OIL',5X,'N2',4X,'O2',4X,'H2O',
     *4X,'CO2',5X,'CO',4X,'H2',3X,'CH4',1X,'C2H4',2X,'C2H6',1X,
     *'G*',2X,'TEMP',1X,'PRESS',1X,'C3H6',1X,'C3H8',1X,'C4H10',1X,
     *'H2S',2X,'NH3',3X,'S',4X,'ASH',4X,'AIR'/)
  150 FORMAT(1X,I2,1X,F7.1,2F7.2,2F6.2,2F7.2,2F6.2,2F5.2,F3.0,F6.0,
     *F7.1,6F5.2,F6.2,F7.2)
  164 FORMAT(52X,'STREAM - COMPONENT DATA**'/)
  165 FORMAT('1')
  167 FORMAT(/ 1X,'* GAS-LIQUID IDENTIFICATION  ''1''= GAS, ''0''',
```

```
     *'= LIQUID'/ 1X,'** ALL COMPONENTS IN TONS/HR, TEMPERATURE ',
     *'IN DEG F, AND PRESSURE IN PSIA')
 174 FORMAT(/////////55X,'MATERIAL BALANCE CHECK'/)
 175 FORMAT(76X,'DIFFERENCE IN TONS/HR'/53X,'UNIT NAME',19X,
     *'(IN-OUT)'/)
 176 FORMAT(43X,7A4,10X,F8.3/)
 180 FORMAT(48X,'PROCESS UNITS STREAMS AND UTILITIES*'/ 52X,
     *'STREAMS ENTERING',18X,'FEUL',11X,'NET'/ 17X,'UNIT NAME',29X,
     *'AND LEAVING',20X,'GAS',4X,'WORK',3X,'STEAM',4X,'COND.',4X,
     *'CW'//)
 185 FORMAT(/ 8X,'* ENTERING STREAM NO. ''+'', LEAVING STREAM NO',
     *'. ''-'','/10X,'STREAM NO.<1.--UNUTILIZED STREAM,'/10X,
     *'STREAM NO.>100.--VALUE ALSO INCLUDED IN UTILITIES'//10X,
     *'UTILITIES:'/18X,'FUEL GAS, MM BTU',9X,'(IN=+)'/18X,'WORK, ',
     *'HP',17X,'(IN=+)'/18X,'STEAM, MM BTU',12X,'(IN=+)'/18X,
     *'CONDENSATE, TONS',9X,'(OUT=+)'/18X,'COOLING WATER, 1000 ',
     *'GPM  (IN=+)')
 200 FORMAT(11F7.2)
 250 FORMAT(8X,7A4,1X,4F7.2,5F5.0,4F8.1/)
 251 FORMAT(1X,21F6.2,4X/)
 299 FORMAT(10X,'STREAM NOT INPUTTED--',I5)
 300 FORMAT(7A4,4F4.0,5F3.0,F5.1,F5.0,2F5.1)
 310 FORMAT('1'///////  50X,'CCEO PROCESS STREAMS ( 1 HR BASIS)'
     *//)
 320 FORMAT(1X,'STREAM #',8X,I2,9(10X,I2)/)
 330 FORMAT(1X,'COMPOSITION-KMOL'/)
 350 FORMAT((1X,A8,3X,10(F10.2,2X)))
 400 FORMAT(20F4.0)
 423 FORMAT('1'////////51X,'TOTAL ENTERING QUANTITIES'//67X,'TOTAL',
     *' ENERGY IN',4X,'TOTAL WORK EQ. IN'/41X,'UNIT NAME',17X,
     *'KCAL (1ST LAW)',7X,'KCAL (2ND LAW)'/)
 450 FORMAT(31X,7A4,9X,E11.4,9X,E11.4/)
 477 FORMAT(15X,7A4,11X,F9.5,11X,F9.5,12X,F9.3/)
 550 FORMAT(1X,'ECH/KCAL',3X,10E12.4/)
 551 FORMAT(/1X,'ACH/KCAL',3X,10E12.4/)
 650 FORMAT(1X,'EPH/KCAL',3X,10E12.4/)
 651 FORMAT(1X,'APH/KCAL',3X,10E12.4/)
 670 FORMAT('1'///////29X,'THERMODYNAMIC EFFICIENCIES AND ENERGY',
     *' BALANCE CLOSURE FOR THE CCEO PROCESS'//)
 675 FORMAT(24X,'UNIT NAME',22X,'FIRST LAW',10X,'SECOND LAW',10X,
     *'ENERGY BALANCE')
 680 FORMAT(55X,'EFFICIENCY', 9X,'EFFICIENCY',12X,'CLOSURE (%)'//)
 750 FORMAT(1X,'E/KCAL',5X,10E12.4/)
 751 FORMAT(1X,'A/KCAL',5X,10E12.4/)
     STOP
     END
```

```
      FUNCTION CPI(A,B,T)
C
C     ****************************************************************
C
C             THIS FUNCTION SUBPROGRAM CALCULATES THE CHANGE
C               IN WORK EQUIVALENT/KMOL AS A COMPONENT IS
C                ADJUSTED TO THE STANDARD STATE (298.15K)
C
C     ****************************************************************
C
      C=B/1000.
      TI=298.15
      CPI=(A-TI*C)*(T-TI)+C/2*(T**2.-TI**2.)-A*TI*ALOG(T/TI)
      RETURN
      END
```

```
      FUNCTION CPA(A,B,T)
C
C     ****************************************************************
C
C                THIS FUNCTION SUBPROGRAM CALCULATES THE
C              ENTHALPY CHANGE AS A COMPONENT IS ADJUSTED
C                   TO ITS STANDARD STATE (298.15K)
C
C     ****************************************************************
C
      C=B/1000.
      TI=298.15
      CPA=A*(T-TI)+C/2.*(T**2-TI**2)
      RETURN
      END
```

ECHO CHECK OF DATA

NO. STREAMS= 75 NO. UNITS= 19

STREAM - COMPONENT DATA**

NO.	COAL	OIL	N2	O2	H2O	CO2	CO	H2	CH4	C2H4	C2H6	G*	TEMP	PRESS	C3H6	C3H8	C4H10	H2S	NH3	S	ASH	AIR
1	1031.0	0.0	0.0	0.0	167.80	0.0	0.0	0.0	0.0	0.0	0.0	0.	70.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	31.0	0.0	0.0	0.0	2.00	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	24.91	0.0	0.16	0.84	19.34	0.61	0.13	0.0	0.0	1.	70.	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	70.	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	72.14
5	0.0	0.0	78.78	0.0	110.56	31.59	0.0	0.0	0.0	0.0	0.0	1.	150.	16.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	1000.0	0.0	0.0	0.0	63.00	0.0	0.0	0.0	0.0	0.0	0.0	0.	70.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	65.32	0.0	0.0	0.0	0.0	0.0	0.0	0.	112.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	0.0	0.0	71.64	0.0	0.49	2.43	55.62	1.75	0.36	0.0	0.0	1.	100.	30.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	200.	24.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	208.61
10	0.0	0.0	227.63	0.0	18.95	92.75	0.0	0.0	0.0	0.0	0.0	1.	110.	15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	0.0	0.0	0.16	0.0	2.62	27.38	9.48	1.13	3.77	0.17	0.45	1.	550.	23.6	0.16	0.11	0.31	1.32	0.0	0.0	0.0	0.0
12	-977.3	0.0	0.16	0.0	2.62	27.38	9.48	1.13	3.77	0.17	0.45	1.	550.	23.6	0.16	0.11	0.31	1.32	0.0	0.0	0.0	0.0
13	10.6	0.40	0.0	0.0	11.00	0.0	0.0	0.0	0.0	0.0	0.0	0.	110.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.0	0.0	0.31	0.0	5.07	52.89	18.31	2.19	7.27	0.33	0.87	1.	1000.	29.2	0.31	0.21	0.60	2.56	0.0	0.0	0.0	0.0
15	0.0	0.0	0.0	156.50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	72.	30.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	0.0	0.0	0.0	0.0	336.85	0.0	0.0	0.0	0.0	0.0	0.0	1.	1000.	30.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	-7.9	197.00	2.20	0.0	285.21	378.56	131.02	15.67	52.07	2.37	6.20	1.	850.	20.2	2.18	1.52	4.28	18.30	0.0	0.0	0.0	0.0
18	-539.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	1550.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	1.32	0.0
19	0.0	0.0	0.47	0.0	7.69	80.27	27.79	3.32	11.04	0.50	1.32	1.	1000.	30.4	0.47	0.32	0.91	3.88	0.0	0.0	0.0	0.0
20	-7.9	197.00	0.0	0.0	0.99	0.0	0.0	0.0	0.0	0.0	0.0	0.	250.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	0.0	0.0	0.0	0.0	247.95	0.0	0.0	0.0	0.0	0.0	0.0	0.	183.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
22	0.0	0.0	1.73	0.0	28.58	298.29	103.23	12.35	41.03	1.87	4.88	1.	110.	16.0	1.71	1.20	3.37	14.42	0.0	0.0	0.0	0.0
23	0.0	0.0	0.0	0.0	5.74	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	100.	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	402.69
25	0.0	0.0	0.88	0.0	7.42	15.12	52.30	6.25	20.79	0.95	2.47	1.	100.	16.0	0.87	0.61	1.71	4.17	0.0	0.0	0.0	0.0
26	0.0	0.0	301.12	90.92	10.65	0.0	0.0	0.0	0.0	0.0	0.0	1.	100.	16.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	0.0	0.0	0.0	0.0	33.74	0.0	0.0	0.0	0.0	0.0	0.0	0.	90.	14.7	0.0	0.0	0.0	0.0	2.44	0.0	0.0	0.0
28	0.0	0.0	2.61	0.0	2.26	313.41	155.53	10.60	61.82	2.82	7.35	1.	90.	150.0	2.58	1.81	5.08	10.59	0.0	0.0	0.0	0.0
29	0.0	0.0	0.0	0.0	0.0	268.52	0.0	0.0	0.0	0.0	0.0	1.	220.	30.0	0.0	0.0	0.0	18.56	0.0	0.0	0.0	0.0
30	0.0	0.0	2.61	0.0	2.26	44.09	155.53	18.60	61.82	2.82	7.35	1.	110.	140.0	2.58	1.81	5.08	0.03	0.0	0.0	0.0	0.0
31	0.0	0.0	2.33	0.0	2.02	40.12	139.02	16.62	55.25	2.52	6.57	1.	110.	140.0	2.31	1.62	4.54	0.03	0.0	0.0	0.0	0.0
32	0.0	0.0	0.28	0.0	0.24	4.77	16.51	1.98	6.57	0.30	0.78	1.	110.	140.0	0.27	0.19	0.54	0.0	0.0	0.0	0.0	0.0
33	0.0	0.0	2.33	0.0	2.02	40.12	139.02	16.62	55.25	2.52	6.57	1.	100.	30.0	2.31	1.62	4.54	0.03	0.0	0.0	0.0	0.0
34	0.0	0.0	1.45	0.0	1.26	25.01	86.72	10.37	34.46	1.57	4.10	1.	100.	30.0	1.44	1.01	2.83	0.02	0.0	0.0	0.0	0.0
35	0.0	0.0	0.88	0.0	0.76	15.11	52.30	6.25	20.79	0.95	2.47	1.	100.	30.0	0.87	0.61	1.71	0.01	0.0	0.0	0.0	0.0
36	0.0	0.0	0.0	0.0	107.26	0.0	0.0	0.0	0.0	0.0	0.0	1.	440.	415.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
37	0.0	0.0	0.0	0.0	11.70	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
38	0.0	0.0	0.0	0.0	74.73	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
39	0.0	0.0	1.31	0.0	0.84	0.01	0.01	9.75	3.33	0.0	0.0	1.	125.	215.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
40	0.0	0.0	0.55	0.0	0.01	0.0	0.0	0.0	0.0	0.0	0.0	1.	100.	60.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
41	-7.9	5.82	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	350.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	1.32	0.0
42	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	70.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	1.32	0.0

NO.	COAL	OIL	N2	O2	H2O	CO2	CO	H2	CH4	C2H4	C2H6	G*	TEMP	PRESS	C3H6	C3H8	C4H10	H2S	NH3	S	ASH	AIR
43	0.0	0.0	0.55	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	70.	69.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
44	0.0	191.18	0.0	0.0	0.98	0.0	0.0	0.0	0.0	0.0	0.0	0.	300.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
45	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	0.	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
46	0.0	0.0	0.0	0.0	14.71	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
47	0.0	-175.80	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
48	0.0	0.0	1.31	0.0	0.08	0.01	0.34	14.88	9.24	0.05	0.97	1.	100.	1700.0	0.19	0.77	1.18	3.42	0.09	0.0	0.0	0.0
49	0.0	0.0	0.88	0.0	1.62	15.11	52.30	6.25	20.79	0.95	2.47	1.	100.	26.0	0.87	0.61	1.71	0.75	2.35	0.0	0.0	0.0
50	0.0	0.0	0.0	0.0	0.06	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
51	0.0	0.0	0.0	0.0	0.06	0.01	0.0	0.0	0.0	0.0	0.0	1.	100.	26.0	0.0	0.0	0.0	3.42	0.09	0.0	0.0	0.0
52	0.0	0.0	1.31	0.0	0.08	0.0	0.34	14.88	9.24	0.05	0.97	1.	100.	1690.0	0.19	0.77	1.18	0.0	0.0	0.0	0.0	0.0
53	0.0	0.0	0.0	0.0	0.08	0.0	0.0	14.88	4.62	0.0	0.0	1.	100.	1680.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
54	0.0	0.0	1.31	0.0	0.92	0.01	0.01	24.63	7.55	0.0	0.0	1.	200.	1800.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
55	0.0	0.0	1.31	0.0	0.0	0.0	0.34	0.0	4.62	0.05	0.97	1.	100.	30.0	0.19	0.77	1.18	0.0	0.0	0.0	0.0	0.0
56	0.0	0.0	0.0	0.0	290.93	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
57	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	200.	27.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1388.14
58	0.0	0.0	0.0	0.0	234.40	0.0	0.0	0.0	0.0	0.0	0.0	1.	275.	27.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
59	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	350.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	136.87	0.0
60	0.0	0.0	0.0	0.0	215.52	0.0	0.0	0.0	0.0	0.0	0.0	0.	115.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
61	0.0	0.0	1084.63	0.0	100.24	58.78	842.14	26.41	5.46	0.0	0.0	1.	110.	20.0	0.0	0.0	0.0	17.56	0.0	0.0	0.0	0.0
62	0.0	0.0	0.0	0.0	92.87	0.0	0.0	0.0	0.0	0.0	0.0	0.	90.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
63	0.0	0.0	1084.63	0.0	7.37	58.78	842.14	26.41	5.46	0.0	0.0	1.	90.	150.0	0.0	0.0	0.0	17.56	0.0	0.0	0.0	0.0
64	0.0	0.0	0.0	0.0	0.0	22.06	0.0	0.0	0.0	0.0	0.0	1.	220.	30.0	0.0	0.0	0.0	17.36	0.0	0.0	0.0	0.0
65	0.0	0.0	0.0	0.0	0.0	290.58	0.0	0.0	0.0	0.0	0.0	1.	220.	30.0	0.0	0.0	0.0	35.92	0.0	0.0	0.0	0.0
66	0.0	0.0	101.85	0.0	25.60	309.95	0.0	0.0	0.0	0.0	0.0	1.	285.	16.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
67	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.	100.	14.7	0.0	0.0	0.0	0.0	0.0	33.79	0.0	0.0
68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.	100.	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	117.43
69	0.0	0.0	14.76	0.0	0.10	0.50	11.46	0.36	0.08	0.0	0.0	1.	100.	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
70	0.0	0.0	1084.63	0.0	7.37	36.72	842.14	26.41	5.46	0.0	0.0	1.	110.	140.0	0.0	0.0	0.0	0.20	0.0	0.0	0.0	0.0
71	0.0	0.0	1084.63	0.0	7.37	36.72	842.14	26.41	5.46	0.0	0.0	1.	100.	30.0	0.0	0.0	0.0	0.20	0.0	0.0	0.0	0.0
72	0.0	0.0	184.29	0.0	1.25	6.24	143.09	4.49	0.93	0.0	0.0	1.	100.	30.0	0.0	0.0	0.0	0.03	0.0	0.0	0.0	0.0
73	0.0	0.0	900.34	0.0	6.12	30.48	699.05	21.92	4.55	0.0	0.0	1.	100.	30.0	0.0	0.0	0.0	0.17	0.0	0.0	0.0	0.0
74	0.0	0.0	931.79	0.0	7.36	55.49	785.77	32.29	38.99	1.57	4.10	1.	100.	30.0	1.44	1.01	2.83	0.19	0.0	0.0	0.0	0.0
75	0.0	0.0	0.0	2.22	0.0	68.62	0.0	0.0	0.0	0.0	0.0	1.	110.	14.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

* GAS-LIQUID IDENTIFICATION '1'= GAS, '0'= LIQUID
** ALL COMPONENTS IN TONS/HR, TEMPERATURE IN DEG F, AND PRESSURE IN PSIA

PROCESS UNITS STREAMS AND UTILITIES*

UNIT NAME	STREAMS ENTERING AND LEAVING								FEUL GAS	WORK	NET STEAM	COND.	CW
COAL PREPARATION	-0.05	1.00	3.00	4.00	-2.	-6.	0.	0.	0.	8.0	0.0	0.0	0.0
DRYING & STAGE 1 PYROLYSIS	-0.07	-0.10	6.00	8.00	9.	11.	-12.	-13.	0.	38.3	10.0	5.4	30.7
STAGE 2, 3, AND 4 PYROLYSIS	12.00	13.00	14.00	15.00	16.	41.	-17.	-18.	62.	0.0	0.0	0.0	0.0
PRODUCT RECOVERY	-0.21	-19.00	-20.00	-22.00	17.	0.	0.	0.	88.	5.9	93.0	50.3	79.5
PYROLYSIS GAS COMPRESSION	-0.27	-28.00	22.00	25.00	0.	0.	0.	0.	0.	79.3	-275.0	121.9	0.0
PYROLYSIS ACID GAS REMOVAL	28.00	-29.00	-30.00	0.0	0.	0.	0.	0.	0.	1.7	1281.0	693.7	22.6
PYROLYSIS GAS EXPANSION	31.00	-33.00	0.0	0.0	0.	0.	0.	0.	0.	-24.6	0.0	0.0	-2.5
OIL FILTRATION	-0.40	20.00	0.42	0.43	-41.	-44.	0.	0.	1.	1.2	16.0	8.7	1.1
OIL HYDROTREATING	-0.46	44.00	54.00	35.00	-49.	-47.	-45.	-48.	167.	41.5	-435.0	0.0	0.6
PURGE ACID GAS REMOVAL	48.00	50.00	-51.00	-52.00	0.	0.	0.	0.	0.	2.0	0.0	0.0	0.0
HYDROCARBON REMOVAL	52.00	-53.00	-55.00	0.0	0.	0.	0.	0.	0.	1.8	0.0	0.0	0.0
AMMONIA REMOVAL	-0.26	23.00	24.00	49.00	51.	-25.	0.	0.	0.	5.5	0.0	0.0	0.0
HYDROGEN PLANT	-0.38	-0.75	32.00	37.00	36.	-39.	55.	0.	403.	10.1	-106.0	18.0	13.9
CHAR GASIFICATION	-0.59	-0.60	-61.00	58.00	57.	56.	18.	2.	0.	39.5	-1888.0	0.0	7.5
GASIFIER GAS COMPRESSION	-0.62	61.00	-63.00	0.0	0.	0.	0.	0.	0.	219.1	-668.0	0.0	0.0
GASIFIER ACID GAS REMOVAL	63.00	-64.00	-70.00	0.0	0.	0.	0.	0.	0.	0.3	203.0	110.1	3.6
GASIFIER GAS EXPANSION	70.00	-71.00	0.0	0.0	0.	0.	0.	0.	0.	-113.0	0.0	0.0	-14.4
SULFUR RECOVERY	69.00	-0.66	65.00	68.00	-67.	0.	0.	0.	0.	3.0	-225.0	6.4	0.0
OVERALL COED PROCESS	1.00	4.00	9.00	15.00	0.	24.	0.	42.	0.	320.9	-501.0	-219.0	151.7

0.50 0.55 57.00 68.00 -0.05 -0.07 -0.10 -0.21 -0.26 -0.27 -0.38 -0.40-45.00 -0.46-47.00 -0.59 -0.60 -0.62 -0.66-67.00-74.00

-0.75 43.00 0.03 0.08160.00360.00580.00 0.69 -0.72 0.0 0.0

* ENTERING STREAM NO. '+', LEAVING STREAM NO. '-',
  STREAM NO.<1.--UNUTILIZED STREAM,
  STREAM NO.>100.--VALUE ALSO INCLUDED IN UTILITIES

UTILITIES:

FUEL GAS, MM BTU	(IN=+)
WORK, HP	(IN=+)
STEAM, MM BTU	(IN=+)
CONDENSATE, TONS	(OUT=+)
COOLING WATER, 1000 GPM	(IN=+)

MATERIAL BALANCE CHECK

UNIT NAME	DIFFERENCE IN TONS/HR (IN-OUT)
COAL PREPARATION	-0.001
DRYING & STAGE 1 PYROLYSIS	-0.000
STAGE 2, 3, AND 4 PYROLYSIS	-0.001
PRODUCT RECOVERY	0.001
PYROLYSIS GAS COMPRESSION	-0.001
PYROLYSIS ACID GAS REMOVAL	0.001
PYROLYSIS GAS EXPANSION	0.0
OIL FILTRATION	-0.000
OIL HYDROTREATING	0.001
PURGE ACID GAS REMOVAL	0.0
HYDROCARBON REMOVAL	0.0
AMMONIA REMOVAL	-0.000
HYDROGEN PLANT	0.006
CHAR GASIFICATION	0.000
GASIFIER GAS COMPRESSION	0.000
GASIFIER ACID GAS REMOVAL	-0.000
GASIFIER GAS EXPANSION	0.0
SULFUR RECOVERY	-0.000
OVERALL COED PROCESS	0.043

COEO PROCESS STREAMS (1 HR BASIS)

STREAM #	1	2	3	4	5	6	7	8	9	10
COMPOSITION-KMOL										
COAL-TON	1031.00	31.00	0.0	0.0	0.0	1000.00	0.0	0.0	0.0	0.0
OIL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	2091.34	0.0	0.0	0.0	0.0	6047.60	0.0
N2	0.0	0.0	806.71	0.0	2551.29	0.0	0.0	2320.06	0.0	7371.79
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	8449.90	100.71	8.06	0.0	5567.47	3172.49	3289.32	24.67	0.0	954.26
CO2	0.0	0.0	17.32	0.0	651.20	0.0	0.0	50.09	0.0	1911.95
CO	0.0	0.0	626.38	0.0	0.0	0.0	0.0	1801.42	0.0	0.0
H2	0.0	0.0	274.51	0.0	0.0	0.0	0.0	787.52	0.0	0.0
CH4	0.0	0.0	7.35	0.0	0.0	0.0	0.0	20.36	0.0	0.0
C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	8449.90	100.71	1740.32	2091.34	8769.95	3172.49	3289.32	5004.12	6047.60	10238.00
PRES-PSI	14.70	14.70	20.00	20.00	16.00	14.70	14.70	30.00	24.50	15.00
TEMP-K	294.26	310.93	294.26	294.26	338.71	294.26	317.59	310.93	366.48	316.48
ACH/KCAL	0.6235E 10	0.1075E 09	0.6268E 08	0.0	0.0	0.6048E 10	0.0	0.1800E 09	0.0	0.0
APH/KCAL	-0.1406E 07	0.1037E 06	-0.1327E 06	-0.5833E 05	0.6142E 08	-0.1012E 07	0.1151E 07	0.7133E 06	0.2978E 07	0.1153E 08
A/KCAL	0.6234E 10	0.1876E 09	0.6255E 08	-0.5833E 05	0.6142E 08	0.6047E 10	0.1151E 07	0.1807E 09	0.2978E 07	0.1153E 08
ECH/KCAL	0.6235E 10	0.1875E 09	0.5829E 08	0.0	0.3475E 07	0.6040E 10	0.0	0.1674E 09	0.0	0.1019E 08
EPH/KCAL	0.9255E 04	0.2160E 04	-0.8094E 06	0.3818E 06	0.7689E 07	0.6663E 04	0.3599E 05	-0.1115E 07	0.2127E 07	-0.2549E 07
E/KCAL	0.6235E 10	0.1875E 09	0.5748E 08	0.3818E 06	0.1116E 08	0.6048E 10	0.3599E 05	0.1663E 09	0.2127E 07	0.7636E 07

COED PROCESS STREAMS (1 HR BASIS)

STREAM #	11	12	13	14	15	16	17	18	19	20
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	10.60	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	0.0	0.0	1.21	0.0	0.0	0.0	595.73	0.0	0.0	595.73
AIR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	5.18	5.18	0.0	10.04	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	4436.93	0.0	71.25	0.0	15.22	0.0
H2O	131.94	131.94	553.93	255.31	0.0	0.0	0.0	0.0	0.0	0.0
CO2	564.41	564.41	0.0	1090.27	0.0	16962.75	14362.32	0.0	387.25	49.85
CO	307.04	307.04	0.0	593.02	0.0	0.0	7803.63	0.0	1654.69	0.0
H2	508.51	508.51	0.0	985.53	0.0	0.0	4243.47	0.0	900.06	0.0
CH4	213.19	213.19	0.0	411.10	0.0	0.0	7051.70	0.0	1494.04	0.0
C2H4	5.50	5.50	0.0	10.67	0.0	0.0	2944.45	0.0	624.29	0.0
C2H6	13.58	13.58	0.0	26.25	0.0	0.0	76.64	0.0	16.17	0.0
C3H6	3.45	3.45	0.0	6.68	0.0	0.0	187.05	0.0	39.82	0.0
C4H8	2.26	2.26	0.0	4.32	0.0	0.0	47.00	0.0	10.13	0.0
C4H10	4.84	4.84	0.0	9.36	0.0	0.0	31.27	0.0	6.58	0.0
H2S	35.14	35.14	0.0	68.15	0.0	0.0	66.80	0.0	14.20	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	487.15	0.0	103.29	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	0.0	977.25	0.0	0.0	0.0	0.0	0.0	1.32	0.0	0.0
TOTAL-KM	1795.03	1795.03	555.14	3470.71	4436.93	16962.75	7.88	539.82	0.0	7.88
PRES-PSI	23.64	23.64	14.70	29.18	30.52	30.52	37968.44	0.0	5265.73	645.58
TEMP-K	560.93	560.93	316.48	810.93	295.37	810.93	20.20	14.70	30.38	14.70
							727.59	1116.48	810.93	394.26
ACH/KCAL	0.1187E 09	0.6029E 10	0.6719E 08	0.2295E 09	0.0	0.0	0.3209E 10	0.3020E 10	0.3482E 09	0.1563E 10
APH/KCAL	0.5764E 07	0.5795E 08	0.2253E 06	0.2012E 08	-0.9190E 05	0.2538E 09	0.3373E 09	0.8999E 08	0.3052E 08	0.7570E 07
A/KCAL	0.1245E 09	0.6087E 10	0.6742E 08	0.2496E 09	-0.9190E 05	0.2538E 09	0.3546E 10	0.3110E 10	0.3787E 09	0.1571E 10
ECH/KCAL	0.1129E 09	0.6023E 10	0.6719E 08	0.2182E 09	0.4135E 07	0.0	0.3128E 10	0.3020E 10	0.3310E 09	0.1563E 10
EPH/KCAL	0.2760E 06	0.1504E 08	0.6658E 04	0.6007E 07	0.1921E 07	0.7423E 08	0.7201E 08	0.4670E 08	0.9241E 07	0.1062E 07
E/KCAL	0.1132E 09	0.6038E 10	0.6720E 08	0.2242E 09	0.6056E 07	0.7423E 08	0.3200E 10	0.3067E 10	0.3403E 09	0.1564E 10

COEO PROCESS STREAMS (1 HR BASIS)

STREAM #	21	22	23	24	25	26	27	28	29	30
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	11673.98	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	56.03	0.0	0.0	28.50	9751.76	0.0	84.52	0.0	84.52
O2	0.0	0.0	0.0	0.0	0.0	2577.67	0.0	0.0	0.0	0.0
H2O	12486.02	1439.20	289.05	0.0	373.65	536.30	1699.04	113.81	0.0	113.81
CO2	0.0	6148.95	0.0	0.0	311.68	0.0	0.0	6460.63	5535.27	925.36
CO	0.0	3343.41	0.0	0.0	1693.89	0.0	0.0	5037.30	0.0	5037.30
H2	0.0	5557.66	0.0	0.0	2812.58	0.0	0.0	8370.23	0.0	8370.23
CH4	0.0	2320.16	0.0	0.0	1175.63	0.0	0.0	3495.80	0.0	3495.80
C2H4	0.0	60.47	0.0	0.0	30.72	0.0	0.0	91.19	0.0	91.19
C2H6	0.0	147.22	0.0	0.0	74.52	0.0	0.0	221.74	0.0	221.74
C3H6	0.0	36.86	0.0	0.0	18.76	0.0	0.0	55.62	0.0	55.62
C4H8	0.0	24.69	0.0	0.0	12.55	0.0	0.0	37.24	0.0	37.24
C4H10	0.0	52.60	0.0	0.0	26.69	0.0	0.0	79.29	0.0	79.29
H2S	0.0	383.86	0.0	0.0	111.01	0.0	0.0	494.87	494.07	0.80
NH3	0.0	0.0	0.0	0.0	0.0	129.98	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	12486.02	19571.10	289.05	11673.98	6670.16	12995.71	1699.04	24542.21	6029.33	18512.88
PRES-PSI	14.70	16.00	14.70	20.00	16.00	16.00	14.70	150.00	30.00	140.00
TEMP-K	357.04	316.48	310.93	310.93	310.93	310.93	305.37	305.37	377.59	316.48
ACH/KCAL	0.0	0.1294E 10	0.0	0.0	0.6442E 09	0.0	0.0	0.1938E 10	0.6643E 08	0.1872E 10
APH/KCAL	0.1324E 08	0.1820E 08	0.6648E 05	0.1071E 07	0.4592E 07	0.6042E 07	0.2209E 06	0.2707E 07	0.5306E 07	0.3825E 07
A/KCAL	0.1324E 08	0.1312E 10	0.6648E 05	0.1071E 07	0.6488E 09	0.6842E 07	0.2209E 06	0.1941E 10	0.7174E 08	0.1875E 10
ECH/KCAL	0.0	0.1230E 10	0.0	0.0	0.5940E 09	0.1425E 08	0.0	0.1824E 10	0.1193E 09	0.1705E 10
EPH/KCAL	0.1157E 07	-0.1513E 08	0.1385E 04	0.2152E 07	-0.4968E 07	-0.3718E 07	0.2641E 04	0.1150E 08	0.2139E 07	0.1004E 08
E/KCAL	0.1157E 07	0.1215E 10	0.1385E 04	0.2152E 07	0.5890E 09	0.1053E 08	0.2641E 04	0.1835E 10	0.1215E 09	0.1715E 10

COEO PROCESS STREAMS (1 HR BASIS)

STREAM #	31	32	33	34	35	36	37	38	39	40
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	75.46	9.07	75.46	46.96	28.50	0.0	0.0	0.0	42.42	17.81
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	101.72	12.09	101.72	63.45	38.27	5401.29	589.18	3763.18	42.30	0.50
CO2	827.03	98.33	827.03	515.56	311.48	0.0	0.0	0.0	0.21	0.0
CO	4502.57	534.73	4502.57	2808.69	1693.89	0.0	0.0	0.0	0.32	0.0
H2	7479.21	891.03	7479.21	4666.63	2812.58	0.0	0.0	0.0	4387.63	0.0
CH4	3124.28	371.52	3124.28	1940.64	1175.63	0.0	0.0	0.0	188.30	0.0
C2H4	81.49	9.70	81.49	50.77	30.72	0.0	0.0	0.0	0.0	0.0
C2H6	198.21	23.53	198.21	123.69	74.52	0.0	0.0	0.0	0.0	0.0
C3H6	49.80	5.82	49.80	31.04	18.76	0.0	0.0	0.0	0.0	0.0
C4H8	33.33	3.91	33.33	20.78	12.55	0.0	0.0	0.0	0.0	0.0
C4H10	70.86	0.43	70.86	44.17	26.69	0.0	0.0	0.0	0.0	0.0
H2S	0.80	0.0	0.80	0.53	0.27	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	16544.75	1968.14	16544.75	10320.90	6223.84	5401.29	589.18	3763.18	4661.18	18.32
PRES-PSI	140.00	140.00	30.00	30.00	30.00	415.00	14.70	14.70	215.00	60.00
TEMP-K	316.48	316.48	310.93	310.93	310.93	504.26	310.93	310.93	324.82	310.93
ACH/KCAL	0.1673E 10	0.1989E 09	0.1673E 10	0.1043E 10	0.6293E 09	0.0	0.0	0.0	0.3398E 09	0.0
APH/KCAL	0.3419E 07	0.4065E 06	0.2704E 07	0.1687E 07	0.1017E 07	0.6604E 08	0.1355E 06	0.8655E 06	0.1299E 07	0.6966E 04
A/KCAL	0.1676E 10	0.1993E 09	0.1675E 10	0.1045E 10	0.6303E 09	0.6604E 08	0.1355E 06	0.8655E 06	0.3411E 09	0.6966E 04
ECH/KCAL	0.1523E 10	0.1811E 09	0.1523E 10	0.9503E 09	0.5732E 09	0.0	0.0	0.0	0.2841E 09	0.2547E 04
EPH/KCAL	0.8975E 07	0.1069E 07	-0.6159E 07	-0.3841E 07	-0.2318E 07	0.2402E 08	0.2823E 04	0.1803E 05	0.6777E 07	0.1496E 05
E/KCAL	0.1532 10	0.1822E 09	0.1517E 10	0.9465E 09	0.5708E 09	0.2402E 08	0.2823E 04	0.1803E 05	0.2909E 09	0.1751E 05

COEO PROCESS STREAMS (1 HR BASIS)

STREAM #	41	42	43	44	45	46	47	48	49	50
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	17.60	0.0	0.0	578.13	0.0	0.0	531.62	0.0	0.0	0.0
AIR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	17.81	0.0	0.0	0.0	0.0	42.42	28.50	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	49.35	0.0	740.75	0.0	4.03	81.58	3.02
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.21	311.48	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.01	1653.89	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6696.19	2812.58	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	522.50	1175.63	0.0
C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.62	30.72	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	29.26	74.52	0.0
C3H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.10	18.76	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.84	12.55	0.0
C4H10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	18.42	26.69	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	91.04	19.96	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.79	125.18	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	1.32	1.32	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	7.88	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	17.60	0.0	17.81	627.48	0.0	740.75	531.62	7441.41	6412.02	3.02
PRES-PSI	14.70	14.70	60.00	14.70	0.0	14.70	14.70	1700.00	26.00	14.70
TEMP-K	449.82	294.26	294.26	422.04	255.37	310.93	310.93	310.93	310.93	310.93
ACH/KCAL	0.8897E 08	0.0	0.0	0.1475E 10	0.0	0.0	0.1692E 10	0.6162E 09	0.6320E 09	0.0
APH/KCAL	0.6439E 06	-0.1043E 04	-0.4916E 03	0.9779E 07	0.0	0.1704E 06	0.9170E 06	0.7123E 06	0.1494E 07	0.6949E 03
A/KCAL	0.8962E 08	-0.1043E 04	-0.4916E 03	0.1484E 10	0.0	0.1704E 06	0.1693E 10	0.6169E 09	0.6334E 09	0.6949E 03
ECH/KCAL	0.8896E 08	0.0	0.2547E 04	0.1474E 10	0.0	0.0	0.1692E 10	0.5316E 09	0.5869E 09	0.0
EPH/KCAL	0.1234E 06	0.6866E 01	0.1484E 05	0.1601E 07	0.0	0.3550E 04	0.1911E 05	0.1903E 08	-0.3256E 07	0.1448E 02
E/KCAL	0.8909E 08	0.6866E 01	0.1739E 05	0.1476E 10	0.0	0.3550E 04	0.1692E 10	0.5507E 09	0.5837E 09	0.1448E 02

COED PROCESS STREAMS (1 HR BASIS)

STREAM #	51	52	53	54	55	56	57	58	59	60
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	0.0	0.0	0.0	40242.16	0.0	0.0	0.0
N2	0.0	42.42	0.0	42.42	42.42	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	3.02	4.03	4.03	46.33	0.0	14650.36	0.0	11803.68	0.0	10852.94
CO2	0.21	0.0	0.0	0.21	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	11.01	0.0	0.32	11.01	0.0	0.0	0.0	0.0	0.0
H2	0.0	6696.19	6696.19	11083.81	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	522.50	261.25	449.56	261.25	0.0	0.0	0.0	0.0	0.0
C2H4	0.0	1.62	0.0	0.0	1.62	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	29.26	0.0	0.0	29.26	0.0	0.0	0.0	0.0	0.0
C3H6	0.0	4.10	0.0	0.0	4.10	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	15.84	0.0	0.0	15.84	0.0	0.0	0.0	0.0	0.0
C4H10	0.0	18.42	0.0	0.0	18.42	0.0	0.0	0.0	0.0	0.0
H2S	91.04	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	4.79	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	136.87	0.0
CHAR-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	99.06	7345.38	6961.47	11622.65	383.92	14650.36	40242.16	11803.68	0.0	10852.94
PRES-PSI	26.00	1690.00	1680.00	1800.00	30.00	14.70	27.92	27.92	14.70	14.70
TEMP-K	310.93	310.93	310.93	366.48	310.93	310.93	366.48	408.15	449.82	319.26
ACH/KCAL	0.1224E 08	0.6039E 09	0.5131E 09	0.8529E 09	0.9088E 08	0.0	0.0	0.0	0.0	0.0
APH/KCAL	0.4280E 05	0.7016E 06	0.6506E 06	0.5957E 07	0.5097E 05	0.3370E 07	0.1981E 08	0.1348E 09	0.4219E 07	0.4124E 07
A/KCAL	0.1228E 08	0.6046E 09	0.5137E 09	0.8589E 09	0.9093E 08	0.3370E 07	0.1981E 08	0.1348E 09	0.4219E 07	0.4124E 07
ECH/KCAL	0.1750E 08	0.5141E 09	0.4283E 09	0.7124E 09	0.8582E 08	0.0	0.0	0.0	0.0	0.0
EPH/KCAL	0.1975E 05	0.1905E 08	0.1888E 08	0.3227E 08	-0.9873E 05	0.7021E 05	0.1727E 08	0.3032E 08	0.8081E 06	0.1395E 06
E/KCAL	0.1752E 08	0.5332E 09	0.4472E 09	0.7447E 09	0.8572E 08	0.7021E 05	0.1727E 08	0.3032E 08	0.8081E 06	0.1395E 06

COED PROCESS STREAMS (1 HR BASIS)

STREAM #	61	62	63	64	65	66	67	68	69	70
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3404.29	0.0	0.0
N2	35125.73	0.0	35125.73	0.0	0.0	3298.41	0.0	0.0	478.00	35125.73
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	5047.78	4676.65	371.13	0.0	0.0	1289.14	0.0	0.0	5.04	371.13
CO2	1211.69	0.0	1211.69	454.74	5990.01	6385.30	0.0	0.0	10.31	756.95
CO	27275.21	0.0	27275.21	0.0	0.0	0.0	0.0	0.0	371.17	27275.21
H2	11884.84	0.0	11884.84	0.0	0.0	0.0	0.0	0.0	162.00	11884.84
CH4	308.75	0.0	308.75	0.0	0.0	0.0	0.0	0.0	4.52	308.75
C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	467.45	0.0	467.45	462.12	956.19	0.0	0.0	0.0	0.0	5.32
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	956.02	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	81321.38	4676.65	76644.75	916.87	6946.20	10976.85	956.02	3404.29	1031.04	75727.88
PRES-PSI	20.00	14.70	150.00	30.00	30.00	16.00	14.70	20.00	20.00	140.00
TEMP-K	316.48	305.37	305.37	377.59	377.59	413.71	310.93	310.93	310.93	316.48
ACH/KCAL	0.2785E 10	0.0	0.2785E 10	0.6214E 08	0.1286E 09	0.0	0.6704E 08	0.0	0.3713E 08	0.2723E 10
APH/KCAL	0.6381E 08	0.6080E 06	0.7850E 07	0.7309E 06	0.6037E 07	0.2586E 08	0.6695E 05	0.3123E 06	0.1465E 06	0.1376E 08
A/KCAL	0.2849E 10	0.6080E 06	0.2793E 10	0.6287E 08	0.1346E 09	0.2586E C8	0.6791E 08	0.3123E 06	0.3728E 08	0.2737E 10
ECH/KCAL	0.2622E 10	0.0	0.2622E 10	0.8905E 08	0.2084E 09	0.3099E 08	0.1335E 09	0.0	0.3454E 08	0.2533E 10
EPH/KCAL	-0.3692E 08	0.7269E 04	0.5365E 08	0.9418E 05	0.1973E 07	-0.9234E 06	0.1398E 04	0.6274E 06	-0.4781E 06	0.5237E 08
E/KCAL	0.2585E 10	0.7269E 04	0.2676E 10	0.8914E 08	0.2103E 09	0.3006E 08	0.1335E 09	0.6274E 06	0.3406E 08	0.2585E 10

COEO PROCESS STREAMS (1 HR BASIS)

STREAM #	71	72	73	74	75	76	77	78	79	80
COMPOSITION-KMOL										
COAL-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OIL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AIR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	35125.73	5968.23	29157.50	29204.46	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	62.88	0.0	0.0	0.0	0.0	0.0
H2O	371.13	62.95	308.18	370.63	0.0	0.0	0.0	0.0	0.0	0.0
CO2	756.95	128.63	628.31	1143.87	1414.45	0.0	0.0	0.0	0.0	0.0
CO	27275.21	4634.39	22649.81	25449.50	0.0	0.0	0.0	0.0	0.0	0.0
H2	11884.84	2020.56	9864.28	14530.91	0.0	0.0	0.0	0.0	0.0	0.0
CH4	308.75	52.59	257.29	2204.81	0.0	0.0	0.0	0.0	0.0	0.0
C2H4	0.0	0.0	0.0	50.77	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	123.69	0.0	0.0	0.0	0.0	0.0	0.0
C3H6	0.0	0.0	0.0	31.04	0.0	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	20.78	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	0.0	0.0	0.0	44.17	0.0	0.0	0.0	0.0	0.0	0.0
H2S	5.32	0.80	4.53	5.06	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ASH-TONS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CHAR-TON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOTAL-KM	75727.88	12868.13	62860.91	73179.38	1477.33	0.0	0.0	0.0	0.0	0.0
PRES-PSI	30.00	30.00	30.00	30.00	14.70	0.0	0.0	0.0	0.0	0.0
TEMP-K	310.93	310.93	310.93	310.93	316.48	0.0	0.0	0.0	0.0	0.0
ACH/KCAL	0.2723E 10	0.4628E 09	0.2261E 10	0.3304E 10	0.0	0.0	0.0	0.0	0.0	0.0
APH/KCAL	0.1077E 08	0.1829E 07	0.8942E 07	0.1062E 08	0.2594E 06	0.0	0.0	0.0	0.0	0.0
A/KCAL	0.2734E 10	0.4646E 09	0.2270E 10	0.3314E 10	0.2994E 06	0.0	0.0	0.0	0.0	0.0
ECH/KCAL	0.2533E 10	0.4305E 09	0.2103E 10	0.3053E 10	0.6814E 07	0.0	0.0	0.0	0.0	0.0
EPH/KCAL	-0.1689E 08	-0.2870E 07	-0.1402E 08	-0.2361E 08	-0.1452E 06	0.0	0.0	0.0	0.0	0.0
E/KCAL	0.2516E 10	0.4276E 09	0.2089E 10	0.3029E 10	0.6669E 07	0.0	0.0	0.0	0.0	0.0

TOTAL ENTERING QUANTITIES

UNIT NAME	TOTAL ENERGY IN KCAL (1ST LAW)	TOTAL WORK EQ. IN KCAL (2ND LAW)
COAL PREPARATION	0.6303E 10	0.6300E 10
DRYING & STAGE 1 PYROLYSIS	0.6388E 10	0.6361E 10
STAGE 2, 3, AND 4 PYROLYSIS	0.6763E 10	0.6514E 10
PRODUCT RECOVERY	0.3597E 10	0.3231E 10
PYROLYSIS GAS COMPRESSION	0.2024E 10	0.1867E 10
PYROLYSIS ACID GAS REMOVAL	0.2265E 10	0.1920E 10
PYROLYSIS GAS EXPANSION	0.1676E 10	0.1532E 10
OIL FILTRATION	0.1577E 10	0.1567E 10
OIL HYDROTREATING	0.3049E 10	0.2864E 10
PURGE ACID GAS REMOVAL	0.6185E 09	0.5523E 09
HYDROCARBON REMOVAL	0.6061E 09	0.5346E 09
AMMONIA REMOVAL	0.6513E 09	0.6070E 09
HYDROGEN PLANT	0.4660E 09	0.3945E 09
CHAR GASIFICATION	0.3487E 10	0.3333E 10
GASIFIER GAS COMPRESSION	0.3025E 10	0.2761E 10
GASIFIER ACID GAS REMOVAL	0.2845E 10	0.2689E 10
GASIFIER GAS EXPANSION	0.2737E 10	0.2585E 10
SULFUR RECOVERY	0.1746E 09	0.2474E 09
OVERALL COED PROCESS	0.6530E 10	0.6523E 10

THERMODYNAMIC EFFICIENCIES AND ENERGY BALANCE CLOSURE FOR THE COED PROCESS

UNIT NAME	FIRST LAW EFFICIENCY	SECOND LAW EFFICIENCY	ENERGY BALANCE CLOSURE (%)
COAL PREPARATION	0.98915	0.98980	99.910
DRYING & STAGE 1 PYROLYSIS	0.96345	0.95986	98.457
STAGE 2, 3, AND 4 PYROLYSIS	0.98423	0.96206	98.423
PRODUCT RECOVERY	0.90798	0.96551	99.556
PYROLYSIS GAS COMPRESSION	0.99696	0.99295	100.337
PYROLYSIS ACID GAS REMOVAL	0.88055	0.95882	91.841
PYROLYSIS GAS EXPANSION	1.00710	0.99836	100.332
OIL FILTRATION	0.99856	0.99899	100.132
OIL HYDROTREATING	1.00143	0.99695	100.443
PURGE ACID GAS REMOVAL	0.99746	0.99717	99.798
HYDROCARBON REMOVAL	0.99762	0.99681	99.810
AMMONIA REMOVAL	0.99617	0.96915	100.805
HYDROGEN PLANT	0.79194	0.75519	91.046
CHAR GASIFICATION	0.95346	0.81242	96.574
GASIFIER GAS COMPRESSION	0.97908	0.98495	99.078
GASIFIER ACID GAS REMOVAL	0.98690	0.99485	99.171
GASIFIER GAS EXPANSION	1.02009	0.99564	100.537
SULFUR RECOVERY	0.71613	0.59909	86.662
OVERALL COED PROCESS	0.79657	0.74932	94.206

APPENDIX B

This appendix refers to the optimization of the flue gas heat recovery system in Part III. A computer program listing with sample output corresponding to 8 heat exchangers and a 1 in. tube outside diameter is presented. Throughout the program listing descriptive comments are included which give most of the assumptions. The program may briefly be described in terms of three sections. The first section physically designs the heat exchanger, a counterflow one-pass fixed-tube-sheet shell and tube carbon steel exchanger, once the inside and outside fluid properties have been entered as data and once the independent design variables have been given values. In this section the shell-side heat transfer and pressure drop quantities are calculated from empirical relations given by Perry (16) and the corresponding tube-side quantities are calculated from relations given by Peters and Timmerhaus (24). Because of the moderate stream temperatures, less than 550K, radiation has been neglected in the heat transfer coefficient calculations. The next section of the program estimates all of the equipment costs from correlations given by Guthrie (27) and Peters and Timmerhaus. The final program section calculates the remaining quantities such as power, annual costs, and work equivalents necessary to determine values for the economic and thermodynamic objective functions. The program is structured to print out results for any or all of the objective function optimizations. The results consist of two major sections. The first gives a search table for a specified tube outside diameter and number of heat exchangers. The temperature difference column listed in the table shows the temperature difference that exists at the hot end of the heat exchanger, i.e. inlet flue gas temperature minus exit preheated air temperature. The next section presents the heat exchanger design criteria and objective function values in addition to several intermediate results for one of the objective function optimizations.

```
C
C*****************************************************************
C
C SECOND LAW AND COST OPTIMIZATION OF A FLUE GAS HEAT RECOVERY
C SYSTEM USING A COUNTERFLOW ONE PASS FIXED-TUBE-SHEET SHELL AND
C TUBE HEAT EXCHANGER-ALL CARBON STEEL
C
C WRITTEN BY TERRY L. UNRUH UNDER THE ADVISEMENT OF DR. B. G. KYLE,
C DEPT. OF CHEMICAL ENGINEERING, KANSAS STATE UNIV.
C
C*****************************************************************
C*****************************************************************
C
C                          DATA DESCRIPTION
C
C*****************************************************************
C
C 1. INSIDE FLUID PROPERTIES, WI-KG/HR(MASS FLOW RATE), CPI-
C    KCAL/KG/DEG K(HEAT CAPACITY),VISI-G/CM/S(VISCOSITY),TKI-
C    CAL/S/CM/DEG K(THERMAL CONDUCTIVITY)
C
C 2. OUTSIDE FLUID PROPERTIES, WO-KG/HR(MASS FLOW RATE), CPO-
C    KCAL/KG/DEG K(HEAT CAPACITY), VISO-G/CM/S(VISCOSITY),TKO-
C    CAL/S/CM/DEG K(THERMAL CONDUCTIVITY)
C
C 3. RANGES OF SEARCH, NUMBER OF HEAT EXCHANGERS, TUBE OUTSIDE
C    DIAMETER, EXIT PREHEATED AIR TEMP., INSIDE SHELL DIAMETER,
C    AND OPTIMIZATION OUTPUT CHOICE, NET PRESENT VALUE, WORK
C    EQUIVALINT(COMBINED HEAT RECOVERY SYSTEM), OVERALL SECOND LAW
C    EFFICIENCY(HEAT EXCHANGER ADDITION SYSTEM) (1=YES)
C
C*****************************************************************
      REAL JK,LC,JC,MWTO,NC,NCW,LMTD,LS,K1,MAXLS,LT,JL,JB
      REAL NPVOLD,EFOLD
      REAL EINF(25,25),TDIF(25),NPV(25,25),EFF(25,25)
      INTEGER WNPV,WWE,WEFF
      INTEGER IDS(25)
      DATA EINF,TDIF,NPV,EFF/1900*0./
      DATA IDS/25*0/
      READ(5,100) WI,CPI,VISI,TKI
      READ(5,100) WO,CPO,VISO,TKO
      READ(5,125) NEXCH1,NEXCH2,ITOD1,ITOD2,ITMP4A,ITMP4B,ISID1,
     *ISID2,WNPV,WWE,WEFF
      WRITE(6,150)
      WRITE(6,170)
      WRITE(6,200) WI,CPI,VISI,TKI
      WRITE(6,220) WO,CPO,VISO,TKO
C
C     ***********************************************************
C
C                     INITIATE OPTIMIZATION LOOPS
C
C     ***********************************************************
C
      NXCH1 = NEXCH1
      NXCH2 = NEXCH2
      ITEMPA = ITMP4A
      ITEMPB = ITMP4B
```

```
      ISD1 = ISID1
      ISD2 = ISID2
      TWI = WI
      TWO = WO
      SKIP = 0.
      IECK = 0
      NPVOLD = -9.*10.**8
      EINOLD = 9.*10.**9
      JOPT = 0
      IOPT = 0
   95 CONTINUE
C
C     *  VARY THE NUMBER OF HEAT EXCHANGERS.                           *
C
      DO 50 NEXCH = NEXCH1,NEXCH2
      WI = TWI/NEXCH
      WO = TWO/NEXCH
C
C     *  VARY THE ALLOWABLE TUBE OUTSIDE DIAMETER, TOD IN CM,          *
C     *  FOR THREE POSSIBLE VALUES,5/8, 3/4, OR 1 IN.                  *
C
      DO 40 JTOD = ITOD1,ITOD2
      ITOD = JTOD-2
C
C     *  VARY THE EXIT PREHEATED AIR TEMPERATER, ITEMP4, IN            *
C     *  DEGREES K.  THE ABSOLUTE MAXIMUM IS 533.15 K, THE INLET       *
C     *  FLUE GAS TEMPERATURE.                                         *
C
      J = 0
      DO 10 ITEMP4 = ITMP4A,ITMP4B,20
      J = J+1+JOPT
      TDIF(J) = 533.15-ITEMP4
      ITN = (ITMP4B-ITMP4A)/20+1
C
C     *  VARY THE SHELL INSIDE DIAMETER, SID, IN CM                    *
C
      I = 0
      DO 20 ISID = ISID1,ISID2,25
      I = I+1+IOPT
      SID = ISID
      IDS(I) = ISID
C
C
C     ****************************************************************
C     ****************************************************************
C
C                              H E A T
C                           E X C H A N G E R
C                              D E S I G N
C                             S E C T I O N
C
C     ****************************************************************
C     ****************************************************************
C
C
C     *  RELATE THE TUBE OUTSIDE DIAMETER TO PITCH, P, AND             *
C     *  PARALLEL TO FLOW PITCH, PP.  THE TOTAL NUMBER OF EX-          *
C     *  CHANGER TUBES, NT, ARE CALCULATED FROM DATA CORRELATIONS *
```

```
C       *  ACCURATE WITHIN 3%.                                          *
C
   30 IF(ITOD) 31,32,33
   31 TOD = 1.5875
      P = 2.06375
      PP = 1.7882
      NT = ((8./5.)**2)*.22664*(SID/2.54)**2.19775
      GO TO 35
   32 TOD = 1.905
      P = 2.38125
      PP = 2.0676
      NT = ((4./3.)**2)*.40804*(SID/2.54)**2.071733
      GO TO 35
   33 TOD = 2.54
      P = 3.175
      PP = 2.7483
      NT = .36764*(SID/2.54)**2.09445
   35 CONTINUE
      IF(IECK.NE.0) GO TO 132
      WRITE(6,945)
      WRITE(6,950)
      WRITE(6,960) NXCH1,NXCH2
      WRITE(6,970) TOD,TCO
      WRITE(6,980) ISD1,ISD2
      WRITE(6,990) ITEMPA,ITEMPE
  132 IECK = IECK+1
C
C       *  FIND THE AMOUNT OF HEAT TRANSFERED, Q, IN CAL/HR FROM THE*
C       *  INSIDE FLUID.                                               *
C
      TEMP1 = 533.15
      TEMP3 = 310.93
      TEMP4 = ITEMP4
      Q = WI*1000./28.3*(6.9*(TEMP4-TEMP3)+(.92*10.**(-3))/2.*
     *(TEMP4**2-TEMP3**2))
C
C       *  CALCULATE THE SHELL-SIDE FLUID EXIT TEMPERATURE, TEMP2,    *
C       *  IN DEG K USING AN ENERGY BALANCE AND A TWC PARAMETER HEAT*
C       *  CAPACITY                                                     *
C
      A = 1.14/2.*10.**(-3)
      B = 7.53
      C = -(B*TEMP1+A*TEMP1**2-Q/WO/1000.*30.9)
      TEMP2 = (-B+SQRT(B**2-4*A*C))/(2*A)
C
C       ***************************************************************
C
C                CALCULATE SHELL-SIDE HEAT TRANSFER PARAMETERS
C
C       ***************************************************************
C
C       *  CALCULATE CROSSFLOW AREA, SM, AT OR NEAR CENTERLINE FOR   *
C       *  ONE CROSSFLOW SECTION ASSUMING A 1/2 IN. CLEARANCE          *
C       *  BETWEEN SID AND OUTER TUBE LIMIT, ALSO FIND THE BAFFLE     *
C       *  SPACING, LS, IN CM                                           *
C
      NNN = 0
      LS = SID
```

```
      IF(LS.LT.5.08) LS = 5.08
      MAXLS = (74.*2.54)*(TOD/2.54)**.75
      IF(LS.GT.MAXLS) LS = MAXLS
      DOTL = SID-.5*2.54*2.
   47 SM = LS*(SID-DOTL+(DOTL-TOD)*(P-TOD)/P)
C
C     *  CALCULATE THE FRACTION OF TOTAL TUBES IN CROSSFLOW, FC,   *
C     *  ASSUMING A BAFFLE CUT, LC, OF 49% SID(UNOBSTRUCTED FLOW)  *
C
      PI = 3.1416
      LC = .49*SID
      FCC = (SID-2.*LC)/DOTL
      FC = 1./PI*(PI+2.*FCC*SIN(ARCOS(FCC))-2.*ARCOS(FCC))
C
C     *  CALCULATE SHELL-SIDE REYNOLDS NUMBER,SREYN                *
C
      SREYN = TOD*WO*1000./VISO/SM/3600.
      SPRNDT = CPO*VISO/TKO
C
C     *  CALCULATE SHELL-SIDE HEAT-TRANSFER COEFFICIENT,HO, IN     *
C     *  CAL/(SEC SQCM DEG C) FOR AN IDEA TUBE BANK.               *
C
C     *  FIND JK FROM A TUBE-BANK & REYNOLD NO. RELATION(RE>800.)  *
C
      JK = 0.2236*SREYN**(-.3495)
C
C     *  ASSUME BULK AND WALL AVERAGE VISCOSITIES ARE EQUAL SO     *
C     *  THAT (VISB/VISW)**0.14 = 1.                               *
C
      HO = JK*CPO*WO/SM/3.600*(TKO/CPO/VISO)**(2./3.)
C
C     *  CORRECT HO FOR BAFFLE-CONFIGURATION EFFECTS, JC, USING    *
C     *  FC.                                                       *
C
      IF(FC.GE..9) GO TO 190
      JC = .6125*FC+0.6175
      GO TO 195
  190 JC = -FC+2.05
C
C     *  FIND THE CORRECTION FACTOR, JL, FOR BAFFLE-LEAKAGE        *
C     *  EFFECTS ASSUMING A 1/36 INCH DIAMETRAL CLEARANCE BETWEEN  *
C     *  TUBE AND BAFFLE AND A 1/4 INCH DIAMETRAL SHELL-BAFFLE     *
C     *  CLEARANCE.  THE TUBE-TO-BAFFLE AND SHELL-TO- BAFFLE LEAK-*
C     *  AGE AREAS FOR ONE BAFFLE ARE STB AND SSB RESPECTIVELY.    *
C     *  THE JL CURVE-FIT IS VALID FOR X>.08 WITHIN 3% AND FOR     *
C     *  X<.08 WITHIN 5%.                                          *
C
  195 STB = .0245*TOD*NT*(1.+FC)/2.54
      SSB = SID/2.54/8.*(PI-ARCOS(1.-2*LC/SID))
      X = (SSB+STB)/SM*2.54
      Z = SSB/(SSB+STB)
      IF(X.LT..08) GO TO 196
      JL = (-.4222*Z-.47052)*X+(-.0974*Z+.90817)
      GO TO 197
  196 JL = -2.02*X+.978
C
C     *  FIND THE CORRECTION FACTOR, JB, FOR BUNDLE-BY-PASSING     *
C     *  EFFECTS ASSUMING NO SEALING STRIPS.  THE FRACTION OF      *
```

```
C      *  CROSSFLOW AREA AVAILABLE FOR BY-PASS FLOW IS FBP.          *
C
  197 FBP = (SID-DOTL)*LS/SM
      JB = EXP(-1.2397*FBP-.00254)
C
C      *  CALCULATE FINAL HO.                                          *
C
      HO = HO*JC*JL*JB
C
C     ******************************************************************
C
C              CALCULATE TUBE-SIDE HEAT TRANSFER PARAMETERS
C
C     ******************************************************************
C
C      *  CALCULATE TUBE-SIDE REYNOLDS NUMBER,TREYN, ASSUMING A        *
C      *  BWG OF 14.                                                    *
C
      TID = TOD-.083*2.54*2.
      TREYN = TID*WI*1000./VISI/(PI*(TID**2)/4.)/NT/3600.
C
C      *  CALCULATE THE INSIDE-FLUID PRANDTL NUMBER, PRNDTL.           *
C
      PRNDTL = CPI*VISI/TKI
      MMM = 0
C
C      *  INITIALIZE TUBE LENGTH IN CASE FLOW IS LAMINAR OF IN THE *
C      *  TRANSITION REGION AND ITERATION IS REQUIRED.                 *
C
      LT = 6.
   89 LTI = LT
C
C      *  CALCULATE THE INSIDE HEAT-TRANSFER COEFFICIENT, HI, USING*
C      *  THE SIEDER-TATE CORRELATIONS.  ASSUMING VISB/VISW = 1.   *
C      *  FOR EITHER A TURBULENT, TRANSITION, OF LAMINAR REGION     *
C      *  DEPENDING ON TREYN.                                           *
C
      IF(TREYN.LT.10000.) GO TO 86
      HI = .023*TKI/TID*(TREYN**.8)*(PRNDTL**(1./3.))
      GO TO 88
   86 IF(TREYN.LT.2100.) GO TO 87
      HI = .116*TKI/TID*((TREYN**(2./3.))-125.)*(PRNDTL**(1./3.))*
     *(1.+(TID/LT)*(2./3.))
      GO TO 88
   87 HI = 1.18*TKI/TID*(4.*WI*CPI/3.14/TKI/LT)**(1./3.)
C
C
C     ******************************************************************
C
C                     CALCULATE THE TUBING LENGTH NEEDED TO
C                  TRANSFER THE AMOUNT OF HEAT, Q, DETERMINED
C                    FROM THE TEMPERATURE APPROACH CONDITION
C
C     ******************************************************************
C
C       *  CALCULATE THE LOG MEAN TEMPERATURE DIFFERENCE               *
C
   88 LMTD = (TEMP1-TEMP4-TEMP2+TEMP3)/ALOG((TEMP1-TEMP4)/
```

```
     *(TEMP2-TEMP3))
C
C     *  CALCULATE THE OVERALL HEAT-TRANSFER COEFFICIENT BASED ON *
C     *  THE OUTSIDE TUBE AREA, UC.  FOULING IS ASSUMED NEG-      *
C     *  LIGABLE.                                                 *
C
      TKW = .1075
      UO = 1./(1./HO+TOD/HI/TID+TOD*(TOD-TID)/TKW/((TID+TOD)/2.))
C
C     *  CALCULATE THE OUTSIDE AREA, AO, THE TUBE LENGTH, LT, AND *
C     *  THE NUMBER OF BAFFLES, NB.  IF NB=0 THEN ITERATE BY      *
C     *  REDUCING THE BAFFLE SPACING, LS.                         *
C
      AO = Q/UC/LMTD/3600.
      LT = AO/PI/TOD/NT
      IF(TREYN.GE.10000.) GO TO 77
      IF(ABS(LTI-LT).LT..3) GO TO 77
      MMM = MMM+1
      IF(MMM.GE.15) GO TO 77
      GO TO 89
   77 NB = LT/LS-1
      NNN = NNN+1
      IF(NNN.EQ.20) GO TO 44
      IF(NB.NE.0) GO TO 44
      LS = LT/2.-.1
      GO TO 47
   44 IF(LT.GT.SID) GO TO 45
      NPV(I,J) = 9999999.
      EINF(I,J) = 9999999.
      EFF(I,J) = .99999
      GO TO 20
   45 IF(LT.LT.610.) GO TO 46
      NPV(I,J) = 8888888.
      EINF(I,J) = 8888888.
      EFF(I,J) = .88888
      GO TO 20
C
C     ***********************************************************
C
C                  CALCULATE SHELL-SIDE PRESSURE DROP
C
C     ***********************************************************
C
C     *  FIND THE IDEAL-TUBE-BANK FRICTION FACTOR, FK, FROM A     *
C     *  RELATION VALID FOR SREYN>300.                            *
C
   46 FK = .9187*SREYN**(-.17729)
C
C     *  ITTERATE WITH RESPECT TO THE AVERAGE SHELL PRESSURE,     *
C     *  SPAVG, TO CALCULATE THE SHELL-FLUID DENSITY, RHOS, IN    *
C     *  G/CM**3.  INITIATE THE LOOP WITH A VALUE OF 5 PSI FOR    *
C     *  THE SHELL-SIDE PRESSURE DROP GUESS, DPSG.                *
C
      NN = 1.
      DPSG = 5.
      MWTO = 30.9
      AVGTO = (TEMP1+TEMP2)/2.
    5 SPAVG = (14.7+(14.7+DPSG))/2.
```

```
      RHOS = SPAVG/14.7/(.08205)/AVGTU/1000.*MWTO
C
C     *  CALCULATE THE NUMBER OF TUBE ROWS CROSSED IN ONE CROSS-   *
C     *  FLOW SECTION, NC.                                          *
C
      NC = SID*(1.-2.*LC/SID)/PP
C
C     *  CALCULATE THE PRESSURE DROP, DPC, IN PSI FOR AN IDEAL      *
C     *  CROSSFLOW SECTION ASSUMING VISB/VISW = 1.                  *
C
      DPC = 2.*4.014*10.**(-4)*.03613*((1./3.6)**2)*FK*(WO**2)*NC/
     *RHOS/(SM**2)
C
C     *  CALCULATE THE NUMBER OF EFFECTIVE CROSSFLOW ROWS IN EACH *
C     *  WINDOW, NCW.                                               *
C
      NCW = .8*LC/PP
C
C     *  CALCULATE THE AREA FOR FLOW THROUGH EACH WINDOW, SW, BY   *
C     *  THE DIFFERENCE BETWEEN THE GROSS WINDOW AREA AND THE PART*
C     *  OF THAT AREA OCCUPIED BY TUBES.                            *
C
      SWC = 1.-2*LC/SID
      SW = (SID**2)/4.*(ARCOS(SWC)-SWC*SQRT(1.-SWC**2))-NT/8.*(1.-
     *FC)*PI*TOO
C
C     *  CALCULATE THE PRESSURE DROP, DPW, FOR AN IDEAL WINDOW     *
C     *  SECTION IN PSI.                                            *
C
      DPW = .5*4.014*10.**(-4)*.03613*(WO**2)*(2.+.6*NCW)/SM/SW/
     *RHOS*((1./3.6)**2)
C
C     *  FIND THE CORRECTION FACTOR, RL, FOR EFFECT OF BAFFLE      *
C     *  LEAKAGE ON PRESSURE DROP.  THE LINEAR CURVE-FIT IS VALID *
C     *  FOR X<.7 AND RL>.1.  THE FIT APPROXIMATES THE CURVES      *
C     *  WITHIN 5%.                                                 *
C
      IF(X.LT..1) GO TO 180
      RL = (-.653166*Z-.618674)*X+(-.24038*Z+.75349)
      GO TO 185
  180 RL = -3.5*X+.925
C
C     *  FIND THE CORRECTION FACTOR, RB, FOR BUNDLE BY-PASS        *
C     *  ASSUMING NO SEALING STRIPS.  THE EXPONENTIAL FIT ACCURACY*
C     *  IS WITHIN 1%.                                              *
C
  185 RB = EXP(-3.75404*FBP-.010703)
C
C     *  CALCULATE THE PRESSURE DROP. DPS, IN PSI ACROSS THE SHELL*
C     *  SIDE EXCLUDING NOZZLES.                                    *
C
      DPS = ((NB-1.)*DPC*RB+NB*DPW)*RL+2*DPC*RB*(1.+NCW/NC)
C
C     *  CHECK IF THE CALCULATED PRESSURE DROP IS WITHIN 1. PSI OF*
C     *  THE INITIAL GUESS. IF NOT THEN LET THIS CALCULATED VALUE *
C     *  BE THE NEW GUESS.                                          *
C
      IF(NN.GT.100) GO TO 15
```

```
      PDIFF = ABS(DPS-DPSG)
      IF(PDIFF.LE.0.1) GO TO 15
      DPSG = DPS
      NN = NN+1.
      GO TO 5
C
C     ****************************************************************
C
C                    CALCULATE THE TUBE-SIDE PRESSURE DROP
C
C     ****************************************************************
C
C     *  FIND THE FANNING FRICTION FACTOR, F, FROM THE BLASIUS       *
C     *  FORMULA.                                                     *
C
   15 F = .0791/(TREYN**.25)
C
C     *  CALCULATE BI, THE CORRECTION FACTOR TO ACCOUNT FOR SUDDEN*
C     *  CONTRACTION, SUDDEN EXPANSION, AND REVERSAL OF FLOW         *
C     *  DIRECTION.                                                   *
C
      KI = (1-(TID**2)*NT/SID**2)**2+.05
      FILMDT = (TEMP1+TEMP2)/2.-(TEMP3+TEMP4)/2.
      BI = 1.+(.51*KI*FILMDT)/(TEMP4-TEMP3)/(PRNDTL**(2./3.))
C
C     *  CALCULATE THE PRESSURE DROP, TDP, IN INCHES OF H2O           *
C
      MWTI = 28.8
      AVGTI = (TEMP3+TEMP4)/2.
      RHOI = 1./.08205/AVGTI/1000.*MWTI
      TDP = BI*2.*F*(WI/1000./(PI*(TID**2)/4.)**2)*LT/RHOI/TID/1.01/
     *2490.8*((1./36.)**2)
      TDP = BI*2.*F*((WI*1000./(PI/4.*TID**2)/NT)**2)*LT/RHOI/TID/
     *1.02/(3600.**2)*4.0142*10.**(-4)
C
C     ****************************************************************
C     ****************************************************************
C
C                                   C O S T
C                               E S T I M A T I O N
C                                 S E C T I O N
C
C     ****************************************************************
C     ****************************************************************
C
C
C     ****************************************************************
C
C              CALCULATE THE JAN. 1979 COSTS OF THE AIR BLOWER,
C                  ARBCST, AND THE FLUE GAS BLOWER, FGBCST.
C
C     ****************************************************************
C
C     *  CALCULATE AIR AND FLUE GAS VOLUMETRIC FLOW RATES ARCFM     *
C     *  AND FGCFM RESPECTIVELY, IN CUBIC FT./MIN. ASSUMING AN      *
C     *  INLET PRESSURE OF 1. ATM. ALSO CONVERT TDP TO PSI.          *
C
      ARCFM = WI*1000.*.08205*TEMP3/MWTI*.03532/60.*NEXCH
```

```
      FGCFM = WO*1000.*.08205*TEMP1/MWTO*.03532/60.*NEXCH
      PST = .0361*TOP
      PDS = DPS
C
C     *  USE THE BLOWER CORRELATIONS FOR A PRESSURE INCREASE OF     *
C     *  BETWEEN 3 AND 30 PSI.  IF THE PRESSURE INCREASE IS LESS    *
C     *  THAN 3 PSI THEN SET IT EQUAL TO THAT LOWER LIMIT.  HOW-    *
C     *  EVER, IF THIS INCREASE IS GREATER THAN 30 PSI THEN USE AN*
C     *  AXIAL COMPRESSOR CORRELATION.                              *
C
      IF(PST.LT.3.) PST = 3.
      IF(DPS.LT.3.) PDS = 3.
      IF(PST.LE.30.) GOTO 60
      ARBCST = 3.5*10.**5
      GO TO 65
   60 ARBCST = (13.3847*PST**1.09347)*ARCFM**(.57695*PST**
     *(-.017041))
   65 IF(DPS.LE.30.) GO TO 70
      FGBCST = 6.*10.**5
      GO TO 75
   70 FGBCST = (13.3847*PDS**1.09347)*FGCFM**(.57695*PDS**
     *(-.017041))
   75 CONTINUE
C
C     *  CONVERT THESE JAN. 1967 COSTS TO A JAN. 1979 BASIS BY      *
C     *  USING A COST COEFFICIENT, CSTCF1, DETERMINED FROM THE      *
C     *  CHEMICAL ENGINEERING PLANT COST INDEX.                     *
C
      CSTCF1 = 229./109.1
      ARBCST = ARBCST*CSTCF1
      FGBCST = FGBCST*CSTCF1
C
C     *  APPLY A FIELD INSTALLATION FACTOR TO OBTAIN A TOTAL COST *
C     *  OF THE BLOWERS.                                            *
C
      BWRCST = (ARBCST+FGBCST)*1.1
C
C     ***************************************************************
C
C                        CALCULATE THE JAN. 1979 COST
C                          OF THE HEAT EXCHANGER(S)
C
C     ***************************************************************
C
C     *  CONVERT THE AREA TO SQ. FT., EAO, AND CALCULATE THE HEAT *
C     *  EXCHANGER BASE MID 1970 COST, BASCST.                      *
C
      EAO = AU/10000.*10.764
      BASCST = 73.7*EAO**.701
C
C     *  CALCULATE THE DESIGN FACTOR, FD, FOR A FIXED TUBE SHEET   *
C     *  HEAT EXCHANGER.                                            *
C
      FD = .809*BASCST**(-.007664)
C
C     *  CALCULATE THE JAN. 1979 PURCHASED EQUIPMENT COST, HXCOST,*
C     *  USING A SECOND COST COEFFICIENT, CSTCF2.                   *
C
```

```
      CSTCF2 = 229./122.
      HXCOST = CSTCF2*BASCST*FD*NEXCH
C
C     *  CALCULATE THE TOTAL MATERIAL COST, HXMTL, USING A MATER- *
C     *  IAL FACTOR OF 0.7.  INCLUDED ARE ITEMS SUCH AS PIPING AND*
C     *  INSULATION.
C
      HXMTL = .7*HXCOST
C
C     *  CALCULATE THE TOTAL HEAT EXCHANGER COST INCLUDING LABOR, *
C     *  THXCST, USING A MODULAR FACTOR OF 3.17.                  *
C
      THXCST = 3.17*HXCOST
C
C     *  OBTAIN THE TOTAL COST OF THE HEAT RECOVERY ADDITION,     *
C     *  TOTCST.                                                  *
C
      TOTCST = THXCST+BWRCST
C
C
C     *************************************************************
C     *************************************************************
C
C                          E C O N O M I C
C                               A N D
C                             E N E R G Y
C                       O P T I M I Z A T I O N
C                             S E C T I O N
C     *************************************************************
C     *************************************************************
C
C
C     *************************************************************
C
C               CALCULATE THE NET PRESENT VALUE OF THE HEAT
C              RECOVERY ADDITION FOR A 12 YEAR SERVICE LIFE
C
C
C     *  CALCULATE THE ELECTRIC POWER ANNUAL COST, PWRCST,        *
C     *  ASSUMING:  (1) ISOTHERMAL COMPRESSION, (2) 340 DAYS/YR   *
C     *  OF OPERATION, (3) AN AVERAGE ELECTRIC RATE OF $.032/KWH. *
C     *  BLOWER POWERS ARE IN CAL/HR, (4) 80% ISOTHERMAL          *
C     *  EFFICIENCY.                                              *
C
      POWFGS = WO*1000./MWTO*1.987*TEMP1*ALOG((DPS+14.7)/14.7)/.8*
     *NEXCH
      PCWAIR = WI*1000./MWTI*1.987*TEMP3*ALOG((TOP+406.8)/406.8)/.8*
     *NEXCH
      PWRCST = (PCWAIR+POWFGS)/3600.*4.186*10.**(-3)*24.*340.*.032
C
C     *  CALCULATE THE FUEL OIL ANNUAL SAVINGS, FLSVNG, ASSUMING: *
C     *  (1) 33 A.P.I. (2) 0% SULFUR, (3) AN AVERAGE FUEL COST OF *
C     *  $.85/GAL OR $6.1/MM BTU.  THIS LEADS TO A HIGHER HEATING *
C     *  VALUE OF 19370. BTU/LB OR 10760.CAL/G.                   *
C
      FLSVNG = Q/252.*6.1/(10.**6)*24.*340.*NEXCH
C
C     *  CALCULATE THE ANNUAL COST, ANLCST, ASSUMING THE FOLLOWING*
```

```
C      *  PERCENTAGES OF THE TOTAL ADDITION COST:  MAINTENANCE-4.%,*
C      *  PLANT OVERHEAD-2.6%, AND TAXES & INSURANCE-1.5%.  ALSO   *
C      *  ASSUME NO ADDITIONAL LABOR AND STRAIGHT LINE DEPRECIATION*
C
       ANLCST = PWRCST+((4.+2.6+1.5)/100.+1./12.)*TOTCST
C
C      *  FIND THE NET ANNUAL CASH FLOW, ACF, USING A 48% TAX RATE.*
C
       ACF = (FLSVNG-ANLCST)*(1.-.48)+TOTCST/12.
C
C      *  EVALUATE THE NET PRESENT VALUE, NPV, ASSUMING A 15% RATE *
C      *  OF RETURN, UNIFORM CASH FLOWA, NO WORKING CAPITAL, AND   *
C      *  NO SALVAGE VALUE.                                        *
C
       NPV(I,J) = ACF*((EXP(.15*12.)-1)/.15)*EXP(-.15*12.)-TOTCST
C
C      ************************************************************
C
C                    CALCULATE THE WORK EQUIVALENT INTO
C                    THE FURNACE UNIT ON A ONE HOUR BASIS
C                 RESULTING FROM THE HEAT RECOVERY ADDITION
C
C      ************************************************************
C
C      *  DETERMINE THE WORK EQUIVALENT OF THE SAVED FUEL OIL,     *
C      *  EOIL, IN KCAL.  USE THE HIGH-MOLECULAR-WEIGHT HYDROCARBON*
C      *  ASSUMPTION THAT THE WORK EQUIVALENT IS APPROXIMATELY     *
C      *  EQUAL TO THE HEAT OF COMBUSTION(LIQ. H2O).  ALSO ASSUME  *
C      *  OIL AT REFERENCE TEMPERATURE AND PRESSURE.               *
C
       EOIL = -Q/1000.*NEXCH
C
C      *  CALCULATE THE WORK EQUIVALENT OF THE ELECTRICAL WORK,    *
C      *  EELEC, IN KCAL ASSUMING AN ELECTRICAL GENERATING         *
C      *  EFFECIENCY OF 38%.                                       *
C
       EELEC = (POWAIR+POWFGS)/1000./.38
C
C      *  CALCULATE THE EQUIPMENT AND CONSTRUCTION ENERGY FLOW,    *
C      *  EQCON, IN KCAL FROM ENERGY/$(1963) COEFFICIENTS ASSUMING *
C      *  NO SCRAP VALUE.  USE A THIRD COST COEFFICIENT, CSTSF3,   *
C      *  TO CONVERT TO THE JAN. 1979 BASIS.                       *
C
       CSTCF3 = 229./102.3
       EQCON = (23200.*HXCOST+20700.*HXMTL+(ARBCST+FGBCST)*14700.)/
      *CSTCF3/12./340./24.
C
C      *  CALCULATE THE WORK EQUIVALENT INPUT WITH RESPECT TO THE  *
C      *  ADDITION ASSUMING INPUT AIR AT REFERENCE CONDITIONS FOR  *
C      *  THE COMBINED HEAT RECOVERY SYSTEM.                       *
C
       EAIR = TWI/28.8*CPA(6.6,.92,TEMP4)
       ESGAS = TWO/30.9*CPA(7.53,1.14,TEMP1)
       ESGAS = ESGAS+.013*TWO/30.9*10519
       EINF(I,J) = EOIL+EELEC+EQCON
C
C      *  CALCULATE THE OVERALL SECOND LAW EFFICIENCY OF THE HEAT  *
C      *  EXCHANGER ADDITION SYSTEM.                               *
```

```
C
      EFF(I,J)  = EAIR/(ESGAS+EELEC+EQCON)
C
C     *  ROUTINE TO FIND AND SAVE VARIABLE VALUES CORRESPONDING    *
C     *  TO OPTIMAL OBJECTIVE FUNCTION VALUES.                     *
C
      IF(SKIP.GE.1.) GO TO 90
      IF(NPV(I,J).LT.NPVOLD) GO TO 80
      NPVOLD = NPV(I,J)
      NJ1 = JTOD
      NIA = ITEMP4
      NI1 = ISID
      NE1 = NEXCH
      IO1 = I-1
      JO1 = J-1
   80 IF(EINF(I,J).GT.EINOLD) GO TO 85
      EINOLD = EINF(I,J)
      EJ1 = JTOD
      EIA = ITEMP4
      EI1 = ISID
      EE1 = NEXCH
      IO2 = I-1
      JO2 = J-1
   85 IF(EFF(I,J).LT.EFOLD) GO TO 20
      EFOLD = EFF(I,J)
      EFJ1 = JTOD
      EFIA = ITEMP4
      EFI1 = ISID
      EFE1 = NEXCH
      IO3 = I-1
      JO3 = J-1
   20 CONTINUE
   10 CONTINUE
C
C     ***************************************************************
C
C                             PRINTOUT ROUTINE
C
C     ***************************************************************
C
      IF(WNPV.NE.1) GO TO 120
      WRITE(6,850)
      WRITE(6,860)
      WRITE(6,870) TOD
      WRITE(6,874) NEXCH
      WRITE(6,876)
      WRITE(6,880)
      WRITE(6,900) (IDS(I),I=1,11)
      WRITE(6,910) (TDIF(J),(NPV(I,J),I=1,11),J=1,ITN)
      WRITE(6,940)
      WRITE(6,930)
  120 IF(WWE.NE.1) GO TO 130
      WRITE(6,920)
      WRITE(6,860)
      WRITE(6,870) TOD
      WRITE(6,874) NEXCH
      WRITE(6,878)
      WRITE(6,880)
```

```
      WRITE(6,900) (IDS(I),I=1,11)
      WRITE(6,910) (TDIF(J),(EINF(I,J),I=1,11),J=1,ITN)
      WRITE(6,940)
      WRITE(6,930)
  130 IF(WEFF.NE.1) GO TO 40
      WRITE(6,925)
      WRITE(6,860)
      WRITE(6,870) TOD
      WRITE(6,874) NEXCH
      WRITE(6,876)
      WRITE(6,880)
      WRITE(6,900) (IDS(I),I=1,11)
      WRITE(6,890) (TDIF(J),(EFF(I,J),I=1,11),J=1,ITN)
      WRITE(6,935)
      WRITE(6,943)
   40 CONTINUE
   50 CONTINUE
   90 SKIP = SKIP+1.
      IF(SKIP.NE.1.) GO TO 105
      IF(WNPV.NE.1) GO TO 140
      ITOD1 = NJ1
      ITOD2 = NJ1
      ITMP4A = NIA
      ITMP4B = NIA
      ISID1 = NI1
      ISID2 = NI1
      NEXCH1 = NE1
      NEXCH2 = NE1
      IOPT = IO1
      JOPT = JO1
      WRITE(6,280)
      GO TO 95
C
C     *  CONVERT TO AMERICAN ENGINEERING UNITS AND CHECK VALUES    *
C     *  OF X, RL, AND SREYN.                                      *
C
  105 IF(X.LE..7) GO TO 186
       WRITE(6,992)
  186 IF(RL.GE..1) GO TO 187
      WRITE(6,994)
  187 IF(SREYN.GE.800) GO TO 188
      WRITE(6,996)
  188 AO = AO/10000.
      Q = Q*NEXCH
      LT = LT/100.
      SDPS = DPS/14.696
      STOP = TOP*1.868
      ESID = SID/2.54
      ELT = LT/2.54/12.*100.
      ELS = LS/2.54
      ETOD = TOD/2.54
      EHO = HO/.0001355
      EHI = HI/.0001355
      EUO = UO/.0001355
      EQ = Q/252.
      ETEMP1 = (TEMP1-273.15)*1.8+32.
      ETEMP2 = (TEMP2-273.15)*1.8+32.
      ETEMP3 = (TEMP3-273.15)*1.8+32.
```

```
      ETEMP4 = (TEMP4-273.15)*1.8+32.
      ELMTD = LMTD*1.8
      EAO = AO*10.764
      ARFLOW = ARCFM/2118.9
      FGFLOW = FGCFM/2118.9
      POWFGS = POWFGS/60./252.*.01758
      POWAIR = POWAIR/60./252.*.01758
      ABPWR = POWAIR*.7457
      FGPWR = POWFGS*.7457
      WRITE(6,290)
      WRITE(6,300)
      WRITE(6,310) TOD,ETOD
      WRITE(6,320) SID,ESID
      WRITE(6,330) LT,ELT
      WRITE(6,340) NT
      WRITE(6,350) LS,ELS
      WRITE(6,360) NB
      WRITE(6,370) NEXCH
      WRITE(6,380)
      WRITE(6,400)
      WRITE(6,410) SREYN
      WRITE(6,420) SPRNDT
      WRITE(6,430) HO,EHO
      WRITE(6,440) TREYN
      WRITE(6,450) PRNDTL
      WRITE(6,460) HI,EHI
      WRITE(6,470) UO,EUO
      WRITE(6,480) Q,EQ
      WRITE(6,490) TEMP1,ETEMP1
      WRITE(6,500) TEMP2,ETEMP2
      WRITE(6,510) TEMP3,ETEMP3
      WRITE(6,520) TEMP4,ETEMP4
      WRITE(6,530) LMTD,ELMTD
      WRITE(6,540) AO,EAO
      WRITE(6,550) SOPS,OPS
      WRITE(6,560) STOP,TOP
      WRITE(6,600)
      WRITE(6,610)
      WRITE(6,620) ARFLOW,ARCFM
      WRITE(6,630) FGFLOW,FGCFM
      WRITE(6,640) POWAIR,ABPWR
      WRITE(6,650) POWFGS,FGPWR
      WRITE(6,660)
      WRITE(6,670)
      WRITE(6,680) ARBCST
      WRITE(6,690) FGBCST
      WRITE(6,700) HXCOST
      WRITE(6,710) HXMTL
      WRITE(6,720) THXCST
      WRITE(6,730) TOTCST
      WRITE(6,740) PWRCST
      WRITE(6,750) FLSVNG
      WRITE(6,760) ANLCST
      WRITE(6,770) ACF
      WRITE(6,780) NPV(I,J)
      WRITE(6,790)
      WRITE(6,800)
      WRITE(6,810) EOIL
```

```
      WRITE(6,820) EELEC
      WRITE(6,830) EQCON
      WRITE(6,840) EINF(I,J)
      WRITE(6,845) EFF(I,J)
  140 IF(SKIP.EQ.1) SKIP = 2
      IF(SKIP.NE.2.) GO TO 160
      IF(WWE.NE.1) GO TO 160
      ITOO1 = EJ1
      ITOO2 = EJ1
      ITMP4A = EIA
      ITMP4B = EIA
      ISIO1 = EI1
      ISIO2 = EI1
      NEXCH1 = EE1
      NEXCH2 = EE1
      IOPT = IO2
      JOPT = JO2
      WRITE(6,285)
      GO TO 95
  160 IF(SKIP.EQ.2) SKIP = 3
      IF(SKIP.NE.3) GO TO 999
      IF(WEFF.NE.1) GO TO 999
      ITOO1 = EFJ1
      ITOO2 = EFJ1
      ITMP4A = EFIA
      ITMP4B = EFIA
      ISIO1 = EFI1
      ISIO2 = EFI1
      NEXCH1 = EFE1
      NEXCH2 = EFE1
      IOPT =IO3
      JOPT = JO3
      WRITE(6,287)
      GO TO 95
C
C     ******************************************************************
C
C                                     FORMATS
C
C     ******************************************************************
C
  100 FORMAT(8F10.3)
  125 FORMAT(11I5)
  150 FORMAT(//////////56X,'ECHO CHECK OF DATA'////)
  170 FORMAT(43X,'MASS FLOW RATE',2X,'HEAT CAPACITY',4X,'VISCOSITY',
     *5X,'THERM. COND.'/47X,'KG/HR',7X,'KCAL/KG/DEG K',5X,'G/CM/S',
     *6X,'CAL/S/CM/DEG K'//)
  200 FORMAT(27X,'INSIDE FLUID',5X,4(E12.4,3X)//)
  220 FORMAT(27X,'OUTSIDE FLUID',4X,4(E12.4,3X)//)
  280 FORMAT('1'///40X,'***** SEARCH RESULTS FOR THE ECONOMIC ',
     *'OPTIMUM *****'////)
  285 FORMAT('1'///,37X,'***** SEARCH RESULTS FOR THE OPTIMUM WOR',
     *'K EQUIVALENT *****'////)
  287 FORMAT('1'///30X,'***** SEARCH RESULTS FOR THE OPTIMUM OVER',
     *'ALL SECOND LAW EFFICIENCY *****'////)
  290 FORMAT(///55X,'HEAT-EXCHANGER DESIGN',///)
  300 FORMAT(31X,'HEAT-EXCHANGER SPECIFICATION',26X,'VALUE'//)
  310 FORMAT(32X,'TUBE OUTSIDE DIAMETER',24X,F5.3,1X,'CM',8X,F5.3,1X
```

```
     *'IN'/)
 320 FORMAT(32X,'SHELL INSIDE DIAMETER',22X,F7.3,1X,'CM',6X,F6.2,2X
     *'IN'/)
 330 FORMAT(32X,'TUBE LENGTH',34X,F5.3,1X,'M',8X,F5.2,2X,'FT'/)
 340 FORMAT(32X,'NUMBER OF TUBES',27X,I4/)
 350 FORMAT(32X,'BAFFLE SPACING',29X,F7.3,1X,'CM',7X,F5.2,2X,'IN'/)
 360 FORMAT(32X,'NUMBER OF BAFFLES',27X,I2/)
 370 FORMAT(32X,'NUMBER OF HEAT EXCHANGERS',19X,I2///)
 380 FORMAT('1'//,55X,'HEAT-EXCHANGER DESIGN',///)
 400 FORMAT(7X,'HEAT TRANSFER AND/OR PRESSURE DROP QUANTITY',41X,
     *'VALUE'//)
 410 FORMAT(10X,'SHELL-SIDE REYNOLD''S NUMBER',24X,E12.5/)
 420 FORMAT(10X,'SHELL-SIDE PRANDTL NUMBER',27X,F6.4/)
 430 FORMAT(10X,'SHELL-SIDE HEAT-TRANSFER COEFFICIENT',16X,F9.7,3X,
     *'CAL/S/SQ CM/C',12X,F6.3,7X,'BTU/HR/SQ FT/F'/)
 440 FORMAT(10X,'TUBE-SIDE REYNOLD''S NUMBER',25X,E12.5/)
 450 FORMAT(10X,'TUBE-SIDE PRANDTL NUMBER',28X,F6.4/)
 460 FORMAT(10X,'TUBE-SIDE HEAT-TRANSFER COEFFICIENT',17X,F9.7,3X,
     *'CAL/S/SQ CM/C',12X,F6.3,7X,'BTU/HR/SQ FT/F'/)
 470 FORMAT(10X,'OVERALL HEAT TRANSFER COEFFICIENT',19X,F9.7,3X,
     *'CAL/S/SQ CM/C',12X,F6.3,7X,'BTU/HR/SQ FT/F'/)
 480 FORMAT(10X,'TOTAL AMOUNT OF HEAT TRANSFERED',20X,E12.5,1X,
     *'CAL/HR',19X,E12.5,1X,'BTU/HR'/)
 490 FORMAT(10X,'INLET FLUE GAS TEMPERATURE',24X,F6.2,8X,'DEG K',
     *19X,F6.2,8X,'DEG F'/)
 500 FORMAT(10X,'OUTLET FLUE GAS TEMPERATURE',23X,F6.2,8X,'DEG K',
     *19X,F6.2,8X,'DEG F'/)
 510 FORMAT(10X,'INLET COMBUSTION AIR TEMPERATURE',18X,F6.2,8X,
     *'DEG K',19X,F6.2,8X,'DEG F'/)
 520 FORMAT(10X,'OUTLET COMBUSTION AIR TEMPERATURE',17X,F6.2,8X,
     *'DEG K',19X,F6.2,8X,'DEG F'/)
 530 FORMAT(10X,'LOG MEAN TEMPERATURE DIFFERENCE',19X,F6.2,8X,
     *'DEG C',19X,F6.2,8X,'DEG F'/)
 540 FORMAT(10X,'OUTSIDE TUBULAR AREA/EXCHANGER',21X,E11.4,2X,
     *'SQ M',21X,E11.4,2X,'SQ FT'/)
 550 FORMAT(10X,'SHELL-SIDE PRESSURE DROP',27X,F7.4,6X,'ATM',21X,
     *F7.3,7X,'PSI'/)
 560 FORMAT(10X,'TUBE-SIDE PRESSURE DROP',26X,F7.2,8X,'MM HG',19X,
     *F7.3,7X,'IN H2O'/)
 600 FORMAT(////59X,'BLOWER DESIGNS'///)
 610 FORMAT(35X,'SPECIFICATION',34X,'VALUE'//)
 620 FORMAT(31X,'AIR FLOW RATE',23X,F6.2,1X,'CU M/S',7X,E11.4,1X,
     *'CFM'/)
 630 FORMAT(31X,'FLUE GAS FLOW RATE',18X,F6.2,1X,'CU M/S',7X,E11.4,
     *1X,'CFM'/)
 640 FORMAT(31X,'AIR BLOWER POWER',17X,F9.2,1X,'KW',7X,F9.2,7X,'HP'
     */)
 650 FORMAT(31X,'FLUE GAS BLOWER POWER',12X,F9.2,1X,'KW',7X,F9.2,7X,
     *'HP')
 660 FORMAT('1'///,50X,'HEAT RECOVERY ADDITION ECONOMICS'///)
 670 FORMAT(47X,'QUANTITY',25X,'JAN. 1979 VALUE'//)
 680 FORMAT(36X,'AIR BLOWER',36X,'$',F9.0/)
 690 FORMAT(36X,'FLUE GAS BLOWER',32X,F9.0/)
 700 FORMAT(36X,'HEAT EXCHANGER',33X,F9.0/)
 710 FORMAT(36X,'TOTAL HEAT EXCHANGER MATERIAL',18X,F9.0/)
 720 FORMAT(36X,'HEAT EXCHANGER MODULE',26X,F9.0/)
 730 FORMAT(36X,'HEAT RECOVERY ADDITION',25X,F9.0/)
 740 FORMAT(36X,'AVERAGE ANNUAL POWER',27X,F9.0/)
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750 FORMAT(36X,'ANNUAL FUEL SAVINGS',28X,F9.0/)
760 FORMAT(36X,'ANNUAL COST',36X,F9.0/)
770 FORMAT(36X,'NET ANNUAL CASH FLOW',27X,F9.0/)
780 FORMAT(36X,'NET PRESENT VALUE',28X,F11.0/)
790 FORMAT(////49X,'WORK EQUIVALENTS (ONE HOUR BASIS)'////)
800 FORMAT(48X,'QUANTITY',23X,'VALUE IN KCAL'//)
810 FORMAT(40X,'OIL SAVED',30X,E12.5/)
820 FORMAT(40X,'ELECTRICITY',28X,E12.5/)
830 FORMAT(40X,'EQUIPMENT & CONSTRUCTION',15X,E12.5/)
840 FORMAT(40X,'TOTAL',34X,E12.5/)
845 FORMAT(////45X,'OVERALL SECOND LAW EFFICIENCY',3X,F8.5)
850 FORMAT('1'///,44X,'NET PRESENT VALUES FOR A RANGE OF TEMPER',
   *'ATURES'/)
860 FORMAT(46X,'AND SHELL INSIDE DIAMETERS WITH A CONSTANT'/)
870 FORMAT(50X,'TUBE OUTSIDE DIAMETER OF',F6.3,' CM'/)
874 FORMAT(55X,'AND',I3,' HEAT EXCHANGERS'/)
876 FORMAT(60X,'(JAN. 1979 $)'////)
878 FORMAT(61X,'(KCAL/HR)'////)
880 FORMAT(7X,'TEMP.',45X,'SHELL INSIDE DIAMETER (CM)'/7X,'DIFF.')
890 FORMAT(6X,F6.2,3X,11F10.5/)
900 FORMAT(7X,'DEG C',7X,11(I3,7X)/)
910 FORMAT(6X,F6.2,3X,11F10.0/)
920 FORMAT('1'///,45X,'WORK EQUIVALENTS FOR A RANGE OF TEMPERAT',
   *'URES'/)
925 FORMAT('1'///37X,'OVERALL SECOND LAW EFFICIENCIES FOR A RAN',
   *'GE OF TEMPERATURES'/)
930 FORMAT(20X,'ERROR CONDITION 9999999.:  LENGTH OF TUBES LESS',
   *' THAN SHELL INSIDE DIAMETER')
935 FORMAT(////20X,'ERROR CONDITION .88888:  LENGTH OF TUBES ',
   *'EXCEED 6.1 M (20 FT)'//)
940 FORMAT(////20X,'ERROR CONDITION 8888888.:  LENGTH OF TUBES ',
   *'EXCEED 6.1 M (20 FT)'//)
943 FORMAT(20X,'ERROR CONDITION .99999:  LENGTH OF TUBES LESS ',
   *'THAN SHELL INSIDE DIAMETER')
945 FORMAT(58X,'RANGE OF SEARCH'///)
950 FORMAT(35X,'INDEX VARIABLE',25X,'INITIAL VALUE',8X,'FINAL V',
   *'ALUE'//)
960 FORMAT(26X,'NUMBER OF HEAT EXCHANGERS',25X,I3,16X,I3/)
970 FORMAT(26X,'TUBE OUSIDE DIAMETER',31X,F5.3,1X,'CM',12X,F5.3,1X,
   *'CM'/)
980 FORMAT(26X,'SHELL INSIDE DIAMETER',28X,I3,5X,'CM',10X,I3,5X,
   *'CM'/)
990 FORMAT(26X,'OUTLET COMBUSTION AIR TEMPERATURE',16X,I3,5X,'K',
   *11X,I3,5X,'K'///)
992 FORMAT(' X GREATER THAN .7')
994 FORMAT(' RL GREATER THAN .1')
996 FORMAT(' SREYN LESS THAN 800')
999 STOP
    END
```

```
      FUNCTION CPA(A,B,T)
C
C     ******************************************************************
C
C             THIS FUNCTION SUBPROGRAM CALCULATES THE CHANGE
C               IN WORK EQUIVALENT/KMOL AS A COMPONENT IS
C                ADJUSTED TO THE STANDARD STATE (298.15K)
C
C     ******************************************************************
C
      C = B/1000.
      TI = 298.15
      CPA = (A-TI*C)*(T-TI)+C/2*(T**2.-TI**2.)-A*TI*ALOG(T/TI)
      RETURN
      END
```

ECHO CHECK OF DATA

	MASS FLOW RATE KG/HR	HEAT CAPACITY KCAL/KG/DEG K	VISCOSITY G/CM/S	THERM. COND. CAL/S/CM/DEG K
INSIDE FLUID	0.2880E 06	0.2517E 00	0.2173E-03	0.7564E-04
OUTSIDE FLUID	0.3473E 06	0.2613E 00	0.2480E-03	0.8667E-04

RANGE OF SEARCH

INDEX VARIABLE	INITIAL VALUE	FINAL VALUE
NUMBER OF HEAT EXCHANGERS	8	8
TUBE OUSIDE DIAMETER	2.540 CM	2.540 CM
SHELL INSIDE DIAMETER	50 CM	300 CM
OUTLET COMBUSTION AIR TEMPERATURE	330 K	530 K

NET PRESENT VALUES FOR A RANGE OF TEMPERATURES
AND SHELL INSIDE DIAMETERS WITH A CONSTANT
TUBE OUTSIDE DIAMETER OF 2.540 CM
AND 8 HEAT EXCHANGERS
(JAN. 1979 $)

TEMP. DIFF. DEG C	SHELL INSIDE DIAMETER (CM) 50	75	100	125	150	175	200	225	250	275	300
203.15	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
183.15	-12488079.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
163.15	-10056931.	-7231442.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
143.15	-14317363.	-3279299.	-3678976.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
123.15	-15549486.	-2544414.	-522817.	-939832.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
103.15	-18278672.	-4799310.	764701.	1488444.	1155520.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
83.15	-20247488.	-5264464.	458321.	2650180.	2974742.	2750206.	2443713.	9999999.	9999999.	9999999.	9999999.
63.15	8888888.	-7313977.	277981.	2698272.	3781512.	3592527.	3774350.	3572305.	3359826.	3121549.	9999999.
43.15	8888888.	8888888.	8888888.	8888888.	3872172.	4138533.	4365006.	4131516.	3834808.	3460210.	2984347.
23.15	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.
3.15	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.

ERROR CONDITION 8888888.: LENGTH OF TUBES EXCEED 6.1 M (20 FT)

ERROR CONDITION 9999999.: LENGTH OF TUBES LESS THAN SHELL INSIDE DIAMETER

WORK EQUIVALENTS FOR A RANGE OF TEMPERATURES
AND SHELL INSIDE DIAMETERS WITH A CONSTANT
TUBE OUTSIDE DIAMETER OF 2.540 CM
AND 8 HEAT EXCHANGERS
(KCAL/HR)

TEMP. DIFF. DEG C	SHELL INSIDE DIAMETER (CM) 50	75	100	125	150	175	200	225	250	275	300
203.15	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
183.15	36264032.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
163.15	30438672.	22289104.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
143.15	42629744.	11982191.	12904360.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
123.15	46490992.	10637357.	4644311.	5558148.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
103.15	55402080.	17596736.	1602662.	-779853.	-235198.	9999999.	9999999.	9999999.	9999999.	9999999.	9999999.
83.15	61940064.	15502192.	2905910.	-3716768.	-5129648.	-4843875.	-4224523.	9999999.	9999999.	9999999.	9999999.
63.15	8888888.	25643472.	3957982.	-3475869.	-7313959.	-8573327.	-8289593.	-8356259.	-8512912.	-8752881.	9999999.
43.15	8888888.	8888888.	8888888.	8888888.	-7673692.	-9298227.	-10621699.	-10838930.	-11005220.	-11130852.	-11225238.
23.15	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.
3.15	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.	8888888.

ERROR CONDITION 8888888.: LENGTH OF TUBES EXCEED 6.1 M (20 FT)

ERROR CONDITION 9999999.: LENGTH OF TUBES LESS THAN SHELL INSIDE DIAMETER

OVERALL SECOND LAW EFFICIENCIES FOR A RANGE OF TEMPERATURES
AND SHELL INSIDE DIAMETERS WITH A CONSTANT
TUBE OUTSIDE DIAMETER OF 2.540 CM
AND 8 HEAT EXCHANGERS
(JAN. 1979 $)

TEMP. DIFF. DEG C	SHELL INSIDE DIAMETER (CM) 50	75	100	125	150	175	200	225	250	275	300
203.15	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999
183.15	0.00665	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999
163.15	0.01237	0.01537	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999
143.15	0.01472	0.03291	0.03173	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999
123.15	0.01927	0.04700	0.06189	0.05892	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999
103.15	0.02216	0.04729	0.09091	0.10540	0.10169	0.99999	0.99999	0.99999	0.99999	0.99999	0.99999
83.15	0.02562	0.05525	0.10087	0.15043	0.16804	0.16416	0.15632	0.99999	0.99999	0.99999	0.99999
63.15	0.88888	0.05692	0.11149	0.16607	0.22225	0.24999	0.24315	0.24473	0.24850	0.25452	0.99999
43.15	0.88888	0.88888	0.88888	0.88888	0.24529	0.28208	0.32135	0.32886	0.33486	0.33953	0.34313
23.15	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.80888	0.88888	0.88888	0.88888
3.15	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.88888	0.86888

ERROR CONDITION .88888: LENGTH OF TUBES EXCEED 6.1 M (20 FT)

ERROR CONDITION .99999: LENGTH OF TUBES LESS THAN SHELL INSIDE DIAMETER

***** SEARCH RESULTS FOR THE ECONOMIC OPTIMUM *****

HEAT-EXCHANGER DESIGN

HEAT-EXCHANGER SPECIFICATION	VALUE	
TUBE OUTSIDE DIAMETER	2.540 CM	1.000 IN
SHELL INSIDE DIAMETER	200.000 CM	78.74 IN
TUBE LENGTH	4.655 M	15.27 FT
NUMBER OF TUBES	3442	
BAFFLE SPACING	187.960 CM	74.00 IN
NUMBER OF BAFFLES	1	
NUMBER OF HEAT EXCHANGERS	8	

HEAT-EXCHANGER DESIGN

HEAT TRANSFER AND/OR PRESSURE DROP QUANTITY	VALUE			
SHELL-SIDE REYNOLD'S NUMBER	0.15825E 05			
SHELL-SIDE PRANDTL NUMBER	0.7477			
SHELL-SIDE HEAT-TRANSFER COEFFICIENT	0.0019911	CAL/S/SQ CM/C	14.695	BTU/HR/SQ FT/F
TUBE-SIDE REYNOLD'S NUMBER	0.80360E 04			
TUBE-SIDE PRANDTL NUMBER	0.7231			
TUBE-SIDE HEAT-TRANSFER COEFFICIENT	0.0010299	CAL/S/SQ CM/C	7.601	BTU/HR/SQ FT/F
OVERALL HEAT TRANSFER COEFFICIENT	0.0005986	CAL/S/SQ CM/C	4.417	BTU/HR/SQ FT/F
TOTAL AMOUNT OF HEAT TRANSFERED	0.13016E 11	CAL/HR	0.51649E 08	BTU/HR
INLET FLUE GAS TEMPERATURE	533.15	DEG K	500.00	DEG F
OUTLET FLUE GAS TEMPERATURE	389.40	DEG K	241.25	DEG F
INLET COMBUSTION AIR TEMPERATURE	310.93	DEG K	100.00	DEG F
OUTLET COMBUSTION AIR TEMPERATURE	490.00	DEG K	422.33	DEG F
LOG MEAN TEMPERATURE DIFFERENCE	59.06	DEG C	106.31	DEG F
OUTSIDE TUBULAR AREA/EXCHANGER	0.1278E 04	SQ M	0.1376E 05	SQ FT
SHELL-SIDE PRESSURE DROP	0.0579	ATM	0.851	PSI
TUBE-SIDE PRESSURE DROP	2.35	MM HG	1.258	IN H2O

BLOWER DESIGNS

SPECIFICATION	VALUE			
AIR FLOW RATE	72.90	CU M/S	0.1545E 06	CFM
FLUE GAS FLOW RATE	136.59	CU M/S	0.2894E 06	CFM
AIR BLOWER POWER	28.51	KW	21.26	HP
FLUE GAS BLOWER POWER	973.64	KW	726.04	HP

HEAT RECOVERY ADDITION ECONOMICS

QUANTITY	JAN. 1979 VALUE
AIR BLOWER	$ 81005.
FLUE GAS BLOWER	115593.
HEAT EXCHANGER	654146.
TOTAL HEAT EXCHANGER MATERIAL	457902.
HEAT EXCHANGER MODULE	2073642.
HEAT RECOVERY ADDITION	2239899.
AVERAGE ANNUAL POWER	261699.
ANNUAL FUEL SAVINGS	2570384.
ANNUAL COST	638006.
NET ANNUAL CASH FLOW	1195921.
NET PRESENT VALUE	4365006.

WORK EQUIVALENTS (ONE HOUR BASIS)

QUANTITY	VALUE IN KCAL
OIL SAVED	-0.13016E 08
ELECTRICITY	0.22682E 07
EQUIPMENT & CONSTRUCTION	0.12566E 06
TOTAL	-0.10622E 08

OVERALL SECOND LAW EFFICIENCY 0.32135

***** SEARCH RESULTS FOR THE OPTIMUM WORK EQUIVALENT *****

HEAT-EXCHANGER DESIGN

HEAT-EXCHANGER SPECIFICATION	VALUE	
TUBE OUTSIDE DIAMETER	2.540 CM	1.000 IN
SHELL INSIDE DIAMETER	300.000 CM	118.11 IN
TUBE LENGTH	4.516 M	14.82 FT
NUMBER OF TUBES	8048	
BAFFLE SPACING	187.960 CM	74.00 IN
NUMBER OF BAFFLES	1	
NUMBER OF HEAT EXCHANGERS	8	

HEAT-EXCHANGER DESIGN

HEAT TRANSFER AND/OR PRESSURE DROP QUANTITY	VALUE			
SHELL-SIDE REYNOLD'S NUMBER	0.10680E 05			
SHELL-SIDE PRANDTL NUMBER	0.7477			
SHELL-SIDE HEAT-TRANSFER COEFFICIENT	0.0015229	CAL/S/SQ CM/C	11.239	BTU/HR/SQ FT/F
TUBE-SIDE REYNOLD'S NUMBER	0.34365E 04			
TUBE-SIDE PRANDTL NUMBER	0.7231			
TUBE-SIDE HEAT-TRANSFER COEFFICIENT	0.0003832	CAL/S/SQ CM/C	2.828	BTU/HR/SQ FT/F
OVERALL HEAT TRANSFER COEFFICIENT	0.0002638	CAL/S/SQ CM/C	1.947	BTU/HR/SQ FT/F
TOTAL AMOUNT OF HEAT TRANSFERED	0.13016E 11	CAL/HR	0.51649E 08	BTU/HR
INLET FLUE GAS TEMPERATURE	533.15	DEG K	500.00	DEG F
OUTLET FLUE GAS TEMPERATURE	389.40	DEG K	241.25	DEG F
INLET COMBUSTION AIR TEMPERATURE	310.93	DEG K	100.00	DEG F
OUTLET COMBUSTION AIR TEMPERATURE	490.00	DEG K	422.33	DEG F
LOG MEAN TEMPERATURE DIFFERENCE	59.06	DEG C	106.31	DEG F
OUTSIDE TUBULAR AREA/EXCHANGER	0.2900E 04	SQ M	0.3122E 05	SQ FT
SHELL-SIDE PRESSURE DROP	0.0408	ATM	0.599	PSI
TUBE-SIDE PRESSURE DROP	0.51	MM HG	0.275	IN H2O

BLOWER DESIGNS

SPECIFICATION	VALUE	
AIR FLOW RATE	72.90 CU M/S	0.1545E 06 CFM
FLUE GAS FLOW RATE	136.59 CU M/S	0.2894E 06 CFM
AIR BLOWER POWER	6.23 KW	4.65 HP
FLUE GAS BLOWER POWER	691.10 KW	515.35 HP

HEAT RECOVERY ADDITION ECONOMICS

QUANTITY	JAN. 1979 VALUE
AIR BLOWER	$ 81005.
FLUE GAS BLOWER	115593.
HEAT EXCHANGER	1156419.
TOTAL HEAT EXCHANGER MATERIAL	809493.
HEAT EXCHANGER MODULE	3665847.
HEAT RECOVERY ADDITION	3882104.
AVERAGE ANNUAL POWER	182100.
ANNUAL FUEL SAVINGS	2570384.
ANNUAL COST	820059.
NET ANNUAL CASH FLOW	1233937.
NET PRESENT VALUE	2984347.

WORK EQUIVALENTS (ONE HOUR BASIS)

QUANTITY	VALUE IN KCAL
OIL SAVED	-0.13016E 08
ELECTRICITY	0.15783E 07
EQUIPMENT & CONSTRUCTION	0.21203E 06
TOTAL	-0.11225E 08

OVERALL SECOND LAW EFFICIENCY 0.34313

HEAT-EXCHANGER DESIGN

HEAT TRANSFER AND/OR PRESSURE DROP QUANTITY	VALUE			
SHELL-SIDE REYNOLD'S NUMBER	0.10680E 05			
SHELL-SIDE PRANDTL NUMBER	0.7477			
SHELL-SIDE HEAT-TRANSFER COEFFICIENT	0.0015229	CAL/S/SQ CM/C	11.239	BTU/HR/SQ FT/F
TUBE-SIDE REYNOLD'S NUMBER	0.34365E 04			
TUBE-SIDE PRANDTL NUMBER	0.7231			
TUBE-SIDE HEAT-TRANSFER COEFFICIENT	0.0003832	CAL/S/SQ CM/C	2.828	BTU/HR/SQ FT/F
OVERALL HEAT TRANSFER COEFFICIENT	0.0002638	CAL/S/SQ CM/C	1.947	BTU/HR/SQ FT/F
TOTAL AMOUNT OF HEAT TRANSFERED	0.13016E 11	CAL/HR	0.51649E 08	BTU/HR
INLET FLUE GAS TEMPERATURE	533.15	DEG K	500.00	DEG F
OUTLET FLUE GAS TEMPERATURE	389.40	DEG K	241.25	DEG F
INLET COMBUSTION AIR TEMPERATURE	310.93	DEG K	100.00	DEG F
OUTLET COMBUSTION AIR TEMPERATURE	490.00	DEG K	422.33	DEG F
LOG MEAN TEMPERATURE DIFFERENCE	59.06	DEG C	106.31	DEG F
OUTSIDE TUBULAR AREA/EXCHANGER	0.2900E 04	SQ M	0.3122E 05	SQ FT
SHELL-SIDE PRESSURE DROP	0.0400	ATM	0.599	PSI
TUBE-SIDE PRESSURE DROP	0.51	MM HG	0.275	IN H2O

BLOWER DESIGNS

SPECIFICATION	VALUE	
AIR FLOW RATE	72.90 CU M/S	0.1545E 06 CFM
FLUE GAS FLOW RATE	136.59 CU M/S	0.2894E 06 CFM
AIR BLOWER POWER	6.23 KW	4.65 HP
FLUE GAS BLOWER POWER	691.10 KW	515.35 HP

***** SEARCH RESULTS FOR THE OPTIMUM OVERALL SECOND LAW EFFICIENCY *****

HEAT-EXCHANGER DESIGN

HEAT-EXCHANGER SPECIFICATION	VALUE	
TUBE OUTSIDE DIAMETER	2.540 CM	1.000 IN
SHELL INSIDE DIAMETER	300.000 CM	118.11 IN
TUBE LENGTH	4.516 M	14.82 FT
NUMBER OF TUBES	8048	
BAFFLE SPACING	187.960 CM	74.00 IN
NUMBER OF BAFFLES	1	
NUMBER OF HEAT EXCHANGERS	8	

HEAT RECOVERY ADDITION ECONOMICS

QUANTITY	JAN. 1979 VALUE
AIR BLOWER	$ 81005.
FLUE GAS BLOWER	115593.
HEAT EXCHANGER	1156419.
TOTAL HEAT EXCHANGER MATERIAL	809493.
HEAT EXCHANGER MODULE	3665847.
HEAT RECOVERY ADDITION	3882104.
AVERAGE ANNUAL POWER	182100.
ANNUAL FUEL SAVINGS	2570864.
ANNUAL COST	820059.
NET ANNUAL CASH FLOW	1233937.
NET PRESENT VALUE	2984347.

WORK EQUIVALENTS (ONE HOUR BASIS)

QUANTITY	VALUE IN KCAL
OIL SAVED	-0.13016E 08
ELECTRICITY	0.15783E 07
EQUIPMENT & CONSTRUCTION	0.21203E 06
TOTAL	-0.11225E 08

OVERALL SECOND LAW EFFICIENCY 0.34313

ANALYSIS OF THE COED PROCESS AND OPTIMIZATION OF FLUE GAS HEAT RECOVERY FROM A SECOND LAW PERSPECTIVE

by

TERRY LEE UNRUH

B.S., Kansas State University, 1978

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1979

ABSTRACT

The basis for second law thermodynamic analysis of processes involving chemical transformations is reviewed and the COED process and its attendant chemistry is described. The energetics of this process and of each step therein are calculated from a commercial plant design study and are examined from a second law perspective. Two efficiencies, an incremental and an absolute, are found to be useful in this analysis. The incremental efficiency is most useful with physical processes while the absolute or second law efficiency is most useful with processes involving chemical transformations. The second law (absolute) efficiency is shown to be 0.75. In contrast, the thermal or first law efficiency is 0.80. When the inefficiencies of oxygen production and electricity generation are charged to the COED process the second law efficiency decreases to 0.68. An energy cost assigned to the equipment and construction is evaluated using energy/dollar data obtained from an economic Input-Output analysis for the U.S. economy. When this energy cost plus an energy credit for salvage is included in the analysis a final overall second law efficiency of 0.67 is found.

In addition, the optimization of a flue gas heat recovery system from a second law perspective is performed. This system is described and two thermodynamic and one economic objective function are determined. These objective functions are optimized from the standpoint of four independent design variables, the number of heat exchangers, the tube outside diameter, the shell inside diameter, and the exit preheated air temperature. Results are compared on the basis of the number of heat exchangers. The thermodynamic optimums are found at approximately 30 heat exchangers but are taken at 13 heat exchangers since the objective function values of these two amounts are within 5% of each other. In contrast, a distinct economic

optimum is found at 8 heat exchangers. The design conditions of the economic optimum are determined to produce a thermodynamic objective function value within 20% of the optimal value. The converse, however, is found to not be true.