MASTER

HYDRGN - A COMPUTERIZED TECHNIQUE FOR THE
ANALYSIS OF THERMOCHEMICAL WATER-SPLITTING CYCLES

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COMPUTER PROGRAM FOR THE ANALYSIS OF CLOSED
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SUMMARY

The HYDRGN computer program was designed to analyze closed thermochemical cycles for the production of hydrogen from water. This report includes the basic theory, assumptions, and methods of calculation used in this analysis along with a description of the program and its use.

The source program and necessary data bank are available from the University of Kentucky. These may be obtained by sending a magnetic tape (minimum length 1200 ft) and a written request specifying the type of computer and recording characteristics of the tape. A small fee is charged for the recording and handling of the tape.

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INTRODUCTION

Recently the United States and other industrialized nations have found themselves in an energy crisis. This has been due to an increasing need for portable fuels and a dwindling of the supplies of petroleum and natural gas from which these fuels are derived. As a result, interest in hydrogen as an alternative transportable fuel has been growing (1,2).

While hydrogen may be produced from water by electrolysis, it has been shown (3) that it is theoretically possible to produce it more efficiently by closed cycle thermochemical water-splitting processes. Such a process consists of a series of chemical reactions formulated such that the net results are the consumption of heat and water and the production of hydrogen and oxygen. All reactants, other than water, in a single step within the process are regenerated as the products of the other steps. Likewise, all products of a single step, other than hydrogen and oxygen, are consumed as reactants elsewhere within the cycle.

Many such closed cycles have already been proposed (4,5,6) and several investigators are at work producing others. Since the number of possible cycles is almost limitless, a quick and relatively simple method for rating them is needed. The purpose of the HYDRGN computer program is to provide such a ranking of these cycles so that obviously poor ones may be eliminated from further consideration.

An analysis of any process may be made in various degrees of detail. One extreme is a complete description of the process including a flow sheet, sizing of equipment, and costing. In the present case, it was necessary to analyze the processes with a minimum amount of data. This meant that many idealizations of actual mechanisms had to be made.

The HYDRGN Program uses thermodynamic data for the pure components involved in each chemical reaction to calculate the standard state enthalpy, entropy, and Gibbs-free energy changes for each chemical reaction as well as for the material transfer steps, which take the materials from the conditions where they appear as products to the conditions where they are to be used as reactants. Using these properties and the extent of reaction at equilibrium, the heat and useful work needed for each step is calculated. The program also calculates the number of moles of each reactant in the recycle stream at various fractions of equilibrium conversion. The total process heat needed by the cycle which must be supplied by external sources is obtained by a heat exchange routine that determines the amount of heat liberated by the exothermic steps in the cycle which cannot be either utilized internally by the endothermic steps or used to produce useful work. Finally, the program calculates figures of merit and loss coefficients which are used in evaluating the process.

In the next section, the definitions, limitations, and theory on which the program is based will be presented.

THEORY

The theory on which the HYDRGN Program is based is taken from references 7-10.

Consider a reaction of the form:

We now assume that this reaction is conducted as shown in Fig. 1 and is

isothermal, isobaric, and all products and reactants are ideal gases and form ideal gaseous solutions.

FIGURE 1 Reaction Scheme

Defining

ΔH° = Standard state enthalpy change for reaction

ΔS° = Standard state entropy change for reaction

ΔG° = Standard state Gibbs Free Energy change for reaction

Q_T = Total heat input

T = Temp. of the reaction

W_T = Total useful work input

the first law of thermodynamics for a flow system, neglecting kinetic and potential energy, is:

$$(2) \quad \Delta H^\circ = Q_T - W_T$$

where: $Q_T = Q_M + Q_R + Q_S$

$$W_T = W_M + W_R + W_S$$

We can now analyze each element within Figure 1 to determine the heat and work requirements.

Mixer

Since the pure gaseous reactants are mixed to form an ideal solution at constant temperature and pressure,

$$\Delta H_M = 0 = Q_M - W_M$$

If the mixing is conducted in a manner such that no work other than p_v work is done on the process, $W_M = 0$ and

$$(3) \quad Q_M = \Delta H_M = 0.$$

Separator

For an ideal solution,

$$\Delta H_S = 0 = Q_S - W_S$$

The minimum amount of energy which must be expended in this separation will be for the case of a completely reversible process. Therefore,

$$(4) \quad Q_S = T\Delta S_S = W_S$$

and for an ideal mixture of gases;

$$(5) \quad \Delta S_S = R \sum_i n_i \ln X_i$$

where:

R = gas constant

n_i = number of moles of species i in mixture

x_i = mole fraction of species i in mixture

combining equations 4 and 5, we get:

$$(6) \quad W_S = RT \sum_i n_i \ln X_i = Q_S$$

This relationship shows that an amount of work, W_S , must be added to the separator and an equal amount of heat, Q_S , is extracted from the process.

Reactor

Assuming no work other than pv work is done within the reactor itself,

$$W_R = 0$$

and from the first law:

$$(7) \quad \Delta H_R = Q_R$$

combining the heat and work terms for each element of the process,

$$\begin{aligned} Q_T &= Q_M + Q_R + Q_S \\ &= 0 + \Delta H_R + RT \sum_i n_i \ln X_i \end{aligned}$$

If it is further assumed that the heat liberated by the separation process is unrecoverable as would probably be the case,

$$Q_T = \Delta H_R$$

and since,

$$\Delta H^\circ = \Delta H_M + \Delta H_R + \Delta H_S$$

and

$$\Delta H_M = \Delta H_S = 0$$

then

$$(8) \quad Q_T = \Delta H^\circ$$

That is, the total heat of the reaction is equal to the standard state enthalpy change. Also,

$$W_T = W_M + W_R + W_S$$

$$= 0 + 0 + RT \sum_i n_i \ln X_i$$

$$(9) \quad W_T = RT \sum_i n_i \ln X_i$$

If all elements of the reaction are conducted reversibly such as in an electrochemical cell, the heat and work relationships become:

$$(10) \quad Q_T = Q_M + Q_R + Q_S$$

$$Q_T = T(\Delta S_M + \Delta S_R + \Delta S_S) = T\Delta S^\circ$$

$$(11) \quad W_T = W_M + W_R + W_S$$

$$W_T = -(\Delta G_M + \Delta G_R + \Delta G_S) = -\Delta G^\circ$$

Heterogeneous Reactions

For a heterogeneous reaction, equations 8 and 9 are applicable with a modification to the work of separation. In this case, the work of separation is based only on the gas phase. This results from the assumption that the work to separate the various phases is negligible and that it will be unnecessary to separate the components in the condensed phases. Therefore, n_i and X_i in equation 9 refer to the number of moles and the mole fractions based on the gas phase.

Referring to equation 1, we shall derive the general equations for the work of separation for gases. If we define

L_i = relative number of moles of species i in reactor mixture

ϵ = number of moles of component R_1 reacting/mole of R_1 entering the reactor

and require that stoichiometric amounts of products be produced, then:

$$\text{moles of } R_1 \text{ entering separator} = r_1 \frac{1-\epsilon}{\epsilon}$$

$$\text{moles of } R_i \text{ entering separator} = \frac{r_1 \frac{L_i}{L_1} - \epsilon r_i}{\epsilon}$$

R_1 will be referred to as the "base reactant". The choice of the base reactant is optional so long as consistency is maintained throughout the calculations.

For a heterogeneous chemical reaction in which each condensed compound is assumed to be present as a pure phase, the change in the standard state Gibbs free energy is given by:

$$(12) \quad \Delta G^\circ = -RT \left[\sum_j p_j \ln x_{p_j} - \sum_i r_i \ln x_{R_i} \right] \\ - RT \left(\sum_j p_j - \sum_i r_i \right) \ln P_T$$

where the summations are over all gaseous species. For the complete separation of all the gases in the equilibrium reaction mixture, the work of separation is:

$$(13) \quad W_{\text{sep}} = RT \left[\sum_j p_j \ln x_{p_j} + \sum_i \left(\frac{r_1 \left(\frac{L_i}{L_1} \right) - \epsilon r_i}{\epsilon} \right) \ln x_{R_i} \right]$$

adding 12 and 13, we get

$$(14) \quad W_{\text{sep}} = -\Delta G^\circ + RT \sum_i \left(\frac{r_1 L_i}{L_1 \epsilon} \right) \ln x_{R_i} - RT \left(\sum_j p_j - \sum_i r_i \right) \ln P_T$$

From equation 14, it is seen that for a complete separation of the gaseous species, at one atmosphere, the work needed for separation must be greater than or equal to the standard state Gibbs free energy change.

Since the reactants will be recycled and remixed before entering the reactor, all the gaseous reactants may be summed and treated as a single component in calculating the work of separation. This has been done in the analysis of the HYDRGN program. In this case, equation 13 becomes:

$$(15) \quad W_{\text{sep}} = RT \left\{ \sum_j p_j \ln X_{p_j} + \left[\ln \left(\sum_i X_{R_i} \right) \right] \left[\sum_i \left(\frac{r_i L_i}{L_{\text{E}}} - r_i \right) \right] \right\}$$

If there is a single gaseous product, the pressure of the gas at equilibrium is:

$$(16) \quad P_T = e^{-\Delta G^\circ / RT p_i}$$

If ΔG° is negative, the pressure of the gas, P_T , is greater than one atmosphere and no work is needed to remove the pure product. However, if ΔG° is positive, the pressure as given by equation 16 is less than one atmosphere. Therefore, in order to cause the reaction to proceed, work of compression must be expended in pumping the gas from P_T to one atmosphere. The work of separation in this case becomes:

$$(17) \quad W_{\text{sep}} = -p_i \cdot RT \ln (P_{\text{atm}}/P_T) = -(p_i \cdot RT) \frac{\Delta G^\circ}{RT p_i} = -\Delta G^\circ$$

By a similar analysis, if there is only one gaseous reactant, equation 16 becomes:

$$(18) \quad P_T = e^{\Delta G^\circ / RT r_i}$$

From this relationship, it is seen that if ΔG° is less than zero, P_T is less than one atmosphere and no work of compression is needed. Likewise, if ΔG° is greater than zero, the equilibrium pressure of the reaction is greater than one atmosphere and an amount of work equal to $-\Delta G^\circ$ must be expended to compress the gaseous reactant to this higher pressure.

For a reaction in which there are more than one gaseous product and no gaseous reactants, the HYDRGN program assumes that the reaction is conducted at a temperature where the equilibrium pressure of the reaction is one atmosphere so that there is no work of compression. Likewise, the program assumes the pressure is one atmosphere for the case of multiple gaseous reactants and no gaseous products.

If there are no gaseous species in the reaction, either as reactants or product, the program assumes the minimum amount of work expended is $-\Delta G^\circ$ if ΔG° is greater than zero.

Individual Reaction Figures of Merit

The definition of thermal efficiency, η , (called the figure of merit by Funk [3,10]) is

$$(19) \quad \eta = \frac{\Delta H^\circ_{298.15}}{Q_{\text{total}}}$$

where

$$(20) \quad Q_{\text{total}} = \sum \left(Q_j + \frac{W_j}{\text{EFF}} \right)$$

and where

$H^\circ_{298.15}$ = enthalpy change for decomposition of liquid water to hydrogen and oxygen at 298.15 K and 1 atm. (68.3 kcal/g mole H_2)

Q_{total} = total thermal energy required by process

Q_j = direct thermal energy input from primary heat source

W_j = direct useful work input

EFF = efficiency of converting thermal energy to useful work.

It has been shown several times [14] that the upper limit on η is

$$\eta \leq \begin{cases} 1.0 \\ \frac{\Delta H^\circ_{298.15}}{\Delta G^\circ_{298.15}} \frac{T_H - T_C}{T_H} \end{cases}$$

where

T_H = the high temperature in the process

T_C = heat rejection temperature

$\Delta G^\circ_{298.15}$ = free energy change for decomposition of liquid water at 298.15 K and 1 atm.

In the analysis using the HYDRGN program T_C is taken at 298.15 K and since the raw material is liquid water, the "higher heating value" of hydrogen is used in the calculation of the figure of merit. The analysis is designed to consider all processes in exactly the same manner so that a relative ranking can be obtained.

In most water decomposition processes there will be two or more reactions. The efficiency (figure of merit) of each reaction will have an effect on the overall efficiency of the process. In order to maintain consistency of analysis, the individual step (stage) efficiency will be defined as

$$(21) \quad \eta_j = \frac{\Delta H_j}{\theta_j}$$

where

ΔH_j = the enthalpy change for the stage at 298.15 K and 1 atm.

θ_j = the total heat requirement (including that necessary to produce the required useful work) for the stage.

then

$$(22) \quad \sum_j \Delta H_j = \Delta H^\circ_{298.15}$$

and

$$(23) \quad \sum_j \theta_j = Q_{\text{total}}$$

then since

$$(19) \quad \eta = \frac{\Delta H^\circ_{298.15}}{Q_{\text{total}}}$$

(2), (22), and (23) may be substituted into (19) to give

$$(24) \quad \eta = \frac{\sum_j \eta_j \theta_j}{Q_{\text{total}}}$$

or

$$(25) \quad \eta = \sum_j \eta_j \frac{\theta_j}{Q_{\text{total}}}$$

The $\theta_j/Q_{\text{total}}$ act as weighting factors for the individual stage figures of merit.

By themselves the values of the individual stage efficiencies have little meaning. In fact, if ΔH_j is negative for a given step, the "stage efficiency" can be negative. It is the combination of the stage efficiency and its weighting factor which has real meaning in this analysis. This combination shows the contribution of the stage to the total process efficiency. Therefore, it is desirable that the combination of the stage efficiency and its weighting factor be a large positive number. It is unlikely that each step in a multi-step purely thermochemical process will make a positive contribution to the efficiency.

Loss Coefficients

A second approach to the efficiency of a process or an individual stage considers the heat losses. The losses, which can be determined using the HYDRGN program are the rejected heat (Q_{rej}) and the heat necessary to produce the work of separation ($Q_s = \frac{W_s}{\text{EFF}}$).

We define a loss coefficient as

$$(26) \quad E = \frac{Q_s + Q_{rej}}{\Delta H^\circ_{298.15}}$$

This quantity can be used to compare the relative losses of several processes. It is desirable for this loss coefficient to be small and in the extreme zero.

If we now apply the loss coefficient concept to the individual steps of a process, as was done for the figure of merit, we obtain

$$(27) \quad E_j = \frac{(Q_s + Q_{rej})_j}{\Delta H^\circ_{298.15}}$$

where the $(Q_s + Q_{rej})_j$ are the heat necessary for separation and the heat rejected for stage j . The total loss coefficient is then the sum of the individual loss coefficients such that

$$(28) \quad E = \sum_j E_j = \sum_j \frac{(Q_s + Q_{rej})_j}{\Delta H^\circ_{298.15}}$$

and for the whole process

$$(29) \quad \sum_j Q_{rej_j} = Q_{rej} = Q - \Delta H^\circ_{298.15}$$

where Q is the heat requirement other than the heat equivalent of the work of separation of the process.

In addition, the sum of the heats of separation of the various steps sum to the total heat of separation of the process:

$$(30) \quad \sum_j Q_{s_j} = Q_s = \frac{W_s}{EFF}$$

Then equation (26) becomes

$$(31) \quad E = \frac{Q - \Delta H^\circ_{298.15} + \frac{W_s}{EFF}}{\Delta H^\circ_{298.15}}$$

While it is the overall loss coefficient, E , which allows comparison of losses between processes, it is the individual loss coefficients, E_j , which allow comparison of individual steps in the process and show the steps which need most attention if process efficiency is to be improved.

CALCULATION OF THERMODYNAMIC PROPERTIES

For each species involved in the cycle the heat capacity, enthalpy, entropy, and Gibbs free energy are computed by the following relationships:

$$(32) \quad \frac{C_p^\circ}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$(33) \quad \frac{H^\circ}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T}$$

$$(34) \quad \frac{S^\circ}{R} = a_1 \ln T + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7$$

$$(35) \quad G^\circ = H^\circ - TS^\circ$$

The coefficients are obtained from either molecular constant data or thermodynamic data using the PAC-2 computer program (ref. 12). For each species, two sets of coefficients are obtained for temperature intervals of 300 to 1000K and 1000 to 5000K. A library of these thermodynamic coefficients is included with the program for 740 species (solid, liquid, and gas phases of a compound are counted as separate species).

We have arbitrarily assumed $H^\circ_{298.15} = (\Delta H^\circ_f)_{298.15}$ for each compound. For reference elements, $H^\circ_{298.15} = 0$.

HEAT TRANSFER

The total theoretical amount of heat necessary to complete any thermochemical cycle which decomposes one gram mole of water is 68.31 kcal. This

figure assumes that all heat released by the exothermic steps can be used by the endothermic parts of the process. Since the exothermic chemical reactions usually occur at the lower temperatures of the cycle, this assumption is seldom, if ever, true. Therefore, an analysis of the temperatures and enthalpy changes of all of the steps in the cycle is necessary in order to determine which exothermic and endothermic steps are compatible for the exchange of heat. This process of "matching" the steps in the cycle for the purpose of heat exchange is based on the first and second laws of thermodynamics and is done in the MATCH subroutine.

Considering the heat exchange between two steps of the cycle to take place in a constant pressure-countercurrent heat exchanger as shown in Figure 2, the following relationship follows from the first law of thermodynamics:

$$(36) \quad n_A (H_{A_1} - H_{A_2}) + n_B (H_{B_2} - H_{B_1}) + Q = 0$$

where n is the number of moles of material in the stream and Q is the amount of heat exchanged with the surroundings (assumed to equal zero).

If A is the endothermic stream, the second law requires that at every point in the exchanger the following inequality holds:

$$(37) \quad t_B > t_A$$

It is however, assumed that t_A may equal t_B at either the inlet or the outlet of the heat exchanger (no temperature offset).

In order to maximize the amount of heat recovered from the exothermic steps, the total enthalpy change for a step may have to be accomplished by matching with more than one of the other appropriate steps within the cycle. The HYDRGN program uses two methods for this division of the total enthalpic change of a step between multiple heat exchange matches.

FIGURE 2 Heat Exchanger Setup

As seen in equation 36, one method is to change the number of moles of one or both of the streams involved in a match. This is called stream splitting and is used primarily for isothermal steps but may also be used for some nonisothermal cases.

In the second method, which is used only for nonisothermal steps, the number of moles remains constant for all the heat exchanges in which the step is involved. However, the total temperature change required by the step is divided between the various matches according to the requirements imposed by equations 36 and 37 for each exchange.

If there is to be any heat from exothermic steps which cannot be applied to the endothermic steps, it is desirable to have this excess heat available at the higher temperatures. Therefore, the exothermic steps must be matched in ascending order of their temperatures. Using 298 K as the first value, a listing in ascending order is made of the temperatures at which the isothermal steps occur. The temperatures in this list are referred to as the "temperature levels" of the process and determine the order in which matching of the steps is to be done.

At each level, all exothermic steps with initial temperatures equal to this level are found. An attempt is then made to match all of this available heat to the appropriate endothermic parts of the process before proceeding to the next higher temperature level.

Using the criteria imposed by equations 36 and 37 and the assumptions described above, the order of matching at each temperature level is as follows:

- (1) The heat liberated by nonisothermal steps is first matched to the appropriate isothermal steps. If all of the available heat from these steps cannot be matched in this manner, attempts are made to apply it to appropriate nonisothermal steps in the cycle.

- (2) The heat liberated by isothermal steps is now matched in the same manner.

As part of the matching process, the constraint expressed by equation 37 is initially imposed only at the inlet and outlet conditions of the two streams. If either or both of the steps involved in the match are isothermal, no further calculations are needed. In the case of two non-isothermal streams being matched, it is possible to meet these conditions and still have a violation of the second law at some point within the heat exchanger.

This possibility usually but not always occurs if there is a phase change in one of the streams. For this reason, the ROUTE subroutine sets up all phase changes as separate isothermal steps. However, it is still necessary to check matches between nonisothermal steps for second law violations. The method used consists of dividing the total heat transferred in the exchanger into 25 increments and determining the temperature of each stream at these points. If $t_B < (t_A + 5.0)$, the match between the two steps is flagged in the output as an indication that there may be a violation of the second law.

In performing the above calculations, a form of equation 33 must be solved for T at a particular value of H for the material involved in the step. It should be noted that each nonisothermal step consists of heating or cooling only a single compound.

If (H_1, T_1) and (H_2, T_2) are the inlet and outlet conditions of one of the steps in the match, the first enthalpy value at which the match is checked is:

$$(38) \quad H^* = H_1 + (H_2 - H_1)/25$$

Using equation 33, the general equation to be solved for T^* at the value H^* is:

$$(39) \quad H = f(T)$$

Subtracting H^* from both sides of equation 39, we get:

$$(40) \quad H - H^* = f(T) - H^*$$

This relationship is now of a form to be solved by the secant method of iteration (ref. 11). The iteration is repeated until the absolute error for the value of H is less than 0.01 cal.

While the above methods will not necessarily lead to the optimum heat exchange matches for the final design of the process, they do give the value for the minimum amount of heat which must be provided from an external source. This minimum value of external heat needed, Q^* , is obtained by summing the heat to be supplied to the endothermic steps after all possible heat matches have been made. Any exothermic heat available above 500 K after the matching process is assumed to be converted into work with a fraction of the Carnot efficiency. This work generated by the process, W_{gen} , is subtracted from the work needed by the cycle.

FIGURES OF MERIT

The overall figure of merit, η , which this program uses to evaluate the relative merits of a thermochemical cycle is defined as:

$$(19) \quad \eta = \frac{\Delta H^\circ_{298.15}}{Q_{\text{total}}}$$

where $\Delta H^\circ_{298.15}$ is the molar heat of decomposition of liquid water at 298.15 K and Q_{total} is the total energy which must be supplied to the cycle from an external source to produce one mole of hydrogen. The value of $\Delta H^\circ_{298.15}$ is

68.31 kcal for all cycles. Q_{total} includes both the heat and work energy required by the process. Since $\Delta H^\circ_{298.15}$ is constant, the value of the figure of merit depends on the method used to calculate Q_{total} .

The HYDRGN program computes a maximum and a minimum value for the figure of merit under two different sets of conditions. The maximum and minimum values for each of the two figures of merit are the result of using the respective minimum and maximum values of the work for each reaction.

As seen in equation 41, the first estimate of the figure of merit is made assuming total recovery of all exothermic heat and 100 percent efficiency for the work of separation. In all calculations the efficiency of conversion of heat to work may be selected by the operator; in the case an efficiency is not specified the program uses 0.3.

The second estimate of η , shown in equation 42, is obtained after heat exchange matching. The heat needed by the cycle, Q^* , is the sum of the endothermic heats remaining after the matching process. The work of separation is reduced by the total work generated by unmatched exothermic heat and it is further assumed that the separation processes are only 50 percent efficient.

$$(41) \quad \eta_1 = \frac{\Delta H^\circ_{298.15}}{\Delta H^\circ_{298.15} + (W_{sep}/EFF)}$$

$$(42) \quad \eta_2 = \frac{\Delta H^\circ_{298.15}}{Q^* + \left(\frac{2W_{sep} - W_{gen}}{EFF} \right)}$$

COMPUTER PROGRAM

The HYDRGN computer program was written in FORTRAN IV and was designed to work on any operating system compatible with FORTRAN IV.

At the University of Kentucky, the program was checked out on an IBM 370/165 computer with a Fortran G compiler. The total program is 175,448 bytes long of which 102,990 bytes are for the source program.

Due to shorter word length, the IBM 370 system required some double precision variables not required by other machines. These are indicated in the list of variables in Appendix B.

In order to provide maximum flexibility, many of the program's computations are optional. The program will always calculate the thermodynamic changes (ΔH° , ΔS° , and ΔG°) for any set of chemical reactions. If the changes for a complete cycle producing one mole of hydrogen are desired, the DRAW option is used. The analysis then includes the material transfer steps which heat or cool the products of the chemical reactions to the temperatures of the reactions in which they appear as reactants. This option also causes the program to set up the matching of steps for heat exchange. By specifying a base reactant and the conversion ratio at equilibrium, the program calculates work of separation for the reaction. Use of the H298 option causes the program to calculate the thermodynamic changes for the chemical reactions at 298.15 K.

Each cycle may be run at multiple temperature schedules and for various ratios of reactants as detailed under input data. Any number of cycles may be stacked for a single run.

Flow of the Program

The general flow of the main program is shown in Appendix C. From this diagram it is evident that:

- (1) The READIN subroutine reads and lists the input cards describing the chemical reactions, the reaction conditions (temperature, pressure, epsilon), and various options for the cycle.
- (2) The DATAS subroutine is called to search either card input or tape unit 4 for the necessary thermodynamic data of the various compounds used in the cycle.

- (3) The ROUTE subroutine sets up material transfer steps between the chemical reactions in order to complete the cycle.
- (4) The main program uses CPHSG subroutine to calculate ΔH° , ΔS° , and ΔG° for each step.
- (5) The first table of output is printed and subroutine REMOVE is called to calculate work of separation for the chemical reactions.
- (6) A table listing the endothermic and exothermic steps is output.
- (7) The MATCH subroutine is called to set up the matching of the steps for heat exchange and to calculate the figures of merit.
- (8) If the thermodynamic changes at room temperature are desired, FZ298 routine is called to determine the phase of the compounds in the chemical reactions at room temperature. The program then recycles throughout the section of the Main program which calculates ΔH° , ΔS° , and ΔG° at these conditions and outputs the results.
- (9) The LOSS subroutine is called to calculate individual step figures of merit and loss coefficients and to set up a summary table for the whole process.
- (10) The program proceeds to the next cycle.

Main Routine and Subroutines

The main routine directs the general flow of the program as given in Appendix C and was discussed under General Flow of Program section.

READIN - This subroutine is called from Main to read and list the cards describing the cycle. These cards are discussed under Cycle Input Data. This reaction input data describes the products and reactants for the chemical reaction steps and the conditions and options for which the cycle is to be analyzed.

This subroutine also checks to see if the reactions are balanced and rationalizes the stoichiometric coefficients to a basis of one mole of hydrogen produced.

DATAS - This routine searches the thermodynamic data list, contained either on card input or tape (unit 4), for all the compounds involved in the cycle. When one of the compounds of the cycle is found in this listing of species, all phases of the species are assigned identifying index numbers and their coefficients are read into core.

The routine then matches the chemical formula and phase of each product and reactant to the appropriate species found in the listing and the identifying index number of this species is associated with the product or reactant. From this point on, the product or reactant is identified by this index number.

ROUTE - This routine completes the cycle by setting up the material transfer steps which are necessary to take the materials from the temperature reaction(s) where they are used as reactants.

If a material makes phase transitions in the process of being transferred, these transitions are set up as separate constant temperature steps.

CPHSG - This routine calculates the enthalpy, entropy, and Gibbs free energy of a material at a particular temperature using equations 32 to 35 of the Theory.

EQNS - This routine forms an alphanumeric array for outputting the chemical reactions in standard chemical notation.

FZ298 - This routine determines the phase of each reactant and product of the chemical reactions at room temperature for computing the thermodynamic changes of these reactions at 298.15 K.

REMOVE - This routine computes the work of separation and moles of reactant recycle of the chemical reactions. Only the work of separation of

the gaseous components is calculated. All gaseous reactants are summed and treated as a single component for this calculation. If there are less than two gaseous components (treating all gaseous reactants as a single component), the work of separation is taken to be equal to ΔG° if it is positive. If ΔG° is negative for this case, there is no work of separation.

The computations are carried out for up to 4 reactant ratios and for various percentages of reaction equilibrium (50 to 100% in increments of 10). These percentages may be changed by alteration of REMO 265 in the REMOVE subroutine. From these results, maximum and minimum works of separation are found. The summations of these maximum and minimum works for all the reactions are used to calculate the respective minimum and maximum figures of merit for the cycle.

MATCH - This routine matches exothermic and endothermic steps for heat exchange purposes as described in the Heat Transfer section. The routine then determines the total amount of external heat required by the cycle and calculates the figures of merit.

CMATCH - This routine sets up the coefficient array used in POLY and SECANT.

SEEK - This routine checks for second law violations and sets up the function which determines the temperature of a stream at a given value of the enthalpy content.

SECANT - This routine finds the roots of the functions set up on the SEEK routine.

LOSS - This routine calculates individual reaction figures of merit and loss coefficients and sets up a summary table for the process for each temperature schedule.

PROGRAM INPUT

Program input data are divided into five categories, one of which is optional. These categories are:

- (a) Data identifying the process (TITLE card).
- (b) Data describing the products and reactants of the cycle (CHEMICAL REACTIONS cards).
- (c) Namelists data which include the temperature, pressure, equilibrium conversions of the base reactants, and options (NAMELISTS input).
- (d) Library of thermodynamic data for the compounds in the process (THERMO data).
- (e) Comments on assumptions or limitations of each chemical reaction (NOTES). This category of data is optional.

The required order of the data cards is:

- (1) Title Card
- (2) CHEMICAL REACTIONS code card
- (3) Chemical reactions cards
- (4) Blank card
- (5) NAMELISTS code card
- (6) Namelists data
- (7) Blank card
- (8) NOTES code card
- (9) Note cards
- (10) Blank card
- (11) THERMO code card
- (12) Thermo data (these cards and the preceeding code card may be omitted if the thermo data for the cycle are to be read from tape)
- (13) END code card

(14) Repeat 1-13 for each process to be analyzed in a single computer run

(15) FINI code card

The words CHEMICAL REACTION, NAMELISTS, NOTES, THERMO, END, and FINI are control codes used by the program to identify succeeding input data. The codes are punched on separate cards beginning in column 1 and precede their appropriate data cards as shown in the above listing.

Examples of input cards for several cases are given in the Sample Problems, Appendix E. Each of the five categories of input data is discussed in detail in the following sections.

Title Card

The first input data is a single card of up to 80 characters which identifies the process to be analyzed. The information on this card such as the name of the cycle and the date becomes part of the heading for the tables of output.

Chemical Reactions Data

As indicated in the order of input listing, the first card in this set is a code card containing the words CHEMICAL REACTIONS punched in columns 1 to 18 and the last card in the set is blank. In between the first and last cards are cards for each reactant and product of the chemical reactions of the cycle. A maximum of 10 chemical reactions, each containing a maximum of 5 reactants and 5 products, may be used. Table 1 gives the format and contents of these cards. The order of the cards within the set is unimportant.

The number of the chemical reaction, the use of the compound (reactant or product), the chemical formula, the stoichiometric coefficient, and the phase (solid, liquid or gas) of the compound are required information for

each reactant and product. The absolute values of the stoichiometric coefficients is not important since the program rationalizes these values so that the process is based on one mole of hydrogen produced. However, the chemical reactions must be balanced and form a cycle with no byproducts.

In addition, the cards for reactants contain the following:

(1) A code letter, 'B', is in column 41 if the compound is the 'base' reactant of the reaction. The 'base' reactant is the reactant on which the extent of reaction at equilibrium (defined as the moles of reactant reacting/mole of reactant entering reactor, epsilon) has been calculated. This may be any reactant of the reaction so long as consistency is maintained.

(2) For each chemical reaction a maximum of four sets of ratios of the reactants entering the reactor may be input. Each ratio set is composed of the respective value of the relative number of moles (L_i) input on each reactant card in columns 42 to 73. The input order of these values must be consistent with the epsilon values of the namelists.

The cards for the products of the reactions contain the basic information plus the temperatures at which any phase changes for the material occur. These are listed in ascending order and are needed only if there is a phase change when the product is heated or cooled to the temperature of the reaction in the cycle where it is used as a reactant.

Namelists Input

The first card in this set has NAMELISTS punched in columns 1 to 9 and the last card in the set is a blank card. The set of required data between these cards contains a namelist (NAM1) input for each chemical reaction. Table II lists the variables of these namelists. The following is a brief description of some of these variables.

Temperatures - Temperatures are in degrees Kelvin. Up to 10 temperatures may be input for each reaction. If more than one temperature per reaction is input, the entire analysis of the process will be repeated using the appropriate temperature for each reaction; i.e. - For Temperature Schedule 1, the first input temperature for each reaction will be used; for Temperature Schedule 2, the second temperature input for each reaction will be used; etc. All reaction namelists must contain an equal number of input temperatures even if the temperature of a particular reaction is the same in all Temperature Schedules.

One limitation on the variation of the temperature for a reaction is that all compounds of the reaction must remain in the phases specified in the Chemical Reactions input.

Pressure - Pressure is given in atmospheres.

Extent of Reaction at Equilibrium - The extent of reaction at equilibrium, epsilon, is defined as the number of moles of base reactant which reacts to produce the stoichiometric amount of products per mole of base reactant entering the reactor. Values of this variable, $EP(I,J)$, must be included for each temperature, $T(I)$, and each set of reaction ratios, $RATIO(J)$.

Efficiency of Conversion of Heat to Work - This is an optional input; the program will default to 0.3 if an efficiency is not specified.

Notes Cards

The first card of this optional set of input data has NOTES punched in columns 1 to 5 and the last card of the set is blank. The main body of this data consists of cards containing any comments the user wishes to make about the reactions. Any assumptions, possible side reactions, sources of information, and limitations of the reactions should be included on these

cards. These comments will be printed above the reactions in the first table of output. A maximum of five cards for each reaction may be used. The format of these cards is given in Table III.

Thermo Data

The library of thermodynamic data consists of the coefficients used in equations 32 to 35 for all compounds used in the cycle. The order and format of these data cards are given in Table IV. These data are in the form as output by PAC-2 (12) and used in the chemical equilibrium program CEC-72 (13).

These data may be input either from cards or from tape. During a computer run, the appropriate data for all phases (solid, liquid, and gas) of the compounds involved in the cycle are selected and stored in core. When the data are to be read from cards, only the data for the compounds used in the cycle being run are included. The tape includes all compounds for which data are available.

If the data are to be read from cards, the first card contains the word THERMO in columns 1 to 6 followed by the cards listed in Table IV. If no THERMO code card is included, the program assumes that the data are contained on tape (unit 4). Therefore, if more than one cycle is to be analyzed in a single run, the THERMO data for each cycle must either be input on cards or be contained on tape.

PROGRAM OUTPUT

The program output consists of the input data cards and tables of results. The input data are listed as they are read into the program. Only the thermodynamic data pertinent to the cycle in question are listed from the data bank.

Chemical Reactions

Table I of the output is an analysis of the chemical reaction steps in the cycle. The title of the cycle, the temperature schedule, and a list of the chemical reactions are at the top of this first table. The main body of the table consists of the following for each chemical reaction:

- (1) The step number and isothermal temperature of the reaction in degrees Kelvin
- (2) The chemical reaction
- (3) The values of ΔH° , ΔS° , ΔG°
- (4) The material which is the base reactant
- (5) Results of the work of separation calculations. These include:
 - (a) In the first column is the equilibrium value of the fraction converted of the base reactant entering the reactor (ϵ)
 - (b) The second column lists the reactants
 - (c) In column three are the relative number of moles of each reactant entering the reactor (L_i)
 - (d) Within the outlined box are twelve columns. The first six contain the moles of recycle for each reactant at various degrees of the equilibrium conversion and the last six columns are values of the work of separation of gases for these respective degrees of conversion

Material Transfer Steps

Table II of the output is a listing of the thermodynamic changes for the material transfer steps of the cycle. Each entry contains:

- (1) The step number and the initial and final temperatures of the material
- (2) The material being transferred

(3) The origin of the material and its destination.

(4) ΔH° , ΔS° , ΔG° for the step

There will be a separate set of Tables I and II for each temperature schedule being run.

The next set of tables contain a summary of the enthalpy changes for all steps in the cycle. These tables contain the step number, the temperatures of the reactants and products, and the enthalpy change for the step entered in either the exothermic or endothermic column depending on the sign of the enthalpy change.

Heat Transfer Output

Internal heat exchange is described in a set of two tables for each temperature schedule. The first table of output of this set describes the conditions for each heat exchange match.

Column one of this table gives the amount of heat to be exchanged between the two steps; and if there is a possible second law violation, this value is preceded by a 'W'. The remainder of the table is divided into two parts, one describing the stream supplying the heat and the other the stream absorbing the heat. In each part, the step number, the temperature change of the step needed to accomplish the heat exchange, and the total enthalpy changes the step must make before and after the heat exchange are given.

The second table for the heat exchanges is a summary of the enthalpy change which each step must still make after all possible internal heat matches have been made.

Figures of Merit

The next table of output gives the total work required, the work generated, and the figures of merit for the cycle at each temperature

schedule. The note at the end of this table contains the assumptions made in the calculation of these values.

Chemical Reactions at 298 K

If the H298 option is used, a table of output will be essentially a duplicate of Table I except that all the reactions will be at 298 K and no work of separation will be calculated.

Process Summary

The last table (one for each temperature schedule) gives a summary of significant information on the process including the individual figures of merit and loss coefficients.

ARRAY SIZES

The HYDRGN program can handle up to:

- (1) 10 chemical reactions with a maximum of 5 reactants and 5 products each.
- (2) 40 material transfer steps (heating, cooling and phase changes of materials). This automatically limits (1). i.e., if the maximum number of reactions and materials are used in (1), there must be a minimum of 50 recycle steps which are limited to 40.
- (3) Four sets of reactant ratios (L_i 's) per reaction.
- (4) Four different atoms per compound.
- (5) Ten different temperature cycles per process.
- (6) Five comments (Notes) per chemical reaction.
- (7) Fifty different compounds per process including all phases of each compound found in the data bank. For example, if there are three phases per compound in the data bank; only sixteen different compounds may be used in the process.

PROGRAM MESSAGES

Warnings

1. "FOR TEMP. SCHEDULE _____, AND REACTION _____, THE TEMP IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR _____"; MAIN Program statement 120.

The temperature of the reaction is more than 10 deg. outside the range of the data on which the thermodynamic coefficients were based.

2. "THE TOTAL NUMBER OF PRODUCTS IN EACH PHASE DO NOT SUM TO THE NUMBER OF PRODUCTS IN REACTION _____, CHECK 960 LOOP ON MAIN"; MAIN program, statement 940.

The sum of the number of products in each of the three phases do not sum to the total number of products for this reaction. Test 1 is set equal to false and no work of separation is calculated for the reaction.

3. "THE SUM OF ALL THE REACTANTS IN REACTION _____ DO NOT EQUAL THE NUMBER OF REACTANTS, CHECK THE 960 DO LOOP IN MAIN". MAIN program, statement 980. Same as for warning 2 except as regards to the reactants instead of the products.

4. "IN REACTION _____ THE MATERIAL _____ HAS NOT BEEN EXACTLY MATCHED FOR ITS PHASE AT 298 K"; FZ298 routine, statement 100; In trying to find the phase of the indicated material at room temp., the lowest temp., range of any phase is above 300 K.

5. " *** WARNING *** THE DIFFERENCE IN EXOTHERMIC AND ENDOTHERMIC HEATS REMAINING ARE IN ERROR. CHECK HEAT MATCHING TABLE CAREFULLY"; MATCH routine, statement 1320. The difference between the exothermic and endothermic heats after heat matching is not equal to 86.3 kcal. This denotes an error in the heat matching and the table of heat exchange steps should be checked carefully.

Errors

For the following errors, TEST 20 = . TRUE. and the program terminates the cycle in question and proceeds to the next cycle to be run.

1. "THE LAST CARD HAS AN UNRECOGNIZABLE CODE"; READIN routine, statement 140; The program is trying to read a "Code" card which indicates the type of input cards which are to follow and the code in columns 1-4 is not one of the following: END; NOTE; CHEM; NAME; THER.
2. "CODE FOR THIS CARD IS IN ERROR"; READIN subroutine statement 300; The program is trying to read the data cards for the chemical reactions and has not recognized the card as a blank card, a product card, or a reactant card.

3. "ERROR IN NUMBER OF TEMPERATURES FOR STEP _____"; READIN sub-routine, statement 660; The program is reading the namelists and has found the number of temperature schedules for the indicated step to be in disagreement with the number found in the first namelist.
4. "DATA CARDS ARE OUT OF ORDER, NAMELISTS MUST BE AFTER REACTION CARDS"; READIN routine, statement 740; The program has encountered a namelist card before the data for the chemical reactions have been read. (Put namelists after Chemical Reaction Cards).
5. "THE ELEMENT _____ IS IN THE PRODUCTS OF REACTION _____ BUT IS NOT IN THE REACTANTS"; READIN routine, statement 880; check to be sure that this element is balanced in this reaction.
6. "REACTION _____ IS NOT BALANCED IN REGARD TO THE ELEMENT _____"; READIN routine, statement 940; see error 5.
7. "FOR REACTION _____ THE FOLLOWING REACTANT HAS NOT BEEN MATCHED TO THE DATA FOR THE SPECIES FOUND ON TAPE 4 _____"; DATAS routine, statement 680; see error 7.
8. "FOR REACTION _____ THE FOLLOWING PRODUCT HAS NOT BEEN MATCHED TO THE DATA FOR THE SPECIES FOUND ON TAPE 4 _____"; DATAS routine, statement 840, see error 7.
9. "IN REACTION _____, _____ HAS NOT BEEN MATCHED"; ROUTE routine, statement 820; The cycle is not balanced so that there are no by-products or extra reactants.
10. "ERROR IN COEFFICIENTS FOR ONE OF THE COMPONENTS IN REACTION _____"; CPHSG routine, statement 40; the a_j Thermodynamic Coefficient is zero. Check the temp. ranges for the materials in the indicated reaction.
11. "PHASE OF A COMPONENT HAS BEEN INCORRECTLY READ IN SUBROUTINE REMOVE"; REMOVE routine, statement 800; The program is seeing a phase other than S, L, or G.
12. "ERROR *** I HAS A NEGATIVE VALUE IN SEEK SUBROUTINE"; SEEK routine, statement 200; check value of first item in list of input to SEEK as called from MATCH.
13. "**** ERROR *** THE MOLE FRACTION OF ONE OF THE REACTANTS IN THE FINAL REACTION MIXTURE IS NEGATIVE FOR RATIO SET _____. CHECK THE EPSILON FOR THIS SET OF RATIOS"; REMOVE routine, statement 40; either the epsilon for this ratio set is too high or the base reactant has been incorrectly specified causing more than the stoichiometric amount of one of the reactants to be reacted.

DETERMINATION OF EXTENT OF REACTION

For the Reaction:

- Z_i = moles of Reactant i initially present
- r_i = Stoic Coeff. of Reactant i
- p_i = Stoic Coeff. of Product i
- ϵ^* = extent of Reaction at equilibrium
(moles of R_1 reacted/moles of R_1 initially present)
- x_{R_i} = mole fraction of Reactant i in equilibrium mixture
- n_{R_i} = no. of moles of Reactant i in final mixture
- n_{P_i} = no. of moles of Product i in final mixture

Then, assuming no moles of Product present initially:

$$(43) \quad x_{R_1} = \frac{n_{R_1}}{\sum n_{R_i} + \sum n_{P_i}}$$

$$(44) \quad n_{R_1} = Z_1 - \epsilon^* Z_1 = Z_1 (1 - \epsilon^*)$$

$$(45) \quad n_{R_i} = Z_i - \frac{r_i}{r_1} \epsilon^* Z_1$$

$$(46) \quad n_{P_i} = \frac{p_i}{r_1} \epsilon^* Z_1$$

Therefore:

$$(47) \quad x_{R_1} = \frac{Z_1 (1 - \epsilon^*)}{\sum (Z_i - \frac{r_i}{r_1} \epsilon^* Z_1) + \sum (\frac{p_i}{r_1} \epsilon^* Z_1)}$$

$$(48) \quad x_{R_1} = \frac{Z_1 (1 - \epsilon^*)}{\sum Z_i - \frac{\epsilon^*}{r_1} Z_1 \sum r_i + \frac{\epsilon^* Z_1}{r_1} \sum p_i}$$

$$(49) \quad Z_1 (1 - \epsilon^*) = x_{R_1} \left(\sum Z_i + \frac{\epsilon^* Z_1}{r_1} (\sum p_i - \sum r_i) \right)$$

$$(50) \quad \epsilon^* \left(Z_1 + \frac{Z_1 x_{R_1}}{r_1} (\sum p_i - \sum r_i) \right) = Z_1 - x_{R_1} \sum Z_i$$

$$(51) \quad \epsilon^* = \frac{\frac{r_1}{Z_1} (Z_1 - x_{R_1} \sum Z_i)}{(r_1 + x_{R_1} (\sum p_i - \sum r_i))}$$

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A P P E N D I X E S

APPENDIX A

Symbols

a_i ($i = 1,7$)	-	least squares coefficients (eqs. 32-35).
G	-	Gibbs Free Energy
H	-	Enthalpy
L_i	-	relative number of moles of species i in reactor mixture
n_i	-	number of moles of species i
P	-	Pressure
P_i	-	i^{th} product
p_i	-	stoichiometric coefficient of the i^{th} product
Q	-	heat (positive if added to the process)
Q^*	-	sum of the heat to the endothermic steps which must be supplied by an external source.
R	-	Gas Constant
R_i	-	i^{th} Reactant
r_i	-	Stoichiometric coefficient of the i^{th} Reactant
S	-	Entropy
T	-	Absolute temperature
t_A	-	Temp. of endothermic stream in heat exchanger
t_B	-	Temp. of exothermic stream in heat exchanger
W	-	Useful work (positive if done by the system)
W_{gen}	-	Work generated by the process from the heat of unmatched exothermic steps.
X_i	-	mole fraction of species i
ϵ	-	number of moles of component R_1 reacting per mole of R_1 entering reactor
η_1	-	First estimate of the figure of merit
η_2	-	Second estimate of the figure of merit

Subscripts

A - Endothermic

B - Exothermic

M - Mixer

R - Reactor

S - Separator

T - Total

Superscript

⁰ - Standard state

APPENDIX B

<u>Variables</u>					
<u>Variable</u>	<u>Type</u>	<u>Common Label</u>	<u>Dimensions</u>	<u>Routines where used</u>	<u>Description</u>
A		----	1	DATAS	A = 4 if THERMO Date is to be read from tape and A = 5 if from cards.
AFACT	real	IND1	1	MAIN CPHSG	Stoichiometric coefficient. (+ if a product; - if a reactant).
APROD	real	MATL3	10, 5	READIN EQNS REMOVE MAIN	Stoichiometric coefficients of products in chemical reaction steps.
AREACT	real	MATL3	10,5	READIN EQNS REMOVE MAIN	Stoichiometric coefficients of reactants in chemical reaction steps.
B	real (double precision)	----	2,6	SEEK	Temporary storage for thermo. coefficients, a_i .
BASE	integer	INDX	10	READIN MAIN REMOVE	Index number of reactant which is base reactant.
BLANK	real	----	1	READIN DATAS	Littoral blank.

C	double precision real	----	2,7	SECANT MATCH CMATCH SEEK POLY	Temporary storage for thermodynamic coefficients used to calculate enthalpy.
CARD	integer	----	1	READIN	Index number of comment cards for reaction.
CARNOT	real	----	1	MATCH	
C1MAX	real	----	1	MATCH	Maximum first estimate of figure of merit.
C2MAX	real	----	1	MATCH	Maximum second estimate of figure of merit.
C1MIN	real	----	1	MATCH	Minimum first estimate of figure of merit.
C2MIN	real	----	1	MATCH	Minimum second estimate of figure of merit.
CNAME	real	----	1	READIN	Alphameric letters 'NAME' indicates beginning of namelists.
COEF	real (double precision)	DOUBLE	2,7,50	TFIND DATAS CPHSG MATCH CMATCH SEEK	Thermodynamic coefficients, a_j , for compounds found on tape unit 4.
COLOS	real	----	10,10	LOSS	Individual loss coefficients

COMM	real	----	1	READIN	Alphameric letters 'NOTE' indicates beginning of comment cards for chemical reactions.
CONST1, CONST2	real	----	1	SEEK	Values of the enthalpy at the cold end of the counter-current heat exchanger. Used to check second law violations.
D	real	----	4	DATAS	Atomic coefficients of compounds in thermodynamic data list.
DAT	real	----	13	READIN DATAS	Temporary storage.
DATE1, DATE2	real	----	1	DATAS	Alphameric data indicating the reference source for thermodynamic data.
DD	real	----	1	DATAS	Alphameric character 'D'.
DRAW	logical	LOGIC	1	MAIN READIN	DRAW = T, means that recycle steps are to be set up in ROUTE routine.
DUMH	real (double precision)	----	6	MAIN	Dummy variable.
EE	real	----	1	DATAS	Alphameric character 'E'.
EFEL	real	WORK	1	MATCH LOSS READIN	Efficiency for heat to work for the heat source heat.

EI	real	----	1	REMOVE	Fractional part of the value of epsilon at equilibrium. Varies from 1.0 to 0.5.
EP	real	----	10,4	READIN	Equilibrium value of epsilon in namelist NAM1. First index refers to Temp. schedule and second index to the reactant ratio.
EPSI	real	WORK	10,10,4	READIN REMOVE LOSS	Equilibrium value of epsilon.
FAZEP	real	FZE	11,5	MAIN READIN DATAS REMOVE	Alphameric letter (S, L, G) indicating phase of product of a chemical reaction.
FAZER	real	FZE	11,5	MAIN READIN DATAS REMOVE	Alphameric letter (S, L, G) indicating phase of reactant of a chemical reaction.
FF	real	----	10,10	LOSS	Weighting factors for stage efficiency
FMERIT	real	----	10,10	LOSS	Individual stage efficiency
FMT	real	----	130	EQNS	Temporary storage of chemical reaction equation in alphameric form for output purposes.
FR	real	----	1	REMOVE	Increment by which the extent of reaction epsilon is varied for calculation of work of separation

FRMOL	real	----	10	REMOVE	Mole fraction in gas phase of gaseous reactants when there are no gaseous products.
FUNT	real	----	1	MATCH	Value of the enthalpy of a material for which the temperature of the material at this enthalpy is sought. See HHET.
G	real (double precision)	----	1	TFIND CPHSG	Gibbs free energy of a compound.
GAS	real	----	1	CPHSG TFIND DATAS ROUTE MAIN REMOVE FZ298	Alphameric letter 'G' indicating the material is a gas.
GASSUM	real (double precision)	----	1	REMOVE	Total number of moles of all gases in a reaction which enter the separator.
GO	real	----	11	MAIN	Storage array.
GPRIME	real	----	1	TFIND	Derivative used in finding the transition temperatures.
GS	real (double precision)	DOUBLE	50,10	MAIN CPHSG REMOVE	Gibbs free energy change of a step.
GTOT	real (double precision)	----	10	MAIN	Total Gibbs free energy change for a cycle.
H	real (double precision)	----	1	CPHSG	Enthalpy of a compound.

H298	logical	LOGIC	1	MAIN READIN	If H298 = T, the thermo- dynamic properties of the chemical reactions are to be calculated at 298 K.
HAM	real	WORK	10	MAIN REMOVE MATCH	Maximum total work needed for the cycle at each temperature schedule.
HB HB1 HB2	real	----	1	MATCH	Enthalpy change of a non-chemical reaction step.
HBF HBF1 HBF2	real	----	1	MATCH	Final enthalpy of a non-chemical reaction step.
HBI HBI1 HBI2	real	----	1	MATCH	Initial enthalpy of a non-chemical reaction step.
HEAT	real	----	1	MATCH	Amount of heat which is exchanged between two steps in the cycle.
HEATR HEATR2	real	----	1	MATCH	Temporary storage for the amount of heat remaining in the exothermic and endothermic stream respectively.
HEND01 HEND02	real	----	1	MAIN	Temporary storage for total endothermic heat of the cycle, used only for printout.
HHET	real	----	1	SEEK POLY SECANT	The enthalpy of a material for which the corresponding temperature is to be found.

HIM	real	WORK	10	MAIN REMOVE MATCH LOSS	Minimum total work needed for a cycle for each temperature schedule.
HO	real	WGMIN	11	LOSS MAIN	Storage array.
HOT	real	----	1	SEEK	Same as HHET.
HS	real (double precision)	DOUBLE	50,10	MAIN CPHSG MATCH LOSS	Enthalpy change for a step.
HSEX01 HSEX02	real	----	1	MAIN	Total exothermic heats of two temperature schedules in the cycle. Used for printout purposes only.
HSG298	logical	----	1	MAIN	Logical variable which is always false in the first pass thru MAIN. It is redefined as True, if H298 is True, for control purposes during the second pass through Main.
HSII	real	----	1	MATCH	Same as HB.
HSSG	real	----	10	MATCH	Total exothermic heat which cannot be exchanged within the cycle.
HSSL	real	----	10	MATCH	Total endothermic heat which must be supplied to the cycle from outside sources.

HST	real	WGMIN	10,10	LOSS MAIN	Heat of the reaction at Temperature T.
HSTOCP	real	MATL3	50	MAIN ROUTE MATCH	Stoichiometric coefficient of the product in a heating or cooling step.
HSTOCR	real	MATL3	50	MAIN ROUTE MATCH	Stoichiometric coefficient of the reactant in a heating or cooling step.
HTOT	real (double precision)	DOUBLE	10	MAIN MATCH	Total enthalpy change for a cycle (should be about 68.3 kcal).
HYD	real	----	1	READIN DATAS	Alphameric character 'H'.
IBASE	integer	----	1	REMOVE	The reactant number of the base reactant.
IFLAG	integer	----	1	MATCH SEEK	IFLAG = 1, indicates there is a possible second law violation when two streams are matched for heat exchange.
IRoute	integer	MATL2	50,2	MAIN ROUTE LOSS	Used only for heating and cooling steps. IRoute (J, 1 & 2) are the numbers of the steps for which step J is the interlinking step in the cycle.
JSTG	integer	----	11	LOSS	Array to determine number of summary table.

K	integer	INDX	1	MAIN CPHSG REMOVE LOSS	Index denoting the number of the temperature schedule.
KEYNOP	integer	MATL2	11,5	MAIN DATAS REMOVE ROUTE EQNS FZ298	The index number of the species found in the thermo- dynamic data which matches the product in a chemical reaction.
KEYNOR	integer	MATL2	11,5	MAIN DATAS ROUTE EQNS REMOVE FZ298	Same as above except for reactants.
KK	integer	----	1	READIN	Number of the reactant for a chemical reaction.
KYNP	integer	MATL2	50	MAIN ROUTE MATCH	The index number of the species found in the thermodynamic data which matches the product of a heating or cooling step.
KYNR	integer	MATL2	50	MAIN ROUTE MATCH	Same as above for the reactant.
L	integer	----	1	ROUTE	Indicates whether the step is a heating or a cooling step.

LCN	integer	----	1	ROUTE	If LCN = 1, the stoichiometric coefficient as well as the materials are matched. If LCN = 2, the material may be divided among several steps.
LIQUID	real	----	1	DATAS FZ298	Alphameric character 'L'.
LL	integer	----	1	MAIN ROUTE	Value of LNOTE.
LNOTE	integer	MATL3	10	MAIN READIN	The number of comment cards read for each chemical reaction.
MM	integer	----	1	DATAS MATCH	Number of different solid phases of a compound. Number of temperatures in a cycle which are greater than the TLEVEL(J) in question. Used to arrange the temperature levels of the cycle in ascending order.
MT	real	----	4	DATAS	Atomic symbols read from thermo data cards. See Table IV.
MTLO	integer	----	1	DATAS	Species index number of the solid phase of a compound with the lowest temperature range.
MTUP	integer	----	1	DATAS	Species index number of the solid phase of a compound with the highest temperature range.

NARE	integer	----	1	MAIN	Integer value of AREACT or APRD used to determine the number of spaces needed for the stoichiometric coefficient in printing the chemical equation.
NB	integer	----	1	MAIN	Value of BASE(I); the number of the base reactant for the reaction.
NCOUNT	integer	----	1	DATAS	Number of blanks in the twelve spaces reserved for the species name.
NGASP	integer	FZE	1	REMOVE MAIN	Number of gaseous products in a reaction.
NGASR	integer	FZE	1	MAIN REMOVE	Number of gaseous reactants in a reaction.
NIR	integer	----	1	MAIN	Number of spaces allotted for printing stoichiometric coefficients in chemical equations.
NJ	integer	----	1	ROUTE	Species number (KEYNOP) of the product to be heated or cooled.
NJJ	integer	----	1	ROUTE	Species number (KEYNOR) of the reactant which corresponds to NJ.
NLEVEL	integer	----	1	MATCH	Number of temperature levels in the cycle for heat matching routine.

NLIQP	integer	FZE	1	MAIN	Number of liquid products in reaction.
NLIQR	integer	FZE	1	MAIN	Number of liquid reactants in reaction.
NOTE	real	MATL3	10,100	MAIN	Comments on each chemical reaction.
NOTEMP	integer	INDX	1	MAIN READIN ROUTE MATCH LOSS	Number of temperature schedules to be run per cycle.
NPROD	integer	MATL3	11	MAIN FZ298 READIN DATAS ROUTE EQNS REMOVE	Number of products per chemical reaction.
NR	integer	INDX	1	MAIN READIN DATAS ROUTE FZ298 MATCH LOSS	Number of chemical reactions per cycle.
NR1	integer	INDX	1	MAIN DATAS ROUTE MATCH LOSS	Number of chemical reactions per cycle +1.
NRATIO	integer	MATL3	10	READIN REMOVE	Number of reactant ratio sets per chemical reaction. Maximum value is 4.

NREACT	integer	MATL3	11	MAIN FZ298 READIN DATAS ROUTE EQNS REMOVE	Number of reactants in a chemical reaction.
NRXNS	integer	INDX	1	MAIN READIN DATAS ROUTE MATCH LOSS	Total number of steps in a cycle. (Chemical reactions + heating and cooling steps + phase changes).
NSATOM	integer	INDX	50	MAIN DATAS EQNS LOSS	Number of characters in the name of a compound.
NSOLP	integer	FZE	1	MAIN	Number of solid products in a reaction.
NSOLR	integer	FZE	1	MAIN	Number of solid reactants in a reaction.
NSPEC	integer	----	1	DATAS	Number of compounds, including all phases of a single compound, to be considered for a single cycle.
NSUB	integer	----	1	MAIN	Total number of spaces needed to print out one of the chemical reactions.
NTOT	integer	INDX	1	MAIN EQNS	Number of spaces to be skipped before printing out chemical reactions.

NUM	integer	----	8	EQNS	Temporary storage in integer form of each digit in the stoichiometric coefficient of the compound to be printed in a chemical reaction.
OXY	real	----	1	DATAS	Alphameric character 'O'.
P	real	PRESS	50,10,2	CPHSG READIN ROUTE REMOVE FZ298	Pressure of a step in atmospheres.
PATCO	real	FNAME	11,5,4	READIN DATAS	Atomic coefficients for the products of a chemical reaction.
PATOM	real	FNAME	11,5,4	READIN DATAS	Atomic symbols for the products of a chemical reaction.
PEQ	real	----	10,10	REMOVE	Equilibrium pressure of the chemical reaction.
PERW	real	----	10,10	LOSS	Percentage of total work for each step.
PLIQ	real	----	1	MAIN	Alphameric character 'L'.
PRES	real	----	1	READIN	Namelist name for the pressure of the reaction in atmospheres.
PRO	real	----	1	READIN	Alphameric word 'PROD'.
PTRAN	real	----	1	TFIND ROUTE	Pressure at which a phase change occurs.

Q	real	----	10	LOSS	Total endothermic heat required externally.
QOUT	real	----	10	LOSS	Total exothermic heat not used internally.
QS	real	----	10,10	LOSS	Heat necessary to generate the net work at 50% separation efficiency and the input value of efficiency of heat to work.
QST	real	----	10	LOSS	Total heat necessary to generate the net work.
QTOT	real	----	10,10	LOSS	Total endothermic heat plus heat needed to produce work.
R	real	INDX	1	MAIN TFIND CPHSG REMOVE CMATCH	Gas constant = 1.987165.
RATCO	real	FNAME	11,5,4	READIN DATAS	Atomic coefficients for the reactants in a chemical reaction.
RATIO	real	MATL3	10,5,4	READIN REMOVE	Relative number of moles of reactant entering reactor.
RATOM	real	FNAME	11,5,4	READIN DATAS	Atomic symbols of reactant.
REAC	real	----	1	READIN	Alphameric word 'REAC'.
RMOLES	real	----	10,4,10,6	REMOVE	Moles of each gaseous reactant in mixture leaving reactor.

ROOT ROOT1 ROOT2	real	----	1	MATCH SECANT SEEK	Temperature found in SEEK for a known value of the enthalpy.
S	real (double precision)	----	1	CPHSG	Value of entropy for a material.
SAME	logical	LOGIC	1	MAIN READIN	If true, the thermo data from tape 4 is the same as for previous cycle and it is not necessary to read tape 4 again.
SO	real	----	11	MAIN	Storage array.
SOL SOLID	real	----	1	MAIN FZ298 DATAS	Alphameric character 'S'.
SPATCO	real	MATL1	50,4	DATAS ROUTE FZ298	Atomic coefficients for the species necessary for the cycle.
SPATOM	real	MATL1	50,4	DATAS ROUTE FZ298	Atomic symbols of the necessary species of the cycle.
SPEC	real	MATL1	50,12	MAIN DATAS ROUTE EQNS REMOVE	Formula name of the specie.
SPFAZE	real	MATL1	50	DATAS CPHSG TFIND ROUTE FZ298	Phase of a species (S, L, or G).

SS	real (double precision)	DOUBLE	50,10	MAIN CPHSG TFIND	Entropy change for a step in the cycle.
STOICP	real	FNAME	11,5	READIN DATAS ROUTE	Stoichiometric coefficients of the products of a chemical reaction step.
STOICR	real	FNAME	11,5	READIN DATAS ROUTE	Stoichiometric coefficients of the reactants of a chemical reaction step.
STOT	real (double precision)	----	10	MAIN	Entropy change for entire cycle.
SUMPG	real (double precision)	FZE	1	MAIN REMOVE	Total moles of gaseous products entering separator.
SUMPL	real (double precision)	FZE	1	MAIN	Total moles of liquid products entering separator.
SUMPS	real	FZE	1	MAIN	Total moles of solid products entering separator.
SUMRG	real (double precision)	----	1	REMOVE	Total moles of gaseous reactants entering separator.
SUMRL	real (double precision)	----	1	REMOVE	Total moles of liquid reactants entering separator.
SUMRS	real	----	1	REMOVE	Total moles of solid reactants entering separator.
SUMW	real (double precision)	----	1	REMOVE	Total moles of gaseous reactants in separator times ln (mole fraction of gaseous reactants).
T	real	----	20	READIN	Namelist, NAM1, name of temperatures of chemical reaction. Also used for the number of atoms of the elements in checking to see if the chemical reaction is balanced.

T1,T2	real	----	1	DATAS	Temporary storage.
T	real	----	2,2	MATCH SEEK	Inlet and outlet temperatures of the heating and cooling streams being matched for heat transfer.
TAB	real	----	1	READIN	Absolute value of T in READIN.
T1T, T2T	real	----	1	MAIN	Temperature range of the thermodynamic data $\pm 10^\circ\text{K}$. Used to check if the reaction is being run outside this range.
TCOLOS	real	----	10	LOSS	Loss coefficient of cycle.
TEMP1, TEMP2	real	TMP	50,10	MAIN READIN DATAS ROUTE CPHSG REMOVE FZ298 MATCH LOSS	Initial and final temperatures of a step in the process, TEMP1 is the temperature of the products of the step and TEMP2 is the temperature of reactants.
TEST1	logical	LOGIC	10	MAIN READIN	TEST1(I) = TRUE, indicates that the work of separation is to be calculated for Step I.
TEST3	logical	----	1	REMOVE	TEST3 = TRUE, indicates that the moles of recycle for one of the reactants is greater than 1000. Used to control printout format.

TEST15	logical	----	1	READIN	TEST15 = TRUE, indicates the reactant and product cards have been read and allows the reading of the namelists.
TEST20	logical	LOGIC	1	MAIN READIN DATAS ROUTE CPHSG	TEST20 = TRUE, indicates a serious error has been encountered and computation for the cycle is to be terminated and the next cycle read.
TGUESS			1	ROUTE TFIND	Estimate of temperature for finding temperature of phase change.
THER	real	----	1	READIN	Alphameric 'THER'.
THERM	logical	LOGIC	1	READIN DATAS	THERM = TRUE, indicates that the thermo data is to be read from cards.
THIGH	real	----	1	DATAS	Highest possible temperature of the thermo data (5000K).
TITLE	real	MISC	20	MAIN MATCH LOSS	Alphameric name of the cycle being evaluated.
TLEVEL	real	----	30	MATCH	Temperature levels of cycle arranged in ascending order for use in heat matching routine. TLEVEL (1) = 298.15K.
TLN	real	IND1	1	MAIN CPHSG	Natural logarithm of TT; used to calculate thermo-dynamic properties.

TLOW	real	----	1	DATAS	Lowest temperature in temperature range of species in the thermo data. (300K).
TMAX	real	----	1	MATCH	Maximum temperature of the steps in a process for one temperature schedule.
TMERIT	real	----	10	LOSS	Cycle figure of merit.
TMID	real	TMP	1	DATAS CPHSG	Common temperature of the two temperature ranges of the THERMO data. (usually 1000K).
TNEXT	real	----	1	MATCH	The next highest temperature in the cycle greater than TLEVEL(J). Used to arrange the TLEVEL(J) in ascending order.
TOTMOL	real	----	10,10	REMOVE	Moles of all species.
TPHASE	real	TMP	11,5,4	READIN DATAS	Temperatures of phase changes of a product. Used to set up heating and cooling steps of the cycle so that the phase changes occur at constant temp.
TQTOT	real	----	10	LOSS	Total external heat needed by cycle.
TRANGE	real	TMP	2,50	MAIN DATAS FZ298 ROUTE	Temperature range of the original thermodynamic data taken from the literature.

TRY	real	----	1	READIN	Total number of moles of H_2 gas produced by the cycle as written. Used to normalize the stoichiometric coefficients.
TRY	real	----	1	MATCH	Difference between total exothermic and endothermic heats for the cycle after heat matching. (Should equal 68.3 kcal).
TT	real	IND1	1	MAIN CPHSG MATCH	Temporary storage of the value of temperature.
WEND	real	----	1	READIN	Alphameric word 'END'.
WG	real	WLOS	50,10	LOSS MATCH	The work generated internally.
WGMAX	real	----	10,10	REMOVE	Maximum amount of work of separation for each chemical reaction at each temperature.
WGMAX1	real	----	4	REMOVE	Maximum work of separation for a reaction for each ratio set.
WGMIN	real	DTABLE	10,10	MAIN REMOVE LOSS	Same as WGMAX except for minimum value.
WGMIN1	real	----	4	REMOVE	Same as WGMAX1 except for minimum value.
WILDP	real	----	50	MATCH	Original values of HSTOCP before heat matching.

WILDR	real	----	50	MATCH	Original values of HSTOCR before heat matching.
WOMAX	real	----	1	MATCH	Maximum heat requirement to provide the necessary work, HAM, for the cycle at a particular temperature schedule.
WOMIN	real	----	1	MATCH	Minimum heat requirement to provide the necessary work, HIM, for the cycle at a particular temperature schedule.
WORKC	real	----	10	REMOVE	Work requirement for a chemical reaction when there is either a single gaseous product and no gaseous reactants or there are gaseous reactants but no gaseous products.
WORKG	real	----	10,6,4	REMOVE	Works of separation of a chemical reaction for 4 ratios of reactants and 6 fractions of the equilibrium conversion.
WTFAC	real	----	10,10	LOSS	Individual weighing factor.
WTGEN	real	----	10	LOSS	Total work generated internally.
X	real	----		POLY	Temperature at which the value of the enthalpy is to be calculated by the POLY subroutine.

X1,X2	real	----	1	SECANT	Iterative values of the temperature being sought by the SECANT routine for a known value of the enthalpy.
X	real	----	50	MATCH	Moles of material in heating or cooling streams. (Same as XMOLES).
X	real	----	2	SEEK SECANT	Temperature limits of the interval in which the temperature at a known value of the enthalpy is to be found by the SECANT routine.
XCR	real	----	1	SEEK MATCH	Incremental values of the enthalpy change at which Second Law violations are checked.
XMOLES	real	----	50	SEEK MATCH	Moles of material in heating and cooling streams being matched for heat exchange.
XPROD	real (double precision)	----	10	REMOVE	Mole fraction of gaseous products in separator mixture.
XREACT	real (double precision)	----	1	REMOVE	Mole fraction of the gaseous reactants, considered as a single component, in the separator.
XT1,XT2	real	----	1	SEEK	Temperatures of the heating and cooling streams at corresponding points along the counter-current heat exchanger. If XT1 is less than 5 degrees larger than XT2, a Second Law violation is considered to be possible.

Y	real	----	2	SEEK	End point temperatures of the stream being cooled.
Z	real	----	1	POLY	Enthalpy value at a single temperature.
ZERO, ZER01, ZER02	real	----	1	DATAS	Alphameric character '0'.

APPENDIX C
Flow Chart of MAIN

APPENDIX D
HYDRGN Program

DOUBLE PRECISION SUMPG,SUMRG,SUML,SUMRL	MAIN	5
INTEGER CARD,STEP,BASE	MAIN	10
REAL NOTE	MAIN	15
LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298,HSG298	MAIN	20
DOUBLE PRECISION DUMH(6)	MAIN	25
DIMENSION SU(11),GO(11)	MAIN	30
DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF	MAIN	35
DIMENSION BASE(10),NSATOM(50),SPEC(50,12),KEYNOR(11,5),KEYNOP(11,5)	MAIN	40
1),KYNR(50),KYNP(50),IROUTE(50,2),TEMP1(50,10),TEMP2(50,10),TRANGE(	MAIN	45
22,50),TPHASE(11,5,4),HS(50,10),SS(50,10),GS(50,10),HTOT(10),	MAIN	50
3COEF(2,7,50),TEST1(10),AREACT(10,5),APROD(10,5),NPROD(11),NREACT(1	MAIN	55
41),NRATIO(10),RATIO(10,5,4),LNOTE(10),NOTE(10,100),HSTOCR(50),	MAIN	60
SHSTOCP(50),FAZER(11,5),FAZEP(11,5),HIM(10),HAM(10),EPSI(10,10,4)	MAIN	65
DIMENSION SPATCH(50,4),SPATCO(50,4),SPFAZE(50)	MAIN	70
DIMENSION STOT(10),GTOT(10)	MAIN	75
COMMON/MISC/TITLE(20)	MAIN	80
COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN	MAIN	85
COMMON/IND1/AFAC,TI,TLN	MAIN	90
COMMON/MATL1/SPEC,SPATOM,SPATCO,SPFAZE	MAIN	95
COMMON/MATL2/KEYNOR,KEYNOP,KYNR,KYNP,IROUTE	MAIN	100
COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TM1D	MAIN	105
COMMON/DOUBLE/HS,SS,GS,HTOT,COEF	MAIN	110
COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298	MAIN	115
COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,	MAIN	120
INRATIO,LNOTE	MAIN	125
COMMON/FZE/SUML,SUMPG,SUMPS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR,	MAIN	130
INLIQR,NSOLR	MAIN	135
COMMON/WORK/HIM,HAM,EPSI,EFEL	MAIN	140
COMMON/PRESS/P(50,10,2)	MAIN	145
COMMON/DTABLE/HGMIN(10,10),HST(10,10),HO(11)	MAIN	150
DATA GAS/1HG/,PLIQ/1HL/,SOL/1HS/,FINI/4HFINI/	MAIN	155
DATA PSOLID/1HS/	MAIN	160
*****	MAIN	165
C FOR EACH CYCLE TO BE PRECESSED, THE MAIN PROGRAM:	MAIN	170
C 1. READS A TITLE CARD FOR THE PROCESS	MAIN	175
C (IT IS HELPFUL TO INCLUDE THE DATE)	MAIN	180
C 2. CALLS THE SUBROUTINE READIN TO READ AND PROCESS THE CARDS	MAIN	185
C DESCRIBING THE PROCESS.	MAIN	190
C 3. CALLS THE SUBROUTINE DATAS WHICH READS THE THERMODYNAMIC	MAIN	195
C DATA FROM EITHER CARDS OR THE DATA FILE ON TAPE UNIT 4	MAIN	200
C WHICH IS ALSO USED FOR THE CEC-72 PROGRAM.	MAIN	205
C 4. IF THE HEATING AND COOLING STEPS ARE TO BE DETERMINED	MAIN	210
C (DRAW=.TRUE.), THE SUBROUTINE ROUTE IS CALLED TO SET UP	MAIN	215
C THESE STEPS.	MAIN	220
C 5. THE MAIN PROGRAM NOW CALCULATES THE ENTHALPY, ENTROPY, AND	MAIN	225
C GIBBS FREE ENERGY CHANGE FOR EACH STEP. (SUBROUTINE CPHSG	MAIN	230
C IS USED IN THIS PROCEDURE)	MAIN	235
C 6. THE FIRST TABLE OF OUTPUT IS NOW PRINTED AND IF THE WORK	MAIN	240
C OF SEPARATION IS TO BE CALCULATED, THE SUBROUTINE REMOVE	MAIN	245
C IS CALLED.	MAIN	250
C 7. THE TABLE LISTING THE EXOTHERMIC AND ENDOTHERMIC STEPS	MAIN	255
C IS PRINTED.	MAIN	260
C 8. IF DRAW=.TRUE., THE MATCH SUBROUTINE IS CALLED TO SET UP	MAIN	265
C THE MATCHES FOR HEAT EXCHANGE.	MAIN	270
C 9. THE ENTHALPY, ENTROPY, AND GIBBS FREE ENERGY CHANGES FOR THE	MAIN	275
C CHEMICAL REACTIONS ARE CALCULATED. THE SUBROUTINE FZ298	MAIN	280
C IS CALLED TO DETERMINE THE FAZES OF THE MATERIALS AT 298K.	MAIN	285
C	MAIN	290

C	THE PROGRAM THEN RECYCLES THROUGH THAT PART OF THE MAIN	MAIN 295
C	PROGRAM WHICH CALCULATES THESE VALUES.	MAIN 300
C		MAIN 305
C	*****	MAIN 310
	R=1.987165	MAIN 315
20	READ(5,40) (TITLE(I),I=1,20)	MAIN 320
40	FORMAT(20A4)	MAIN 325
	IF(TITLE(1).EQ.FINI) GO TO 1620	MAIN 330
	WRITE(6,60) (TITLE(I),I=1,20)	MAIN 335
60	FORMAT('1','BEGINNING OF INPUT DATA FOR ',20A4)	MAIN 340
	HSG298=.FALSE.	MAIN 345
C		MAIN 350
C	READIN IS NOW CALLED TO READ AND PROCESS THE INPUT CARDS FOR THE	MAIN 355
C	PROGRAM.	MAIN 360
C		MAIN 365
	CALL READIN	MAIN 370
	IF(TEST20) GO TO 20	MAIN 375
	80 CONTINUE	MAIN 380
C		MAIN 385
C	DATAS IS CALLED TO READ THE THERMODYNAMIC DATA FILE.	MAIN 390
C		MAIN 395
	CALL DATAS	MAIN 400
	IF(TEST20) GO TO 20	MAIN 405
	WRITE(6,100) (TITLE(I),I=1,20)	MAIN 410
100	FORMAT('0','END OF INPUT DATA FOR ',20A4)	MAIN 415
C		MAIN 420
C	IF DRAW=.TRUE., ROUTE IS CALLED TO SET UP THE	MAIN 425
C	MATERIAL TRANSFER STEPS.	MAIN 430
C		MAIN 435
	IF(DRAW) CALL ROUTE	MAIN 440
	IF(TEST20) GO TO 20	MAIN 445
120	FORMAT(' ','FOR TEMP. SCHEDULE',I3,' AND REACTION',I3,' THE TEMP.	MAIN 450
	IT'S MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR',5X,12A1)	MAIN 455
140	NX=NRXNS	MAIN 460
	IF(.NOT.DRAW) NX=NR	MAIN 465
	N=NOTEMP	MAIN 470
	IF(HSG298) N=1	MAIN 475
C		MAIN 480
C	THIS SECTION CALCULATES THE THERMODYNAMIC PROPERTY CHANGES	MAIN 485
C	FOR EACH STEP USING THE CPHSG SUBROUTINE.	MAIN 490
C		MAIN 495
	DO 440 K=1,N	MAIN 500
	ILM=1	MAIN 505
	IF(HSG298) GO TO 180	MAIN 510
	HAM(K)=0.0	MAIN 515
	HIM(K)=0.0	MAIN 520
	DO 160 NRX=1,NR	MAIN 525
160	WGMIN(NRX,K)=0.0	MAIN 530
	GO TO 200	MAIN 535
180	DUMH(1)=HTOT(K)	MAIN 540
	DUMH(2)=STOT(K)	MAIN 545
	DUMH(3)=GTOT(K)	MAIN 550
	ILM=5	MAIN 555
200	HTOT(K)=0.0	MAIN 560
	STOT(K)=0.0	MAIN 565
	GTOT(K)=0.0	MAIN 570
	IF(ILM.EQ.5) GO TO 220	MAIN 575
	GO TO 180	MAIN 580

220	CONTINUE	MAIN 585
	DO 420 NRX=1,NX	MAIN 590
	IF(.NOT.HSG298) GO TO 240	MAIN 595
	DUMH(4)=SS(NRX,K)	MAIN 600
	DUMH(5)=HS(NRX,K)	MAIN 605
	DUMH(6)=GS(NRX,K)	MAIN 610
240	SS(NRX,K)=0.0	MAIN 615
	HS(NRX,K)=0.0	MAIN 620
	GS(NRX,K)=0.0	MAIN 625
	IF(NRX.GT.NR) GO TO 340	MAIN 630
	NPN=NPRD(NRX)	MAIN 635
	DO 280 NPR=1,NPN	MAIN 640
260	TT=TEMP1(NRX,K)	MAIN 645
	TLN=ALOG(TT)	MAIN 650
	AFACT=APRUD(NRX,NPR)	MAIN 655
	M=KEYNCP(NRX,NPR)	MAIN 660
	T1T=TRANGE(1,M)-10.	MAIN 665
	T2T=TRANGE(2,M)+10.	MAIN 670
	IF(TT.LT.T1T.OR.TT.GT.T2T) WRITE(6,120) K,NRX,(SPEC(M,NN),NN=1,12)	MAIN 675
	CALL CPHSG	MAIN 680
	IF(TEST20) GO TO 20	MAIN 685
280	CONTINUE	MAIN 690
	NPN=NREACT(NRX)	MAIN 695
	DO 320 NPR=1,NPN	MAIN 700
300	TT=TEMP2(NRX,K)	MAIN 705
	TLN=ALOG(TT)	MAIN 710
	AFACT=-AREACT(NRX,NPR)	MAIN 715
	M=KEYNOR(NRX,NPR)	MAIN 720
	T1T=TRANGE(1,M)-10.	MAIN 725
	T2T=TRANGE(2,M)+10.	MAIN 730
	IF(TT.LT.T1T.OR.TT.GT.T2T) WRITE(6,120) K,NRX,(SPEC(M,NN),NN=1,12)	MAIN 735
	CALL CPHSG	MAIN 740
	IF(TEST20) GO TO 20	MAIN 745
320	CONTINUE	MAIN 750
	IF(.NOT.HSG298) HST(NRX,K)=HS(NRX,K)	MAIN 755
	GO TO 400	MAIN 760
340	CONTINUE	MAIN 765
360	TT=TEMP1(NRX,K)	MAIN 770
	TLN=ALOG(TT)	MAIN 775
	AFACT=HSTOCP(NRX)	MAIN 780
	M=KYNP(NRX)	MAIN 785
	T1T=TRANGE(1,M)-10.	MAIN 790
	T2T=TRANGE(2,M)+10.	MAIN 795
	IF(TT.LT.T1T.OR.TT.GT.T2T) WRITE(6,120) K,NRX,(SPEC(M,NN),NN=1,12)	MAIN 800
	CALL CPHSG	MAIN 805
	IF(TEST20) GO TO 20	MAIN 810
380	TT=TEMP2(NRX,K)	MAIN 815
	TLN=ALOG(TT)	MAIN 820
	AFACT=-HSTOCR(NRX)	MAIN 825
	M=KYNR(NRX)	MAIN 830
	T1T=TRANGE(1,M)-10.	MAIN 835
	T2T=TRANGE(2,M)+10.	MAIN 840
	IF(TT.LT.T1T.OR.TT.GT.T2T) WRITE(6,120) K,NRX,(SPEC(M,NN),NN=1,12)	MAIN 845
	CALL CPHSG	MAIN 850
	IF(TEST20) GO TO 20	MAIN 855
400	STOT(K)=STOT(K)+SS(NRX,K)	MAIN 860
	HTOT(K)=HTOT(K)+HS(NRX,K)	MAIN 865
	GTOT(K)=GTOT(K)+GS(NRX,K)	MAIN 870

IF(.NOT.HSG298) GO TO 420	MAIN 875
HO(NRX)=HS(NRX,K)	MAIN 880
SU(NRX)=SS(NRX,K)	MAIN 885
GO(NRX)=GS(NRX,K)	MAIN 890
SS(NRX,K)=DUMH(4)	MAIN 895
HS(NRX,K)=DUMH(5)	MAIN 900
GS(NRX,K)=DUMH(6)	MAIN 905
420 CONTINUE	MAIN 910
HO(11)=HTOT(K)	MAIN 915
SO(11)=STOT(K)	MAIN 920
GO(11)=GTOT(K)	MAIN 925
IF(.NOT.HSG298) GO TO 440	MAIN 930
HTOT(K)=DUMH(1)	MAIN 935
STOT(K)=DUMH(2)	MAIN 940
GTOT(K)=DUMH(3)	MAIN 945
440 CONTINUE	MAIN 950
IF(HSG298) GO TO 520	MAIN 955
NTOT=0	MAIN 960
C	MAIN 965
C THIS SECTION PRINTS THE FIRST TABLE OF OUTPUT.	MAIN 970
C	MAIN 975
DO 500 I=1,NR	MAIN 980
NSUB=0	MAIN 985
NPN=NREACT(I)	MAIN 990
DO 460 NPR=1,NPN	MAIN 995
M=KEYNDR(I,NPR)	MAIN1000
NARE=AREACT(I,NPR)	MAIN1005
NIR=5	MAIN1010
IF((AREACT(I,NPR)-NARE).EQ.0.0) NIR=3	MAIN1015
IF((AREACT(I,NPR)-NARE).EQ.0.0.AND.NARE.LT.10) NIR=2	MAIN1020
460 NSUB=NSUB+3+NIR+NSATOM(M)	MAIN1025
NPN=NPROD(I)	MAIN1030
DO 480 NPR=1,NPN	MAIN1035
M=KEYNOP(I,NPR)	MAIN1040
NARE=APROD(I,NPR)	MAIN1045
NIR=5	MAIN1050
IF((APROD(I,NPR)-NARE).EQ.0.0) NIR=3	MAIN1055
IF((APROD(I,NPR)-NARE).EQ.0.0.AND.NARE.LT.10) NIR=2	MAIN1060
480 NSUB=NSUB+3+NIR+NSATOM(M)	MAIN1065
500 IF(NSUB.GT.NTOT) NTOT=NSUB	MAIN1070
NSUB=NTOT	MAIN1075
IF(NSUB.GE.125) NTOT=1	MAIN1080
IF(NSUB.LT.125) NTOT=(132-NSUB)/2	MAIN1085
NSUB=NTOT	MAIN1090
IF(.NOT.HSG298) GO TO 640	MAIN1095
C	MAIN1100
C THIS SECTION PRINTS THE TABLE FOR THE RESULTS AT 298 K.	MAIN1105
C	MAIN1110
520 WRITE(6,540) (TITLE(I),I=1,20)	MAIN1115
540 FORMAT('0',T45,'PROPERTIES OF THE BASE REACTIONS AT 298 K FOR',/T4	MAIN1120
15,20A4)	MAIN1125
DO 580 I=1,NR	MAIN1130
WRITE(6,780) I,TEMP2(I,1),P(I,1,1)	MAIN1135
NTOT=1	MAIN1140
CALL EQNS	MAIN1145
560 WRITE(6,820) HO(1),SO(1),GO(1)	MAIN1150
580 CONTINUE	MAIN1155
WRITE(6,600) HO(11),SO(11),GO(11)	MAIN1160

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600 FORMAT(' ',130(' '),/T2,'TOTALS ',T10,'DELTA-H=',-3PF11.5,' KCAL, MAIN1165
1DELTA-S=',0PF12.5,' CAL/DEG, DELTA-G=',-3PF11.5,' KCAL',/' ',130(' MAIN1170
2-')) MAIN1175
DO 620 K=1,NUTEMP MAIN1180
NR10=NR+10 MAIN1185
DO 620 I=11,NR10 MAIN1190
II=I-10 MAIN1195
620 TEMP1(II,K)=TEMP1(I,K) MAIN1200
CALL LOSS MAIN1205
GO TO 20 MAIN1210
640 CONTINUE MAIN1215
DO 1260 K=1,NUTEMP MAIN1220
WRITE(6,660) (TITLE(I),I=1,20),K MAIN1225
660 FORMAT('1',T62,'TABLE I',/T45,'ANALYSIS OF THE CHEMICAL REACTION S MAIN1230
1TEPS IN',/T45,20A4,/T50,' TEMPERATURE SCHEDULE ',12,'.') MAIN1235
DO 680 I=1,NR MAIN1240
NTOT=NSUB MAIN1245
680 CALL EQNS MAIN1250
WRITE(6,700) MAIN1255
700 FORMAT('0','TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE MAIN1260
1BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H2. EPS1 EQ. IS THE',MAIN1265
2/' FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUMMAIN1270
3. CALCULATIONS ARE MADE FOR THE FRACTION',/' CONVERTED AT 100, 90MAIN1275
4, ETC. PERCENT OF THIS EQUILIBRIUM VALUE') MAIN1280
WRITE(6,760) MAIN1285
WRITE(6,720) MAIN1290
720 FORMAT(' ',T4,'EPSI EQ. REACTANT RATIO* MOLES OF REACTANMAIN1295
1T IN RECYCLE STREAM * WORK OF SEPARATION OF GAMAIN1300
2SES',/T33,'*',T82,'*',T105,'(KCAL)') MAIN1305
WRITE(6,760) MAIN1310
WRITE(6,740) MAIN1315
740 FORMAT(' ',T33,'* EXTENT OF REACTION AS PERCENT OF MAIN1320
1EPSI EQ. * EXTENT OF REACTION AS PERCENT OF EPSI EQ.',/T33, MAIN1325
2* 100 90 80 70 60 50 * 100 90 MAIN1330
3 80 70 60 50') MAIN1335
WRITE(6,760) MAIN1340
760 FORMAT(' ',T33,'*',48(' '),*',48(' '), MAIN1345
DO 1000 I=1,NR MAIN1350
WRITE(6,780) I,TEMP2(I,K),P(I,K,1) MAIN1355
780 FORMAT('0','STEP ',I2,'. AT ',F7.2,'DEG., AND ',F7.2,'ATM.') MAIN1360
NTOT=1 MAIN1365
CALL EQNS MAIN1370
800 WRITE(6,820) HS(I,K),SS(I,K),GS(I,K) MAIN1375
820 FORMAT(' ',T10,'DELTA-H=',-3PF11.5,' KCAL, DELTA-S=',0PF12.5,' MAIN1380
1CAL/DEG, DELTA-G=',-3PF11.5,' KCAL') MAIN1385
840 IF(LNOTE(1).EQ.0) GO TO 880 MAIN1390
LL=LNOTE(1) MAIN1395
WRITE(6,860) (NOTE(I,NO),NO=1,LL) MAIN1400
860 FORMAT(' ',19A4) MAIN1405
880 NB=BASE(I) MAIN1410
IF(NB.LE.0) TEST1(I)=.FALSE. MAIN1415
IF(.NOT.TEST1(I)) GO TO 1000 MAIN1420
NB=KEYNUR(I,NB) MAIN1425
WRITE(6,900) (SPEC(NB,LL),LL=1,I2) MAIN1430
900 FORMAT(' ',3X,12A1,'IS THE BASE REACTANT FOR THIS REACTION') MAIN1435
IF(.NOT.TEST1(I)) GO TO 1000 MAIN1440
SUMPG=0.0 MAIN1445
SUMPS=0.0 MAIN1450

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SUMPL=0.0
NGASP=0
NLIQP=0
NSOLP=0
NGASR=0
NLIQR=0
NSOLR=0
NPN=NPROD(1)
DO 920 NPR=1,NPN
  IF(FAZEP(1,NPR).EQ.GAS) NGASP=NGASP+1
  IF(FAZEP(1,NPR).EQ.GAS) SUMPGE=SUMPGE+APRUD(1,NPR)
  IF(FAZEP(1,NPR).EQ.PLIQ) NLIQP=NLIQP+1
  IF(FAZEP(1,NPR).EQ.PLIQ) SUMPL=SUMPL+APROD(1,NPR)
  IF(FAZEP(1,NPR).EQ.SOL) NSOLP=NSOLP+1
  IF(FAZEP(1,NPR).EQ.SOL) SUMPS=SUMPS+APROD(1,NPR)
920 CONTINUE
  IF((NGASP+NLIQP+NSOLP).NE.NPN) WRITE(6,940) 1
940 FORMAT('0','THE TOTAL NUMBER OF PRODUCTS IN EACH PHASE DO NOT SUM
  ITO THE NUMBER OF PRODUCTS IN REACTION',2X,I2,/' CHECK BEGINNING
  2F THE 820 DO LOOP IN MAIN PROGRAM')
  IF((NGASP+NLIQP+NSOLP).NE.NPN) TEST1(1)=.FALSE.
  NPN=NREACT(1)
  DO 960 NPR=1,NPN
    IF(FAZER(1,NPR).EQ.GAS) NGASR=NGASR+1
    IF(FAZER(1,NPR).EQ.PLIQ) NLIQR=NLIQR+1
    IF(FAZER(1,NPR).EQ.SOL) NSOLR=NSOLR+1
960 CONTINUE
    IF((NGASR+NLIQR+NSOLR).NE.NPN) WRITE(6,980) 1
980 FORMAT('0','THE SUM OF ALL THE REACTANTS IN REACTION ',I2,2X,'DO
  101 EQUAL THE NUMBER OF REACTANTS, CHECK THE 860 DO LOOP IN MAIN')
    IF((NGASR+NLIQR+NSOLR).NE.NPN) TEST1(1)=.FALSE.
C
C REMOVE CALCULATES THE WORK OF SEPARATION.
C
  IF(TEST1(1)) CALL REMOVE
1000 CONTINUE
  IF(.NOT.DRAW) GO TO 1240
  NR1=NR+1
C
C THIS SECTION PRINTS THE RESULTS FOR THE HEATING AND COOLING STEPS.
C
  WRITE(6,1020) (TITLE(I),I=1,20),K
1020 FORMAT('1',I62,'TABLE 11',/T50,'ANALYSIS OF THE HEATING AND COOLIN
  1G STEPS IN',/T45,20A4,/T55,' TEMPERATURE SCHEDULE ',I2,.',',/T80,
  2' DELTA-H DELTA-S DELTA-G',/T80,' (KCAL) (CAL/DEG)
  3(KCAL)')
  DO 1220 I=NR1,NKXNS
    M=KYNR(I)
    NM=KYNP(I)
    WRITE(6,1060) 1,TEMP2(I,K),TEMP1(I,K)
    WRITE(6,1040) P(1,K,2),P(I,K,1)
1040 FORMAT(' ',T26,F7.2,' ATM. ---> ',F7.2,' ATM.')
1060 FORMAT(' ',T26,F7.2,' DEG. ---> ',F7.2,' DEG.')
    IF(ROUTE(1,1).EQ.0) GO TO 1100
    IF(ROUTE(1,2).EQ.0) GO TO 1140
    WRITE(6,1080) HSTOCR(1),(SPEC(M,NN),NN=1,12),ROUTE(1,1),HSTOCP(1)
    1,(SPEC(M,NN),NN=1,12),ROUTE(1,2),HS(1,K),SS(1,K),GS(1,K)
1080 FORMAT(' ',I4,F5.2,1X,I2A1,'FROM REACTION ',I2,' ---> ',F5.2,1X,

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MAIN1455
 MAIN1460
 MAIN1465
 MAIN1470
 MAIN1475
 MAIN1480
 MAIN1485
 MAIN1490
 MAIN1495
 MAIN1500
 MAIN1505
 MAIN1510
 MAIN1515
 MAIN1520
 MAIN1525
 MAIN1530
 MAIN1535
 MAIN1540
 MAIN1545
 MAIN1550
 MAIN1555
 MAIN1560
 MAIN1565
 MAIN1570
 MAIN1575
 MAIN1580
 MAIN1585
 MAIN1590
 MAIN1595
 MAIN1600
 MAIN1605
 MAIN1610
 MAIN1615
 MAIN1620
 MAIN1625
 MAIN1630
 MAIN1635
 MAIN1640
 MAIN1645
 MAIN1650
 MAIN1655
 MAIN1660
 MAIN1665
 MAIN1670
 MAIN1675
 MAIN1680
 MAIN1685
 MAIN1690
 MAIN1695
 MAIN1700
 MAIN1705
 MAIN1710
 MAIN1715
 MAIN1720
 MAIN1725
 MAIN1730
 MAIN1735
 MAIN1740

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112A1, ' IN REACTION ',I2,T80,-3PF11.5,0PF12.4,-3PF11.5) MAIN1745
GO TO 1180 MAIN1750
1100 WRITE(6,1120) HSTOCR(I),(SPEC(M,NN),NN=1,12),HSTOCP(I),(SPEC(MM,NN) MAIN1755
1),NN=1,12),IROUTE(I,2),HS(I,K),SS(I,K),GS(I,K) MAIN1760
1120 FORMAT(' ',T4,F5.2,1X,12A1,'RAW MATERIAL',T39,'---> ',F5.2,1X,12A1 MAIN1765
1,' IN REACTION ',I2,T80,-3PF11.5,0PF12.4,-3PF11.5) MAIN1770
GO TO 1180 MAIN1775
1140 WRITE(6,1160) HSTOCR(I),(SPEC(M,NN),NN=1,12),IROUTE(1,1),HSTOCP(I) MAIN1780
1,(SPEC(MM,NN),NN=1,12),HS(I,K),SS(I,K),GS(I,K) MAIN1785
1160 FORMAT(' ',T4,F5.2,1X,12A1,'FROM REACTION ',I2,' ---> ',F5.2,1X, MAIN1790
12A1,' FINAL PRDUCET',T80,-3PF11.5,0PF12.4,-3PF11.5) MAIN1795
1180 WRITE(6,1200) MAIN1800
1200 FORMAT(' ',130(' ')) MAIN1805
1220 CONTINUE MAIN1810
1240 CONTINUE MAIN1815
WRITE(6,1260) NRXNS,HTOT(K),STOT(K),GTOT(K) MAIN1820
1260 FORMAT(' ',T2,'TOTALS FOR STEPS 1 TO ',I2,T80,-3PF11.5,0PF12.4, MAIN1825
1-3PF11.5,' ',130(' ')) MAIN1830
1280 CONTINUE MAIN1835
IF(.NOT.DRAW) GO TO 1580 MAIN1840
C MAIN1845
C THIS SECTION PRINTS THE TABLE OF THE EXOTHERMIC AND ENDOTHERMIC STEPS. MAIN1850
C MAIN1855
DO 1560 J=1,NOTEMP,2 MAIN1860
JJ=1+J MAIN1865
WRITE(6,1300) (TITLE(I),I=1,20),J,JJ MAIN1870
1300 FORMAT(' ',T40,20A4,/T40,'COMPARISON OF EXOTHERMIC AND ENDOTHERMIC MAIN1875
1 STEPS',/T10,'*',53(' '),*',53(' '),*',/T10,'*',15X,'TEMPERATUR MAIN1880
2E SCHEDULE',13,15X,'*',15X,'TEMPERATURE SCHEDULE',13,15X,'*',/T10, MAIN1885
3,'*',5(' '),*',21(' '),*',25(' '),*',5(' '),*',21(' '),*',25(' MAIN1890
4'),*',/9X,'*STEP * TEMPERATURES (K) ',7X,'HEAT (KCAL)',7X,'* MAIN1895
5STEP * TEMPERATURES (K) ',7X,'HEAT (KCAL)',7X,'*',/9X,'*',5(' MAIN1900
6'),*',10(' '),*',10(' '),*',12(' '),*',12(' '),*',5(' '),*', MAIN1905
710(' '),*',10(' '),*',12(' '),*',12(' '),*',/T10,'* *REACT MAIN1910
8ANTS * PRODUCTS * EXOTHERMIC * ENDOTHERMIC* *REACTANTS * PRODUMAIN1915
9CTS * EXOTHERMIC * ENDOTHERMIC*) MAIN1920
1320 FORMAT(' ',T10,'*',5(' '),*',10(' '),*',10(' '),*',12(' '),*', MAIN1925
112(' '),*',5(' '),*',10(' '),*',10(' '),*',12(' '),*',12(' ') MAIN1930
2,'*') MAIN1935
WRITE(6,1320) MAIN1940
HSEX01=0.0 MAIN1945
HSEX02=0.0 MAIN1950
HEND01=0.0 MAIN1955
HEND02=0.0 MAIN1960
DO 1500 I=1,NRXNS MAIN1965
IF(JJ.GT.NOTEMP) GO TO 1340 MAIN1970
IF(HS(I,J).LE.0.0.AND.HS(I,JJ).LE.0.0) WRITE(6,1360) I,TEMP2(I,J), MAIN1975
ITEMP1(I,J),HS(I,J),I,TEMP2(I,JJ),TEMP1(I,JJ),HS(I,JJ) MAIN1980
IF(HS(I,J).GT.0.0.AND.HS(I,JJ).GT.0.0) WRITE(6,1380) I,TEMP2(I,J), MAIN1985
ITEMP1(I,J),HS(I,J),I,TEMP2(I,JJ),TEMP1(I,JJ),HS(I,JJ) MAIN1990
IF(HS(I,J).LE.0.0.AND.HS(I,JJ).GT.0.0) WRITE(6,1400) I,TEMP2(I,J), MAIN1995
ITEMP1(I,J),HS(I,J),I,TEMP2(I,JJ),TEMP1(I,JJ),HS(I,JJ) MAIN2000
IF(HS(I,J).GT.0.0.AND.HS(I,JJ).LE.0.0) WRITE(6,1420) I,TEMP2(I,J), MAIN2005
ITEMP1(I,J),HS(I,J),I,TEMP2(I,JJ),TEMP1(I,JJ),HS(I,JJ) MAIN2010
GO TO 1480 MAIN2015
1340 IF(HS(I,J).LE.0.0) WRITE(6,1440) I,TEMP2(I,J),TEMP1(I,J),HS(I,J) MAIN2020
IF(HS(I,J).GT.0.0) WRITE(6,1460) I,TEMP2(I,J),TEMP1(I,J),HS(I,J) MAIN2025
1360 FORMAT(' ',T10,2(' ',1X,I2,' * ',0PF7.2,1X,'*',2X,F7.2,1X,'*',-3MAIN2030

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1PF10.4,2X,'*',12X),'*')
1380 FORMAT(' ',T10,2(' ',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',12X,MAIN2035
1X,'*',-3PF10.4,2X),'*')
MAIN2040
1400 FORMAT(' ',T10,'*',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',-3PFMAIN2045
110.4,2X,'*',12X,'*',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',12XMAIN2050
2,'*',-3PF10.4,2X,'*')
MAIN2055
1420 FORMAT(' ',T10,'*',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',12X,MAIN2060
1,'*',-3PF10.4,2X,'*',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',-3PFMAIN2065
2F10.4,2X,'*',12X,'*')
MAIN2070
1440 FORMAT(' ',T10,'*',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',-3PFMAIN2075
110.4,2X,'*',12X,'*',5X,'*',10X,'*',10X,'*',12X,'*',12X,'*')
MAIN2080
1460 FORMAT(' ',T10,'*',1X,I2,' * ',OPF7.2,1X,'*',2X,F7.2,1X,'*',12X,MAIN2085
1,'*',-3PF10.4,2X,'*',5X,'*',10X,'*',10X,'*',12X,'*',12X,'*')
MAIN2090
1480 CONTINUE
MAIN2095
IF(HS(1,J).LE.0.0) HSEX01=HSEX01+HS(1,J)
MAIN2100
IF(HS(1,J).GT.0.0) HEND01=HEND01+HS(1,J)
MAIN2105
IF(JJ.GT.NOTEMP) GO TO 1500
MAIN2110
IF(HS(1,JJ).LE.0.0) HSEX02=HSEX02+HS(1,JJ)
MAIN2115
IF(HS(1,JJ).GT.0.0) HEND02=HEND02+HS(1,JJ)
MAIN2120
1500 CONTINUE
MAIN2125
WRITE(6,1320)
MAIN2130
IF(JJ.LE.NOTEMP) WRITE(6,1520) HSEX01,HEND01,HSEX02,HEND02
MAIN2135
IF(JJ.GT.NOTEMP) WRITE(6,1540) HSEX01,HEND01
MAIN2140
WRITE(6,1320)
MAIN2145
1520 FORMAT(' ',T10,'*',11X,'TOTALS',10X,'*',-3PF10.4,2X,'*',F10.4,2X,'MAIN2150
1,'*',27X,'*',F10.4,2X,'*',F10.4,2X,'*')
MAIN2155
1540 FORMAT(' ',T10,'*',11X,'TOTALS',10X,'*',-3PF10.4,2X,'*',F10.4,2X,'MAIN2160
1,'*',27X,'*',12X,'*',12X,'*')
MAIN2165
1560 CONTINUE
MAIN2170
C
MAIN2175
C SUBROUTINE MATCH IS NOW CALLED TO SET UP THE HEAT EXCHANGE STEPS.
MAIN2180
C
MAIN2185
CALL MATCH
MAIN2190
1580 CONTINUE
MAIN2195
IF(HSG298) H298=.FALSE.
MAIN2200
IF(H298) HSG298=.TRUE.
MAIN2205
IF(H298) SAME=.TRUE.
MAIN2210
IF(H298) DRAW=.FALSE.
MAIN2215
C
MAIN2220
C FZ298 IS CALLED TO DETERMINE THE PHASES OF THE MATERIALS AT 298K
MAIN2225
C IN ORDER TO CALCULATE THE PROPERTY CHANGES OF THE CHEMICAL REACTIONS
MAIN2230
C
MAIN2235
DO 1600 K=1,NOTEMP
MAIN2240
NR10=NR+10
MAIN2245
DO 1600 I=11,NR10
MAIN2250
II=I-10
MAIN2255
1600 TEMP1(I,K)=TEMP1(II,K)
MAIN2260
IF(H298) CALL FZ298
MAIN2265
IF(H298) GO TO 140
MAIN2270
GO TO 20
MAIN2275
1620 CONTINUE
MAIN2280
STOP
MAIN2285
END
MAIN2290
MAIN2295

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SUBROUTINE ROUTE		ROUT 5
C	*****	ROUT 10
C	THIS ROUTINE SETS UP THE MATERIAL TRANSFER STEPS	ROUT 15
C	*****	ROUT 20
C		ROUT 25
C	THE PROGRAM FIRSTS TRIES TO MATCH THE PRODUCTS TO REACTANTS IN STEPS	ROUT 30
C	FOR WHICH THE STOICHIOMETRIC COEFFICIENTS ARE EQUAL (LCN=1).	ROUT 35
C	IF THIS IS NOT POSSIBLE, IT BREAKS UP THE STREAMS TO MAKE THE MATCH	ROUT 40
C	(LCN=2).	ROUT 45
C		ROUT 50
C	THE MATCHING CONSISTS OF TAKING EACH PRODUCT OF EACH REACTION AND	ROUT 55
C	COMPARING IT WITH THE REACTANTS OF ALL OTHER REACTIONS.	ROUT 60
C		ROUT 65
	REAL NOTE	ROUT 70
	INTEGER BASE	ROUT 75
	LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298,TEST3,TEST4	ROUT 80
	DIMENSION FAZER(11,5),FAZEP(11,5),RATOM(11,5,4),PATOM(11,5,4),	ROUT 85
	IRATCO(11,5,4),PATCO(11,5,4),TG(10),PDUM1(10),PDUM2(10)	ROUT 90
	DIMENSION BASE(10),NSATOM(50),SPEC(50,12),SPATOM(50,4),SPATCO(50,4)	ROUT 95
	1),SPFAZE(50),KEYNOR(11,5),KEYNOP(11,5),KYNR(50),KYNP(50),	ROUT 100
	2)ROUTE(50,2),TEMP1(50,10),TEMP2(50,10),TRANGE(2,50),TPHASE(11,5,4)	ROUT 105
	3,TEST1(10),AREACT(10,5),APROD(10,5),NPROD(11),NREACT(11),NRATIO(10	ROUT 110
	4),RATIO(10,5,4),LNOTE(10),NOTE(10,100),HSTOCR(50),HSTOCP(50),	ROUT 115
	5)STOICR(11,5),STOICP(11,5)	ROUT 120
	COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN	ROUT 125
	COMMON/MATL1/SPEC,SPATCM,SPATCO,SPFAZE	ROUT 130
	COMMON/MATL2/KEYNOR,KEYNOP,KYNR,KYNP,IROUTE	ROUT 135
	COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID	ROUT 140
	COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298	ROUT 145
	COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,	ROUT 150
	INRATIO,LNOTE	ROUT 155
	COMMON/FNAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO	ROUT 160
	COMMON/PRESS/P(50,10,2)	ROUT 165
	DATA GAS/1HG/,BLANK/1H /,SOL/'S'/	ROUT 170
	LCN=1	ROUT 175
	NRXNS=NR	ROUT 180
	NR1=NR+1	ROUT 185
20	DO 720 I=1,NR1	ROUT 190
	NPP=NPROD(I)	ROUT 195
	DO 700 J=1,NPP	ROUT 200
	NJ=KEYNOP(I,J)	ROUT 205
	IF(STOICP(I,J).EQ.0.0) GO TO 700	ROUT 210
	DO 680 II=1,NR1	ROUT 215
	NPR=NREACT(II)	ROUT 220
	DO 660 JJ=1,NPR	ROUT 225
	TEST3=.FALSE.	ROUT 230
	TEST4=.FALSE.	ROUT 235
	NJJ=KEYNOR(II,JJ)	ROUT 240
	IF(STOICR(II,JJ).EQ.0.0) GO TO 660	ROUT 245
	DO 40 NN=1,4	ROUT 250
	IF(SPATUM(NJ,1).EQ.SPATOM(NJJ,1).AND.SPATOM(NJ,2).EQ.BLANK.AND.SPAREACT	ROUT 255
	UM(NJJ,2).EQ.BLANK.AND.SPATCO(NJ,1).NE.SPATCO(NJJ,1)) GO TO 60	ROUT 260
	IF(SPATOM(NJ,NN).NE.SPATOM(NJJ,NN).OR.SPATCO(NJ,NN).NE.SPATCO(NJJ,	ROUT 265
	NN)) GO TO 660	ROUT 270
40	CONTINUE	ROUT 275
	IF(LCN.EQ.1.AND.STOICR(II,JJ).NE.STOICP(I,J)) GO TO 660	ROUT 280
	GO TO 80	ROUT 285
C		ROUT 290

C THE FOLLOWING SECTION SETS UP THE STEPS TO HEAT OR COOL THE PRODUCTS	ROUT 295
C TO THE TEMPERATURE WHERE THEY ARE USED AS REACTANTS.	ROUT 300
C PHASE CHANGES ARE SEPARATE STEPS CONDUCTED AT CONSTANT TEMPERATURE.	ROUT 305
C THIS IS DONE IN ORDER TO MINIMIZE THE POSSIBILITY OF SECOND	ROUT 310
C LAW VIOLATIONS IN THE HEAT TRANSFER MATCHING	ROUT 315
C	ROUT 320
C	ROUT 325
60 TEST3=.TRUE.	ROUT 330
X1=SPATCO(NJ,1)*STOICP(1,J)	ROUT 335
X2=SPATCO(NJJ,1)*STOICR(II,JJ)	ROUT 340
IF(LCN.EQ.1.AND.X1.NE.X2) GO TO 660	ROUT 345
IF(LCN.EQ.1) HDUM=X1	ROUT 350
IF(LCN.NE.1) HDUM=AMIN1(X1,X2)	ROUT 355
80 NL=NJ	ROUT 360
DO 100 LT=1,NOTEMP	ROUT 365
PDUM1(LT)=1.0	ROUT 370
IF(1.NE.NR1) PDUM1(LT)=P(I,LT,1)	ROUT 375
PDUM2(LT)=1.0	ROUT 380
IF(11.NE.NR1) PDUM2(LT)=P(II,LT,2)	ROUT 385
100 CONTINUE	ROUT 390
DO 120 LT=1,NOTEMP	ROUT 395
TG(LT)=298.15	ROUT 400
IF(11.NE.NR1) TG(LT)=TEMP2(II,LT)	ROUT 405
120 CONTINUE	ROUT 410
IF(NJ.EQ.NJJ) GO TO 220	ROUT 415
LIT=1	ROUT 420
L=1	ROUT 425
LL=0	ROUT 430
IF(NJ.GT.NJJ) L=-1	ROUT 435
140 NL=NJ+(LL*L*(LIT-1))	ROUT 440
NLL=NL+L	ROUT 445
IF(.NOT.TEST3) GO TO 160	ROUT 450
NTOP=MAX0(NJ,NJJ)	ROUT 455
NBOT=MING(NJ,NJJ)	ROUT 460
IF(SPFAZE(NJ).EQ.SOL.OR.SPFAZE(NJJ).EQ.SOL) NBOT=NBOT+1	ROUT 465
IF(L.LT.0.AND.NL.LT.NTOP.AND.NL.GT.NBOT) NL=NTOP	ROUT 470
IF(L.GT.0.AND.NL.LT.NTOP.AND.NL.GT.NBOT) NL=NBOT	ROUT 475
IF(L.GT.0.AND.NLL.LT.NTOP.AND.NLL.GT.NBOT) NLL=NTOP	ROUT 480
IF(L.LT.0.AND.NLL.LT.NTOP.AND.NLL.GT.NBOT) NLL=NBOT	ROUT 485
160 CONTINUE	ROUT 490
NTG=NL	ROUT 495
IF(L.LT.0) NTG=NLL	ROUT 500
NLF=1	ROUT 505
NLLF=1	ROUT 510
TG(1)=(TRANGE(2,NTG)+TRANGE(1,NTG))/2.	ROUT 515
C	ROUT 520
C THE TEMPERATURE OF A PHASE TRANSITION IS TO BE FOUND	ROUT 525
C	ROUT 530
DO 200 LI=1,NOTEMP	ROUT 535
IF(NLF.EQ.0.AND.NLLF.EQ.0) GO TO 180	ROUT 540
PTRAN=PDUM1(LI)	ROUT 545
IF(L.GT.0.AND.PDUM2(LI).GT.PDUM1(LI)) PTRAN=PDUM2(LI)	ROUT 550
IF(SPFAZE(NL).NE.GAS) NLF=0	ROUT 555
IF(SPFAZE(NLL).NE.GAS) NLLF=0	ROUT 560
TGUESS=TG(LI)	ROUT 565
CALL TFIND(TGUESS,NL,NLL,PTRAN,NLF,NLLF)	ROUT 570
IF(TEST20) RETURN	ROUT 575
200 TG(LI)=TGUESS	ROUT 580

LIN=L1+1	ROUT 585
IF(LIN.GT.10) LIN=10	ROUT 590
TG(LIN)=TGUESS	ROUT 595
200 CONTINUE	ROUT 600
220 NRXNS=NRXNS+1	ROUT 605
KYNR(NRXNS)=NL	ROUT 610
KYNP(NRXNS)=NL	ROUT 615
DO 280 LT=1,NOTEMP	ROUT 620
P(NRXNS,LT,2)=PDUM1(LT)	ROUT 625
IF(NJ.EQ.NJJ) GO TO 240	ROUT 630
IF(NL.EQ.NJ.AND.SPFAZE(NJ).EQ.GAS) GO TO 260	ROUT 635
240 PDUM1(LT)=PDUM2(LT)	ROUT 640
260 P(NRXNS,LT,1)=PDUM1(LT)	ROUT 645
280 CONTINUE	ROUT 650
IF(NL.NE.NJ) GO TO 320	ROUT 655
DO 300 LT=1,NOTEMP	ROUT 660
TEMP2(NRXNS,LT)=TEMP1(1,LT)	ROUT 665
IF(1.EQ.NR1) TEMP2(NRXNS,LT)=298.15	ROUT 670
300 TEMP1(NRXNS,LT)=TG(LT)	ROUT 675
IROUTE(NRXNS,1)=0	ROUT 680
IF(1.NE.NR1) IROUTE(NRXNS,1)=1	ROUT 685
IROUTE(NRXNS,2)=NRXNS+1	ROUT 690
IF(NJ.EQ.NJJ) IROUTE(NRXNS,2)=11	ROUT 695
IF(11.EQ.NR1) IROUTE(NRXNS,2)=0	ROUT 700
GO TO 440	ROUT 705
320 DO 340 LT=1,NOTEMP	ROUT 710
TEMP2(NRXNS,LT)=TEMP1(NRXNS-1,LT)	ROUT 715
340 TEMP1(NRXNS,LT)=TG(LT)	ROUT 720
IROUTE(NRXNS,1)=NRXNS-1	ROUT 725
IROUTE(NRXNS,2)=NRXNS+1	ROUT 730
GO TO 440	ROUT 735
360 IF(NJ.EQ.NJJ) GO TO 640	ROUT 740
NRXNS=NRXNS+1	ROUT 745
KYNR(NRXNS)=NL	ROUT 750
KYNP(NRXNS)=NLL	ROUT 755
IROUTE(NRXNS,1)=NRXNS-1	ROUT 760
IROUTE(NRXNS,2)=NRXNS+1	ROUT 765
DO 380 LT=1,NOTEMP	ROUT 770
TEMP2(NRXNS,LT)=TEMP1(NRXNS-1,LT)	ROUT 775
P(NRXNS,LT,2)=PDUM1(LT)	ROUT 780
P(NRXNS,LT,1)=PDUM1(LT)	ROUT 785
380 TEMP1(NRXNS,LT)=TEMP2(NRXNS,LT)	ROUT 790
IF(TEST3) GO TO 400	ROUT 795
HSTOCR(NRXNS)=HSTOCP(NRXNS-1)	ROUT 800
HSTOCP(NRXNS)=HSTOCP(NRXNS-1)	ROUT 805
GO TO 420	ROUT 810
400 HSTOCR(NRXNS)=HDUM/SPATCO(NL,1)	ROUT 815
HSTOCP(NRXNS)=HDUM/SPATCO(NLL,1)	ROUT 820
420 CONTINUE	ROUT 825
L1=L1+1	ROUT 830
LL=1	ROUT 835
IF(NLL.EQ.NJJ) GO TO 600	ROUT 840
GO TO 140	ROUT 845
440 CONTINUE	ROUT 850
IF(TEST3) GO TO 520	ROUT 855
IF(NL.NE.NJ) GO TO 500	ROUT 860
IF(STOICP(1,J)-STOICR(11,JJ)) 460,460,460	ROUT 865
460 HSTOCP(NRXNS)=STOICP(1,J)	ROUT 870
760 CONTINUE	ROUT1165
DO 780 J=1,NPR	ROUT1170
N=KEYNOK(1,J)	ROUT1175
IF(STOICR(1,J).GE.SMALL) WRITE(6,820) 1,(SPEC(N,NN),NN=1,12)	ROUT1180
IF(STOICR(1,J).GE.SMALL) TEST20=.TRUE.	ROUT1185
780 CONTINUE	ROUT1190
800 CONTINUE	ROUT1195
820 FORMAT('0','IN REACTION',I3,5X,12A1,' HAS NOT BEEN MATCHED')	ROUT1200
840 RETURN	ROUT1205
END	ROUT1210

HSTOCR(NRXNS)=STOICP(I,J)	ROUT 875
STOICR(II,JJ)=STOICR(II,JJ)-STOICP(I,J)	ROUT 880
STOICP(I,J)=0.0	ROUT 885
GO TO 360	ROUT 890
480 HSTOCR(NRXNS)=STOICR(II,JJ)	ROUT 895
HSTOCP(NRXNS)=STOICP(II,JJ)	ROUT 900
STOICP(I,J)=STOICP(I,J)-STOICR(II,JJ)	ROUT 905
STOICR(II,JJ)=0.0	ROUT 910
GO TO 360	ROUT 915
500 HSTOCP(NRXNS)=HSTOCP(NRXNS-1)	ROUT 920
HSTOCR(NRXNS)=HSTOCR(NRXNS)	ROUT 925
GO TO 360	ROUT 930
520 CONTINUE	ROUT 935
IF(NL.NE.NJ) GO TO 580	ROUT 940
IF(X1-X2) 540,540,560	ROUT 945
540 HSTOCP(NRXNS)=X1/SPATCO(NL,1)	ROUT 950
HSTOCR(NRXNS)=HSTOCP(NRXNS)	ROUT 955
STOICR(II,JJ)=(X2-X1)/SPATCO(NJJ,1)	ROUT 960
STOICP(I,J)=0.0	ROUT 965
GO TO 360	ROUT 970
560 HSTOCR(NRXNS)=X2/SPATCO(NL,1)	ROUT 975
HSTOCP(NRXNS)=HSTOCR(NRXNS)	ROUT 980
STOICP(I,J)=(X1-X2)/SPATCO(NJ,1)	ROUT 985
STOICR(II,JJ)=0.0	ROUT 990
GO TO 360	ROUT 995
580 HSTOCR(NRXNS)=HDUM/SPATCO(NL,1)	ROUT1000
HSTOCP(NRXNS)=HSTOCR(NRXNS)	ROUT1005
GO TO 360	ROUT1010
600 NRXNS=NRXNS+1	ROUT1015
HSTOCP(NRXNS)=HSTOCP(NRXNS-1)	ROUT1020
HSTOCR(NRXNS)=HSTOCP(NRXNS-1)	ROUT1025
IRROUTE(NRXNS,1)=NRXNS-1	ROUT1030
IRROUTE(NRXNS,2)=II	ROUT1035
KYNR(NRXNS)=NLL	ROUT1040
KYNP(NRXNS)=NLL	ROUT1045
DO 620 LT=1,NOTEMP	ROUT1050
P(NRXNS,LT,1)=P(II,LT,2)	ROUT1055
P(NRXNS,LT,2)=PDUM1(LT)	ROUT1060
IF(II.EQ.NR1) TEMP1(NRXNS,LT)=298.15	ROUT1065
IF(II.NE.NR1) TEMP1(NRXNS,LT)=TEMP2(II,LT)	ROUT1070
620 TEMP2(NRXNS,LT)=TG(LT)	ROUT1075
640 CONTINUE	ROUT1080
660 CONTINUE	ROUT1085
680 CONTINUE	ROUT1090
700 CONTINUE	ROUT1095
720 CONTINUE	ROUT1100
IF(LCN.EQ.2) GO TO 740	ROUT1105
LCN=2	ROUT1110
GO TO 20	ROUT1115
740 CONTINUE	ROUT1120
DO 800 I=1,NR1	ROUT1125
NPP=NPROD(I)	ROUT1130
NPR=NREACT(I)	ROUT1135
SMALL=0.0005	ROUT1140
DO 760 J=1,NPP	ROUT1145
N=KEYNOP(I,J)	ROUT1150
IF(STOICP(I,J).GE.SMALL) WRITE(6,820) I,(SPEC(N,NN),NN=1,12)	ROUT1155
IF(STOICP(I,J).GE.SMALL) TEST20=.TRUE.	ROUT1160

SUBROUTINE TFIND(TGUESS,NL,NLL,PTRAN,NLF,NLLF)	TFIN 5
LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298	TFIN 10
DOUBLE PRECISION HS,SS,GS,HTOT,COEF	TFIN 15
DIMENSION TX(30)	TFIN 20
COMMON/LUGIC/PLINE,TEST20,DRAW,SAME,TEST1(10),THERM,H298	TFIN 25
COMMON/DOUBLE/HS(50,10),SS(50,10),GS(50,10),HTOT(10),COEF(2,7,50)	TFIN 30
COMMON/MATL1/SPEC(50,12),SPATOM(50,4),SPATCU(50,4),SPFAZE(50)	TFIN 35
DATA GAS/1HG/	TFIN 40
IF(SPFAZE(NL).NE.GAS) P1FUN=0.0	TFIN 45
IF(SPFAZE(NLL).NE.GAS) P2FUN=0.0	TFIN 50
IF(SPFAZE(NL).EQ.GAS) P1FUN=ALOG(PTRAN)	TFIN 55
IF(SPFAZE(NLL).EQ.GAS) P2FUN=ALOG(PTRAN)	TFIN 60
R=1.987165	TFIN 65
TX(1)=TGUESS	TFIN 70
DO 100 L=2,30	TFIN 75
I=L-1	TFIN 80
T=TX(1)	TFIN 85
TT=T*1	TFIN 90
VART=1.	TFIN 95
M=1	TFIN 100
IF(T.LE.1000.) M=2	TFIN 105
IF(COEF(M,1,NL).LE.0.0) M=-(M-3)	TFIN 110
N=1	TFIN 115
IF(T.LE.1000.) N=2	TFIN 120
IF(COEF(N,1,NLL).LE.0.0) N=-(N-3)	TFIN 125
RAT=SPATCU(NLL,1)/SPATCO(NL,1)	TFIN 130
DO 20 J=1,5	TFIN 135
VART=T*VART	TFIN 140
XJ=J	TFIN 145
HS(1,J)=(COEF(N,J,NLL)-RAT*COEF(M,J,NL))*(VART/XJ)	TFIN 150
20 SS(2,J)=(COEF(N,J,NLL)-RAT*COEF(M,J,NL))*(VART/TT)	TFIN 155
HS(1,6)=COEF(N,6,NLL)-RAT*COEF(M,6,NL)	TFIN 160
SS(1,1)=(COEF(N,1,NLL)-RAT*COEF(M,1,NL))*ALOG(T)	TFIN 165
HS(1,7)=0.0	TFIN 170
VART=1.0	TFIN 175
DO 40 J=2,5	TFIN 180
VART=T*VART	TFIN 185
XJ=J-1	TFIN 190
SS(1,J)=(COEF(N,J,NLL)-RAT*COEF(M,J,NL))*(VART/XJ)	TFIN 195
40 HS(2,J)=(COEF(N,J,NLL)-RAT*COEF(M,J,NL))*VART	TFIN 200
SS(1,6)=COEF(N,7,NLL)-RAT*COEF(M,7,NL)	TFIN 205
HS(2,1)=COEF(N,1,NLL)-RAT*COEF(M,1,NL)	TFIN 210
SS(1,7)=-(P2FUN-P1FUN)	TFIN 215
DO 60 J=6,7	TFIN 220
HS(2,J)=0.0	TFIN 225
60 SS(2,J)=0.0	TFIN 230
G=0.0	TFIN 235
GPRIME=0.0	TFIN 240
DO 80 J=1,7	TFIN 245
G=G+R*(HS(1,J)-T*SS(1,J))	TFIN 250
80 GPRIME=GPRIME+R*(HS(2,J)-T*SS(2,J)-SS(1,J))	TFIN 255
DIFG=ABS(G)	TFIN 260
IF(DIFG.LE.0.001) GO TO 120	TFIN 265
TX(L)=TX(1)-(G/GPRIME)	TFIN 270
DIFT=ABS(TX(L)-TX(1))	TFIN 275
IF(DIFT.LE.0.5) GO TO 120	TFIN 280
IF(TX(L).LE.0.0) TX(L)=1000.0	TFIN 285
100 CONTINUE	TFIN 290
120 CONTINUE	TFIN 295
TGUESS=TX(1)	TFIN 300
RETURN	TFIN 305
END	TFIN 310

C	SUBROUTINE READIN	*****	READ 5
C	THIS SUBROUTINE READS AND PROCESSES ALL DATA CARDS FOR THE CYCLE	*****	READ 10
C			READ 15
C			READ 20
C			READ 25
C	FOR EACH CYCLE, THERE ARE THREE TYPES OF INPUT DATA CARDS. THE		READ 30
C	FIRST CARD IN EACH GROUP CONTAINS THE CODE WORD INDICATING THE		READ 35
C	TYPE OF INPUT DATA WHICH IS TO FOLLOW. THIS CODE WORD IS THE FIRST		READ 40
C	WORD IN THE FOLLOWING LIST AND IS TYPED BEGINNING IN COLUMN ONE.		READ 45
C	THE END OF EACH GROUP OF CARDS IS A BLANK CARD. THE END OF THE INPUT		READ 50
C	FOR EACH CYCLE IS DENOTED BY A CARD WITH 'END' IN COLUMNS 1-3. THE		READ 55
C	END OF ALL CYCLES TO BE RUN IS DENOTED WITH A CARD CONTAINING		READ 60
C	'FINISH' IN COLUMNS 1-6 (THIS CARD FOLLOWS THE 'END' CARD		READ 65
C	OF THE LAST CYCLE).		READ 70
C	1. CHEMICAL REACTION - CARDS CONTAIN THE FORMULA OF THE VARIOUS		READ 75
C	REACTANTS AND PRODUCTS ALONG WITH THEIR PHASE AND		READ 80
C	STOICHIOMETRIC COEFFICIENTS. THE CARDS FOR THE REACTANTS ALSO		READ 85
C	CONTAIN THEIR RATIOS IN THE REACTION MIXTURE.		READ 90
C	2. NOTES - CARDS CONTAIN ANY COMMENTS ABOUT EACH REACTION WHICH ARE		READ 95
C	TO BE PRINTED IN THE OUTPUT.		READ 100
C	3. NAMELISTS - CARDS. FOR EACH REACTION THERE IS A NAMELIST (NAM1)		READ 105
C	WHICH CONTAINS THE SYEP (REACTION NUMBER), PRES (PRESSURE),		READ 110
C	T (TEMPERATURES), AND EP (EPSIES). ALSO, ON ONE OF THE NAMELIST		READ 115
C	CARDS ARE ANY OF THE FOLLOWING OPTIONS:		READ 120
C	DRAW=.TRUE. MEANS THAT MATERIAL TRANSFER STEPS ARE TO BE SET UP.		READ 125
C	SAME=.TRUE. MEANS THAT THE SAME CHEMICAL SPECIES AS IN THE		READ 130
C	PREVIOUS CYCLE ARE TO BE USED AND THAT TAPE 4 WILL NOT HAVE TO		READ 135
C	BE READ FOR THE THERMODYNAMIC DATA.		READ 140
C	H298=.FALSE. MEANS THAT THE THERMODYNAMIC PROPERTIES OF THE		READ 145
C	CHEMICAL REACTIONS AT 298K ARE NOT TO BE CALCULATED.		READ 150
C			READ 155
C	INTEGER CARD,STEP,BASE,A,B		READ 160
C	REAL NOTE		READ 165
C	LOGICAL TEST15		READ 170
C	LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298		READ 175
C	DOUBLE PRECISION XREACT,XPROD,SUMW,SUMRG,GASSUM		READ 180
C	DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF,SUMPG,SUML		READ 185
C	DIMENSION STOICR(11,5),STOICP(11,5),RATOM(11,5,4),PATOM(11,5,4),		READ 190
C	IRATCO(11,5,4),PATCO(11,5,4),RATIO(10,5,4)		READ 195
C	DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TRANGE(2,5		READ 200
C	10),T(20),TPHASE(11,5,4),TEST1(10),AREACT(10,5),APROD(10,5),		READ 205
C	2NPROD(11),NREACT(11),NRATIO(10),DAT(25),LNNOTE(10),NOTE(10,100)		READ 210
C	3,HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),EP(10,4),EPSI(10,10		READ 215
C	4,4),HIM(10),HAM(10),PRES(10)		READ 220
C	COMMON/FNAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO		READ 225
C	COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,1,K,J,M,NRX,NTOT,BASE,NSATOM,NN		READ 230
C	COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TM10		READ 235
C	COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298		READ 240
C	COMMON/PRESS/P(50,10,2)		READ 245
C	COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,		READ 250
C	INRATIO,LNNOTE		READ 255
C	COMMON/FZE/SUML,SUMPG,SUMPS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR,		READ 260
C	INL1QR,NSOLR		READ 265
C	COMMON/WORK/HIM,HAM,EPSI,EFEI		READ 270
C	DATA PRU/4HPRUD/,REAC/4HREAC/,BLANK/4H /,WEND/3HEND/		READ 275
C	1,COMM/4HNOTE/,CHEM/4HCHEM/,CNAME/4HNAME/,THER/4HTHER/,BA/1H6/		READ 280
C	DATA HYD/1HH/		READ 285
C	NAMELIST/NAM1/STEP,T,EP,PRES,DRAW,SAME,H298,EFF		READ 290

EFEL=0.3	READ 295
H298=.TRUE.	READ 300
SAME=.FALSE.	READ 305
EFF=0.3	READ 310
TRY=0.0	READ 315
URAW=.FALSE.	READ 320
THERM=.FALSE.	READ 325
TEST15=.FALSE.	READ 330
TEST20=.FALSE.	READ 335
DO 40 I=1,10	READ 340
BASE(I)=0	READ 345
DO 20 J=1,10	READ 350
JJ=J+10	READ 355
T(JJ)=0.0	READ 360
J5=J	READ 365
IF(J.GT.5) J5=1	READ 370
FAZER(1,J5)=BLANK	READ 375
TEMP1(1,J)=0.0	READ 380
TEMP2(1,J)=0.0	READ 385
20 FAZER(1,J5)=BLANK	READ 390
TEST1(1)=.FALSE.	READ 395
NREACT(1)=0	READ 400
NPROD(1)=0	READ 405
NRATIO(1)=0	READ 410
LNCTE(1)=0	READ 415
40 CONTINUE	READ 420
NR=0	READ 425
C	READ 430
C A CODE CARD IS READ INDICATING THE TYPE OF INPUT CARDS TO FOLLOW	READ 435
C *****NOTE*****	READ 440
C THE ONLY STIPULATION AS TO THE ORDER OF EACH SECTION OF CARDS IS THAT	READ 445
C CHEMICAL REACTION CARDS MUST BE READ BEFORE THE NAMELISTS.	READ 450
C	READ 455
C	READ 460
60 READ(5,80) (DAT(I),I=1,10)	READ 465
80 FORMAT(20A4)	READ 470
WRITE(6,100) (DAT(I),I=1,10)	READ 475
100 FORMAT(' ',20A4)	READ 480
120 IF(DAT(1).EQ.WEND) GO TO 760	READ 485
IF(DAT(1).EQ.BLANK) GO TO 60	READ 490
C TEST20=.TRUE. MEANS THAT AN ERROR HAS BEEN FOUND IN THE INPUT AND THE	READ 495
C SKIPS TO THE NEXT CYCLE.	READ 500
IF(TEST20) GO TO 60	READ 505
IF(DAT(1).EQ.COMM) GO TO 160	READ 510
IF(DAT(1).EQ.CHEM) GO TO 240	READ 515
IF(DAT(1).EQ.CNAME) GO TO 520	READ 520
IF(DAT(1).EQ.THER) THERM=.TRUE.	READ 525
IF(DAT(1).EQ.THER.AND.TEST15) GO TO 760	READ 530
WRITE(6,140)	READ 535
140 FORMAT('0','THE LAST CARD HAS AN UNRECONIZABLE CODE')	READ 540
TEST20=.TRUE.	READ 545
GO TO 60	READ 550
C	READ 555
C THIS SECTION READS THE NOTE CARDS FOR EACH REACTION. THE FIRST TWO	READ 560
C ITEMS ON EACH NOTE CARD ARE IN I2 FORMAT. THE FIRST NUMBER IS THE	READ 565
C NUMBER OF THE CARD FOR THIS REACTION (1, 2, UP TO 5 FOR EACH REACTION)	READ 570
C THE SECOND IS THE NUMBER OF THE CHEMICAL REACTION (UP TO 10). THE	READ 575
C REMAINDER OF THE CARD IS IN A4 FORMAT AND IS USED FOR THE COMMENTS.	READ 580

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C
160 READ(5,180) CARD,STEP,(DAT(I),I=1,19)
180 FORMAT(2I2,19A4)
WRITE(6,200) CARD,STEP,(DAT(I),I=1,19)
200 FORMAT(' ',2I2,19A4)
IF(CARD.EQ.0) GO TO 60
LNOTE(STEP)=CARD*19
DO 220 I=1,19
J=((CARD-1)*19)+I
220 NNOTE(STEP,J)=DAT(I)
GO TO 160

C
C THIS SECTION READS AND PROCESSES THE CHEMICAL REACTION CARDS.
C*****THESE CARDS MUST COME BEFORE THE NAMELISTS*****
C
240 READ(5,260) STEP,(DAT(I),I=1,17)
260 FORMAT(12,2A4,*(A2,F3.0),A1,F9.4,A1,4F8.3,7X)
WRITE(6,280) STEP,(DAT(I),I=1,17)
280 FORMAT(' ',12,2A4,4(A2,F3.0),A1,F9.4,A1,4F8.3,7X)
IF(DAT(1).EQ.BLANK) GO TO 500
IF(DAT(1).EQ.REAC) GO TO 320
IF(DAT(1).EQ.PROD) GO TO 420
WRITE(6,300)
300 FORMAT('0','CODE FOR THIS CARD IS IN ERROR')
TEST20=.TRUE.
GO TO 120
320 K=NREACT(STEP) + 1
NREACT(STEP)=K
DO 340 I=1,4
RATOM(STEP,K,I)=DAT(2*I+1)
340 RATCO(STEP,K,I)=DAT(2*I+2)
IF(STEP.GI.NR) NR=STEP
DO 360 I=1,4
NRXNS=NR
AREACT(STEP,K)=DAT(12)
IF(DAT(14).EQ.0.0) DAT(14)=AREACT(STEP,K)
360 RATIO(STEP,K,I)=DAT(I+13)
380 STOICK(STEP,K)=AREACT(STEP,K)
IF(DAT(13).EQ.BA) BASE(STEP)=K
FAZER(STEP,K)=DAT(11)
IF(NRATIO(STEP).GE.1) GO TO 240
DO 400 I=1,4
400 IF(RATIO(STEP,K,I).NE.0.0) NRATIO(STEP)=NRATIO(STEP)+1
GO TO 240
420 KK=NPROD(STEP)+1
NPROD(STEP)=KK
DO 440 I=1,4
PATOM(STEP,KK,I)=DAT(2*I+1)
440 PATCO(STEP,KK,I)=DAT(2*I+2)
FAZER(STEP,KK)=DAT(11)
APROD(STEP,KK)=DAT(12)
DO 460 I=1,4
460 TPHASE(STEP,KK,I)=DAT(I+13)
480 STOICP(STEP,KK)=APROD(STEP,KK)
GO TO 240
500 CONTINUE
TEST15=.TRUE.
GO TO 60

```

```

READ 585
READ 590
READ 595
READ 600
READ 605
READ 610
READ 615
READ 620
READ 625
READ 630
READ 635
READ 640
READ 645
READ 650
READ 655
READ 660
READ 665
READ 670
READ 675
READ 680
READ 685
READ 690
READ 695
READ 700
READ 705
READ 710
READ 715
READ 720
READ 725
READ 730
READ 735
READ 740
READ 745
READ 750
READ 755
READ 760
READ 765
READ 770
READ 775
READ 780
READ 785
READ 790
READ 795
READ 800
READ 805
READ 810
READ 815
READ 820
READ 825
READ 830
READ 835
READ 840
READ 845
READ 850
READ 855
READ 860
READ 865
READ 870

```

```

C THIS SECTION READS THE NAMELISTS.
520 IF(.NOT.TEST15) GO TO 720
    DO 700 I=1,NK
    DO 560 K=1,10
        T(K)=0.0
        PRES(K)=1.0
        DO 540 J=1,4
540 EP(K,J)=0.0
560 CONTINUE
        READ(5,NAM1)
        WRITE(6,NAM1)
        IF(EFF.GT.0.0) EFEL=EFF
        DO 620 J=1,10
        DO 580 K=1,4
            EPS1(STEP,J,K)=EP(J,K)
            IF(EPS1(STEP,J,K).NE.0.0) TEST1(STEP)=.TRUE.
580 CONTINUE
            IF(1.EQ.1) GO TO 600
            IF(T(J).EQ.0.0.AND.(J-1).NE.NOTEMP) GO TO 640
600 IF(T(J).EQ.0.0.AND.1.EQ.1) NOTEMP=J-1
            IF(T(J).EQ.0.0) GO TO 680
            IF(PRES(J).LE.0.0) PRES(J)=1.0
            P(STEP,J,1)=PRES(J)
            P(STEP,J,2)=PRES(J)
            TEMP1(STEP,J)=T(J)
620 TEMP2(STEP,J)=T(J)
            NOTEMP=10
            GO TO 680
640 WRITE(6,660) STEP
660 FORMAT('1', 'ERROR IN NUMBER OF TEMPERATURES FOR STEP',12)
            TEST2=.TRUE.
680 CONTINUE
700 CONTINUE
            GO TO 60
720 WRITE(6,740)
740 FORMAT(' ', 'DATA CARDS ARE OUT OF ORDER, NAMELISTS MUST BE AFTER
    1REACTION CARDS')
            TEST2=.TRUE.
            GO TO 60
760 CONTINUE

C
C THIS SECTION CHECKS TO SEE IF THE REACTIONS ARE BALANCED.
C
    DO 980 NRX=1,NR
    NPR=NREACT(NRX)
    DO 840 I=1,NPR
        IF(RATOM(NRX,1,1).EQ.HYD.AND.RATOM(NRX,1,2).EQ.BLANK) TRY=TRY-
        1STOICR(NRX,1)
    DO 820 J=1,4
        IF(RATOM(NRX,1,J).EQ.BLANK) GO TO 840
        IF(1.EQ.1.AND.J.EQ.1) GO TO 800
    DO 780 N=1,NN
        IF(RATOM(NRX,1,J).NE.DAT(N)) GO TO 780
        T(N)=T(N)+RATCO(NRX,1,J)*STOICR(NRX,1)
        GO TO 820
780 CONTINUE
    NN=NN+1
    DAT(NN)=RATOM(NRX,1,J)

```

```

READ 875
READ 880
READ 885
READ 890
READ 895
READ 900
READ 905
READ 910
READ 915
READ 920
READ 925
READ 930
READ 935
READ 940
READ 945
READ 950
READ 955
READ 960
READ 965
READ 970
READ 975
READ 980
READ 985
READ 990
READ 995
READ1000
READ1005
READ1010
READ1015
READ1020
READ1025
READ1030
READ1035
READ1040
READ1045
READ1050
READ1055
READ1060
READ1065
READ1070
READ1075
READ1080
READ1085
READ1090
READ1095
READ1100
READ1105
READ1110
READ1115
READ1120
READ1125
READ1130
READ1135
READ1140
READ1145
READ1150
READ1155
READ1160

```

T(NN)=RATCO(NRX,I,J)*STOICR(NRX,I)	READ1165
GO TO 820	READ1170
800 NN=1	READ1175
DAT(1)=RATOM(NRX,1,1)	READ1180
T(1)=RATCO(NRX,1,1)*STOICR(NRX,1)	READ1185
820 CONTINUE	READ1190
840 CONTINUE	READ1195
NPP=NPROD(NRX)	READ1200
DO 920 I=1,NPP	READ1205
IF(PATOM(NRX,I,1).EQ.HYD.AND.PATOM(NRX,I,2).EQ.BLANK) TRY=TRY+	READ1210
1 STOICP(NRX,I)	READ1215
DO 900 J=1,4	READ1220
IF(PATOM(NRX,I,J).EQ.BLANK) GO TO 920	READ1225
DO 860 N=1,NN	READ1230
IF(PATOM(NRX,I,J).NE.DAT(N)) GO TO 860	READ1235
T(N)=T(N)-PATCO(NRX,I,J)*STOICP(NRX,I)	READ1240
GO TO 900	READ1245
860 CONTINUE	READ1250
WRITE(6,860) PATOM(NRX,I,J),NRX	READ1255
880 FORMAT('0','THE ELEMENT ',A2,' IS IN THE PRODUCTS OF REACTION',13,	READ1260
1', BUT IS NOT IN THE REACTANTS')	READ1265
IF(DRAW) TEST20=.TRUE.	READ1270
900 CONTINUE	READ1275
920 CONTINUE	READ1280
SMALL=0.00001	READ1285
DO 960 N=1,NN	READ1290
TAB=ABS(T(N))	READ1295
IF(TAB.LE.SMALL) GO TO 960	READ1300
WRITE(6,940) NRX,DAT(N)	READ1305
940 FORMAT('0','REACTION ',13,' IS NOT BALANCED IN REGARD TO THE ELEMENT',A2)	READ1310
IF(DRAW) TEST20=.TRUE.	READ1315
960 CONTINUE	READ1320
980 CONTINUE	READ1325
IF(.NOT.DRAW.OR.(TRY.GT.0.999.AND.TRY.LT.1.001)) GO TO 1060	READ1330
DO 1040 I=1,NKXNS	READ1335
NPR=NREACT(I)	READ1340
DO 1000 J=1,NPR	READ1345
AREACT(I,J)=AREACT(I,J)/TRY	READ1350
1000 STOICR(I,J)=AREACT(I,J)	READ1355
NPP=NPROD(I)	READ1360
DO 1020 J=1,NPP	READ1365
APROD(I,J)=APROD(I,J)/TRY	READ1370
1020 STOICP(I,J)=APROD(I,J)	READ1375
1040 CONTINUE	READ1380
1060 RETURN	READ1385
END	READ1390
	READ1395

SUBROUTINE FZ298	FZ29	5
DOUBLE PRECISION SUMPG, SUMRG, SUMPL, SUMRL	FZ29	10
INTEGER CARD, STEP, BASE	FZ29	15
LOGICAL TEST3, TEST4	FZ29	20
REAL NOTE, LIQUID	FZ29	25
DIMENSION BASE(10), NSATOM(50), SPEC(50,12), SPATOM(50,4), SPATCO(50,4)	FZ29	30
1), SPFAZE(50), KEYNOR(11,5), KEYNOP(11,5), KYNR(50), KYNP(50), IROUTE(50)	FZ29	35
2,2), TEMP1(50,10), TEMP2(50,10), TRANGE(2,50), TPHASE(11,5,4), AREACT(11,5,4)	FZ29	40
30,5), APROD(10,5), RATIO(10,5,4), NOTE(10,100), HSTOCR(50), HSTOCP(50)	FZ29	45
4NPROD(11), NREACT(11), NRATIO(10), LNOTE(10)	FZ29	50
COMMON/INDX/R, NR, NR1, NRXNS, NOTEMP, I, K, J, M, NRX, NTOT, BASE, NSATOM, NN	FZ29	55
COMMON/MATL1/SPEC, SPATOM, SPATCO, SPFAZE	FZ29	60
COMMON/MATL2/KEYNOR, KEYNOP, KYNR, KYNP, IROUTE	FZ29	65
COMMON/TEMP/TEMP1, TEMP2, TRANGE, TPHASE, TMID	FZ29	70
COMMON/MATL3/AREACT, APROD, RATIO, NOTE, HSTOCR, HSTOCP, NPROD, NREACT,	FZ29	75
INRATIO, LNOTE	FZ29	80
COMMON/PRESS/P(50,10,2)	FZ29	85
DATA GAS/1HG/, SOLID/1HS/, LIQUID/1HL/, BLANK/1H /	FZ29	90
WRITE(6,20)	FZ29	95
20 FORMAT('1', ' ')	FZ29	100
DO 200 I=1, NR	FZ29	105
IF(TEMP1(I,1).LE.301.) GO TO 180	FZ29	110
NPR=NREACT(I)	FZ29	115
DO 160 LL=1,2	FZ29	120
DO 140 J=1, NPR	FZ29	125
IF(LL.EQ.1) N=KEYNOR(I,J)	FZ29	130
IF(LL.EQ.2) N=KEYNOP(I,J)	FZ29	135
IF(SPFAZE(N).EQ.SOLID.AND.TRANGE(1,N).LE.301.) GO TO 140	FZ29	140
IF(SPFAZE(N).EQ.LIQUID.AND.TRANGE(1,N).LE.301.) GO TO 140	FZ29	145
NN=N	FZ29	150
TEST4=.FALSE.	FZ29	155
40 NN=NN-1	FZ29	160
IF(NN.EQ.0) GO TO 140	FZ29	165
TEST3=.FALSE.	FZ29	170
DO 60 K=1,4	FZ29	175
IF(SPATOM(N,1).EQ.SPATOM(NN,1).AND.SPATOM(N,2).EQ.BLANK.AND.SPATOM(N,2).EQ.BLANK.AND.SPATCO(N,1).NE.SPATCO(NN,1)) TEST3=.TRUE.	FZ29	180
IF(TEST3) GO TO 60	FZ29	185
IF(SPATOM(N,K).NE.SPATOM(NN,K).OR.SPATCO(N,K).NE.SPATCO(NN,K))	FZ29	190
1 GO TO 80	FZ29	200
60 CONTINUE	FZ29	205
TEST4=.FALSE.	FZ29	210
IF(SPFAZE(N).EQ.GAS) GO TO 120	FZ29	215
IF(TRANGE(1,NN).LE.301..AND.LL.EQ.1) KEYNOR(I,J)=NN	FZ29	220
IF(TRANGE(1,NN).LE.301..AND.LL.EQ.2) KEYNOP(I,J)=NN	FZ29	225
IF(TRANGE(1,NN).LE.301..AND.LL.EQ.1.AND.TEST3) AREACT(1,J)=(AREACT(1,J)+	FZ29	230
1(I,J)*SPATCO(N,1))/SPATCO(NN,1)	FZ29	235
IF(TRANGE(1,NN).LE.301..AND.LL.EQ.2.AND.TEST3) APROD(1,J)=(APROD(1,J)+	FZ29	240
1(J)*SPATCO(N,1))/SPATCO(NN,1)	FZ29	245
IF(TRANGE(1,NN).LE.301.) GO TO 140	FZ29	250
GO TO 40	FZ29	255
80 N1=NN+1	FZ29	260
IF(N.EQ.N1.AND.SPFAZE(N).EQ.GAS) TEST4=.TRUE.	FZ29	265
IF(SPATOM(N,2).NE.BLANK) TEST4=.FALSE.	FZ29	270
IF(TEST4) GO TO 40	FZ29	275
IF(SPFAZE(N1).NE.GAS) WRITE(6,100) 1, (SPEC(N,L), L=1,12)	FZ29	280
IF(LL.EQ.1) KEYNOR(1,J)=NN+1	FZ29	285
IF(LL.EQ.2) KEYNOP(1,J)=NN+1	FZ29	290

GO TO 140	FZ29 295
100 FORMAT(' ', 'IN REACTION ', I2, ' THE MATERIAL ', I2A1, ' HAS NOT BEEN	FZ29 300
1 EXACTLY MATCHED FOR ITS PHASE AT 298 K.')	FZ29 305
120 IF(TRAN(1,NN).LE.301..AND.TRAN(2,NN).GE.300..AND.LL.EQ.1)	FZ29 310
1 KEYNO(1,J)=NN	FZ29 315
IF(TRAN(1,NN).LE.301..AND.TRAN(2,NN).GE.300..AND.LL.EQ.2)	FZ29 320
1 KEYNO(1,J)=NN	FZ29 325
IF(SFAZE(NN).EQ.GAS) GO TO 40	FZ29 330
IF(TRAN(1,NN).LE.301..AND.TRAN(2,NN).GE.300.) GO TO 140	FZ29 335
IF(TRAN(2,NN).LT.301.) GO TO 140	FZ29 340
GO TO 40	FZ29 345
140 CONTINUE	FZ29 350
NPR=NPROD(1)	FZ29 355
160 CONTINUE	FZ29 360
180 TEMP1(1,1)=298.15	FZ29 365
TEMP2(1,1)=298.15	FZ29 370
P(1,1,1)=1.0	FZ29 375
P(1,1,2)=1.0	FZ29 380
200 CONTINUE	FZ29 385
RETURN	FZ29 390
END	FZ29 395

SUBROUTINE DATAS	DATA 5
C THIS SUBROUTINE FINDS THE NECESSARY DATA ON TAPE 4 FOR ALL SPECIES	DATA 10
C WITH THE SAME TYPE AND NUMBER OF ATOMS AS THOSE OF THE REACTANTS AND	DATA 15
C PRODUCTS IN THE CHEMICAL REACTIONS. IT READS IN THE DATA FOR ALL	DATA 20
C PHASES OF THESE SPECIES.	DATA 25
C	DATA 30
C	DATA 35
C****ALL DATA CARDS FOR A SPECIES MUST BE IN ASCENDING ORDER AS TO THEIR	DATA 40
C TEMPERATURE RANGES (GASE PHASE COMES LAST).*****	DATA 45
C	DATA 50
C EACH SET OF DATA READ IN IS ASSIGNED A SPECIES NUMBER FOR	DATA 55
C IDENTIFICATION PURPOSES. THE PROGRAM THEN MATCHES THE SPECIES FOUND	DATA 60
C TO THE PRODUCTS AND REACTANTS AND ASSIGNS THE NUMBER OF THE SPECIES	DATA 65
C TO THE KEYNOR(I,J) FOR THE REACTANT AND TO THE KEYNOP(I,J) FOR EACH	DATA 70
C PRODUCT. THESE KEYNUMBERS ARE USED FOR ALL FURTHER CALCULATIONS AND	DATA 75
C REFERENCES.	DATA 80
C	DATA 85
INTEGER BASE,A	DATA 90
REAL NOTE,MT,NNN,LIQUID	DATA 95
LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298	DATA 100
DOUBLE PRECISION HS,SS,GS,HTOT,COEF,SUML,SUMPG	DATA 105
DIMENSION DAT(13),MT(4),D(4)	DATA 110
DIMENSION BASE(10),NSATOM(50),SPEC(50,12),SPATOM(50,4),SPATCO(50,4)	DATA 115
1),SPFAZE(50),KEYNOR(11,5),KEYNOP(11,5),KYNR(50),KYNP(50),IROUTE(50)	DATA 120
1,2),TEMP1(50,10),TEMP2(50,10),TRANGE(2,50),TPHASE(11,5,4),HS(50,10)	DATA 125
2),SS(50,10),GS(50,10),HTOT(10),COEF(2,7,50),TEST1(10),AREACT(10,5)	DATA 130
3,APROD(10,5),NPROD(11),NREACT(11),NRATIO(10),RATIO(10,5,4),LNOTE(10)	DATA 135
40),NOTE(10,100),HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),	DATA 140
5STOICR(11,5),STOICP(11,5),RATOM(11,5,4),PATOM(11,5,4),RATCO(11,5,4)	DATA 145
6),PATCO(11,5,4)	DATA 150
COMMON/INDX/K,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN	DATA 155
COMMON/HATL1/SPEC,SPATOM,SPATCO,SPFAZE	DATA 160
COMMON/HATL2/KEYNOR,KEYNOP,KYNR,KYNP,IROUTE	DATA 165
COMMON/THP/TEMP1,TEMP2,TRANGE,TPHASE,TMID	DATA 170
COMMON/DOUBLE/HS,SS,GS,HTOT,COEF	DATA 175
COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298	DATA 180
COMMON/HATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,	DATA 185
1NRATIO,LNOTE	DATA 190
COMMON/FZE/SUML,SUMPG,SUMPS,FAZER,FAZEP,NGASP,NLIQP,NSOLP,NGASR,	DATA 195
1NLIQR,NSOLR	DATA 200
COMMON/FNAME/STOICR,STOICP,RATOM,PATOM,RATCO,PATCO	DATA 205
DATA EE/1HE/,NNN/1HN/,OD/1HD/,BLANK/1H /	DATA 210
DATA SOLID/1HS/,LIQUID/1HL/,GAS/1HG/	DATA 215
DATA HYD/1HH/,OXY/1HO/	DATA 220
DATA ZERO/2H00/,ZER01/2H0 /,ZER02/2H 0/	DATA 225
NR1=NR+1	DATA 230
NRXNS=NR	DATA 235
C	DATA 240
C THE PROGRAM FIRST SETS UP A DUMMY REACTION WITH OXYGEN AND HYDROGEN AS	DATA 245
C THE REACTANTS AND LIQUID WATER AS THE PRODUCT. THIS IS DONE SO THAT	DATA 250
C THE ROUTE SUBROUTINE WILL MATCH THESE MATERIALS.	DATA 255
C	DATA 260
NRXNS=NRXNS+1	DATA 265
NPROD(NRXNS)=1	DATA 270
NREACT(NRXNS)=2	DATA 275
RATOM(NRXNS,1,1)=HYD	DATA 280
RATOM(NRXNS,1,2)=BLANK	DATA 285
RATOM(NRXNS,1,3)=BLANK	DATA 290

RATOM(NRXNS,2,1)=OXY	DATA 295
RATOM(NRXNS,2,2)=BLANK	DATA 300
RATOM(NRXNS,2,3)=BLANK	DATA 305
RATCO(NRXNS,1,1)=2.0	DATA 310
RATCO(NRXNS,1,2)=0.0	DATA 315
RATCO(NRXNS,1,3)=0.0	DATA 320
RATCO(NRXNS,2,1)=2.0	DATA 325
RATCO(NRXNS,2,2)=0.0	DATA 330
RATCO(NRXNS,2,3)=0.0	DATA 335
PATOM(NRXNS,1,1)=HYD	DATA 340
PATOM(NRXNS,1,2)=UXY	DATA 345
PATOM(NRXNS,1,3)=BLANK	DATA 350
PATCO(NRXNS,1,1)=2.0	DATA 355
PATCO(NRXNS,1,2)=1.0	DATA 360
PATCO(NRXNS,1,3)=0.0	DATA 365
RATOM(NRXNS,1,4)=BLANK	DATA 370
RATOM(NRXNS,2,4)=BLANK	DATA 375
RATCO(NRXNS,1,4)=0.0	DATA 380
RATCO(NRXNS,2,4)=0.0	DATA 385
PATOM(NRXNS,1,4)=BLANK	DATA 390
PATCO(NRXNS,1,4)=0.0	DATA 395
FAZER(NRXNS,1)=GAS	DATA 400
FAZER(NRXNS,2)=GAS	DATA 405
FAZEP(NRXNS,1)=LIQUID	DATA 410
STOICR(NRXNS,1)=1.0	DATA 415
STOICR(NRXNS,2)=0.5	DATA 420
STOICP(NRXNS,1)=1.0	DATA 425
TPHASE(NR1,1,1)=0.0	DATA 430
TPHASE(NR1,1,2)=0.0	DATA 435
TPHASE(NR1,1,3)=273.15	DATA 440
TPHASE(NR1,1,4)=373.15	DATA 445
C	DATA 450
C IF SAME=.TRUE. IT MEANS THAT THE SAME SPECIES ARE TO BE USED AS IN THE	DATA 455
C PREVIOUS CYCLE AND THAT THERE IS NO NEED TO READ TAPE 4 AGAIN.	DATA 460
C THEREFORE THE PROGRAM TRANSFERS TO STATEMENT 540 TO MATCH THE SPECIES	DATA 465
C WITH THE PRODUCTS AND REACTANTS.	DATA 470
C	DATA 475
IF(SAME) GO TO 540	DATA 480
NSPEC=0	DATA 485
A=4	DATA 490
C	DATA 495
C IF THERM=.TRUE., THE THERMO DATA IS TO BE READ IN FROM THE CARD READER	DATA 500
C THE THERMO DATA FOLLOWS THE LAST BLANK CARD IN THE CARD INPUT FOR THE	DATA 505
C CYCLE AND FIRST CARD HAS 'THER' IN COLUMNS 1-4. THE LAST CARD MUST BE	DATA 510
C AN 'END' CARD	DATA 515
C	DATA 520
IF(THERM) A=5	DATA 525
IF(THERM) GO TO 40	DATA 530
REWIND 4	DATA 535
WRITE(6,20)	DATA 540
20 FORMAT('0',T10,'THERMO DATA FOUND ON TAPE 4')	DATA 545
GO TO 80	DATA 550
40 WRITE(6,60)	DATA 555
60 FORMAT('0',T10,'THERMO DATA READ IN FROM CARDS')	DATA 560
80 READ(A,100) TLW,TMID,THIGH	DATA 565
100 FORMAT(3F10.3,50X)	DATA 570
WRITE(6,120) TLW,TMID,THIGH	DATA 575
120 FORMAT(' ',3F10.3)	DATA 580

C		DATA 585
C	THE IDENTIFICATION CARD FOR A DATA SET ON TAPE 4 IS READ. THE TYPE	DATA 590
C	AND NUMBER OF ATOMS FOR THE SET IS COMPARED TO THE PRODUCTS AND	DATA 595
C	REACTANTS FOR A MATCH.	DATA 600
C	IF THERE IS A MATCH, THE DATA FOR ALL PHASES OF THE MATERIAL IS READ	DATA 605
C	IN AND ASSIGNED A SPECIES NUMBER.	DATA 610
C		DATA 615
140	READ(A,160) (DAT(I),I=1,12),DATE1,DATE2,(MT(J),D(J),J=1,4),DAT(13)	DATA 620
	1,T1,T2	DATA 625
160	FORMAT(12A1,6X,2A3,4(A2,F3.0),A1,2F10.3)	DATA 630
	IF(DAT(1).EQ.EE.AND.DAT(2).EQ.NNN.AND.DAT(3).EQ.DD) GO TO 540	DATA 635
	GO TO 220	DATA 640
180	READ(A,200) (DAT(I),I=1,12),DATE1,DATE2,(MT(J),D(J),J=1,4),DAT(13)	DATA 645
	1,T1,T2	DATA 650
200	FORMAT(///12A1,6X,2A3,4(A2,F3.0),A1,2F10.3)	DATA 655
	IF(DAT(1).EQ.EE.AND.DAT(2).EQ.NNN.AND.DAT(3).EQ.DD) GO TO 540	DATA 660
220	DO 320 I=1,NRXNS	DATA 665
	NPR=NPRG(I)	DATA 670
	DO 260 J=1,NPR	DATA 675
	DO 240 NN=1,4	DATA 680
	IF(MT(NN).EQ.ZERO.OR.MT(NN).EQ.ZERO1.OR.MT(NN).EQ.ZERO2)	DATA 685
	1 MT(NN)=BLANK	DATA 690
	IF(MT(NN).NE.PATUM(I,J,NN).OR.D(NN).NE.PATCU(I,J,NN)) GO TO 260	DATA 695
240	CONTINUE	DATA 700
	GO TO 340	DATA 705
260	CONTINUE	DATA 710
	NPR=NREACT(I)	DATA 715
	DO 300 J=1,NPR	DATA 720
	DO 280 NN=1,4	DATA 725
	IF(MT(NN).EQ.ZERO.OR.MT(NN).EQ.ZERO1.OR.MT(NN).EQ.ZERO2)	DATA 730
	1 MT(NN)=BLANK	DATA 735
	IF(MT(NN).NE.RATOM(I,J,NN).OR.D(NN).NE.RATCU(I,J,NN)) GO TO 300	DATA 740
280	CONTINUE	DATA 745
	GO TO 340	DATA 750
300	CONTINUE	DATA 755
320	CONTINUE	DATA 760
	GO TO 180	DATA 765
340	NSPEC=NSPEC+1	DATA 770
	WRITE(6,360) NSPEC,(DAT(I),I=1,12),DATE1,DATE2,(MT(J),D(J),J=1,4),	DATA 775
	1 DAT(13),T1,T2	DATA 780
360	FORMAT(' ',12,2X,12A1,6X,2A3,4(A2,F3.0),A1,2F10.3)	DATA 785
	NCOUNT=0	DATA 790
	DO 380 NN=1,12	DATA 795
	SPEC(NSPEC,NN)=DAT(NN)	DATA 800
	IF(DAT(NN).EQ.BLANK) NCOUNT=NCOUNT+1	DATA 805
	IF(DAT(NN).EQ.BLANK.AND.NCOUNT.EQ.1) NSATOM(NSPEC)=NN-1	DATA 810
380	CONTINUE	DATA 815
	IF(NCOUNT.EQ.0) NSATOM(NSPEC)=12	DATA 820
400	SPFAZE(NSPEC)=DAT(13)	DATA 825
	TRANGE(1,NSPEC)=T1	DATA 830
	TRANGE(2,NSPEC)=T2	DATA 835
	DO 420 NN=1,4	DATA 840
	SPATOM(NSPEC,NN)=MT(NN)	DATA 845
420	SPATCU(NSPEC,NN)=D(NN)	DATA 850
	READ(A,460) ((CDEF(K,KK,NSPEC),KK=1,7),K=1,2)	DATA 855
	WRITE(6,440) ((CDEF(K,KK,NSPEC),KK=1,7),K=1,2)	DATA 860
440	FORMAT(' ',4X,5E15.8,/5X,5E15.8,/5X,4E15.8)	DATA 865
460	FORMAT(5E15.8/5E15.8/4E15.8)	DATA 870

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      READ(A,160) (DAT(1),I=1,12),DATE1,DATE2,(MT(J),D(J),J=1,4),DA1(13) DATA 875
      1,T1,T2 DATA 880
      IF(DAT(1).EQ.EE.AND.DAT(2).EQ.NNN.AND.DAT(3).EQ.UU) GO TO 540 DATA 885
      DO 480 NN=1,4 DATA 890
      IF(MT(NN).EQ.ZERO.OR.MT(NN).EQ.ZERO1.OR.MT(NN).EQ.ZERO2) DATA 895
      1 MT(NN)=BLANK DATA 900
480 CONTINUE DATA 905
      IF(MT(2).EQ.BLANK.AND.SPATOM(NSPEC,2).EQ.BLANK) GO TO 520 DATA 910
      DO 500 NN=1,4 DATA 915
      IF(MT(NN).EQ.EE) GO TO 220 DATA 920
      IF(MT(NN).NE.SPATOM(NSPEC,NN).OR.D(NN).NE.SPATCO(NSPEC,NN)) GO TO DATA 925
      1 220 DATA 930
500 CONTINUE DATA 935
      GO TO 340 DATA 940
520 IF(MT(1).NE.SPATOM(NSPEC,1)) GO TO 220 DATA 945
      GO TO 340 DATA 950
C DATA 955
C THE PRODUCTS AND REACTANTS ARE NOW MATCHED TO THE SPECIES FOUND AND DATA 960
C THE NUMBER OF THE SPECIES IS ASSIGNED TO THEIR KEYNUP(I,J) OR DATA 965
C KEYNOR(I,J) RESPECTIVELY. I REFERS TO THE NUMBER OF THE REACTION AND DATA 970
C J REFERS TO THE NUMBER OF THE PRODUCT OR REACTANT OF THAT REACTION. DATA 975
C IF ANY PRODUCT OR REACTANT IS NOT MATCHED, AN ERROR MESSAGE IS PRINTED DATA 980
C AND THE PROGRAM SKIPS TO THE NEXT CYCLE. DATA 985
C DATA 990
540 DO 880 I=1,NRXNS DATA 995
      NPR=NREACT(I) DATA1000
      DO 700 J=1,NPR DATA1005
      MTLO=0 DATA1010
      MTUP=0 DATA1015
      MM=0 DATA1020
      DO 660 N=1,NSPEC DATA1025
      DO 560 NN=1,4 DATA1030
      IF(SPATOM(N,NN).NE.RATOM(I,J,NN).OR.SPATCO(N,NN).NE.RATCO(I,J,NN)) DATA1035
      1 GO TO 640 DATA1040
560 CONTINUE DATA1045
      IF(SPFAZE(N).NE.FAZER(I,J)) GO TO 640 DATA1050
      IF(FAZER(I,J).NE.SOLID) GO TO 620 DATA1055
      IF(TEMP1(1,1).GE.TRANGE(1,N).AND.TEMP1(I,1).LE.TRANGE(2,N)) DATA1060
      1 GO TO 620 DATA1065
      MM=MM+1 DATA1070
      IF(MM.GT.1) GO TO 580 DATA1075
      TLO=TRANGE(1,N) DATA1080
      MTLO=N DATA1085
      TUP=TRANGE(2,N) DATA1090
      MTUP=N DATA1095
      IF(N.EQ.NSPEC) GOTO 600 DATA1100
      GO TO 660 DATA1105
580 IF(TRANGE(1,N).LT.TLO) MTLO=N DATA1110
      IF(TRANGE(1,N).LT.TLO) TLO=TRANGE(1,N) DATA1115
      IF(TRANGE(2,N).GT.TUP) MTUP=N DATA1120
      IF(TRANGE(2,N).GT.TUP) TUP=TRANGE(2,N) DATA1125
      IF(N.EQ.NSPEC) GOTO 600 DATA1130
      GO TO 660 DATA1135
600 IF(MM.LT.1) GO TO 620 DATA1140
      IF(TEMP1(1,1).LT.TLO) KEYNOR(I,J)=MTLO DATA1145
      IF(TEMP1(1,1).GT.TUP) KEYNOR(I,J)=MTUP DATA1150
      GO TO 700 DATA1155
620 KEYNOR(I,J)=N DATA1160

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GO TO 700	DATA1165
640 IF(MM.GE.1) GO TO 600	DATA1170
660 CONTINUE	DATA1175
TEST20=.TRUE.	DATA1180
WRITE(6,860) 1,(RATOM(I,J,NN),RATCO(I,J,NN),NN=1,4)	DATA1185
680 FORMAT('0','FOR REACTION',I3,' THE FOLLOWING REACTANT HAS NOT BEEN	DATA1190
1 MATCHED TO THE DATA FOR THE SPECIES FOUND ON TAPE 4',/1X,4(A2,F3.	DATA1195
20))	DATA1200
700 CONTINUE	DATA1205
NPR=NPROD(1)	DATA1210
DO 860 J=1,NPR	DATA1215
MTLO=0	DATA1220
MTUP=0	DATA1225
MM=0	DATA1230
DO 820 N=1,NSPEC	DATA1235
DO 720 NN=1,4	DATA1240
IF(SPATOM(N,NN).NE.PATOM(1,J,NN).OR.SPATCO(N,NN).NE.PATCO(1,J,NN))	DATA1245
160 TO 800	DATA1250
720 CONTINUE	DATA1255
IF(SPEFAZE(N).NE.FAZEP(1,J)) GO TO 800	DATA1260
IF(FAZEP(1,J).NE.SOLID) GO TO 780	DATA1265
IF(TEMP1(1,1).GE.TRANGE(1,N).AND.TEMP1(1,1).LE.TRANGE(2,N))	DATA1270
1 GO TO 780	DATA1275
MM=MM+1	DATA1280
IF(MM.GT.1) GO TO 740	DATA1285
TLO = TRANGE(1,N)	DATA1290
MTLO=N	DATA1295
TUP=TRANGE(2,N)	DATA1300
MTUP=N	DATA1305
IF(N.EQ.NSPEC) GOTO 760	DATA1310
GO TO 820	DATA1315
740 IF(TRANGE(1,N).LT.TLO) MTLO=N	DATA1320
IF(TRANGE(1,N).LT.TLO) TLO=TRANGE(1,N)	DATA1325
IF(TRANGE(2,N).GT.TUP) MTUP=N	DATA1330
IF(TRANGE(2,N).GT.TUP) TUP=TRANGE(2,N)	DATA1335
GO TO 820	DATA1340
760 IF(MM.LT.1) GO TO 780	DATA1345
IF(TEMP1(1,1).LT.TLO) KEYNOP(1,J)=MTLO	DATA1350
IF(TEMP1(1,1).GT.TUP) KEYNOP(1,J)=MTUP	DATA1355
GO TO 860	DATA1360
780 KEYNOP(1,J)=N	DATA1365
GO TO 860	DATA1370
800 IF(MM.GE.1) GO TO 760	DATA1375
820 CONTINUE	DATA1380
TEST20=.TRUE.	DATA1385
WRITE(6,840) 1,(PATOM(I,J,NN),PATCO(1,J,NN),NN=1,4)	DATA1390
840 FORMAT('0','FOR REACTION',I3,' THE FOLLOWING PRODUCT HAS NOT BEEN	DATA1395
1 MATCHED TO THE DATA FOR THE SPECIES FOUND ON TAPE 4',/1X,4(A2,F3.	DATA1400
1))	DATA1405
860 CONTINUE	DATA1410
880 CONTINUE	DATA1415
RETURN	DATA1420
END	DATA1425

SUBROUTINE EQNS	EQNS	5
REAL NOTE	EQNS	10
INTEGER BASE	EQNS	15
DIMENSION NUM(8),RNUM(8),VARA(16),FMT(130)	EQNS	20
COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,1,N,J,M,NRX,NTOT,BASE(10),NSATOME	EQNS	25
1(50),NN	EQNS	30
COMMON/MATL1/SPEC(50,12),SPATOM(50,4),SPATCO(50,4),SPFAZE(50)	EQNS	35
COMMON/MATL2/KEYNOR(11,5),KEYNOP(11,5),KYNR(50),KYNP(50),	EQNS	40
1ROUTE(50,2)	EQNS	45
COMMON/MATL3/AREACT(10,5),APROD(10,5),RATIO(10,5,4),NOTE(10,100),	EQNS	50
1HSTOCR(50),HSTOCP(50),NPROD(11),NREACT(11),NRATIO(10),LNOTE(10)	EQNS	55
DATA VARA/'1','2','3','4','5','6','7','8','9','0','+', '-', '>', ' ',	EQNS	60
1'.,', ' /	EQNS	65
DO 20 K=1,NTOT	EQNS	70
20 FMT(K)=VARA(1+)	EQNS	75
K=NTOT	EQNS	80
NPR=NREACT(1)	EQNS	85
DO 140 J=1,NPR	EQNS	90
DIV=10	EQNS	95
LBEGIN=0	EQNS	100
MINUS=0	EQNS	105
LEND=0	EQNS	110
DO 40 L=1,7	EQNS	115
NUM(L)=(AREACT(1,J)/DIV)-MINUS	EQNS	120
IF(NUM(L).LT.0) NUM(L)=0	EQNS	125
MINUS=(MINUS+NUM(L))*10	EQNS	130
DIV=DIV/10.	EQNS	135
IF(NUM(L).NE.0.AND.LBEGIN.EQ.0) LBEGIN=L	EQNS	140
IF(LBEGIN.LE.2.AND.L.GE.6) NUM(L)=0	EQNS	145
LL=NUM(L)	EQNS	150
IF(NUM(L).EQ.0) LL=10	EQNS	155
RNUM(L)=VARA(LL)	EQNS	160
IF(NUM(L).NE.0) LEND=L	EQNS	165
40 CONTINUE	EQNS	170
IF(LBEGIN.GE.2) GO TO 60	EQNS	175
FMT(K)=RNUM(1)	EQNS	180
K=K+1	EQNS	185
60 FMT(K)=RNUM(2)	EQNS	190
IF(NUM(2).EQ.1.AND.LEND.EQ.2.AND.LBEGIN.EQ.2) K=K-1	EQNS	195
K=K+1	EQNS	200
IF(LEND.LE.2) GO TO 100	EQNS	205
FMT(K)=VARA(15)	EQNS	210
K=K+1	EQNS	215
DO 80 L=3,LEND	EQNS	220
FMT(K)=RNUM(L)	EQNS	225
80 K=K+1	EQNS	230
100 FMT(K)=VARA(14)	EQNS	235
K=K+1	EQNS	240
NB=KEYNOR(1,J)	EQNS	245
NRA=NSAIGM(NB)	EQNS	250
DO 120 L=1,NKA	EQNS	255
FMT(K)=SPEC(NB,L)	EQNS	260
120 K=K+1	EQNS	265
FMT(K)=VARA(14)	EQNS	270
IF(J.EQ.NREACT(1)) GO TO 140	EQNS	275
K=K+1	EQNS	280
FMT(K)=VARA(11)	EQNS	285
K=K+1	EQNS	290

FMT(K)=VARA(14)	EQNS 295
140 K=K+1	EQNS 300
DO 160 L=1,3	EQNS 305
FMT(K)=VARA(12)	EQNS 310
160 K=K+1	EQNS 315
FMT(K)=VARA(13)	EQNS 320
K=K+1	EQNS 325
FMT(K)=VARA(14)	EQNS 330
IF(K.GE.105) WRITE(6,180) (FMT(L),L=1,K)	EQNS 335
K=K+1	EQNS 340
180 FORMAT(' ',130A1)	EQNS 345
IF(K.GE.105) K=NTOT	EQNS 350
NPP=NPROD(1)	EQNS 355
DO 300 J=1,NPP	EQNS 360
DIV=10	EQNS 365
LBEGIN=0	EQNS 370
MINUS=0	EQNS 375
LEND=0	EQNS 380
DO 200 L=1,7	EQNS 385
NUM(L)=(APROD(1,J)/DIV)-MINUS	EQNS 390
IF(NUM(L).LT.0) NUM(L)=0	EQNS 395
MINUS=(MINUS+NUM(L))*10	EQNS 400
DIV=DIV/10.	EQNS 405
IF(NUM(L).NE.0.AND.LBEGIN.EQ.0) LBEGIN=L	EQNS 410
IF(LBEGIN.LE.2.AND.L.GE.6) NUM(L)=0	EQNS 415
LL=NUM(L)	EQNS 420
IF(NUM(L).EQ.0) LL=10	EQNS 425
RNUM(L)=VARA(LL)	EQNS 430
IF(NUM(L).NE.0) LEND=L	EQNS 435
200 CONTINUE	EQNS 440
IF(LBEGIN.GE.2) GO TO 220	EQNS 445
FMT(K)=RNUM(1)	EQNS 450
K=K+1	EQNS 455
220 FMT(K)=RNUM(2)	EQNS 460
IF(NUM(2).EQ.1.AND.LEND.EQ.2.AND.LBEGIN.EQ.2) K=K-1	EQNS 465
K=K+1	EQNS 470
IF(LEND.LE.2) GO TO 260	EQNS 475
FMT(K)=VARA(15)	EQNS 480
K=K+1	EQNS 485
DO 240 L=3,LEND	EQNS 490
FMT(K)=RNUM(L)	EQNS 495
240 K=K+1	EQNS 500
260 FMT(K)=VARA(14)	EQNS 505
K=K+1	EQNS 510
NB=KEYNOP(1,J)	EQNS 515
NRA=NSATUM(NB)	EQNS 520
DO 280 L=1,NRA	EQNS 525
FMT(K)=SPEC(NB,L)	EQNS 530
280 K=K+1	EQNS 535
FMT(K)=VARA(14)	EQNS 540
K=K+1	EQNS 545
FMT(K)=VARA(14)	EQNS 550
IF(J.EQ.NPROD(1)) GO TO 300	EQNS 555
FMT(K)=VARA(11)	EQNS 560
K=K+1	EQNS 565
FMT(K)=VARA(14)	EQNS 570
IF(K.GE.105) WRITE(6,180) (FMT(L),L=1,K)	EQNS 575
IF(K.GE.105) K=NTOT-1	EQNS 580
300 K=K+1	EQNS 585
FMT(K)=VARA(14)	EQNS 590
WRITE(6,180) (FMT(L),L=1,K)	EQNS 595
K=K+1	EQNS 600
RETURN	EQNS 605
END	EQNS 610

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SUBROUTINE CMATCH(M,C,COEF)
DOUBLE PRECISION C(2,6),COEF(2,7,50)
R=1.987165
DO 40 NN=1,2
C(NN,1)=COEF(NN,6,M)*R
DO 20 JJ=2,6
XJ=JJ-1
JJ1=JJ-1
20 C(NN,JJ)=COEF(NN,JJ1,M)*R/XJ
40 CONTINUE
RETURN
END

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CMAT 5
CMAT 10
CMAT 15
CMAT 20
CMAT 25
CMAT 30
CMAT 35
CMAT 40
CMAT 45
CMAT 50
CMAT 55
CMAT 60

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SUBROUTINE CPHSG	CPHS 5
REAL NOTE	CPHS 10
LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298	CPHS 15
INTEGER BASE	CPHS 20
DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF	CPHS 25
DIMENSION BASE(10),NSATOM(50),TEMP1(50,10),TEMP2(50,10),TEST1(10),CPHS	30
1TRANGE(2,50),TPHASE(11,5,4),HS(50,10),SS(50,10),GS(50,10),HTOT(10)CPHS	35
2,COEF(2,7,50)	CPHS 40
COMMON/MATL1/SPEC(50,12),SPATOM(50,4),SPATCO(50,4),SPFAZE(50)	CPHS 45
COMMON/PRESS/P(50,10,2)	CPHS 50
COMMON/INDX/R,NR,NR1,NRXNS,MOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN	CPHS 55
COMMON/IND1/AFACT,TT,TLN	CPHS 60
COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID	CPHS 65
COMMON/DOUBL/HS,SS,GS,HTOT,COEF	CPHS 70
COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298	CPHS 75
DATA GAS/1HG/	CPHS 80
IF(K.EQ.1) GO TO 20	CPHS 85
IF(TEMP1(NRX,K).EQ.TEMP1(NRX,K-1).AND.TEMP2(NRX,K).EQ.TEMP2(NRX,K-CPHS	90
11).AND.P(NRX,K,1).EQ.P(NRX,K-1,1).AND.P(NRX,K,2).EQ.P(NRX,K-1,2))	CPHS 95
2 GO TO 80	CPHS 100
20 N=1	CPHS 105
IF(AFACT.LT.0.0) N=2	CPHS 110
PL=ALOG(P(NRX,K,N))	CPHS 115
IF(SPFAZE(N).NE.GAS) PL=0.0	CPHS 120
L=1	CPHS 125
IF(TT.LE.TMID) L=2	CPHS 130
IF(COEF(L,1,M).NE.0.0) GO TO 60	CPHS 135
WRITE(6,40) NRX	CPHS 140
40 FORMAT(' ', 'ERROR IN COEFFICIENTS FOR ONE OF THE COMPONENTS IN REACPHS	145
CTION ',12)	CPHS 150
TEST20=.TRUE.	CPHS 155
RETURN	CPHS 160
60 S=((((COEF(L,5,M)/4.)*TT+COEF(L,4,M)/3.)*TT+COEF(L,3,M)/2.)*TT+	CPHS 165
1COEF(L,2,M))*TT+COEF(L,1,M)*TLN+COEF(L,7,M)-PL)*R	CPHS 170
H=((((COEF(L,5,M)/5.)*TT+COEF(L,4,M)/4.)*TT+COEF(L,3,M)/3.)	CPHS 175
1*TT+COEF(L,2,M)/2.)*TT+COEF(L,1,M)+COEF(L,6,M)/TT)*R*TT	CPHS 180
G=H-TT*S	CPHS 185
SS(NRX,K)=SS(NRX,K)+S*AFACT	CPHS 190
HS(NRX,K)=HS(NRX,K)+H*AFACT	CPHS 195
GS(NRX,K)=GS(NRX,K)+G*AFACT	CPHS 200
GO TO 100	CPHS 205
80 SS(NRX,K)=SS(NRX,K-1)	CPHS 210
HS(NRX,K)=HS(NRX,K-1)	CPHS 215
GS(NRX,K)=GS(NRX,K-1)	CPHS 220
100 CONTINUE	CPHS 225
RETURN	CPHS 230
END	CPHS 235

	SUBROUTINE REMOVE	REMO 5
C	*****	REMO 10
C	THIS SUBROUTINE CALCULATES THE WORK OF SEPARATION	REMO 15
C	*****	REMO 20
	INTEGER BASE	REMO 25
	REAL NOTE	REMO 30
	DOUBLE PRECISION HS,SS,GS,HTOT,COEF	REMO 35
	DOUBLE PRECISION XREACT,XPROD,SUMW,GASSUM	REMO 40
	DOUBLE PRECISION SUMP, SUMRG, SUMPL, SUMRL	REMO 45
	LOGICAL TEST3	REMO 50
	LOGICAL TEST1,TEST2,TEST20,PLINE,DRAW,SAME,THERM,H298	REMO 55
	DIMENSION SPATUM(50,4),SPATCO(50,4),SPFAZE(50)	REMO 60
	DIMENSION TEST3(10),RMOLES(10,4,10,6),XPROD(10),WORKG(10,6,4),	REMO 65
	WGMAX(4),WGMIN(4),WGMAX(10,10),WGMIN(10,10),EPSI(10,10,4),	REMO 70
	ZPEQ(10,10),FMUL(10),TOTMOL(10,10),WORKC(50),GRMOL(10),TEST2(10)	REMO 75
	DIMENSION BASE(10),NSATOM(50),SPEC(50,12),KEYNOR(11,5),KEYNUP(11,5)	REMO 80
	1),KYNR(50),KYNP(50),1ROUTE(50,2),TEMP1(50,10),TEMP2(50,10),	REMO 85
	ZTRANGE(2,50),TPHASE(11,5,4),HS(50,10),SS(50,10),GS(50,10),	REMO 90
	3HTOT(10),COEF(2,7,50),TEST1(10),AREACT(10,5),APROD(10,5),NPROD(11)	REMO 95
	4,NREACT(11),NRATIO(10),RATIO(10,5,4),LNOTE(10),NOTE(10,100),	REMO 100
	5HSTOCR(50),HSTOCP(50),FAZER(11,5),FAZEP(11,5),HIM(10),HAM(10)	REMO 105
	COMMON/PRESS/P(50,10,2)	REMO 110
	COMMON/INDX/R,NK,NR1,NRXNS,NOTEMP,1,K,J,M,NRX,NTOT,BASE,NSATOM,NN	REMO 115
	COMMON/MATL1/SPEC,SPATOM,SPATCO,SPFAZE	REMO 120
	COMMON/MATL2/KEYNOR,KEYNUP,KYNR,KYNP,1ROUTE	REMO 125
	COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID	REMO 130
	COMMON/DOUBLE/HS,SS,GS,HTOT,COEF	REMO 135
	COMMON/LOGIC/PLINE,TEST20,DRAW,SAME,TEST1,THERM,H298	REMO 140
	COMMON/MATL3/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,	REMO 145
	1NRATIO,LNOTE	REMO 150
	COMMON/FZE/SUMPL,SUMP,SUMPS,FAZER,FAZEP,NGASP,NLIQ,NSOLP,NGASR,	REMO 155
	1NLIQ,NSOLP	REMO 160
	COMMON/WORK/HIX,HAM,EPSI,EFEL	REMO 165
	COMMON/DIABLE/WGMIN,HST(10,10),HO(11)	REMO 170
	DATA LINE/'I',GAS/IHG/,PLIQ/IHL/,SOL/IHS/	REMO 175
	IF(NGASP.EQ.1.AND.NGASR.EQ.0) GO TO 260	REMO 180
	IF(NGASR.GT.0.AND.NGASP.EQ.0) GO TO 340	REMO 185
	IF(K.EQ.1) GO TO 20	REMO 190
	IF(TEMP1(1,K).EQ.TEMP1(1,K-1)) GO TO 220	REMO 195
	20 TEST3(1)=.FALSE.	REMO 200
	JJ=NRATIO(1)	REMO 205
	IF(NGASP.EQ.0.AND.NGASR.EQ.0) GO TO 860	REMO 210
C		REMO 215
C	THE MOLES OF ALL REACTANTS IN THE RECYCLE STREAM ARE CALCULATED AND	REMO 220
C	SUMMED ACCORDING TO THEIR PHASE.	REMO 225
C		REMO 230
	DO 200 J=1,JJ	REMO 235
	DU 160 NN=1,6	REMO 240
	SUMRG=0.	REMO 245
	SUMRL=0.	REMO 250
	SUMRS=0.	REMO 255
	FR=NN	REMO 260
	E1=EPSI(1,K,J)*(1.1-0.1*FR)	REMO 265
	NPN=NREACT(1)	REMO 270
	IBASE=BASE(1)	REMO 275
	DO 60 M=1,NPN	REMO 280
	RMOLES(1,J,M,NN)=(AREACT(1,IBASE) *RATIO(1,M,J)/RATIO(1,IBASE,J)	REMO 285
	1-EI*AREACT(1,M))/E1	REMO 290

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      IF(RMOLES(I,J,M,NN).LT.-0.0001) WRITE(6,40) J REMO 295
      IF(RMOLES(I,J,M,NN).LT.-0.0001) RETURN REMO 300
40  FORMAT(' ',15X,'**ERROR** THE MOLE FRACTION OF ONE OF THE REACTANTREMO 305
      IS IN THE FINAL REACTION MIXTURE IS NEGATIVE FOR RATIO SET',12,/25XREMO 310
      2,'CHECK THE EPSILON FOR THIS SET OF RATIOS.') REMO 315
      IF(RMOLES(I,J,M,NN).GE.1000.) TEST3(1)=.TRUE. REMO 320
      IF(FAZER(I,M).EQ.GAS) SUMRG=SUMRG+RMOLES(I,J,M,NN) REMO 325
      IF(FAZER(I,M).EQ.PLIQ) SUMRL=SUMRL+RMOLES(I,J,M,NN) REMO 330
      IF(FAZER(I,M).EQ.SOL) SUMRS=SUMRS+RMOLES(I,J,M,NN) REMO 335
      IF(FAZER(I,M).NE.GAS.AND.FAZER(I,M).NE.PLIQ.AND.FAZER(I,M).NE.SOL)REMO 340
1  GO TO 780 REMO 345
60  CONTINUE REMO 350
      NPN=NPRUD(I) REMO 355
      GASSUM=SUMPG+SUMRG REMO 360
      XRLACT=SUMRG/GASSUM REMO 365
      IF(XREACT.EQ.0.0) GO TO 80 REMO 370
      SUMW=SUMRG*DLOG(XREACT) REMO 375
      GO TO 100 REMO 380
80  SUMW=0.0 REMO 385
100 DO 120 M=1,NPN REMO 390
      IF(FAZER(I,M).NE.GAS) GO TO 120 REMO 395
      XPROD(M)=APRUD(I,M)/GASSUM REMO 400
      SUMW=SUMW+APRUD(I,M)*DLOG(XPROD(M)) REMO 405
120 CONTINUE REMO 410
      WORKG(I,NN,J)=-(SUMW*R*TEMP1(I,K))/1000. REMO 415
      IF((WORKG(I,NN,J)*1000.).LT.GS(I,K)) GO TO 820 REMO 420
      IF(NN.NE.1) GO TO 140 REMO 425
      WGMAX1(J)=WORKG(I,NN,J) REMO 430
      WGMIN1(J)=WORKG(I,NN,J) REMO 435
      GO TO 160 REMO 440
140 IF(WORKG(I,NN,J).GT.WGMAX1(J)) WGMAX1(J)=WORKG(I,NN,J) REMO 445
      IF(WORKG(I,NN,J).LT.WGMIN1(J)) WGMIN1(J)=WORKG(I,NN,J) REMO 450
160 CONTINUE REMO 455
      IF(J.NE.1) GO TO 180 REMO 460
      WGMAX(I,K)=WGMAX1(J) REMO 465
      WGMIN(I,K)=WGMIN1(J) REMO 470
      GO TO 200 REMO 475
180 IF(WGMAX1(J).GT.WGMAX(I,K)) WGMAX(I,K)=WGMAX1(J) REMO 480
      IF(WGMIN1(J).LT.WGMIN(I,K)) WGMIN(I,K)=WGMIN1(J) REMO 485
200 CONTINUE REMO 490
      HIM(K)=WGMIN(I,K)*1000.+HIM(K) REMO 495
      HAM(K)=WGMAX(I,K)*1000.+HAM(K) REMO 500
      GO TO 400 REMO 505
220 CONTINUE REMO 510
      DO 240 J=1,JJ REMO 515
240 EPS1(I,K,J)=EPS1(I,K-1,J) REMO 520
      WGMIN(I,K)=WGMIN(I,K-1) REMO 525
      WGMAX(I,K)=WGMAX(I,K-1) REMO 530
      HIM(K)=WGMIN(I,K-1)*1000.+HIM(K) REMO 535
      HAM(K)=WGMAX(I,K-1)*1000.+HAM(K) REMO 540
      GO TO 400 REMO 545
C REMO 550
C THIS SECTION DEALS WITH THE SITUATION WHERE THERE IS A SINGLE GASEOUS REMO 555
C PRODUCT AND NO GASEOUS REACTANTS. IT IS ASSUMED THAT THE REACTION CAN REMO 560
C BE DRIVEN TO COMPLETION BY KEEPING THE PRESSURE IN THE REACTOR BELOW REMO 565
C THE EQUILIBRIUM PRESSURE FOR THE REACTION. THIS SECTION CALCULATES REMO 570
C THIS EQUILIBRIUM PRESSURE. REMO 575
C THE WORK OF THE REACTION IS EQUAL TO THE FREE ENERGY CHANGE IF IT IS REMO 580

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C POSITIVE.	REMO 585
C	REMO 590
260 NPN=NPROD(I)	REMO 595
DO 280 NPR=1,NPN	REMO 600
IF(FAZER(1,NPR).NE.GAS) GO TO 280	REMO 605
SG=GS(I,K)	REMO 610
PEQ(I,K)= EXP((-SG)/(R*TEMP1(I,K)*APROD(I,NPR)))	REMO 615
GO TO 300	REMO 620
280 CONTINUE	REMO 625
300 P(I,K,1)=PEQ(I,K)	REMO 630
P(I,K,2)=PEQ(I,K)	REMO 635
WORKC(I)= GS(I,K)/1000.	REMO 640
IF(WORKC(I).LT.0.0) WORKC(I)=0.0	REMO 645
HIM(K)=HIM(K)+WORKC(I) *1000.	REMO 650
HAM(K)=HAM(K)+ WORKC(I) *1000.	REMO 655
WGMIN(I,K)=WORKC(I)	REMO 660
WRITE(6,320) PEQ(I,K),WORKC(I)	REMO 665
320 FORMAT(' ',T33.97(' '),/' ',T33,'* THE EQUILIBRIUM PRESSURE FOR	REMO 670
THIS REACTION = ',E16.6,/T33,'* THE WORK OF SEPARATION = ',F8.4,	REMO 675
2/' ',T33.97(' '),)	REMO 680
GO TO 900	REMO 685
C	REMO 690
C THIS SECTION CALCULATES THE WORK OF SEPARATION FOR THE CASE WHERE	REMO 695
C THERE ARE ONE OR MORE GASEOUS REACTANTS AND NO GASEOUS PRODUCTS.	REMO 700
C	REMO 705
340 NPN=NREACT(I)	REMO 710
SUMA=0.0	REMO 715
DO 360 NPR=1,NPN	REMO 720
IF(FAZER(1,NPR).NE.GAS) GO TO 360	REMO 725
SUMA=SUMA+AREACT(I,NPR)	REMO 730
360 CONTINUE	REMO 735
PIENU=0.0	REMO 740
DO 380 NPR=1,NPN	REMO 745
IF(FAZER(1,NPR).NE.GAS) GO TO 380	REMO 750
FRMOL(NPR)=AREACT(I,NPR)/SUMA	REMO 755
PIENU=AREACT(I,NPR)**FRMOL(NPR)+PIENU	REMO 760
380 CONTINUE	REMO 765
SG=GS(I,K)	REMO 770
PEQ(I,K)=SUMA* EXP(SG/(R*TEMP1(I,K)*SUMA))/PIENU	REMO 775
IF(P(I,K,1).LT.PEQ(I,K)) P(I,K,1)=2.*PEQ(I,K)	REMO 780
P(I,K,2)=P(I,K,1)	REMO 785
TOTMOL(I,K)=(PEQ(I,K)/P(I,K,1))*SUMA*(1.-PEQ(I,K)/P(I,K,1))	REMO 790
WORKC(I)= GS(I,K)/1000.	REMO 795
IF(WORKC(I).LT.0.0) WORKC(I)=0.0	REMO 800
HIM(K)=HIM(K)+WORKC(I) *1000.	REMO 805
HAM(K)=HAM(K)+WORKC(I) *1000.	REMO 810
WGMIN(I,K)=WORKC(I)	REMO 815
WRITE(6,320) PEQ(I,K),WORKC(I)	REMO 820
GO TO 900	REMO 825
C	REMO 830
C THIS SECTION PRINTS THE OUTPUT FOR THE WORK OF SEPARATION	REMO 835
C	REMO 840
400 NPN=NREACT(I)	REMO 845
IF(TEST3(I)) GO TO 600	REMO 850
IF(NPN.GT.1) GO TO 440	REMO 855
NB=KEYNOR(1,1)	REMO 860
WRITE(6,460)	REMO 865
WRITE(6,420) EPS1(I,K,1),(SPEC(NB,I1),I1=1,12) ,RATIO(I,1,1),	REMO 870

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1(RMOLES(1,1,1,NN),NN=1,6),(WORKG(I,NN,1),NN=1,6) REMO 875
420 FORMAT(' ',F9.5,1X,12A1,F9.3,'*',6F8.3,'*',6F8.3,/' ',T33,'*',48(' REMO 880
1-'),'*',48('1-')) REMO 885
GO TO 900 REMO 890
440 JJ=NRATIO(1) REMO 895
NPN1=NPN-1 REMO 900
WRITE(6,460) REMO 905
460 FORMAT(' ',T33,'*',48('1-'),'*',48('1-')) REMO 910
DO 580 J=1,JJ REMO 915
NB=KEYNOR(1,1) REMO 920
WRITE(6,460) EPS1(I,K,J),(SPEC(NB,II),II=1,12),RATIO(I,1,J), REMO 925
1(RMOLES(1,J,1,NN),NN=1,6) REMO 930
480 FORMAT(' ',F9.5,1X,12A1,F9.3,'*',6F8.3,'*') REMO 935
IF(NPN.EQ.2) GO TO 540 REMO 940
DO 500 M=2,NPN1 REMO 945
NB=KEYNOR(1,M) REMO 950
500 WRITE(6,520) (SPEC(NB,II),II=1,12),RATIO(I,M,J),(RMOLES(1,J,M,NN) REMO 955
1),NN=1,6) REMO 960
520 FORMAT(' ',10X,12A1,F9.3,'*',6F8.3,'*') REMO 965
540 NB=KEYNOR(1,NPN) REMO 970
WRITE(6,560) (SPEC(NB,II),II=1,12),RATIO(I,NPN,J),(RMOLES(1,J, REMO 975
1,NPN,NN),NN=1,6),(WORKG(I,NN,J),NN=1,6) REMO 980
560 FORMAT(' ',10X,12A1,F9.3,'*',6F8.3,'*',6F8.3) REMO 985
580 CONTINUE REMO 990
WRITE(6,460) REMO 995
GO TO 900 REMO1000
600 IF(NPN.GT.1) GO TO 640 REMO1005
NB=KEYNOR(1,1) REMO1010
WRITE(6,460) REMO1015
WRITE(6,620) EPS1(1,K,1),(SPEC(NB,II),II=1,12),RATIO(1,1,1), REMO1020
1(RMOLES(1,1,1,NN),NN=1,6),(WORKG(1,NN,1),NN=1,6) REMO1025
620 FORMAT(' ',E9.3,1X,12A1,F9.3,'*',6E8.1,'*',6F8.2,/' ',T33,'*',4 REMO1030
18('1-'),'*',48('1-')) REMO1035
GO TO 900 REMO1040
640 JJ=NRATIO(1) REMO1045
NPN1=NPN-1 REMO1050
WRITE(6,460) REMO1055
DO 760 J=1,JJ REMO1060
NB=KEYNOR(1,1) REMO1065
WRITE(6,660) EPS1(1,K,J),(SPEC(NB,II),II=1,12),RATIO(1,1,J), REMO1070
1(RMOLES(1,J,1,NN),NN=1,6) REMO1075
660 FORMAT(' ',E9.3,1X,12A1,F9.3,'*',6E8.1,'*') REMO1080
IF(NPN.EQ.2) GO TO 720 REMO1085
DO 680 M=2,NPN1 REMO1090
NB=KEYNOR(1,M) REMO1095
680 WRITE(6,700) (SPEC(NB,II),II=1,12),RATIO(1,M,J),(RMOLES(1,J,M,NN) REMO1100
1),NN=1,6) REMO1105
700 FORMAT(' ',10X,12A1,F9.3,'*',6E8.1,'*') REMO1110
720 NB=KEYNOR(1,NPN) REMO1115
WRITE(6,740) (SPEC(NB,II),II=1,12),RATIO(1,NPN,J), REMO1120
1(RMOLES(1,J,NPN,NN),NN=1,6),(WORKG(1,NN,J),NN=1,6) REMO1125
740 FORMAT(' ',10X,12A1,F9.3,'*',6E8.1,'*',6F8.2) REMO1130
760 CONTINUE REMO1135
WRITE(6,460) REMO1140
GO TO 900 REMO1145
780 WRITE(6,800) REMO1150
800 FORMAT(' ', "PHASE OF A COMPONENT HAS BEEN INCORRECTLY READ IN REMO1155
1 SUBROUTINE REMOVE") REMO1160

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TEST20=.TRUE.	REMO1165
GO TO 900	REMO1170
820 WRITE(6,840) GS(1,K)	REMO1175
840 FORMAT(' ',T33,97(' '),/ ' ',T33,'* THE CALCULATED WORK OF SEPARATION	REMO1180
FOR THE GASES IS LESS THAN DELTA-G,*,/T33,'* THE EQUILIBRIUM PURE	REMO1185
2INT FOR THIS REACTION IS PROBABLY IN ERROR,*,/T33,'* THE WORK OF SEPARATION	REMO1190
IS TAKEN TO BE EQUAL TO DELTA-G,*,/T33,'* WORK= ',-3PF1	REMO1195
40.3,' KCAL',/T33,97(' '))	REMO1200
HIM(K)=HIM(K)+ GS(1,K)	REMO1205
HAM(K)=HAM(K)+ GS(1,K)	REMO1210
WGMIN(1,K)=GS(1,K)/1000.	REMO1215
GO TO 900	REMO1220
860 CONTINUE	REMO1225
WORKC(1)= GS(1,K)/1000.	REMO1230
IF(WORKC(1).LT.0.0) WORKC(1)=0.0	REMO1235
WGMIN(1,K)=WORKC(1)	REMO1240
HAM(K)=HAM(K)+ WORKC(1)	REMO1245
HIM(K)=HIM(K)+WORKC(1)	REMO1250
WRITE(6,880) WORKC(1)	REMO1255
880 FORMAT(' ',T33,97(' '),/T32,' * NO GASES ARE PRESENT, THE WORK =	REMO1260
1',F8.4,/ ' ',T33,97(' '))	REMO1265
900 RETURN	REMO1270
END	REMO1275

SUBROUTINE LOSS	LOSS 5
DOUBLE PRECISION H,S,G,HS,SS,GS,HTOT,STOT,GTOT,COEF	LOSS 10
INTEGER BASE	LOSS 15
DIMENSION QST(10),QOUT(10),WNET(10),TQTOT(10),TCOLOS(10),WTGEN(10)	LOSS 20
1),G(10),TMERIT(10),QTOT(10,10),COLOS(10,10),WTFAC(10,10),	LOSS 25
2FF(10,10),FMERIT(10,10)	LOSS 30
DIMENSION QS(10,10),WNET(10,10),PERW(10,10),JSTG(11)	LOSS 35
COMMON/DIABLE/WGMIN(10,10),HST(10,10),HU(11)	LOSS 40
COMMON/MISC/TITLE(20)	LOSS 45
COMMON/TMP/TEMP1(50,10),TEMP2(50,10),TRANGE(2,50),TPHASE(11,5,4),	LOSS 50
1THID	LOSS 55
COMMON/WLGS/WG(50,10)	LOSS 60
COMMON/WORK/HIM(10),HAM(10),EPSI(10,10,4),EFEL	LOSS 65
COMMON/DOUBLE/HS(50,10),SS(50,10),GS(50,10),HTOT(10),COEF(2,7,50)	LOSS 70
COMMON/MAILZ/KEYNOR(11,5),KEYNOP(11,5),KYNR(50),KYNP(50),IROUTE(50)	LOSS 75
1,2)	LOSS 80
COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE(10),NSATOM	LOSS 85
1(50),NN	LOSS 90
DATA JSTG/1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,2H10,3HSUM/	LOSS 95
DO 20 K=1,NOTEMP	LOSS 100
DO 20 I=1,NR	LOSS 105
DO 20 J=1,4	LOSS 110
20 EPSI(1,K,J)=0.0	LOSS 115
C	LOSS 120
C THIS SECTION DETERMINES THE CHEMICAL REACTION NUMBERS WHICH ARE TO BE	LOSS 125
C ASSOCIATED WITH EACH OF THE MATERIAL TRANSFER STEPS.	LOSS 130
C	LOSS 135
J=NR1	LOSS 140
C	LOSS 145
C NR1 IS THE FIRST MATERIAL TRANSFER STEP.	LOSS 150
C	LOSS 155
40 CONTINUE	LOSS 160
I1=IROUTE(J,1)	LOSS 165
I2=IROUTE(J,2)	LOSS 170
C	LOSS 175
C IF I1 IS ZERO, THE TRANSFER STEP INVOLVES A RAW MATERIAL.	LOSS 180
C	LOSS 185
IF(I1.EQ.0) GO TO 60	LOSS 190
IF(I1.LE.NR.AND.I2.LE.NR) GO TO 160	LOSS 195
60 CONTINUE	LOSS 200
C	LOSS 205
C THE 30 LOOP IS USED TO SEARCH FOR THE CHEMICAL REACTION NUMBER TO	LOSS 210
C WHICH THE MATERIAL IS BEING TRANSFERRED.	LOSS 215
C	LOSS 220
DO 80 L=J,NRXNS	LOSS 225
IF(IROUTE(L,2).GT.NR) GO TO 80	LOSS 230
I2=IROUTE(L,2)	LOSS 235
NL=L	LOSS 240
GO TO 120	LOSS 245
80 CONTINUE	LOSS 250
WRITE(6,100)	LOSS 255
100 FORMAT(' ', 'AN ERROR HAS OCCURRED IN THE LOSS SUBROUTINE DURING THLOSS	LOSS 260
1E SCANNING PROCESS TO FIND THE CORRECT REACTION NUMBER FOR EACH OFLOSS	LOSS 265
2 THE MATERIAL TRANSFER STEPS')	LOSS 270
120 CONTINUE	LOSS 275
IF(IROUTE(J,1).EQ.0) I1=IROUTE(NL,2)	LOSS 280
C	LOSS 285
C THE 50 LOOP ASSIGNS THE CHEMICAL REACTION NUMBERS WHICH ARE TO BE	LOSS 290

C ASSOCIATED WITH EACH OF THE MATERIAL TRANSFER STEPS.	LOSS 295
C	LOSS 300
DO 140 L=J,NL	LOSS 305
IRROUTE(L,1)=11	LOSS 310
140 IRROUTE(L,2)=12	LOSS 315
J=NL+1	LOSS 320
GO TO 180	LOSS 325
160 IF(I2.EQ.0) IRROUTE(J,2)=11	LOSS 330
J=J+1	LOSS 335
180 CONTINUE	LOSS 340
IF(J.LT.NRXNS) GO TO 40	LOSS 345
C	LOSS 350
C EPSI(1,K,1)=ENDOTHERMIC HEAT	LOSS 355
C EPSI(1,K,2)= EXOTHERMIC HEAT	LOSS 360
C EPSI(1,K,3)= WORK GENERATED INTERNALLY	LOSS 365
C	LOSS 370
DO 260 K=1,NUTEMP	LOSS 375
DO 240 J=1,NRXNS	LOSS 380
I1=J	LOSS 385
I2=J	LOSS 390
IF(J.LE.NR) GO TO 200	LOSS 395
I1=IRROUTE(J,1)	LOSS 400
I2=IRROUTE(J,2)	LOSS 405
200 CONTINUE	LOSS 410
IF(HS(J,K).LE.0.0) GO TO 220	LOSS 415
EPSI(I1,K,1)=EPSI(I1,K,1)+(0.5*HS(J,K))	LOSS 420
EPSI(I2,K,1)=EPSI(I2,K,1)+(0.5*HS(J,K))	LOSS 425
GO TO 240	LOSS 430
220 EPSI(I1,K,3)=EPSI(I1,K,3)+(0.5*WG(J,K))	LOSS 435
C	LOSS 440
C WG(1,K) IS THE WORK GENERATED INTERNALLY	LOSS 445
C	LOSS 450
EPSI(I2,K,3)=EPSI(I2,K,3)+(0.5*WG(J,K))	LOSS 455
EPSI(I1,K,2)=EPSI(I1,K,2)+(0.5*HS(J,K))	LOSS 460
EPSI(I2,K,2)=EPSI(I2,K,2)+(0.5*HS(J,K))	LOSS 465
240 CONTINUE	LOSS 470
260 CONTINUE	LOSS 475
EFEL=EFEL/100.	LOSS 480
DO 320 K=1,NUTEMP	LOSS 485
HIM(K)=HIM(K)/1000.	LOSS 490
QST(K)=0.0	LOSS 495
QOUT(K)=0.0	LOSS 500
WTNET(K)=0.0	LOSS 505
TQTOT(K)=0.0	LOSS 510
TCOLUS(K)=0.0	LOSS 515
WTGEN(K)=0.0	LOSS 520
Q(K)=0.0	LOSS 525
IMERIT(K)=0.0	LOSS 530
DO 280 I=1,NK	LOSS 535
C HIM(K) IS THE TOTAL MINIMUM WORK OF SEPARATION FOR THE CYCLE	LOSS 540
C WGMIN(1,K) IS THE MINIMUM WORK OF SEPARATION FOR EACH REACTION	LOSS 545
C PERW(1,K) IS THE WORK OF SEPARATION AS A PERCENTAGE	LOSS 550
PERW(1,K)=WGMIN(1,K)/HIM(K)	LOSS 555
C Q(K) IS TOTAL ENDOTHERMIC HEAT REQUIRED EXTERNALLY	LOSS 560
Q(K)=Q(K)+EPSI(1,K,1)	LOSS 565
C QS(1,K) IS THE HEAT NECESSARY TO GENERATE THE NET WORK AT 50(EFF. OF	LOSS 570
C SEPARATION AND THE INPUT VALUE OF THE HEAT TO WORK EFFICIENCY	LOSS 575
C QST(K) IS THE TOTAL HEAT NECESSARY TO GENERATE THE NET WORK	LOSS 580

QST(1,K)=((2.0*WGMIN(I,K)*1000.0)-EPSI(1,K,3))/EFEL	LOSS 585
QST(K)=QST(K)+QST(1,K)	LOSS 590
C QOUT(K) IS THE TOTAL EXOTHERMIC HEAT NOT USED INTERNALLY	LOSS 595
C QTOT(1,K) IS THE TOTAL OF ENDOTHERMIC HEAT PLUS THE HEAT NEEDED	LOSS 600
C TO PRODUCE WORK	LOSS 605
C QTOT(K) IS THE TOTAL EXTERNAL HEAT NEEDED BY THE CYCLE	LOSS 610
QOUT(K)=QOUT(K)+EPSI(1,K,2)	LOSS 615
QTOT(1,K)=QS(1,K)+EPSI(1,K,1)	LOSS 620
QTOT(K)= QTOT(K)+QTOT(1,K)	LOSS 625
C FMERIT(1,K) ARE THE INDIVIDUAL STAGE EFFICIENCIES	LOSS 630
C COLOS(1,K) ARE THE INDIVIDUAL LOSS COEFFICIENTS	LOSS 635
C TCOLOS(K) IS THE LOSS COEFFICIENT FOR THE CYCLE	LOSS 640
FMERIT(1,K)=HO(1)/QTOT(1,K)	LOSS 645
COLOS(1,K)=(QS(1,K)-EPSI(1,K,2))/68300.	LOSS 650
TCOLUS(K)=TCOLUS(K)+COLOS(1,K)	LOSS 655
C WTGEN(K) IS TOTAL WORK GENERATED INTERNALLY	LOSS 660
C WFACT(1,K) ARE THE INDIVIDUAL WEIGHING FACTORS	LOSS 665
WTGEN(K)=WTGEN(K)+EPSI(1,K,3)	LOSS 670
C FF(1,K) ARE THE WEIGHING FACTORS TIMES THE STAGE EFFICIENCIES	LOSS 675
C TMERIT(K) IS THE CYCLE FIGURE OF MERIT	LOSS 680
280 CONTINUE	LOSS 685
DO 300 I=1,NR	LOSS 690
WFACT(1,K)=QTOT(1,K)/TOTOT(K)	LOSS 695
FF(1,K)=WFACT(1,K)*FMERIT(1,K)	LOSS 700
300 TMERIT(K)=TMERIT(K)+FF(1,K)	LOSS 705
320 CONTINUE	LOSS 710
DO 660 K=1,NOTEMP	LOSS 715
JSTG(NR1)=JSTG(11)	LOSS 720
WRITE(6,340) (TITLE(I),I=1,20),K,(JSTG(J),J=1,NR1)	LOSS 725
340 FORMAT('1',T10,'PROCESS SUMMARY',/T10,20A4,/T10,'TEMPERATURE SCHED	LOSS 730
ULE','12,/0','13C(''-')',/0',T18,'STAGE',144,11A8)	LOSS 735
WRITE(6,360)	LOSS 740
360 FORMAT('0',130(''-'))	LOSS 745
WRITE(6,380) (HO(1),I=1,NR),HO(11)	LOSS 750
380 FORMAT('0','(1) H298, HEAT OF REACTION AT 298K (KCAL)',-3P11F8.2)	LOSS 755
WRITE(6,400) (HST(1,K),I=1,NR)	LOSS 760
400 FORMAT('0','(2) HT, HEAT OF REACTION AT TEMP T (KCAL)',-3P11F8.2)	LOSS 765
WRITE(6,420) (TEMP1(1,K),I=1,NR)	LOSS 770
420 FORMAT('0','(3) T, TEMP. OF REACTION (K)',T41,10F8.0)	LOSS 775
WRITE(6,440) (WGMIN(1,K),I=1,NR),H1M(K)	LOSS 780
440 FORMAT('0','(4) WS, THEO. WORK OF SEPARATION (KCAL) ',11F8.2)	LOSS 785
WRITE(6,460) (PERK(1,K),I=1,NR)	LOSS 790
460 FORMAT('0','(5) THEO. WORK OF SEPARATION (') ',10F8.2)	LOSS 795
WRITE(6,480) (EPSI(1,K,3),I=1,NR),WTGEN(K)	LOSS 800
480 FORMAT('0','(6) WG, WORK GENERATED INTERNALLY (KCAL) ',-3P11F8.2)	LOSS 805
WRITE(6,500) EFEL,(QS(1,K),I=1,NR),QST(K)	LOSS 810
500 FORMAT('0','(7) HEAT REQUIRED TO GENERATE WORK (KCAL)',/' ',T6,	LOSS 815
1'QS=(2WS-WG)/',F4.2,T43,-3P11F8.2)	LOSS 820
WRITE(6,520) (EPSI(1,K,1),I=1,NR),Q(K)	LOSS 825
520 FORMAT('0','(8) Q, HEAT REQUIREMENT (KCAL) ',-3P11F8.2)	LOSS 830
WRITE(6,540) (QTOT(1,K),I=1,NR),QTOT(K)	LOSS 835
540 FORMAT('0','(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL) ',-3P11F8.2)	LOSS 840
WRITE(6,560) (WFACT(1,K),I=1,NR)	LOSS 845
560 FORMAT('0','(10) WEIGHING FACTOR (9)/SUM(9) ',10F8.3)	LOSS 850
WRITE(6,580) (EPSI(1,K,2),I=1,NR),QOUT(K)	LOSS 855
580 FORMAT('0','(11) QREJ, HEAT REJECTED (KCAL) ',-3P11F8.2)	LOSS 860
WRITE(6,600) (FMERIT(1,K),I=1,NR)	LOSS 865
600 FORMAT('0','(12) NUJ, INDIVIDUAL FIGURES OF MERIT ',10F8.3)	LOSS 870
WRITE(6,620) (FF(1,K),I=1,NR),TMERIT(K)	LOSS 875
620 FORMAT('0','(13) WEIGHING FACTOR TIMES FIGURES OF MERIT',/' ',	LOSS 880
1 (10)X(12), SUM(13)=OVERALL FIG. MERIT',11F8.3)	LOSS 885
WRITE(6,640) (COLOS(1,K),I=1,NR),TCOLUS(K)	LOSS 890
640 FORMAT('0','(14) LOSS COEFFICIENT, ((7)+(11))/68.3 ',11F8.3)	LOSS 895
WRITE(6,360)	LOSS 900
660 CONTINUE	LOSS 905
RETURN	LOSS 910
END	LOSS 915

SUBROUTINE SECANT(X,C,ROOT,HHET)	SECA 5
C	SECA 10
C SUBROUTINE SECANT FINDS IRRATIONAL ROOTS OF THE EQUATIONS FORMULATED	SECA 15
C IN SEEK	SECA 20
C	SECA 25
DOUBLE PRECISION C	SECA 30
DIMENSION X(2),C(2,6)	SECA 35
X1=X(1)	SECA 40
X2=X(2)	SECA 45
DO 20 IN=1,15	SECA 50
IF(ABS(X2-X1) .LE. .01)	SECA 55
GO TO 40	SECA 60
ROOT=(POLY(X2,C,HHET)*X1-POLY(X1,C,HHET)*X2)/(POLY(X2,C,HHET)-POLY(X1,C,HHET))	SECA 65
IF(ABS(POLY(ROOT,C,HHET)) .LE. .01)	SECA 70
RETURN	SECA 75
X1=X2	SECA 80
20 X2=ROOT	SECA 85
RETURN	SECA 90
40 ROOT=(X1+X2)/2.	SECA 95
RETURN	SECA 100
END	

SUBROUTINE SEEK(I,J,T,XMOLES,ROOT,HHET,IFLAG)	SEEK 5
C	SEEK 10
C SUBROUTINE SEEK SETS UP POLYNOMIAL COEFFICIENTS FOR SECANT AND CHECKS	SEEK 15
C FOR SECOND LAW VIOLATIONS WITH THE HELP OF SECANT.	SEEK 20
C	SEEK 25
C INPUT TO SEEK SHOULD BE AS FOLLOWS--	SEEK 30
C	SEEK 35
C 1. FOR SECOND LAW VIOLATION CHECK	SEEK 40
C I=SPECIES NUMBER OF STREAM BEING COOLED	SEEK 45
C J=SPECIES NUMBER OF STREAM BEING HEATED	SEEK 50
C T=A 2X2 ARRAY WITH THE FOLLOWING VALUES	SEEK 55
C T(1,1)=TEMPERATURE AT HOT END OF THE STREAM BEING COOLED	SEEK 60
C T(1,2)=TEMPERATURE AT COLD END OF STREAM BEING COOLED	SEEK 65
C T(2,1)=TEMPERATURE AT HOT END OF STREAM BEING HEATED	SEEK 70
C T(2,2)=TEMPERATURE AT COLD END OF STREAM BEING HEATED	SEEK 75
C XMOLES(K)=NUMBER OF MOLES IN STREAM K (K=1 OR J)	SEEK 80
C IFLAG= FLAG FOR SECOND LAW VIOLATION	SEEK 85
C IFLAG=0 NO SECOND LAW VIOLATION	SEEK 90
C IFLAG=1 SECOND LAW VIOLATION	SEEK 95
C	SEEK 100
C 2. INPUT TO SEEK WHEN USING TEMPERATURE SEEKING ROUTINE	SEEK 105
C	SEEK 110
C I=0	SEEK 115
C J=SPECIES NUMBER OF STREAM IN QUESTION	SEEK 120
C T= A 2X2 ARRAY CONTAINING THE FOLLOWING VALUES	SEEK 125
C T(1,1)=LOWER END OF TEMPERATURE RANGE	SEEK 130
C T(1,2)=UPPER END OF TEMPERATURE RANGE	SEEK 135
C OTHER TWO VALUES ARE NOT USED IN THIS ROUTINE	SEEK 140
C XMOLES IS NOT USED	SEEK 145
C ROOT=TEMPERATURE OF STREAM IN QUESTION - ANSWER	SEEK 150
C HHET=RIGHT HAND SIDE CONSTANT OF EQUATION - INPUT TO SUBROUTINE	SEEK 155
DOUBLE PRECISION COEF,B,C,HS,SS,GS,HTOT	SEEK 160
DIMENSION XMOLES(50),C(2,6),DERC(2,6),X(2),COEF(2,7,50)	SEEK 165
DIMENSION T(2,2),B(2,6),Y(2)	SEEK 170
DIMENSION HS(50,10),SS(50,10),GS(50,10),HTOT(10)	SEEK 175
COMMON/DOUBLE/HS,SS,GS,HTOT,COEF	SEEK 180
X(1)=T(1,1)	SEEK 185
X(2)=T(1,2)	SEEK 190
IF(1) 160,20,80	SEEK 195
20 DO 60 I1=1,2	SEEK 200
C(11,I1)=COEF(11,6,I1)*1.987165	SEEK 205
DO 40 JJ=2,6	SEEK 210
XJMI=JJ-1	SEEK 215
40 C(11,JJ)=COEF(11,JJ-1,I1)*1.987165/XJMI	SEEK 220
60 CONTINUE	SEEK 225
CALL SECANT(X,C,ROOT,HHET)	SEEK 230
RETURN	SEEK 235
80 DO 120 I1=1,2	SEEK 240
C(11,I1)=COEF(11,6,I1)*1.987165*XMOLES(I1)	SEEK 245
B(11,I1)=COEF(11,6,I1)*1.987165*XMOLES(J)	SEEK 250
DO 100 JJ=2,6	SEEK 255
XJMI=JJ-1	SEEK 260
C(11,JJ)=COEF(11,JJ-1,I1)*1.987165*XMOLES(I1)/XJMI	SEEK 265
100 B(11,JJ)=COEF(11,JJ-1,I1)*1.987165*XMOLES(J)/XJMI	SEEK 270
120 CONTINUE	SEEK 275
CONST1=POLY(T(2,2),B,0.)	SEEK 280
CONST2=POLY(T(1,2),C,0.)	SEEK 285
HHET=POLY(T(2,1),B,0.)-CONST1	SEEK 290

XCR=HMET/25.	SEEK 295
Y(1)=1(1,2)	SEEK 300
Y(2)=1(1,1)	SEEK 305
X(1)=1(2,2)	SEEK 310
X(2)=1(2,1)	SEEK 315
DO 140 11=2,24	SEEK 320
HOT=CONST1+11*XCR	SEEK 325
CALL SECANT(X,B,XT2,HOT)	SEEK 330
HOT=CONST2+11*XCR	SEEK 335
CALL SECANT(Y,C,XT1,HOT)	SEEK 340
IF(XT1-XT2-5.)160,140,140	SEEK 345
140 CONTINUE	SEEK 350
IFLAG=0	SEEK 355
RETURN	SEEK 360
160 IFLAG=1	SEEK 365
RETURN	SEEK 370
180 WRITE(6,200)	SEEK 375
200 FORMAT('0','ERROR *** I HAS A NEGATIVE VALUE IN SEEK SUBROUTINE')	SEEK 380
RETURN	SEEK 385
END	SEEK 390

SUBROUTINE MATCH	MATC	5
INTEGER BASE	MATC	10
REAL NOTE	MATC	15
DOUBLE PRECISION HS,SS,GS,HTOT,COEF	MATC	20
DOUBLE PRECISION C(2,6)	MATC	25
DIMENSION WILDR(50),WILDP(50)	MATC	30
DIMENSION HSSG(10),HSSL(10),WGEN(10)	MATC	35
DIMENSION T(2,2),TLEVEL(30),X(50),XMOLES(50)	MATC	40
DIMENSION HS(50,10),SS(50,10),GS(50,10),HTGT(10),COEF(2,7,50)	MATC	45
DIMENSION TEMP1(50,10),TEMP2(50,10),TRANGE(2,50),TPHASE(11,5,4)	MATC	50
DIMENSION KEYNOR(11,5),KEYNOP(11,5),KYNR(50),KYNP(50),IRROUTE(50,2)	MATC	55
DIMENSION BASE(10),NSATOM(50)	MATC	60
DIMENSION AREACT(10,5),APROD(10,5),RATIO(10,5,4),NOTE(10,100),	MATC	65
HSTOCK(50),HSTOCP(50),NPROD(11),NREACT(11),NRATIO(10),LNOTE(10)	MATC	70
DIMENSION HIM(10),HAM(10),EPSI(10,10,4)	MATC	75
COMMON/MISC/TITLE(20)	MATC	80
COMMON/WORK/HIM,HAM,EPSE,EFEL	MATC	85
COMMON/MATLS/AREACT,APROD,RATIO,NOTE,HSTOCR,HSTOCP,NPROD,NREACT,	MATC	90
INRATIO,LNOTE	MATC	95
COMMON/INDX/R,NR,NR1,NRXNS,NOTEMP,I,K,J,M,NRX,NTOT,BASE,NSATOM,NN	MATC	100
COMMON/MATL2/KEYNOR,KEYNOP,KYNR,KYNP,IRROUTE	MATC	105
COMMON/TMP/TEMP1,TEMP2,TRANGE,TPHASE,TMID	MATC	110
COMMON/DOUBLE/HS,SS,GS,HTOT,COEF	MATC	115
COMMON/WLOS/WG(50,10)	MATC	120
C *****	MATC	125
C THIS SUBROUTINE MATCHES THE EXOTHERMIC AND ENDOTHERMIC STEP FOR HEAT	MATC	130
C EXCHANGE PURPOSES	MATC	135
C *****	MATC	140
C NR1=NR+1	MATC	145
C	MATC	150
C THE FOLLOWING DIAGRAM WILL BE HELPFUL IN UNDERSTANDING THE FLOW OF	MATC	155
C THE ROUTINE AND WILL DEFINE THE NOTATION USED ON THE COMMENT CARDS.	MATC	160
C THIS NOTATION HAS NO RELATIONSHIP TO THE ACTUAL VARIABLE NAMES USED	MATC	165
C IN THE PROGRAM	MATC	170
C	MATC	175
C POINT 2	MATC	180
C	MATC	185
C)-----*	MATC	190
C TC2 * TC1	MATC	195
C * *	MATC	200
C -->-----*	MATC	205
C TH2 *-----* TH1	MATC	210
C	MATC	215
C FROM THIS DIAGRAM, IT IS SEEN THAT TC2 IS THE TEMP. OF THE COLD END OF	MATC	220
C THE STREAM BEING COOLED, TH1 IS THE TEMP. AT THE HOT END OF THE	MATC	225
C STREAM BEING HEATED, ETC.	MATC	230
C	MATC	235
C DO 20 I=NR1,NRXNS	MATC	240
C WILDR(I)=HSTOCK(I)	MATC	245
C 20 WILDP(I)=HSTOCP(I)	MATC	250
C DO 1340 K=1,NOTEMP	MATC	255
C NR1=NR+1	MATC	260
C DO 40 I=NR1,NRXNS	MATC	265
C HSTOCK(I)=WILDR(I)	MATC	270
C 40 HSTOCP(I)=WILDP(I)	MATC	275
C WRITE(6,60) (TITLE(J),J=1,20),K	MATC	280
C 60 FORMAT('1',T32,20A4,'T32',MATCHING OF STREAMS FOR HEAT EXCHANGE FOMATC	MATC	285
C 1R TEMPERATURE SCHEDULE ',I2)	MATC	290

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      WRITE(6,80)
80  FORMAT(' ',11,113(' '),/4X,'HEAT  *',15X,'STREAM SUPPLYING HEAT *MATC 295
1,13X,'*',15X,'STREAM ABSORBING HEAT',/' ',10X,2(' ',6(' '),**',21(MATC 305
2(' '),**',21(' '),/ ' ',EXCHANGED * STEP *',5X,'TEMPERATURES * MATC 310
3  AMOUNT OF HEAT * STEP *',5X,'TEMPERATURES * AMOUNT OF H MATC 315
4EAT',/' ',10X,2(' ',6X,4(' ', '-----')),/3X,'(KCAL) * * MATC 320
5 INITIAL * FINAL * INITIALLY* REMAINING* * INITIAL * FIMATC 325
6NAL * INITIALLY* REMAINING',/11X,2(' ',6X,4(' ',10X)),/11X,'*',6XMATC 330
7,'*',10X,'*',10X,'* AVAILABLE*',10X,'*',6X,'*',10X,'*',10X,'* NEEMATC 335
8DED *',/' ',10(' '),2(' *-----',4(' *-----'))
      NLEVEL=1
      MATC 340
C
C THIS PART OF THE SUBROUTINE DETERMINES THE MAXIMUM TEMPERATURE LEVEL
C OF THE PROCESS
C
      TMAX=298.15
      TLEVEL(1)=298.15
      DO 100 I=1,NRXNS
      IF(TEMP1(I,K).NE.TEMP2(I,K)) GO TO 100
      IF(TEMP1(I,K).LE.TMAX) GO TO 100
      TMAX=TEMP1(I,K)
      MATC 345
      MATC 350
      MATC 355
      MATC 360
      MATC 365
      MATC 370
      MATC 375
      MATC 380
      MATC 385
      MATC 390
      MATC 395
      MATC 400
      MATC 405
C THE OTHER TEMPERATURE LEVELS ARE NOW DETERMINED AND PUT IN ASCENDING
C ORDER
C
      J=1
      120 MM=0
      DO 160 I=1,NRXNS
      IF(TEMP1(I,K).NE.TEMP2(I,K).OR.TEMP1(I,K).LE.TLEVEL(J)) GO TO 160
      MM=MM+1
      IF(MM.GT.1) GO TO 140
      TNEXT=TEMP1(I,K)
      GO TO 160
      MATC 410
      MATC 415
      MATC 420
      MATC 425
      MATC 430
      MATC 435
      MATC 440
      MATC 445
      MATC 450
      MATC 455
      MATC 460
      MATC 465
      MATC 470
      MATC 475
      MATC 480
      MATC 485
      MATC 490
      MATC 495
      140 IF(TEMP1(I,K).GE.TNEXT) GO TO 160
      TNEXT=TEMP1(I,K)
      MATC 500
      MATC 505
      MATC 510
      MATC 515
      MATC 520
      MATC 525
      MATC 530
      MATC 535
      MATC 540
      MATC 545
      MATC 550
      MATC 555
      MATC 560
      MATC 565
      MATC 570
      MATC 575
      MATC 580
      160 CONTINUE
      J=J+1
      TLEVEL(J)=TNEXT
      IF(TLEVEL(J).NE.TMAX) GO TO 120
      MATC 585
C
C THE FOLLOWING IS A BRIEF DESCRIPTION OF THE GENERAL FLOW OF THIS
C ROUTINE BEGINNING WITH THE NEXT TO THE LOWEST TEMP. LEVEL FOR THE
C TEMPERATURE OF THE ROUTINE :
C 1. FINDS THE EXOTHERMIC STEPS WHICH ARE NOT CONSTANT TEMP.
C (COOLING) AND WHOSE INITIAL TEMP. TC1, IS EQUAL TO THE TEMP.
C LEVEL IN QUESTION. THE ROUTINE THEN TRIES TO MATCH THE HEAT
C FROM THESE COOLING STEPS WITH ENDOTHERMIC STEPS IN THE
C FOLLOWING ORDER:
C 1. CONSTANT TEMP. ENDOTHERMIC STEPS.
C 2. ENDOTHERMIC HEATING STEPS.
C
C 11. AT THE SAME TEMP. LEVEL, THE ROUTINE FINDS THE EXOTHERMIC STEPS
C OF CONSTANT TEMP. AND TRIES TO MATCH THEM TO ENDOTHERMIC STEPS
C IN THE FOLLOWING ORDER:
C 1.ENDOTHERMIC STEPS OF CONSTANT TEMP.
C 2. ENDOTHERMIC HEATING STEPS.
C

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C THE ROUTINE THEN REPEATS THIS PROCESS FOR ALL THE TEMPERATURE LEVELS. MATC 585
C MATC 590
      NLEVEL=J MATC 595
C MATC 600
C THE 1100 LOOP SEARCHES FOR EXOTHERMIC STEPS, BEGINNING AT THE NEXT TO MATC 605
C THE LOWEST TEMPERATURE LEVEL AND PROCEEDS UP THE SCALE OF THE TEMP. MATC 610
C LEVELS MATC 615
C MATC 620
      DO 1120 J=2,NLEVEL MATC 625
C MATC 630
C THE 800 LOOP SEARCHES FOR THOSE EXOTHERMIC STEPS WHICH ARE NOT MATC 635
C CONSTANT (COOLING STEPS). MATC 640
C MATC 645
      DO 820 I=1,NRXNS MATC 650
160 IF(HS(I,K).GE.0.0.OR.TEMP2(I,K).NE.TLEVEL(J)) GO TO 820 MATC 655
      IF(TEMP1(I,K).EQ.TEMP2(I,K)) GO TO 820 MATC 660
C MATC 665
C THE 280 LOOP SEARCHES FOR ENDOTHERMIC CONSTANT TEMP. STEPS WHOSE TEMP. MATC 670
C ARE BELOW THE TC1 OF THE EXOTHERMIC STEP TO BE MATCHED. MATC 675
      DO 300 II=1,NRXNS MATC 680
      IF(HS(II,K).LE.0.0.OR.TEMP2(II,K).GE.TEMP2(I,K)) GOTO 300 MATC 685
      IF(TEMP1(II,K).NE.TEMP2(II,K)) GO TO 300 MATC 690
      IF(TEMP1(I,K).LT.TEMP1(II,K)) GO TO 240 MATC 695
C MATC 700
C THIS SECTION MATCHES THE HEAT FROM A COOLING STEP TO A CONSTANT TEMP. MATC 705
C ENDOTHERMIC STEP WHOSE TEMP. IS BELOW TC2. MATC 710
C MATC 715
      IF(HS(I,K)+HS(II,K)) 200,200,220 MATC 720
200 HEATR=HS(I,K)+HS(II,K) MATC 725
      IF(HEATR.GE.(-10.0)) HEATR=0.0 MATC 730
      HEATR2=0.0 MATC 735
      WRITE(6,320) HS(II,K),I,TEMP2(I,K),TEMP1(I,K),HS(I,K),HEATR,II, MATC 740
      1 TEMP2(II,K),TEMP1(II,K),HS(II,K),HEATR2 MATC 745
      HSTOCP(I)=(HEATR*HSTOCP(I))/HS(I,K) MATC 750
      HSTOCP(II)=HSTOCP(I) MATC 755
      HS(I,K)=HEATR MATC 760
      HS(II,K)=0.0 MATC 765
      IF(HS(I,K).EQ.0.0) GO TO 820 MATC 770
      GO TO 300 MATC 775
220 HEAT=-HS(I,K) MATC 780
      HEATR=0.0 MATC 785
      HEATR2=HS(II,K)+HS(I,K) MATC 790
      IF(HEATR2.LE.10.0) HEATR2=0.0 MATC 795
      WRITE(6,320) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),HEATR,II, MATC 800
      1 TEMP2(II,K),TEMP1(II,K),HS(II,K),HEATR2 MATC 805
      HS(II,K)=HEATR2 MATC 810
      HS(I,K)=0.0 MATC 815
      GO TO 820 MATC 820
C MATC 825
C THIS SECTION MATCHES THE COOLING STEP TO AN ENDOTHERMIC CONSTANT TEMP. MATC 830
C STEP WITH A TEMP. BETWEEN TC1 AND TC2. DEPENDING ON THE RELATIVE MATC 835
C AMOUNTS OF EXOTHERMIC AND ENDOTHERMIC HEAT, THE EXOTHERMIC STREAM MAY MATC 840
C BE COOLED TO THE TEMP. OF THE ENDOTHERMIC STEP OR TO SOME TEMP. MATC 845
C BETWEEN THIS TEMP. AND TC1. MATC 850
C MATC 855
240 TT=TEMP2(II,K) MATC 860
      M=KYNR(I) MATC 865
      CALL CMATCH(M,C,COEF) MATC 870

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HBF=POLY(TT,C,0.0)	MATC 875
TT=TEMP2(1,K)	MATC 880
HBI=POLY(TT,C,0.0)	MATC 885
HB=(HBF-HBI)*HSTOCR(1)	MATC 890
IF(HS(11,K)+HB) 280,260,260	MATC 895
260 HEAT=-HB	MATC 900
HEATR=HS(1,K)-HB	MATC 905
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC 910
HEATR2=HS(11,K)+HB	MATC 915
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC 920
WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP1(11,K),HS(1,K),HEATR,11,	MATC 925
1TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC 930
HS(1,K)=HEATR	MATC 935
HS(11,K)=HEATR2	MATC 940
TEMP2(1,K)=TEMP1(11,K)	MATC 945
IF(HS(1,K).EQ.0.0) GO TO 820	MATC 950
GO TO 300	MATC 955
280 HEAT=HS(11,K)	MATC 960
FUNT=(-HS(11,K)/HSTOCR(1))+WBI	MATC 965
T(1,1)=TEMP1(11,K)	MATC 970
T(1,2)=TEMP2(1,K)	MATC 975
CALL SEEK(0,M,T,XMOLES,ROOT,FUNT,IFLAG)	MATC 980
HEATR=HS(1,K)+HS(11,K)	MATC 985
HEATR2=HS(11,K)-HEAT	MATC 990
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC 995
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC1000
WRITE(6,320) HEAT,1,TEMP2(1,K),ROOT,HS(1,K),HEATR,11,TEMP2(11,K),	MATC1005
1TEMP1(11,K),HS(11,K),HEATR2	MATC1010
TEMP2(1,K)=ROOT	MATC1015
HS(1,K)=HEATR	MATC1020
HS(11,K)=0.0	MATC1025
300 CONTINUE	MATC1030
320 FORMAT(' ',1X,-3PF8.3,' * ',I2,' * ',0PF7.2,' * ',F7.2,' * ',	MATC1035
1-3PF8.3,' * ',F8.3,' * ',I2,' * ',0PF7.2,' * ',F7.2,' * ',	MATC1040
2-3PF8.3,' * ',F8.3)	MATC1045
IF(HS(1,K).EQ.0.0) GO TO 820	MATC1050
C	MATC1055
C THIS SECTION (460 LOOP) MATCHES COOLING AND HEATING STREAMS FOR THE	MATC1060
C CASE 1H1.LE.TC1 AND 1H2.LE.TC2	MATC1065
C	MATC1070
DO 500 11=1,NRXNS	MATC1075
IF(HS(11,K).LE.0.0) GO TO 500	MATC1080
IF(TEMP2(11,K).EQ.TEMP1(11,K)) GOTO 500	MATC1085
IF(TEMP2(11,K).GE.TEMP2(1,K)) GO TO 500	MATC1090
IF(TEMP1(11,K).LT.TEMP2(1,K).AND.TEMP2(11,K).LT.TEMP1(1,K)) GO TO	MATC1095
1 340	MATC1100
IF(TEMP2(11,K).LE.TEMP1(1,K).AND.TEMP1(11,K).LE.TEMP2(1,K)) GO TO	MATC1105
1 420	MATC1110
GO TO 500	MATC1115
340 IF(HS(1,K)+HS(11,K)) 360,360,400	MATC1120
360 M=KYNR(1)	MATC1125
MM=KYNR(11)	MATC1130
X(M)=(-HS(11,K))/(HS(1,K)/HSTOCR(1))	MATC1135
X(MM)=HSTOCR(11)	MATC1140
T(1,1)=TEMP2(1,K)	MATC1145
T(1,2)=TEMP1(1,K)	MATC1150
T(2,1)=TEMP1(11,K)	MATC1155
T(2,2)=TEMP2(11,K)	MATC1160

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CALL SEEK(M,MM,T,X,ROOT,HHET,IFLAG)
380 FURMAT(' ','W',-3PF8.3,' * ',I2,' * ',0PF7.2,' * ',F7.2,' * ',MATC1165
1-3PF8.3,' * ',F8.3,' * ',I2,' * ',0PF7.2,' * ',F7.2,' * ',MATC1170
2-3PF8.3,' * ',F8.3)MATC1175
HEATR=HS(I,K)+HS(II,K)MATC1180
IF(HEATR.GE.(-10.0)) HEATR=0.0MATC1185
HEATR2=0.0MATC1190
IF(IFLAG.NE.1) WRITE(6,320) HS(II,K),I,TEMP2(I,K),TEMP1(I,K),MATC1195
1HS(I,K),HEATR,II,TEMP2(II,K),TEMP1(II,K),HS(II,K),HEATR2MATC1200
IF(IFLAG.EQ.1) WRITE(6,380) HS(II,K),I,TEMP2(I,K),TEMP1(I,K),MATC1205
1HS(I,K),HEATR,II,TEMP2(II,K),TEMP1(II,K),HS(II,K),HEATR2MATC1210
HS(I,K)=HEATRMATC1215
HS(II,K)=HEATR2MATC1220
HSTOCR(I)=HSTOCR(I)-X(M)MATC1225
HSTOCR(II)=HSTOCR(II)MATC1230
IF(HS(I,K).EQ.0.0) GO TO 820MATC1235
GO TO 500MATC1240
400 M=KYNR(I)MATC1245
MM=KYNR(II)MATC1250
X(MM)=(-HS(I,K)/(HS(II,K)/HSTOCR(II)))MATC1255
X(M)=HSTOCR(I)MATC1260
T(1,1)=TEMP2(I,K)MATC1265
T(1,2)=TEMP1(I,K)MATC1270
T(2,1)=TEMP1(II,K)MATC1275
T(2,2)=TEMP2(II,K)MATC1280
CALL SEEK(M,MM,T,X,ROOT,HHET,IFLAG)MATC1285
HEAT=-HS(I,K)MATC1290
HEATR=HS(I,K)+HEATMATC1295
HEATR2=HS(II,K)+HS(I,K)MATC1300
IF(HEATR.GE.(-10.0)) HEATR=0.0MATC1305
IF(HEATR2.LE.10.0) HEATR2=0.0MATC1310
IF(IFLAG.NE.1) WRITE(6,320) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),MATC1315
1HEATR,II,TEMP2(II,K),TEMP1(II,K),HS(II,K),HEATR2MATC1320
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),MATC1325
1HEATR,II,TEMP2(II,K),TEMP1(II,K),HS(II,K),HEATR2MATC1330
HSTOCR(II)=HSTOCR(II)-X(MM)MATC1335
HSTOCR(II)=HSTOCR(II)MATC1340
HS(II,K)=HEATR2MATC1345
HS(I,K)=HEATRMATC1350
GO TO 820MATC1355
420 IF(TEMP2(II,K).EQ.TEMP1(I,K).AND.TEMP1(II,K).NE.TEMP2(I,K))MATC1360
1 GO TO 340MATC1365
IF(TEMP2(II,K).NE.TEMP1(I,K).AND.TEMP1(II,K).EQ.TEMP2(I,K))MATC1370
1 GO TO 340MATC1375
IF(HS(I,K)+HS(II,K)) 440,440,460MATC1380
440 HEAT=-(HS(II,K)*0.9)MATC1385
GO TO 480MATC1390
460 HEAT=HS(I,K)MATC1395
480 II=TEMP2(II,K)MATC1400
MM=KYNR(II)MATC1405
CALL CMATCH(MM,C,COEF)MATC1410
HB1=POLY(TT,C,0.0)MATC1415
FUNT=(-HEAT+(HB1*HSTOCR(II)))/HSTOCR(II)MATC1420
T(1,1)=TEMP2(II,K)MATC1425
T(1,2)=TEMP1(II,K)MATC1430
CALL SEEK(0,MM,T,XMOLES,ROOT,FUNT,IFLAG)MATC1435
HEAT=-HEATMATC1440
HEATR=HS(I,K)+HEATMATC1445
MATC1450

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HEATRZ=HS(11,K)-HEAT	MATC1455
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC1460
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC1465
M=KYNK(1)	MATC1470
X(M)=HSTOCK(1)*(1.-HEATR/HS(1,K))	MATC1475
X(MM)=HSTOCK(11)	MATC1480
T(1,1)=TEMP2(1,K)	MATC1485
T(1,2)=TEMP1(1,K)	MATC1490
T(2,1)=ROOT	MATC1495
T(2,2)=TEMP2(11,K)	MATC1500
CALL SEEK(M,MM,T,X,ROU,FUNT,IFLAG)	MATC1505
IF(IFLAG.NE.1) WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP1(1,K),HS(1,K),	MATC1510
HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC1515
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,1,TEMP2(1,K),TEMP1(1,K),HS(1,K),	MATC1520
HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC1525
HSTOCK(1)=HSTOCK(1)*(HEATR/HS(1,K))	MATC1530
HSTOCK(1)=HSTOCK(1)	MATC1535
HS(1,K)=HEATR	MATC1540
HS(11,K)=HEATR2	MATC1545
TEMP2(11,K)=ROOT	MATC1550
IF(HS(1,K).EQ.0.0) GO TO 820	MATC1555
500 CONTINUE	MATC1560
C	MATC1565
C IN THIS SECTION, HEATING AND COOLING STREAMS WITH THE FOLLOWING	MATC1570
C CRITERIA MATCHED: TC1)TH1 AND TC2)TH2.	MATC1575
C	MATC1580
DO 800 11=1,NRXNS	MATC1585
IF(HS(11,K).LE.0.0) GO TO 800	MATC1590
IF(TEMP2(11,K).EQ.TEMP1(11,K)) GO TO 800	MATC1595
IF(TEMP2(11,K).LE.TEMP1(1,K).AND.TEMP1(11,K).LE.TEMP2(1,K))	MATC1600
1 GO TO 800	MATC1605
IF(TEMP2(11,K).GE.TEMP2(1,K)) GO TO 800	MATC1610
IF(TEMP2(1,K).LT.TEMP1(11,K).AND.TEMP2(11,K).LE.TEMP1(1,K))	MATC1615
1 GO TO 600	MATC1620
IF(TEMP2(1,K).LT.TEMP1(11,K).AND.TEMP1(1,K).LT.TEMP2(11,K))	MATC1625
1 GO TO 720	MATC1630
M=KYNR(1)	MATC1635
TI=TEMP2(11,K)	MATC1640
CALL CMATCH(M,C,COEF)	MATC1645
HBF=POLY(TI,C,0.0)	MATC1650
TI=TEMP2(1,K)	MATC1655
HBI=POLY(TI,C,0.0)	MATC1660
HEAT=(HBF-HBI)*HSTOCK(1)	MATC1665
MM=KYNR(11)	MATC1670
X(M)=HSTOCK(1)	MATC1675
X(MM)=HSTOCK(11)	MATC1680
IF(HEAT+HS(11,K)) 520,540,580	MATC1685
520 HEAT=HS(11,K)	MATC1690
T(1,1)=TEMP2(11,K)	MATC1695
T(1,2)=TEMP2(1,K)	MATC1700
FUNT=-HS(11,K)/HSTOCK(1)+HBI	MATC1705
CALL SEEK(0,M,T,XHOLES,ROOT,FUNT,IFLAG)	MATC1710
HBF=POLY(ROOT,C,0.0)	MATC1715
HEATR=HS(1,K)-(HBF-HBI)*HSTOCK(1)	MATC1720
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC1725
HEATR2=0.0	MATC1730
T(1,1)=TEMP2(1,K)	MATC1735
T(1,2)=ROOT	MATC1740

T(2,1)=TEMP1(11,K)	MATC1745
T(2,2)=TEMP2(11,K)	MATC1750
CALL SEEK(M,MM,T,X,RDUM,FUNT,IFLAG)	MATC1755
IF(IFLAG.NE.1) WRITE(6,320) HEAT,I,TEMP2(1,K),ROOT,HS(1,K),HEATR,	MATC1760
111,TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC1765
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,I,TEMP2(1,K),ROOT,HS(1,K),HEATR,	MATC1770
111,TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC1775
TEMP2(1,K)=ROOT	MATC1780
HS(1,K)=HEATR	MATC1785
HS(11,K)=0.0	MATC1790
GO TO 600	MATC1795
540 IF(TEMP1(11,K).EQ.TEMP2(1,K)) GO TO 560	MATC1800
HEAT=-HEAT	MATC1805
HEATR=HS(1,K)+HEAT	MATC1810
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC1815
HEATR2=0.0	MATC1820
T(1,1)=TEMP2(1,K)	MATC1825
T(1,2)=TEMP2(11,K)	MATC1830
T(2,1)=TEMP1(11,K)	MATC1835
T(2,2)=TEMP2(11,K)	MATC1840
CALL SEEK(M,MM,T,X,RDUM,FUNT,IFLAG)	MATC1845
IF(IFLAG.NE.1) WRITE(6,320) HEAT,I,TEMP2(1,K),TEMP2(11,K),HS(1,K),	MATC1850
1HEATR,11,TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC1855
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,I,TEMP2(1,K),TEMP2(11,K),HS(1,K),	MATC1860
1HEATR,11,TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC1865
HS(1,K)=HEATR	MATC1870
HS(11,K)=0.0	MATC1875
TEMP2(1,K)=TEMP2(11,K)	MATC1880
GO TO 600	MATC1885
560 HEAT=-(0.9*HEAT)	MATC1890
HEATR=HS(1,K)+HEAT	MATC1895
HEATR2=HS(11,K)-HEAT	MATC1900
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC1905
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC1910
T(1,1)=TEMP2(11,K)	MATC1915
T(1,2)=TEMP2(1,K)	MATC1920
FUNT=-(HEAT/HSTUCK(1))+HBI	MATC1925
CALL SEEK(0,M,T,XMOLES,ROOT1,FUNT,IFLAG).	MATC1930
MM=KYNR(11)	MATC1935
CALL CHATCH(NN,C,COEF)	MATC1940
TT=TEMP2(11,K)	MATC1945
HBI=POLY(TT,C,0.0)	MATC1950
FUNT=HEAT/HSTUCK(11)+HBI	MATC1955
CALL SEEK(0,MM,I,XMOLES,ROOT2,FUNT,IFLAG)	MATC1960
T(1,1)=TEMP2(1,K)	MATC1965
T(1,2)=ROOT1	MATC1970
T(2,1)=ROOT2	MATC1975
T(2,2)=TEMP2(11,K)	MATC1980
CALL SEEK(M,MM,T,X,RDUM,FUNT,IFLAG)	MATC1985
IF(IFLAG.NE.1) WRITE(6,320) HEAT,I,TEMP2(1,K),ROOT1,HS(1,K),HEATR,	MATC1990
111,TEMP2(11,K),ROOT2,HS(11,K),HEATR2	MATC1995
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,I,TEMP2(1,K),ROOT1,HS(1,K),HEATR,	MATC2000
111,TEMP2(11,K),ROOT2,HS(11,K),HEATR2	MATC2005
HS(1,K)=HEATR	MATC2010
HS(11,K)=HEATR2	MATC2015
TEMP2(1,K)=ROOT1	MATC2020
TEMP2(11,K)=ROOT2	MATC2025
GO TO 800	MATC2030

580	HEAT=-HEAT	MATC2035
	HEATR=HS(1,K)+HEAT	MATC2040
	IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC2045
	MM=KYNR(11)	MATC2050
	CALL CMATCH(MM,C,COEF)	MATC2055
	TT=TEMP2(11,K)	MATC2060
	HB=POLY(TT,C,0.0)	MATC2065
	T(1,1)=TEMP2(11,K)	MATC2070
	T(1,2)=TEMP1(11,K)	MATC2075
	FUNT=HEAT/HSTOCR(11)+HB	MATC2080
	CALL SEEK(0,MM,1,XMOLES,ROOT,FUNT,IFLAG)	MATC2085
	HEATR2=HS(11,K)-HEAT	MATC2090
	IF(HEATR2.LE.10.0) HEATR2=0.0	MATC2095
	T(1,1)=TEMP2(1,K)	MATC2100
	T(1,2)=TEMP2(11,K)	MATC2105
	T(2,1)=ROOT	MATC2110
	T(2,2)=TEMP2(11,K)	MATC2115
	CALL SEEK(M,MM,1,X,RDUM,FUNT,IFLAG)	MATC2120
	IF(IFLAG.NE.1) WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP2(11,K),HS(1,K),	MATC2125
	HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2130
	IF(IFLAG.EQ.1) WRITE(6,380) HEAT,1,TEMP2(1,K),TEMP2(11,K),HS(1,K),	MATC2135
	HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2140
	TEMP2(1,K)=TEMP2(11,K)	MATC2145
	HS(1,K)=HEATR	MATC2150
	TEMP2(11,K)=ROOT	MATC2155
	HS(11,K)=HEATR2	MATC2160
	GO TO 800	MATC2165
C		MATC2170
C	IN THIS SECTION, HEATING AND COOLING STREAMS WITH THE FOLLOWING	MATC2175
C	CRITERIA MATCHED: TC1)TH1 AND TH2)TC2.	MATC2180
C		MATC2185
600	MM=KYNR(11)	MATC2190
	M=KYNR(1)	MATC2195
	X(MM)=HSTOCR(11)	MATC2200
	TT=TEMP2(1,K)	MATC2205
	CALL CMATCH(MM,C,COEF)	MATC2210
	HBF=POLY(TT,C,0.0)	MATC2215
	TT=TEMP2(11,K)	MATC2220
	HBI=POLY(TT,C,0.0)	MATC2225
	HS11=(HBF-HBI)*HSTOCR(11)	MATC2230
	IF(HS11+HS(1,K)) 620,620,680	MATC2235
620	HEAT=HS11	MATC2240
	IF(TEMP2(11,K).EQ.TEMP1(1,K)) HEAT=0.9*HS11	MATC2245
	HEATR=HS(1,K)+HEAT	MATC2250
	HEATR2=HS(11,K)-HEAT	MATC2255
	IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC2260
	IF(HEATR2.LE.10.0) HEATR2=0.0	MATC2265
	ROOT=TEMP2(1,K)	MATC2270
	IF(TEMP2(11,K).NE.TEMP1(1,K)) GO TO 640	MATC2275
	FUNT=(HEAT/HSTOCR(11))+HBI	MATC2280
	T(1,1)=TEMP2(11,K)	MATC2285
	T(1,2)=TEMP2(1,K)	MATC2290
	CALL SEEK(0,MM,1,XMOLES,ROOT,FUNT,IFLAG)	MATC2295
640	IF(HEATR.EQ.0.0) X(M)=HSTOCR(1)	MATC2300
	IF(HEATR.NE.0.0) X(M)=HSTOCR(1)*(1.-HEATR/HS(1,K))	MATC2305
	T(1,1)=TEMP2(1,K)	MATC2310
	T(1,2)=TEMP1(1,K)	MATC2315
	T(2,1)=ROOT	MATC2320

T(2,2)=TEMP2(11,K)	MATC2325
CALL SEEK(M,MM,T,X,RDUM,FUNT,IFLAG)	MATC2330
IF(IFLAG.NE.1) WRITE(6,320) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),	MATC2335
1HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2340
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),	MATC2345
1HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2350
TEMP2(11,K)=ROOT	MATC2355
IF(HEATR.EQ.0.0) GO TO 660	MATC2360
HSTOCR(1)=(HEATR*HSTOCR(1))/HS(I,K)	MATC2365
HSTOCP(1)=HSTOCR(1)	MATC2370
660 HS(I,K)=HEATR	MATC2375
HS(11,K)=HEATR2	MATC2380
IF(HEATR.EQ.0.0) GO TO 820	MATC2385
GO TO 800	MATC2390
680 HEAT=-HS(I,K)	MATC2395
IF(TEMP2(11,K).EQ.TEMP1(I,K)) HEAT=0.9*HEAT	MATC2400
HEATR=HS(I,K)+HEAT	MATC2405
HEATR2=HS(11,K)-HEAT	MATC2410
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC2415
IF(HEATR.LE.10.0) HEATR2=0.0	MATC2420
T(1,1)=TEMP2(11,K)	MATC2425
T(1,2)=TEMP2(1,K)	MATC2430
FUNT=(HEAT/HSTOCR(1))+HBI	MATC2435
CALL SEEK(0,MM,T,XHOLES,ROOT,FUNT,IFLAG)	MATC2440
IF(HEATR.EQ.0.0) X(M)=HSTOCR(1)	MATC2445
IF(HEATR.NE.0.0) X(M)=HSTOCR(1)*(1.-HEATR/HS(I,K))	MATC2450
T(1,1)=TEMP2(1,K)	MATC2455
T(1,2)=TEMP1(I,K)	MATC2460
T(2,1)=ROOT	MATC2465
T(2,2)=TEMP2(11,K)	MATC2470
CALL SEEK(M,MM,1,X,RDUM,FUNT,IFLAG)	MATC2475
IF(IFLAG.NE.1) WRITE(6,320) HEAT,I,TEMP2(1,K),TEMP1(I,K),HS(I,K),	MATC2480
1HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2485
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,I,TEMP2(1,K),TEMP1(I,K),HS(I,K),	MATC2490
1HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2495
HS(11,K)=HEATR2	MATC2500
TEMP2(11,K)=ROOT	MATC2505
IF(HEATR.EQ.0.0) GO TO 700	MATC2510
HSTOCR(1)=HEATR*HSTOCR(1)/HS(I,K)	MATC2515
HSTOCP(1)=HSTOCR(1)	MATC2520
700 HS(I,K)=HEATR	MATC2525
IF(HEATR.EQ.0.0) GO TO 820	MATC2530
GO TO 800	MATC2535
720 N=KYNR(1)	MATC2540
TT=TEMP2(11,K)	MATC2545
CALL CMATCH(M,C,COEF)	MATC2550
HBF1=POLY(TT,C,0.0)	MATC2555
TI=TEMP2(1,K)	MATC2560
HBI1=POLY(TI,C,0.0)	MATC2565
HBI=(HBF1-HBI1)*HSTOCR(1)	MATC2570
MM=KYNR(11)	MATC2575
TI=TEMP2(1,K)	MATC2580
CALL CMATCH(MM,C,COEF)	MATC2585
HBF2=POLY(TI,C,0.0)	MATC2590
TI=TEMP2(11,K)	MATC2595
HBI2=POLY(TI,C,0.0)	MATC2600
HBI2=(HBF2-HBI2)*HSTOCR(11)	MATC2605
X(N)=HSTOCR(1)	MATC2610

X(MM)=HSTOCR(11)	MATC2615
IF(HB1+HB2) 740,760,780	MATC2620
740 HEAT=HB2	MATC2625
HEATR=HS(1,K)+HEAT	MATC2630
HEATR2=HS(11,K)-HEAT	MATC2635
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC2640
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC2645
T(1,1)=TEMP2(11,K)	MATC2650
T(1,2)=TEMP2(1,K)	MATC2655
FUNT=(-HEAT/HSTOCR(1))+HB11	MATC2660
CALL SEEK(0,M,T,XMOLES,ROOT,FUNT,IFLAG)	MATC2665
T(1,1)=TEMP2(1,K)	MATC2670
T(1,2)=ROOT	MATC2675
T(2,1)=TEMP2(1,K)	MATC2680
T(2,2)=TEMP2(11,K)	MATC2685
CALL SEEK(M,MM,1,X,RODM,FUNT,IFLAG)	MATC2690
IF(IFLAG.NE.1) WRITE(6,320) HEAT,1,TEMP2(1,K),ROOT,HS(1,K),HEATR,	MATC2695
11,TEMP2(11,K),TEMP2(1,K),HS(11,K),HEATR2	MATC2700
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,1,TEMP2(1,K),ROOT,HS(1,K),HEATR,	MATC2705
11,TEMP2(11,K),TEMP2(1,K),HS(11,K),HEATR2	MATC2710
TEMP2(11,K)=TEMP2(1,K)	MATC2715
HS(11,K)=HEATR2	MATC2720
TEMP2(1,K)=ROOT	MATC2725
HS(1,K)=HEATR	MATC2730
GO TO 800	MATC2735
760 HEAT=0.9*HB2	MATC2740
HEATR=HS(1,K)+HEAT	MATC2745
HEATR2=HS(11,K)-HEAT	MATC2750
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC2755
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC2760
T(1,1)=TEMP2(11,K)	MATC2765
T(1,2)=TEMP2(1,K)	MATC2770
FUNT=(-HEAT/HSTOCR(1))+HB11	MATC2775
CALL SEEK(0,M,T,XMOLES,ROOT1,FUNT,IFLAG)	MATC2780
FUNT=(HEAT/HSTOCR(11))+HB12	MATC2785
CALL SEEK(0,MM,T,XMOLES,ROOT2,FUNT,IFLAG)	MATC2790
T(1,1)=TEMP2(1,K)	MATC2795
T(1,2)=ROOT1	MATC2800
T(2,1)=ROOT2	MATC2805
T(2,2)=TEMP2(11,K)	MATC2810
CALL SEEK(M,MM,T,X,RODM,FUNT,IFLAG)	MATC2815
IF(IFLAG.NE.1) WRITE(6,320) HEAT,1,TEMP2(1,K),ROOT1,HS(1,K),HEATR,	MATC2820
11,TEMP2(11,K),ROOT2,HS(11,K),HEATR2	MATC2825
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,1,TEMP2(1,K),ROOT1,HS(1,K),HEATR,	MATC2830
11,TEMP2(11,K),ROOT2,HS(11,K),HEATR2	MATC2835
HS(1,K)=HEATR	MATC2840
HS(11,K)=HEATR2	MATC2845
TEMP2(1,K)=ROOT1	MATC2850
TEMP2(11,K)=ROOT2	MATC2855
GO TO 800	MATC2860
780 HEAT=-HB1	MATC2865
T(1,1)=TEMP2(11,K)	MATC2870
T(1,2)=TEMP2(1,K)	MATC2875
FUNT=(HEAT/HSTOCR(11))+HB12	MATC2880
CALL SEEK(0,MM,T,XMOLES,ROOT,FUNT,IFLAG)	MATC2885
HEATR=HS(1,K)+HEAT	MATC2890
HEATR2=HS(11,K)-HEAT	MATC2895
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC2900

IF(HEATR2.LE.10.0) HEATR2=0.0	MATC2905
T(1,1)=TEMP2(1,K)	MATC2910
T(1,2)=TEMP2(11,K)	MATC2915
T(2,1)=ROOT	MATC2920
T(2,2)=TEMP2(11,K)	MATC2925
CALL SEEK(M,MM,T,X,ROUM,FUNT,IFLAG)	MATC2930
IF(IFLAG.NE.1) WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP2(11,K),HS(1,K),	MATC2935
1HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2940
IF(IFLAG.EQ.1) WRITE(6,380) HEAT,1,TEMP2(1,K),TEMP2(11,K),HS(1,K),	MATC2945
1HEATR,11,TEMP2(11,K),ROOT,HS(11,K),HEATR2	MATC2950
TEMP2(1,K)=TEMP2(11,K)	MATC2955
TEMP2(11,K)=ROOT	MATC2960
HS(1,K)=HEATR	MATC2965
HS(11,K)=HEATR2	MATC2970
800 CONTINUE	MATC2975
820 CONTINUE	MATC2980
C	MATC2985
C IN THIS SECTION, THE EXOTHERMIC STEPS AT CONSTANT TEMPERATURE ARE	MATC2990
C MATCHED.	MATC2995
C	MATC3000
DO 1100 I=1,NRXNS	MATC3005
IF(HS(I,K).GE.0.0.OR.TEMP2(I,K).NE.TLEVEL(J).OR.TEMP1(I,K).NE.TEMP	MATC3010
12(I,K)) GO TO 1100	MATC3015
C	MATC3020
C THIS SECTION MATCHES CONSTANT TEMP. EXOTHERMIC STEPS WITH CONSTANT	MATC3025
C TEMP. ENDOTHERMIC STEPS.	MATC3030
C	MATC3035
DO 920 11=1,NRXNS	MATC3040
IF(HS(11,K).LE.0.0.OR.TEMP1(11,K).GT.TEMP1(1,K).OR.TEMP1(11,K).NE.	MATC3045
1TEMP2(11,K)) GO TO 920	MATC3050
IF(HS(1,K)+HS(11,K)) 840,880,880	MATC3055
840 HEAT=HS(11,K)	MATC3060
HEATR=HS(1,K)+HEAT	MATC3065
HEATR2=HS(11,K)-HEAT	MATC3070
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC3075
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC3080
WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP1(1,K),HS(1,K),HEATR,11,	MATC3085
1TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC3090
IF(1.LE.NR) GO TO 860	MATC3095
HSTOCK(1)=(HEATR*HSTOCR(1))/HS(1,K)	MATC3100
HSTOCK(1)=HSTOCK(1)	MATC3105
860 HS(1,K)=HEATR	MATC3110
HS(11,K)=0.0	MATC3115
GO TO 920	MATC3120
880 HEAT=-HS(1,K)	MATC3125
HEATR=HS(1,K)+HEAT	MATC3130
HEATR2=HS(11,K)-HEAT	MATC3135
IF(HEATR.GE.(-10.0)) HEATR=0.0	MATC3140
IF(HEATR2.LE.10.0) HEATR2=0.0	MATC3145
WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP1(1,K),HS(1,K),HEATR,11,	MATC3150
1TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2	MATC3155
IF(11.LE.NR) GO TO 900	MATC3160
HSTOCK(11)=(HEATR2*HSTOCR(11))/HS(11,K)	MATC3165
HSTOCK(11)=HSTOCK(11)	MATC3170
900 HS(11,K)=HEATR2	MATC3175
HS(1,K)=0.0	MATC3180
GO TO 1100	MATC3185
920 CONTINUE	MATC3190

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      IF(HS(1,K).EQ.0.0) GO TO 1100
C
C IN THIS SECTION, CONSTANT TEMP. EXOTHERMIC STEPS ARE MATCHED WITH
C ENDOTHERMIC HEATING STEPS WHOSE TEMP. TH1 ARE LESS THAN OR EQUAL TO
C THE TEMP. OF THE EXOTHERMIC STEP.
C
      DO 1020 11=NR,NRXNS
      IF(HS(11,K).LE.0.0.OR.TEMP1(11,K).GT.TLEVEL(J)) GO TO 1020
      IF(TEMP1(11,K).EQ.TEMP2(11,K)) GO TO 1020
      IF(HS(1,K)+HS(11,K)) 940,940,980
940  HEAT=HS(11,K)
      HEATR=HS(1,K)+HEAT
      HEATR2=HS(11,K)-HEAT
      IF(HEATR.GE.(-10.0)) HEATR=0.0
      IF(HEATR2.LE.10.0) HEATR2=0.0
      WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP1(1,K),HS(1,K),HEATR,11,
      1TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2
      IF(1.LE.NR) GO TO 960
      HSTOCR(1)=(HEATR*HSTOCR(1))/HS(1,K)
      HSTOCP(1)=HSTOCR(1)
960  HS(1,K)=HEATR
      HS(11,K)=0.0
      GO TO 1020
980  HEAT=-HS(1,K)
      HEATR=0.0
      HEATR2=HS(11,K)-HEAT
      IF(HEATR2.LE.10.0) HEATR2=0.0
      WRITE(6,320) HEAT,1,TEMP2(1,K),TEMP1(1,K),HS(1,K),HEATR,11,
      1TEMP2(11,K),TEMP1(11,K),HS(11,K),HEATR2
      IF(HEATR2.EQ.0.0) GO TO 1000
      HSTOCR(11)=(HEATR2*HSTOCR(11))/HS(11,K)
      HSTOCP(11)=HSTOCR(11)
1000 HS(1,K)=0.0
      HS(11,K)=HEATR2
      GO TO 1100
1020 CONTINUE
      IF(HS(1,K).EQ.0.0) GO TO 1100
C
C IN THIS SECTION, CONSTANT TEMP. EXOTHERMIC STEPS ARE MATCHED WITH
C ENDOTHERMIC HEATING STEPS WHOSE TEMP. TH1 ARE GREATER THAN THE
C EXOTHERMIC STEP TEMP. BUT WHOSE TH2 ARE LESS THAN THIS EXOTHERMIC
C TEMP.
C
      DO 1080 11=NR,NRXNS
      IF(HS(11,K).LE.0.0.OR.TEMP2(11,K).GE.TLEVEL(J)) GO TO 1080
      TT=TEMP1(1,K)
      M=KYNR(11)
      CALL CMATCH(M,C,COEF)
      HBF=POLY(TT,C,0.0)
      TT=TEMP2(11,K)
      HB1=POLY(TT,C,0.0)
      HB=(HBF-HB1)*HSTOCR(11)
      IF(HS(1,K)+HB) 1040,1040,1060
1040 HEAT=HB
      HEATR=HS(1,K)+HB
      HEATR2=HS(11,K)-HB
      IF(HEATR.GE.(-10.0)) HEATR=0.0
      IF(HEATR2.LE.10.0) HEATR2=0.0

```

MATC3195
 MATC3200
 MATC3205
 MATC3210
 MATC3215
 MATC3220
 MATC3225
 MATC3230
 MATC3235
 MATC3240
 MATC3245
 MATC3250
 MATC3255
 MATC3260
 MATC3265
 MATC3270
 MATC3275
 MATC3280
 MATC3285
 MATC3290
 MATC3295
 MATC3300
 MATC3305
 MATC3310
 MATC3315
 MATC3320
 MATC3325
 MATC3330
 MATC3335
 MATC3340
 MATC3345
 MATC3350
 MATC3355
 MATC3360
 MATC3365
 MATC3370
 MATC3375
 MATC3380
 MATC3385
 MATC3390
 MATC3395
 MATC3400
 MATC3405
 MATC3410
 MATC3415
 MATC3420
 MATC3425
 MATC3430
 MATC3435
 MATC3440
 MATC3445
 MATC3450
 MATC3455
 MATC3460
 MATC3465
 MATC3470
 MATC3475
 MATC3480

```

WRITE(6,320) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),HEATR,II,
1TEMP2(II,K),TEMP2(I,K),HS(II,K),HEATR2
TEMP2(II,K)=TEMP1(I,K)
HS(II,K)=HEATR2
HS(I,K)=HEATR
IF (HS(I,K).EQ.0.0) GO TO 1100
GO TO 1080
1060 FUNT=HBI-HS(I,K)/HSTOCR(II)
T(1,1)=TEMP2(II,K)
T(1,2)=TEMP1(I,K)
MM=KYNR(II)
CALL SEEK(0,MM,T,XMOLES,ROOT,FUNT,IFLAG)
HEAT=-HS(I,K)
HEATR=0.0
HEATR2=HS(II,K)+HS(I,K)
IF (HEATR2.LE.10.0) HEATR2=0.0
WRITE(6,320) HEAT,I,TEMP2(I,K),TEMP1(I,K),HS(I,K),HEATR,II,
1TEMP2(II,K),ROOT,HS(II,K),HEATR2
TEMP2(II,K)=ROOT
HS(II,K)=HEATR2
HS(I,K)=0.0
GO TO 1100
1080 CONTINUE
1100 CONTINUE
1120 CONTINUE
WRITE(6,1140)
1140 FORMAT(' ',113('-'),//T5,'W-DENOTES THAT A POSSIBLE SECOND LAW VIOMATC3615
1LATION HAS OCCURRED FOR THIS MATCH.',/T7,'(THE DELTA-H VERSUS TEMPMATC3620
ZERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OMATC3625
3THEK WITHIN FIVE DEGREES)',//' ',113('-'))
WRITE(6,1160) (TITLE(L),L=1,20)
1160 FORMAT('1',T+5,20A4)
WRITE(6,1180) K
1180 FORMAT(' ',T38,'SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHMATC3650
1ING',/T52,'FOR TEMPERATURE SCHEDULE',13,//T20,90('-'),/T35,'HEAT AMATC3655
2AVAILABLE',16X,'*',16X,'HEAT REQUIRED',/T20,6('-'),'*,25('-'),'*,MATC3660
312('-'),'*,6('-'),'*,25('-'),'*,12('-'),/T21,'STEP ',7X,'TEMPEMATC3665
4RATURE',7X,'* HEAT * STEP ',7X,'TEMPERATURE',7X,'* HEAT',MATC3670
5,/T26,'*',2('-----*'),12X,'*',6X,'*',2(12('-'),'*)',/T26,'*MATC3675
6 INITIAL * FINAL * AVAILABLE *,6X,'* INITIAL * FINALMATC3680
7AL * REQUIRED',/T20,'-----*',3('-----*'),'-----',3('*-MATC3685
8-----'))
HSSG(K)=0.0
HSSL(K)=0.0
WGEN(K)=0.0
C
C IN CALCULATING THE AMOUNT OF WORK GENERATED FROM EXOTHERMIC HEAT WHICHMATC3715
C CANNOT BE USED FOR INTERNAL HEAT RECOVERY, THE FOLLOWING ASSUMPTIONS MATC3720
C WERE MADE MATC3725
C (1) T2= TEMP OF REACTANTS MATC3730
C (2) T1= TEMP OF PRODUCTS MATC3735
C (3) ONLY HEAT ABOVE 500K IS USED TO PRODUCE WORK MATC3740
C (4) THE EFFICIENCY OF PRODUCING WORK IS 50% OF CARNOT MATC3745
C (5) THE HIGH TEMP IN THE CARNOT IS TAKEN AS AN AVG. VALUE MATC3750
C T2 IF THE STEP IS CONSTANT TEMP MATC3755
C (T2+T1)/2 IF NOT CONST. TEMP. AND T1 IS GREATER THAN 500K MATC3760
C (T2+500)/2 IF NOT CONST. TEMP. AND T1 IS LESS THAN 500K MATC3765
C (6) THE TEMP. AT WHICH HEAT IS REJECTED (FOR CALC. CARNOT) IS 400K MATC3770

```

```

C
DO 1280 I=1,NRXNS
WG(I,K)=0.0
IF(HS(I,K)) 1200,1280,1240
1200 CONTINUE
HSSG(K)=HSSG(K)+HS(I,K)
IF(HS(I,K).GE.(-5.)) GO TO 1280
WRITE(6,1220) I,TEMP2(I,K),TEMP1(I,K),HS(I,K)
1220 FORMAT(' ',I21,I3,4X,OPF8.2,4X,F8.2,4X,-3PF9.3)
IF(TEMP2(I,K).LE.500.) GO TO 1280
TLU=500.
IF(TEMP1(I,K).GT.500.) TLO=TEMP1(I,K)
THI=(TEMP2(I,K)+TLU)/2.0
CARNOT=(THI-400.)/THI
PROP=1.0
IF(TEMP1(I,K).NE.TEMP2(I,K)) PROP=((TEMP2(I,K)-TLO)/(TEMP2(I,K)-
TEMP1(I,K)))
WG(I,K)=-CARNOT*PROP*HS(I,K)
WGEN(K)=WGEN(K)+WG(I,K)
GO TO 1280
1240 WRITE(6,1260) I,TEMP2(I,K),TEMP1(I,K),HS(I,K)
1260 FORMAT(' ',I6,I3,4X,OPF8.2,4X,OPF8.2,4X,-3PF9.3)
HSSL(K)=HSSL(K)+HS(I,K)
GO TO 1280
1280 CONTINUE
WRITE(6,1300) HSSG(K),HSSL(K)
1300 FORMAT(' ',I20,90(' '),/T30,'TOTALS',16X,-3PF9.3,36X,F9.3,/ ' ',I20,
1,90(' '))
TRY=(HSSG(K)+HSSL(K))/1000.
IF(TRY.LT.68..OR. TRY.GT.68.5) WRITE(6,1320)
1320 FORMAT(' ',I15,'***WARNING*** THE DIFFERENCE IN EXOTHERMIC AND ENDMATC3925
10THERMIC HEATS REMAINING ARE',/T30,'IN ERROR. CHECK HEAT MATCHING MATC3930
2TABLE CAREFULLY')
1340 CONTINUE
WRITE(6,1360) (TITLE(J),J=1,20)
1360 FORMAT('1',I36,20A4,/T57,'FIGURES OF MERIT',// ' ',I23,10(' '),* ,MATC3950
121(' '),* ,10(' '),* ,10(' '),* ,31(' '),/ ' ',I26,'TEMP. * ,7X,MATC3955
2,'WORK OF',7X,* WORK * TOTAL * ,8X,'FIGURES OF MERIT',/T33,MATC3960
3,'*',21X,* ,10X,* ,10X,* ,31(' '),/T24,'SCHEDULE * ,6X,'SEPARATMATC3965
4ION * GENERATED* HEAT * 1ST ESTIMATE * 2ND ESTIMATE',/ ' ',MATC3970
5,I33,* ,10(' '),* ,10(' '),* ,10X,* ,10X,4(' '),/ ' ',I3,MATC3975
63,* MIN * MAX * ,10X,* REQUIRED * MIN * MAX * MIN,MATC3980
7 * MAX',/ ' ',I23,4(' '),10(' '),4(' '))
MATC3985
DO 1380 K=1,NOTEMP
WOMAX=HAM(K)/EFEL
WOMIN=HIM(K)/EFEL
C1MAX=HTOT(K)/(HTOT(K)+WOMIN)
C1MIN=HTOT(K)/(HTOT(K)+WOMAX)
WOMAX=(2.*HAM(K)-WGEN(K))/EFEL
WOMIN=(2.*HIM(K)-WGEN(K))/EFEL
C2MIN=HTOT(K)/(HSSL(K)+WOMAX)
C2MAX=HTOT(K)/(HSSL(K)+WOMIN)
WRITE(6,1400) K,HIM(K),HAM(K),WGEN(K),HSSL(K),C1MIN,C1MAX,C2MIN,C2MAX,MATC4035
1MAX
MATC4040
1380 CONTINUE
MATC4045
1400 FORMAT(' ',I27,I2,4X,* ,,-3PF10.3,* ,F10.3,* ,F10.3,* ,F10.3,* ,MATC4050
1', OPF7.4,* ,F7.4,* ,F7.4,* ,F7.4)
MATC4055
WRITE(6,1420)
MATC4060

```

```

1420 FORMAT(' ',T23,4('-----*'),10('---'),4('*-----'))
      EFEL=EFEL*100.
      WRITE(6,1440) EFEL
1440 FORMAT(' ',T25,'ALL HEAT ABOVE 500 K WHICH IS STILL AVAILABLE AFTER
1R STREAM MATCHING, IS TURNED INTO',/T25,'WORK GENERATED USING A 30
2( EFFICIENCY AND SUBTRACTED FROM THE WORK OF SEPARATION NEEDED.',/MATC4085
3T25,'THE FIRST ESTIMATE FOR A FIGURE OF MERIT ASSUMES PERFECT HEATMATC4095
4 REGENERATION AND 100('',/T25,'EFFICIENCY IN THE WORK OF SEPARATIONMATC4100
5.',/T25,'THE SECOND ESTIMATE USES THE HEAT REQUIRED AFTER STREAM MATC4105
6ATCHING AS THE TOTAL HEAT',/T25,'REQUIRED AND ASSUMES ONLY A 50( EMATC4110
7FFICIENCY FOR THE WORK OF SEPARATION.',/T25,'ALL WORK REQUIRED IS MATC4115
8ASSUMED TO BE GENERATED FROM HEAT AT A ',F3.0,'( EFFICIENCY.')
```

MATC4065
MATC4070
MATC4075
MATC4080
MATC4085
MATC4090
MATC4095
MATC4100
MATC4105
MATC4110
MATC4115
MATC4120
MATC4125
MATC4130

```

      RETURN
      END

```

```

      FUNCTION POLY(X,C,HHET)
C
C SUBROUTINE POLY EVALUATES ENTHALPY FOR SEEK AND SECANT
C
      DOUBLE PRECISION C
      DIMENSION C(2,6)
      I=2
      IF(X .GT. 1000.)      I=1
      Z=C(I,6)
      DO 20 J=1,5
      K=6-J
20  Z=C(1,K)+Z*X
      POLY=Z-HHET
      RETURN
      END

```

```

POLY 5
POLY 10
POLY 15
POLY 20
POLY 25
POLY 30
POLY 35
POLY 40
POLY 45
POLY 50
POLY 55
POLY 60
POLY 65
POLY 70
POLY 75

```

APPENDIX - E

Sample Problems

Sample Problem 1. The Vanadium Chloride Process

For the following process:

Run reaction (1) at 1000 and 800 K and with H_2O as the base reactant, use the following data to compute the work of separation:

T	ratio of $\text{H}_2\text{O}/\text{Cl}_2$	Extent of reaction
1000	1/3	0.8559
"	1/2	.775
"	1/1	.5891
"	2/1	.3875
800	1/3	0.6337
"	1/2	.5408
"	1/1	.3931
"	2/1	.2704

Run reaction (2) at 300 K and with VCl_2 as the base reactant, use the following data to compute the work of separation:

T	ratio of VCl_2/HCl	Extent of reaction
300	1/1	.992
	1/2	1.0
	1/3	1.0
	2/1	.496

Run reaction (3) at 1000 K with an extent of reaction = 1.0.

Run reaction (4) at 300 K with an extent of reaction = 1.0.

Also, calculate the properties of the reactions at 298 K.

Input Data Cards for Sample Problem 1

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976 CHEMICAL REACTIONS

1 REACTANT H	20	1	G 1.	B 1.	1.	1.	2.
1 REACTANT CL	2		G 1.	3.	2.	1.	1.
1 PRODUCT H	1 CL	1	G 2.				
1 PRODUCT O	2		G 0.5				
2 REACTANT V	1 CL	2	S 2.	B 1.	1.	1.	2.
2 REACTANT H	1 CL	1	G 2.	1.	2.	3.	1.
2 PRODUCT V	1 CL	3	S 2.				
2 PRODUCT H	2		G 1.				
3 REACTANT V	1 CL	3	S 4.	B			
3 PRODUCT V	1 CL	4	G 2.	425.			
3 PRODUCT V	1 CL	2	S 2.				
4 REACTANT V	1 CL	4	L 2.	B			
4 PRODUCT V	1 CL	3	S 2.				
4 PRODUCT CL	2		G 1.				

NOTES

1 1 THIS IS THE REVERSE DEACON PROCESS.

NAMELISTS

&NAM1 STEP=1, PRES=1, DRAW=T, H298=T, T=1000, 800, EP=0.8559, 0.6337, 8*0.0,
0.775, 0.5408, 8*0.0, 0.5891, 0.3931, 8*0.0, 0.3875, 0.2704 &END

&NAM1 STEP=2, T=2*300, PRES=1, EP=0.9920, 0.9920, 8*0.0, 2*1, 8*0.2*1, 8*0.2*0.4%0
&END

&NAM1 STEP=3, PRES=1, T=2*1000, EP=2*1 &END

&NAM1 STEP=4, PRES=1, T=2*300, EP=2*1 &END

END

BEGINNING OF INPUT DATA FOR THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976

CHEMICAL REACTIONS

1 REACTANT	2.0	1.	0.	0.0	1.00000	1.000	1.000	1.000	2.000
1 REACTANT CL	2.	0.	0.	0.0	1.0000	3.000	2.000	1.000	1.000
1 PRODUCT H	1.00	1.	0.	0.0	2.0000	0.0	0.0	0.0	0.0
1 PRODUCT G	2.	0.	0.	0.0	0.5000	0.0	0.0	0.0	0.0
2 REACTANT V	1.00	2.	0.	0.0	2.0000	1.000	1.000	1.000	2.000
2 REACTANT H	1.00	1.	0.	0.0	2.0000	1.000	2.000	3.000	1.000
2 PRODUCT V	1.00	3.	0.	0.0	2.0000	0.0	0.0	0.0	0.0
2 PRODUCT H	2.	0.	0.	0.0	1.0000	0.0	0.0	0.0	0.0
3 REACTANT V	1.00	3.	0.	0.0	4.0000	0.0	0.0	0.0	0.0
3 PRODUCT V	1.00	4.	0.	0.0	2.0000	425.000	0.0	0.0	0.0
3 PRODUCT V	1.00	2.	0.	0.0	2.0000	0.0	0.0	0.0	0.0
4 REACTANT V	1.00	4.	0.	0.0	2.0000	0.0	0.0	0.0	0.0
4 PRODUCT V	1.00	3.	0.	0.0	2.0000	0.0	0.0	0.0	0.0
4 PRODUCT CL	2.	0.	0.	0.0	1.0000	0.0	0.0	0.0	0.0
5	0.	0.	0.	0.0	0.0	0.0	0.0	0.0	0.0

NOTES

1 1 THIS IS THE REVERSE DEACON PROCESS.

U U

NAMELISTS

NAME1

STEP=	1,T=	1000.0000	, 800.00000	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.54679998	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.58509994	, 0.39309996	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.38749999	, 0.27039999	, 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
1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000

NAME=1,SAME=F,H298=T,EFF= 0.29999995

END

NAME1

STEP=	2,T=	300.00000	, 300.00000	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
1.0000000	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 1.0000000	, 1.0000000	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.49599999	, 0.49599999	, 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
1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000

NAME=1,SAME=F,H298=T,EFF= 0.29999995

END

NAME1

STEP=	3,T=	1000.0000	, 1000.0000	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 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
1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000

NAME=1,SAME=F,H298=T,EFF= 0.29999995

END

NAME1

STEP=	4,T=	300.00000	, 300.00000	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0

NAME=1,SAME=F,H298=T,EFF= 0.29999995

END

NAME1

0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0	, 0.0
1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000

NAME=1,SAME=F,H298=T,EFF= 0.29999995

END

THEMUM DATA FOUND ON TAPE 4

300.000 1000.000 5000.000

```

1  LL2      J 9/85CL 2.  0.  0.  0.G  300.000  5000.000
   0.43077812D 01 0.31182799D-03-0.15310803D-06 0.44511908D-10-0.43057734D-14
   -0.13435250D 04 0.20886676D 01 0.31316881D 01 0.48997849D-02-0.69411462D-05
   0.44785615D-08-0.10621851D-11-0.10979695D 04 0.77833424D 01
2  nCL      J 9/84H 1.CL 1.  0.  0.G  300.000  5000.000
   0.27005882D 01 0.14381881D-02-0.46992994D-06 0.73499401D-10-0.43731091D-14
   -0.11917485D 05 0.64583540D 01 0.35248165D 01 0.29984862D-04-0.86221888D-06
   0.20979720D-08-0.98658148D-12-0.12150508D 05 0.23957710D 01
3  H2       J 3/61H 2.  0.  0.  0.G  300.000  5000.000
   0.31001892D 01 0.51119458D-03-0.52644207D-07-0.34909964D-10 0.36945341D-14
   -0.87738057D 05-0.19829412D 01 0.30574446D 01 0.26765198D-02-0.58099158D-05
   0.55210378D-08-0.16122734D-11-0.98890454D 03-0.22997055D 01
4  H2U(S)   L11/65H 2.0  1.  0.  0.S  200.000  273.150
   0.0 0.0 0.0 0.0 0.0
   0.0 0.0 -0.39269328D-01 0.16920418D-01 0.0
   0.0 0.0 -0.35949578D 05 0.56932779D 00
5  H2U(L)   L11/65H 2.0  1.  0.  0.L  273.150  1000.000
   0.0 0.0 0.0 0.0 0.0
   0.0 0.0 0.12712782D 02-0.17662790D-01-0.22556647D-04
   0.20820903D-06-0.24078606D-09-0.37483199D 05-0.59115341D 02
6  H2U      J 3/61H 2.0  1.  0.  0.G  300.000  5000.000
   0.27167625D 01 0.29451572D-02-0.80224373D-06 0.10226881D-09-0.48472138D-14
   -0.29905824D 05 0.66305668D 01 0.40701275D 01-0.11084499D-02 0.41521180D-05
   -0.29637404D-08 0.80702101D-12-0.30279719D 05-0.32270044D 00
7  B2       J 9/65U 2.  0.  0.  0.G  300.000  5000.000
   0.36219530D 01 0.73618256D-03-0.19652225D-06 0.36201556D-10-0.28945625D-14
   -0.12019824D 04 0.36150951D 01 0.36255980D 01-0.18782183D-02 0.70554543D-05
   -0.67635106D-08 0.21555986D-11-0.10475225D 04 0.43052769D 01
8  VCL2(S)  V 1.CL 2.  0.  0.S  400.000  1300.000
   0.95526459D 01-0.10050602D-03 0.42804328D-06 0.69741879D-09-0.36384833D-12
   -0.57262891D 05-0.41888397D 02 0.80468121D 01 0.24864080D-02 0.26082876D-06
   -0.16870474D-08 0.90676322D-12-0.56852773D 05-0.34894150D 02
9  VCL3(S)  BM584 V 1.CL 3.  0.  0.S  300.000  900.000
   0.0 0.0 0.0 0.0 0.0
   0.0 0.0 0.90046692D 01 0.77003576D-02 0.29381454D-05
   -0.15691260D-07 0.97001244D-11-0.72872250D 05-0.37855011D 02
10 VCL4(L)  V 1.CL 4.  0.  0.L  300.000  1000.000
   0.0 0.0 0.0 0.0 0.0
   0.0 0.0 0.19360275D 02-0.25150350D-02-0.55687997D-05
   0.0 0.0 -0.74112625D 05-0.79361496D 02
11 VCL4     C 66 V 1.CL 4.  0.  0.G  300.000  1500.000
   0.62806005D 01 0.84980540D-02 0.51972811D-05-0.10863229D-07 0.37297309D-11
   -0.64711138D 05 0.72811947D 01 0.91422043D 01 0.10671981D-01-0.78822186D-05
   -0.25107101D-08 0.34211948D-11-0.66326500D 05-0.10827267D 02

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END OF INPUT DATA FOR THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976

FOR TEMP. SCHEDULE 1 AND REACTION 2 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL2(S)
FOR TEMP. SCHEDULE 1 AND REACTION 3 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL3(S)
FOR TEMP. SCHEDULE 1 AND REACTION 11 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL2(S)

FOR TEMP. SCHEDULE 1 AND REACTION 16 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL3(S)
FOR TEMP. SCHEDULE 1 AND REACTION 17 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL3(S)
FOR TEMP. SCHEDULE 2 AND REACTION 2 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL2(S)
FOR TEMP. SCHEDULE 2 AND REACTION 3 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL3(S)
FOR TEMP. SCHEDULE 2 AND REACTION 11 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL2(S)
FOR TEMP. SCHEDULE 2 AND REACTION 16 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL3(S)
FOR TEMP. SCHEDULE 2 AND REACTION 17 THE TEMP. IS MORE THAN 10 DEG.OUTSIDE THE RANGE OF THE DATA FOR	VCL3(S)

TABLE I
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THE VANADIUM CHLORIDE PROCESS APRIL 26, 1976

TEMPERATURE SCHEDULE 1.
 $H_2O + Cl_2 \rightarrow 2 HCl + 0.5 O_2$
 $2 VCl_2(S) + 2 HCl \rightarrow 2 VCl_3(S) + H_2$
 $4 VCl_3(S) \rightarrow 2 VCl_4 + 2 VCl_2(S)$
 $2 VCl_4(L) \rightarrow 2 VCl_3(S) + Cl_2$

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H_2 . EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

EPSI EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM					WORK OF SEPARATION OF GASES (KCAL)						
			EXTENT OF REACTION AS PERCENT OF EPSI EQ.					EXTENT OF REACTION AS PERCENT OF EPSI EQ.						
			100	90	80	70	60	50	100	90	80	70	60	50

STEP 1. AT 1000.00 DEG., AND 1.00 ATM.

DELTA-H= 14.12652 KCAL, DELTA-S= 16.26844 CAL/DEG, DELTA-G= -2.14792 KCAL

THIS IS THE REVERSE DEACON PROCESS.

H_2O IS THE BASE REACTANT FOR THIS REACTION

0.85590 H_2O	1.000*	0.168	0.298	0.460	0.669	0.947	1.337*							
CL ₂	3.000*	2.505	2.895	3.381	4.007	4.842	6.010*	9.606	10.243	10.937	11.704	12.570	13.572	
0.77500 H_2O	1.000*	0.290	0.434	0.613	0.843	1.151	1.581*							
CL ₂	2.000*	1.581	1.867	2.226	2.687	3.301	4.161*	8.416	9.091	9.818	10.616	11.509	12.536	
0.58910 H_2O	1.000*	0.698	0.886	1.122	1.425	1.829	2.395*							
CL ₂	1.000*	0.698	0.886	1.122	1.425	1.829	2.395*	7.535	8.247	9.006	9.832	10.751	11.800	
0.38750 H_2O	2.000*	1.581	1.867	2.226	2.687	3.301	4.161*							
CL ₂	1.000*	0.290	0.434	0.613	0.843	1.151	1.581*	8.416	9.091	9.818	10.616	11.509	12.536	

STEP 2. AT 300.00 DEG., AND 1.00 ATM.

DELTA-H= -17.48063 KCAL, DELTA-S= -41.91027 CAL/DEG, DELTA-G= -4.90755 KCAL

$VCl_2(S)$ IS THE BASE REACTANT FOR THIS REACTION

0.99200 $VCl_2(S)$	1.000*	0.016	0.240	0.520	0.880	1.360	2.032*							
HCL	1.000*	0.016	0.240	0.520	0.880	1.360	2.032*	0.049	0.363	0.582	0.775	0.959	1.146	
1.00000 $VCl_2(S)$	1.000*	0.000	0.222	0.500	0.857	1.333	2.000*							
HCL	2.000*	2.000	2.444	3.000	3.714	4.667	6.000*	1.138	1.237	1.341	1.452	1.574	1.711	
1.00000 $VCl_2(S)$	1.000*	0.000	0.222	0.500	0.857	1.333	2.000*							
HCL	3.000*	4.000	4.667	5.500	6.571	8.000	10.000*	1.492	1.574	1.664	1.762	1.872	1.998	
0.49600 $VCl_2(S)$	2.000*	2.032	2.480	3.040	3.760	4.720	6.065*							
HCL	1.000*	0.016	0.240	0.520	0.880	1.360	2.032*	0.049	0.363	0.582	0.775	0.959	1.146	

STEP 3. AT 1000.00 DEG., AND 1.00 ATM.

DELTA-H= 79.11398 KCAL, DELTA-S= 81.96803 CAL/DEG, DELTA-G= -2.85405 KCAL

$VCl_3(S)$ IS THE BASE REACTANT FOR THIS REACTION

* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.205058E 01
 * THE WORK OF SEPARATION = 0.0

STEP 4. AT 300.00 DEG., AND 1.00 ATM.

DELTA-H= -5.37749 KCAL, DELTA-S= -3.23116 CAL/DEG, DELTA-G= -4.40615 KCAL

$VCl_4(L)$ IS THE BASE REACTANT FOR THIS REACTION

* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.162679E 04
 * THE WORK OF SEPARATION = 0.0

TABLE II
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
TEMPERATURE SCHEDULE 1.

				DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	1000.00 DEG. --->	300.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 HCL	FROM REACTION 1 --->	2.00 HCL	IN REACTION 2	-10.03429	-17.1224	69.64944
STEP 6	1000.00 DEG. --->	298.15 DEG.				
	1.00 ATM. --->	1.00 ATM.				
0.50 O2	FROM REACTION 1 --->	0.50 O2	FINAL PRODUCT	-2.71354	-4.5937	19.07708
STEP 7	300.00 DEG. --->	298.15 DEG.				
	1.00 ATM. --->	1.00 ATM.				
1.00 H2	FROM REACTION 2 --->	1.00 H2	FINAL PRODUCT	-0.01276	-0.0427	0.05778
STEP 8	1000.00 DEG. --->	379.43 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 VCL4	FROM REACTION 3 --->	2.00 VCL4	IN REACTION 9	-31.08515	-48.3080	132.94199
STEP 9	379.43 DEG. --->	379.43 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 VCL4	FROM REACTION 8 --->	2.00 VCL4(L)	IN REACTION 10	-19.11090	-50.3211	-0.01763
STEP 10	379.43 DEG. --->	300.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 VCL4(L)	FROM REACTION 9 --->	2.00 VCL4(L)	IN REACTION 4	-5.63806	-16.6818	10.18078
STEP 11	1000.00 DEG. --->	300.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 VCL2(S)	FROM REACTION 3 --->	2.00 VCL2(S)	IN REACTION 2	-26.27527	-44.6119	51.01828
STEP 12	300.00 DEG. --->	1000.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
1.00 CL2	FROM REACTION 4 --->	1.00 CL2	IN REACTION 1	6.09859	10.3954	-41.63377
STEP 13	298.15 DEG. --->	373.47 DEG.				
	1.00 ATM. --->	1.00 ATM.				
1.00 H2O(L)	RAW MATERIAL --->	1.00 H2O(L)	IN REACTION 14	1.35771	4.0596	-1.41736
STEP 14	373.47 DEG. --->	373.47 DEG.				
	1.00 ATM. --->	1.00 ATM.				
1.00 H2O(L)	FROM REACTION 13 --->	1.00 H2O	IN REACTION 15	9.77287	26.1454	0.00847
STEP 15	373.47 DEG. --->	1000.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
1.00 H2O	FROM REACTION 14 --->	1.00 H2O	IN REACTION 1	5.60144	8.6684	-32.46456
STEP 16	300.00 DEG. --->	1000.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 VCL3(S)	FROM REACTION 2 --->	2.00 VCL3(S)	IN REACTION 3	34.99055	59.1566	-68.19561
STEP 17	300.00 DEG. --->	1000.00 DEG.				
	1.00 ATM. --->	1.00 ATM.				
2.00 VCL3(S)	FROM REACTION 4 --->	2.00 VCL3(S)	IN REACTION 3	34.99055	59.1566	-68.19561
TOTALS FOR STEPS 1 TO 17				68.31810	38.9954	56.69162

TABLE 1
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THE VANADIUM CHLORIDE PROCESS APRIL 26, 1976
TEMPERATURE SCHEDULE 2.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H₂. EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

EPSI EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM						WORK OF SEPARATION OF GASES (KCAL)					
			100	90	80	70	60	50	100	90	80	70	60	50

STEP 1. AT 800.00DEG., AND 1.00ATM.

DELTA-H= 14.02324 KCAL, DELTA-S= 16.15991 CAL/DEG, DELTA-G= 1.09531 KCAL

THIS IS THE REVERSE DRACON PROCESS.

H₂O IS THE BASE REACTANT FOR THIS REACTION

0.65370 H ₂ O	1.000*	0.578	0.753	0.973	1.254	1.630	2.156*							
Cl ₂	3.000*	3.734	4.260	4.918	5.763	6.890	8.466*	9.107	9.587	10.113	10.701	11.369	12.148	
0.54080 H ₂ O	1.000*	0.849	1.055	1.311	1.642	2.062	2.698*							
Cl ₂	2.000*	2.698	3.109	3.623	4.283	5.164	6.396*	8.508	8.998	9.535	10.133	10.810	11.598	
0.39310 H ₂ O	1.000*	1.544	1.827	2.180	2.634	3.240	4.088*							
Cl ₂	1.000*	1.544	1.827	2.180	2.634	3.240	4.088*	8.097	8.596	9.142	9.747	10.432	11.220	
0.27040 H ₂ O	2.000*	2.698	3.109	3.623	4.283	5.164	6.396*							
Cl ₂	1.000*	0.849	1.055	1.311	1.642	2.062	2.698*	8.508	8.998	9.535	10.133	10.810	11.598	

STEP 2. AT 300.00DEG., AND 1.00ATM.

DELTA-H= -17.48063 KCAL, DELTA-S= -41.91027 CAL/DEG, DELTA-G= -4.90755 KCAL

VCL₂(S) IS THE BASE REACTANT FOR THIS REACTION

0.99200 VCL ₂ (S)	1.000*	0.016	0.240	0.520	0.880	1.360	2.032*							
HCl	1.000*	0.016	0.240	0.520	0.880	1.360	2.032*	0.049	0.363	0.582	0.775	0.959	1.140	
1.00000 VCL ₂ (S)	1.000*	0.000	0.222	0.500	0.857	1.333	2.000*							
HCl	2.000*	2.000	2.444	3.000	3.714	4.667	6.000*	1.138	1.237	1.341	1.452	1.574	1.711	
1.00000 VCL ₂ (S)	1.000*	0.000	0.222	0.500	0.857	1.333	2.000*							
HCl	3.000*	4.000	4.667	5.500	6.571	8.000	10.000*	1.492	1.574	1.664	1.762	1.872	1.998	
0.49600 VCL ₂ (S)	2.000*	2.032	2.480	3.040	3.760	4.720	6.065*							
HCl	1.000*	0.016	0.240	0.520	0.880	1.360	2.032*	0.049	0.363	0.582	0.775	0.959	1.140	

STEP 3. AT 1000.00DEG., AND 1.00ATM.

DELTA-H= 79.11398 KCAL, DELTA-S= 81.96803 CAL/DEG, DELTA-G= -2.85405 KCAL

VCL₃(S) IS THE BASE REACTANT FOR THIS REACTION

* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.205058E 01
* THE WORK OF SEPARATION = 0.0

STEP 4. AT 300.00DEG., AND 1.00ATM.

DELTA-H= -5.37749 KCAL, DELTA-S= -3.23116 CAL/DEG, DELTA-G= -4.40815 KCAL

VCL₄(L) IS THE BASE REACTANT FOR THIS REACTION

* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.162679E 04
* THE WORK OF SEPARATION = 0.0

TABLE II
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THE VANADIUM CHLORIDE PROCESS APRIL 26, 1976
TEMPERATURE SCHEDULE 2.

				DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	800.00 DEG. ---> 300.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 HCL	FROM REACTION 1 ---> 2.00 HCL	IN REACTION 2	-7.06504	-13.8119	48.67109	
STEP 6	800.00 DEG. ---> 298.15 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
0.50 U2	FROM REACTION 1 ---> 0.50 U2	FINAL PRODUCT	-1.89256	-3.6783	13.34653	
STEP 7	300.00 DEG. ---> 298.15 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
1.00 H2	FROM REACTION 2 ---> 1.00 H2	FINAL PRODUCT	-0.01276	-0.0427	0.05778	
STEP 8	1000.00 DEG. ---> 379.43 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 VCL4	FROM REACTION 3 ---> 2.00 VCL4	IN REACTION 9	-31.08515	-48.3080	132.94199	
STEP 9	379.43 DEG. ---> 379.43 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 VCL4	FROM REACTION 8 ---> 2.00 VCL4(L)	IN REACTION 10	-19.11090	-50.3211	-0.01763	
STEP 10	379.43 DEG. ---> 300.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 VCL4(L)	FROM REACTION 9 ---> 2.00 VCL4(L)	IN REACTION 4	-5.63806	-16.6818	10.18078	
STEP 11	1000.00 DEG. ---> 300.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 VCL2(S)	FROM REACTION 3 ---> 2.00 VCL2(S)	IN REACTION 2	-26.27527	-44.6119	51.01828	
STEP 12	300.00 DEG. ---> 800.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
1.00 CL2	FROM REACTION 4 ---> 1.00 CL2	IN REACTION 1	4.31527	8.4060	-29.07881	
STEP 13	298.15 DEG. ---> 373.47 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
1.00 H2O(L)	RAW MATERIAL ---> 1.00 H2O(L)	IN REACTION 14	1.35771	4.0596	-1.41736	
STEP 14	373.47 DEG. ---> 373.47 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
1.00 H2O(L)	FROM REACTION 13 ---> 1.00 H2O	IN REACTION 15	9.77287	26.1454	0.00847	
STEP 15	373.47 DEG. ---> 800.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
1.00 H2O	FROM REACTION 14 ---> 1.00 H2O	IN REACTION 1	3.09181	6.5403	-21.55383	
STEP 16	300.00 DEG. ---> 1000.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 VCL3(S)	FROM REACTION 2 ---> 2.00 VCL3(S)	IN REACTION 3	34.99055	59.1566	-68.19561	
STEP 17	300.00 DEG. ---> 1000.00 DEG.					
	1.00 ATM. ---> 1.00 ATM.					
2.00 VCL3(S)	FROM REACTION 4 ---> 2.00 VCL3(S)	IN REACTION 3	34.99055	59.1566	-68.19561	
TOTALS FOR STEPS 1 TO 17			68.31610	38.9954	56.69162	

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
COMPARISON OF EXOTHERMIC AND ENDOTHERMIC STEPS

TEMPERATURE SCHEDULE 1					TEMPERATURE SCHEDULE 2				
STEP	TEMPERATURES (K)		HEAT (KCAL)		*STEP*	TEMPERATURES (K)		HEAT (KCAL)	
*	*REACTANTS*	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*	*	*REACTANTS*	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*
* 1 *	* 1000.00 *	* 1000.00 *		* 14.1205 *	* 1 *	* 800.00 *	* 800.00 *		* 14.0232 *
* 2 *	* 300.00 *	* 300.00 *	* -17.4806 *		* 2 *	* 300.00 *	* 300.00 *	* -17.4806 *	
* 3 *	* 1000.00 *	* 1000.00 *		* 79.1140 *	* 3 *	* 1000.00 *	* 1000.00 *		* 79.1140 *
* 4 *	* 300.00 *	* 300.00 *	* -5.3775 *		* 4 *	* 300.00 *	* 300.00 *	* -5.3775 *	
* 5 *	* 1000.00 *	* 300.00 *	* -10.0343 *		* 5 *	* 800.00 *	* 300.00 *	* -7.0650 *	
* 6 *	* 1000.00 *	* 298.15 *	* -2.7135 *		* 6 *	* 800.00 *	* 298.15 *	* -1.8926 *	
* 7 *	* 300.00 *	* 298.15 *	* -0.0128 *		* 7 *	* 300.00 *	* 298.15 *	* -0.0128 *	
* 8 *	* 1000.00 *	* 379.43 *	* -31.0851 *		* 8 *	* 1000.00 *	* 379.43 *	* -31.0851 *	
* 9 *	* 379.43 *	* 379.43 *	* -19.1109 *		* 9 *	* 379.43 *	* 379.43 *	* -19.1109 *	
* 10 *	* 379.43 *	* 300.00 *	* -5.6381 *		* 10 *	* 379.43 *	* 300.00 *	* -5.6381 *	
* 11 *	* 1000.00 *	* 300.00 *	* -26.2753 *		* 11 *	* 1000.00 *	* 300.00 *	* -26.2753 *	
* 12 *	* 300.00 *	* 1000.00 *		* 6.0986 *	* 12 *	* 300.00 *	* 800.00 *		* 4.3153 *
* 13 *	* 298.15 *	* 373.47 *		* 1.3577 *	* 13 *	* 298.15 *	* 373.47 *		* 1.3577 *
* 14 *	* 373.47 *	* 373.47 *		* 9.7729 *	* 14 *	* 373.47 *	* 373.47 *		* 9.7729 *
* 15 *	* 373.47 *	* 1000.00 *		* 5.6014 *	* 15 *	* 373.47 *	* 800.00 *		* 3.6918 *
* 16 *	* 300.00 *	* 1000.00 *		* 34.9905 *	* 16 *	* 300.00 *	* 1000.00 *		* 34.9905 *
* 17 *	* 300.00 *	* 1000.00 *		* 34.9905 *	* 17 *	* 300.00 *	* 1000.00 *		* 34.9905 *
TOTALS									
			* -117.7279 *	* 186.0459 *				* -113.9378 *	* 182.2557 *

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 1

HEAT		STREAM SUPPLYING HEAT						STREAM ABSORBING HEAT					
EXCHANGED (KCAL)	STEP	TEMPERATURES		AMOUNT OF HEAT		STEP	TEMPERATURES		AMOUNT OF HEAT				
		INITIAL	FINAL	INITIALLY AVAILABLE	REMAINING		INITIAL	FINAL	INITIALLY NEEDED	REMAINING			
W	0.011	7	300.00	298.15	-0.013	0.0	13	298.15	298.79	1.358	1.346		
	0.022	2	300.00	300.00	-17.481	-17.459	13	298.79	300.00	1.346	1.324		
	0.418	10	379.43	373.47	-5.638	-5.220	14	373.47	373.47	9.773	9.355		
W	1.192	10	373.47	300.00	-5.220	-4.028	13	300.00	366.16	1.324	0.132		
	0.545	10	373.47	300.00	-4.028	-3.483	12	300.00	366.21	6.099	5.553		
W	0.132	10	373.47	370.64	-3.483	-3.351	13	366.16	373.47	0.132	0.0		
W	2.892	10	370.64	300.00	-3.351	-0.459	16	300.00	363.68	34.991	32.099		
W	0.413	10	370.64	300.00	-0.459	-0.046	17	300.00	309.22	34.991	34.578		
	9.355	9	379.43	379.43	-19.111	-9.756	14	373.47	373.47	9.355	0.0		
	0.110	9	379.43	379.43	-9.756	-9.645	12	366.21	379.43	5.553	5.443		
	0.049	9	379.43	379.43	-9.645	-9.597	15	373.47	379.43	5.601	5.553		
	0.729	9	379.43	379.43	-9.597	-8.868	16	363.68	379.43	32.099	31.370		
	3.208	9	379.43	379.43	-8.868	-5.660	17	309.22	379.43	34.578	31.370		
	5.443	5	1000.00	627.85	-10.034	-4.592	12	379.43	1000.00	5.443	0.0		
W	2.095	5	627.85	479.05	-4.592	-2.497	15	379.43	627.85	5.553	3.458		
	1.390	5	479.05	379.43	-2.497	-1.106	16	379.43	409.15	31.370	29.979		
	1.501	6	1000.00	627.85	-2.714	-1.212	15	627.85	794.88	3.458	1.957		
	0.817	6	627.85	409.15	-1.212	-0.395	16	409.15	426.46	29.979	29.162		
W	0.107	6	409.15	379.43	-0.395	-0.288	17	379.43	381.73	31.370	31.263		
	1.957	8	1000.00	961.60	-31.085	-29.128	15	794.88	1000.00	1.957	0.0		
W	26.869	8	961.60	426.46	-29.128	-2.259	16	426.46	957.42	29.162	2.293		
W	2.101	8	426.46	382.75	-2.259	-0.158	17	381.73	426.46	31.263	29.162		
W	1.689	11	1000.00	957.42	-26.275	-24.586	16	957.42	988.85	2.293	0.604		
	20.104	11	957.42	426.46	-24.586	-4.482	17	426.46	828.74	29.162	9.058		

W-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.

(THE DELTA-H VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES)

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 1

HEAT AVAILABLE				HEAT REQUIRED			
STEP	TEMPERATURE		HEAT	STEP	TEMPERATURE		HEAT
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED
2	300.00	300.00	-17.459	1	1000.00	1000.00	14.121
4	300.00	300.00	-5.377	3	1000.00	1000.00	79.114
5	379.43	300.00	-1.106				
6	379.43	298.15	-0.288				
8	382.75	379.43	-0.158				
9	379.43	379.43	-5.660				
10	370.64	300.00	-0.046				
11	426.46	300.00	-4.482				
				16	988.85	1000.00	0.604
				17	828.74	1000.00	9.058
TOTALS			-34.577	102.896			

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 2

HEAT		STREAM SUPPLYING HEAT						STREAM ABSORBING HEAT					
EXCHANGED (KCAL)	STEP	TEMPERATURES		AMOUNT OF HEAT		STEP	TEMPERATURES		AMOUNT OF HEAT				
		INITIAL	FINAL	INITIALLY AVAILABLE	REMAINING		INITIAL	FINAL	INITIALLY NEEDED	REMAINING			
0.011	7	300.00	298.15	-0.013	0.0	13	298.15	298.79	1.358	1.346			
0.022	2	300.00	300.00	-17.481	-17.459	13	298.79	300.00	1.346	1.324			
0.416	10	379.43	373.47	-5.638	-5.220	14	373.47	373.47	9.773	9.355			
1.192	10	373.47	300.00	-5.220	-4.028	13	300.00	366.16	1.324	0.132			
0.545	10	373.47	300.00	-4.028	-3.483	12	300.00	366.21	4.315	3.770			
0.132	10	373.47	370.64	-3.483	-3.351	13	366.16	373.47	0.132	0.0			
2.892	10	370.64	300.00	-3.351	-0.459	16	300.00	363.68	34.991	32.099			
0.413	10	370.64	300.00	-0.459	-0.046	17	300.00	309.22	34.991	34.578			
9.355	9	379.43	379.43	-19.111	-9.756	14	373.47	373.47	9.355	0.0			
0.110	9	379.43	379.43	-9.756	-9.645	12	366.21	379.43	3.770	3.659			
0.049	9	379.43	379.43	-9.645	-9.597	15	373.47	379.43	3.692	3.643			
0.729	9	379.43	379.43	-9.597	-8.868	16	363.68	379.43	32.099	31.370			
3.208	9	379.43	379.43	-8.868	-5.660	17	309.22	379.43	34.578	31.370			
3.659	5	800.00	543.86	-7.065	-3.406	12	379.43	800.00	3.659	0.0			
1.369	5	543.86	446.09	-3.406	-2.036	15	379.43	543.86	3.643	2.274			
0.930	5	446.09	379.43	-2.036	-1.106	16	379.43	399.35	31.370	30.440			
1.001	6	800.00	543.86	-1.893	-0.892	15	543.86	659.19	2.274	1.273			
0.532	6	543.86	399.35	-0.892	-0.359	16	399.35	410.68	30.440	29.908			
0.072	6	399.35	379.43	-0.359	-0.288	17	379.43	380.97	31.370	31.298			
10.161	8	1000.00	800.00	-31.085	-20.924	1	800.00	800.00	14.023	3.862			
1.273	6	800.00	774.87	-20.924	-19.651	15	659.19	800.00	1.273	0.0			
18.069	8	774.87	412.44	-19.651	-1.582	16	410.68	774.87	29.908	11.839			
1.474	8	412.44	381.71	-1.582	-0.109	17	380.97	412.44	31.298	29.824			
3.862	11	1000.00	902.22	-26.275	-22.413	1	800.00	800.00	3.862	0.0			
4.944	11	902.22	774.87	-22.413	-17.469	16	774.87	870.30	11.839	6.895			
13.490	11	774.87	412.44	-17.469	-3.979	17	412.44	686.81	29.824	16.334			

W-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.

(THE DELTA-H VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES)

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 2

HEAT AVAILABLE				HEAT REQUIRED			
STEP	TEMPERATURE		HEAT	STEP	TEMPERATURE		HEAT
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED
2	300.00	300.00	-17.459	3	1000.00	1000.00	79.114
4	300.00	300.00	-5.377				
5	379.43	300.00	-1.106				
6	379.43	298.15	-0.288				
8	381.71	379.43	-0.109				
9	379.43	379.43	-5.660				
10	370.64	300.00	-0.046				
11	412.44	300.00	-3.979				
				16	870.30	1000.00	6.895
				17	686.81	1000.00	16.334
TOTALS			-34.023	102.343			

THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
FIGURES OF MERIT

TEMP.	WORK OF	WORK	TOTAL	FIGURES OF MERIT			
SCHEDULE	SEPARATION	GENERATED	HEAT	1ST ESTIMATE	2ND ESTIMATE		
	MIN	MAX	REQUIRED	MIN	MAX	MIN	MAX
1	7.585	15.570	0.0	102.896	0.5683	0.7299	0.3305 0.4452
2	8.146	14.146	0.0	102.343	0.5916	0.7156	0.3474 0.4361

ALL HEAT ABOVE 500 K WHICH IS STILL AVAILABLE AFTER STREAM MATCHING, IS TURNED INTO WORK GENERATED USING A 30% EFFICIENCY AND SUBTRACTED FROM THE WORK OF SEPARATION NEEDED. THE FIRST ESTIMATE FOR A FIGURE OF MERIT ASSUMES PERFECT HEAT REGENERATION AND 100% EFFICIENCY IN THE WORK OF SEPARATION. THE SECOND ESTIMATE USES THE HEAT REQUIRED AFTER STREAM MATCHING AS THE TOTAL HEAT REQUIRED AND ASSUMES ONLY A 50% EFFICIENCY FOR THE WORK OF SEPARATION. ALL WORK REQUIRED IS ASSUMED TO BE GENERATED FROM HEAT AT A 30% EFFICIENCY.

IN REACTION 3 THE MATERIAL VCL2(S) HAS NOT BEEN EXACTLY MATCHED FOR ITS PHASE AT 298 K.
 FOR TEMP. SCHEDULE 1 AND REACTION 2 THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR
 FOR TEMP. SCHEDULE 1 AND REACTION 3 THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR

VCL2(S)
 VCL2(S)

PROPERTIES OF THE BASE REACTIONS AT 298 K FOR
 THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976

STEP 1. AT 298.15DEG., AND 1.00ATM.
 $\text{H}_2\text{O}(\text{L}) + \text{Cl}_2 \longrightarrow 2 \text{HCl} + 0.5 \text{O}_2$

DELTA-H= 24.19254 KCAL, DELTA-S= 43.78508 CAL/DEG, DELTA-G= 11.13802 KCAL

STEP 2. AT 298.15DEG., AND 1.00ATM.
 $2 \text{VCL}_2(\text{S}) + 2 \text{HCl} \longrightarrow 2 \text{VCL}_3(\text{S}) + \text{H}_2$

DELTA-H= -17.48565 KCAL, DELTA-S= -41.92706 CAL/DEG, DELTA-G= -4.98510 KCAL

STEP 3. AT 298.15DEG., AND 1.00ATM.
 $4 \text{VCL}_3(\text{S}) \longrightarrow 2 \text{VCL}_4(\text{L}) + 2 \text{VCL}_2(\text{S})$

DELTA-H= 66.95313 KCAL, DELTA-S= 40.24965 CAL/DEG, DELTA-G= 54.95270 KCAL

STEP 4. AT 298.15DEG., AND 1.00ATM.
 $2 \text{VCL}_4(\text{L}) \longrightarrow 2 \text{VCL}_3(\text{S}) + \text{Cl}_2$

DELTA-H= -5.34192 KCAL, DELTA-S= -3.11224 CAL/DEG, DELTA-G= -4.41401 KCAL

TOTALS DELTA-H= 68.31806 KCAL, DELTA-S= 38.99542 CAL/DEG, DELTA-G= 56.69162 KCAL

PROCESS SUMMARY
THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
TEMPERATURE SCHEDULE 1

STAGE	1	2	3	4	SUM
(1) H298, HEAT OF REACTION AT 298K (KCAL)	24.19	-17.49	66.95	-5.34	68.32
(2) HT, HEAT OF REACTION AT TEMP T (KCAL)	14.12	-17.48	79.11	-5.38	
(3) T, TEMP. OF REACTION (K)	1000.	300.	1000.	300.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	7.54	0.05	0.0	0.0	7.58
(5) THEO. WORK OF SEPARATION ((	0.99	0.01	0.0	0.0	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	0.0	0.0	0.0	0.0	0.0
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) QS=(2WS-WG)/0.30	50.23	0.33	0.0	0.0	50.56
(8) Q, HEAT REQUIREMENT (KCAL)	14.12	0.30	83.94	4.53	102.90
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	64.35	0.63	83.94	4.53	153.46
(10) WEIGHING FACTOR (9)/SUM(9)	0.419	0.004	0.547	0.030	
(11) QREJ, HEAT REJECTED (KCAL)	-0.84	-20.25	-5.17	-8.31	-34.58
(12) NUJ, INDIVIDUAL FIGURES OF MERIT	0.376	-27.711	0.798	-1.179	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)X(12), SUM(13)=OVERALL FIG. MERIT	0.158	-0.114	0.436	-0.035	0.445
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	0.748	0.301	0.076	0.122	1.247

PROCESS SUMMARY
THE VANADIUM CHLORIDE PROCESS APRIL 28, 1976
TEMPERATURE SCHEDULE 2

STAGE	1	2	3	4	SUM
(1) H298, HEAT OF REACTION AT 298K (KCAL)	24.19	-17.49	66.95	-5.34	68.32
(2) HT, HEAT OF REACTION AT TEMP T (KCAL)	14.02	-17.48	79.11	-5.38	
(3) T, TEMP. OF REACTION (K)	800.	300.	1000.	300.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	8.10	0.05	0.0	0.0	8.15
(5) THEO. WORK OF SEPARATION ((	0.99	0.01	0.0	0.0	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	0.0	0.0	0.0	0.0	0.0
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) QS=(2WS-WG)/0.30	53.98	0.33	0.0	0.0	54.31
(8) Q, HEAT REQUIREMENT (KCAL)	0.0	3.45	90.73	8.17	102.34
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	53.98	3.78	90.73	8.17	156.65
(10) WEIGHING FACTOR (9)/SUM(9)	0.345	0.024	0.579	0.052	
(11) QREJ, HEAT REJECTED (KCAL)	-0.84	-20.00	-4.90	-8.28	-34.02
(12) NUJ, INDIVIDUAL FIGURES OF MERIT	0.448	-4.630	0.738	-0.654	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)x(12), SUM(13)=OVERALL FIG. MERIT	0.154	-0.112	0.427	-0.034	0.436
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	0.803	0.298	0.072	0.121	1.293

Sample Problem 2. The Zinc Sulfur Process

For the following process:

Run reaction (1) at 501 K with the extent of reaction = 1.0 for stoichiometric composition.

Run reaction (2) at 1200, and 1300 K with the extent of reaction = 1.0 for stoichiometric composition, $P = 1/2$ atm.

Run reaction (3) at 850 K (there is no work of separation since this is a dummy reaction to vaporize the sulfur).

Run reaction (4) at 850 K with the extent of reaction = 0.42 at stoichiometric composition and the base reactant being H_2O .

Run reaction (5) at 1100, 1200, and 1300 K with respective extents of reaction being 0.0857, 0.1435, and 0.2179.

Input Data Cards for Sample Problem 2

THE ZINC SULFUR PROCESS CHEMICAL REACTIONS

1 REACTANTS 1.00 2.0	G 1.5	1.5
1 REACTANT ZN 1.00 1.0	S 1.0	B 1.0
2 REACTANTS 1.00 3.0	G 0.143	0.143
2 REACTANT ZN 1.0 S 1.00 4.0	S 1.0	B 1.0
3 REACTANTS 2.0	G 0.75	0.75
3 REACTANT H 2.00 1.0	G 1.0	B 1.0
4 REACTANT H 2.0 S 1.0	G 1.0	B 1.0
1 PRODUCT S 1.0	L 0.5	3.88e36
1 PRODUCT ZN 1.0 S 1.00 4.0	S 1.0	
2 PRODUCT ZN 1.00 1.0	S 1.0	
2 PRODUCT S 1.00 2.0	G 1.0	
2 PRODUCT O 2.0	G 0.5	
2 PRODUCT S 1.00 3.0	G 0.143	
3 PRODUCT H 2.0 S 1.0	G 1.0	
3 PRODUCT S 1.00 2.0	G 0.5	
4 PRODUCT H 2.0	G 1.0	
4 PRODUCT S 2.0	G 0.5	

NAMELISTS

```

&NAM1 STEP=1,PRES=1,DRAW=.TRUE.,T=3*501,EP=3*1 &END
&NAM1 STEP=2,PRES=3*0.5,T=1200,1300,1300,EP=3*1 &END
&NAM1 STEP=3,PRES=1,T=3*850,EP=3*0.42 &END
&NAM1 STEP=4,PRES=1,T=1100,1200,1300,EP=0.0857,0.1435,0.2179 &END

```

END

BEGINNING OF INFO CHEMICAL REACTIONS

NAMELISTS

DEAN=T, SAME=F, H298=T, EFF= 0.29999995

STAN
BEN

UNAN=T, SAME=F, H298=T, ETF= 0.29999995

6510

066H=1, SAME=F, H298=1, EFF= 0.49999999

LEND

0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0
0.0	, 0.0	, 0.0	, 0.0	, 0.0
1.0000000	, 1.0000000	, 1.0000000	, 1.0000000	, 1.0000000

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, 0.0      , 0.0      , 0.0      ,
, 0.0      , 0.0      , 0.0      ,
, 0.0      , 0.0      , 0.0      ,
, 0.0      , 0.0      , 0.0      ,
,PRES= 1.00000000 , 1.00000000 ,
, 1.00000000 , 1.00000000 , 1.00000000

```

THERMO DATA FOUND ON TAPE 4
 300.000 1000.000 5000.000
 1 H2 J 3/61H 2.0 0.0 0.0 300.000 5000.000
 0.310018920 01 0.511194580-03 0.526442070-07 0.249099840-10 0.369453410-14
 -0.671380210 05 -0.196294120 01 0.305744460 01 0.267651980-02 -0.580991580-05
 0.552103780-06 -0.161227340-11 -0.988906450 03 -0.229970550 01
 2 H2O(S) L11/65H 2.0 1.0 0.0 200.000 273.150
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.392693280-01 0.169204160-01 0.0
 0.0 0.0 -0.359495780 05 0.569337790 00
 3 H2O(L) L11/65H 2.0 1.0 0.0 273.150 1000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.127127820 02 -0.176627900-01 -0.225566470-04
 0.206209030-06 -0.246766060-09 -0.374831990 05 -0.591153410 02
 4 H2O J 3/61H 2.0 1.0 0.0 300.000 5000.000
 0.271676250 01 0.294513720-02 -0.802243730-06 0.102266810-09 -0.484721380-14
 -0.249055790 05 0.663056660 01 0.407012750 01 -0.110844990-02 0.415211800-05
 -0.296374040-08 0.807021010-12 -0.302797190 05 -0.322700440 00
 5 H2S J12/65H 2.5 1.0 0.0 300.000 5000.000
 0.264790990 01 0.364159960-02 -0.140993600-05 0.242787350-09 -0.157832800-13
 -0.344697880 04 0.747814080 01 0.388112930 01 -0.132118560-03 0.365177220-05
 -0.218204430-08 0.287837790-12 -0.363509160 04 0.251615050 01
 6 H2 J 9/65U 2.0 0.0 0.0 300.000 5000.000
 0.362195300 01 0.736182560-03 -0.196522250-06 0.362015560-10 -0.289456250-14
 -0.126198240 04 0.361509910 01 0.362559860 01 -0.187821630-02 0.705545430-05
 -0.676551060-08 0.215559860-11 -0.164752250 04 0.430527690 01
 7 S(S) J12/65S 1.0 0.0 0.0 300.000 368.360
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.506370160 01 0.268193510-02 -0.213301970-04
 0.947878600-06 -0.173449650-08 0.714826170 03 0.287140660 02
 8 S(L) J12/65S 1.0 0.0 0.0 328.360 2000.000
 0.360366630 01 0.990333970-03 -0.101144090-05 0.405363080-09 -0.566791320-13
 -0.895368790 05 -0.163446960 02 -0.127063090 02 0.907251630-01 -0.169517650-03
 0.130706330-06 -0.352761430-10 0.123460670 04 0.562101590 02
 9 S J 6/11S 1.0 0.0 0.0 300.000 5000.000
 0.290933230 01 -0.555872680-03 0.278369440-06 -0.501947650-10 0.312546370-14
 0.325315450 05 0.379283240 01 0.292700770 01 0.219825540-03 -0.238086520-05
 0.296348190-08 -0.108466880-11 0.324915740 05 0.351205920 01
 10 H2 J 6/61S 1.0 2.0 0.0 300.000 5000.000
 0.524515630 01 0.197042040-02 -0.603757640-06 0.151499690-09 -0.105580010-13
 -0.37552270 05 -0.108755160 01 0.326653290 01 0.532379000-02 0.664375490-06
 -0.58100230-06 0.255904300-11 -0.369081450 05 0.965134720 01
 11 H2S J 9/65S 1.0 3.0 0.0 300.000 5000.000
 0.707575700 01 0.317633850-02 -0.135357550-05 0.256308970-09 -0.179360410-13
 -0.502113750 05 -0.112007920 02 0.257803820 01 0.145563330-01 -0.917641660-05
 -0.792030220-09 0.197094680-11 -0.489317500 05 0.122518630 02
 12 S J12/65S 2.0 0.0 0.0 300.000 5000.000
 0.420511250 01 0.353091400-03 -0.135430640-06 0.252453610-10 -0.173574860-14
 0.141829060 05 0.320947070 01 0.287242410 01 0.504344330-02 -0.620552690-05
 0.530970210-06 -0.573761040-12 0.144870740 05 0.980823990 01
 13 H2O(S) BM584 ZN 1.0 1.0 0.0 300.000 1600.000
 0.619738770 01 -0.188276370-03 0.318795730-07 0.603574970-09 -0.247513110-12
 -0.439266480 05 -0.305434680 02 0.245558740 01 0.103534090-01 -0.665744850-05
 -0.360410060-08 0.384964460-11 -0.429934260 05 -0.115148050 02
 14 H2O(L) BM584 ZN 1.5 1.0 4.0 300.000 1100.000
 0.162806550 02 0.107009060-02 -0.150532970-05 -0.314333450-09 0.264842750-11
 -0.124563190 06 -0.919893190 02 0.112473240 02 0.757656620-02 0.366147350-05
 -0.394940970-08 0.144354150-11 -0.121422250 06 -0.510817260 02

END OF INPUT DATA FOR THE ZINC SULFUR PROCESS

FOR TEMP. SCHEDULE 1 AND REACTION 2	THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR	ZNSO4(S)
FOR TEMP. SCHEDULE 1 AND REACTION 3	THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR	ZNSO4(S)
FOR TEMP. SCHEDULE 2 AND REACTION 2	THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR	ZNSO4(S)
FOR TEMP. SCHEDULE 2 AND REACTION 3	THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR	ZNSO4(S)
FOR TEMP. SCHEDULE 3 AND REACTION 2	THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR	ZNSO4(S)
FOR TEMP. SCHEDULE 3 AND REACTION 3	THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR	ZNSO4(S)

TABLE I
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THE ZINC SULFUR PROCESS

TEMPERATURE SCHEDULE 1.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H₂. EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

EPSI EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM						WORK OF SEPARATION OF GASES (KCAL)					
			EXTENT OF REACTION AS PERCENT OF EPSI EQ.						EXTENT OF REACTION AS PERCENT OF EPSI EQ.					
			100	90	80	70	60	50	100	90	80	70	60	50

STEP 1. AT 501.00DEG., AND 1.00ATM.

DELTA-H= -42.71829 KCAL, DELTA-S= -60.94596 CAL/DEG, DELTA-G= -12.18437 KCAL

ZNO(S) IS THE BASE REACTANT FOR THIS REACTION

* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.286131E-03
 * THE WORK OF SEPARATION = 0.0

STEP 2. AT 1200.00DEG., AND 0.50ATM.

DELTA-H= 72.93666 KCAL, DELTA-S= 56.50555 CAL/DEG, DELTA-G= 5.13200 KCAL

ZNSO₄(S) IS THE BASE REACTANT FOR THIS REACTION

* THE CALCULATED WORK OF SEPARATION FOR THE GASES IS LESS THAN DELTA-G,
 * THE EQUILIBRIUM POINT FOR THIS REACTION IS PROBABLY IN ERROR,
 * THE WORK OF SEPARATION IS TAKEN TO BE EQUAL TO DELTA-G.
 * WURK= 5.132 KCAL

STEP 3. AT 850.00DEG., AND 1.00ATM.

DELTA-H= -5.70502 KCAL, DELTA-S= -7.37816 CAL/DEG, DELTA-G= 0.56642 KCAL

H₂O IS THE BASE REACTANT FOR THIS REACTION

0.42000 S ₂	0.750*	1.036	1.234	1.482	1.801	2.226	2.821*							
H ₂ O	1.000*	1.381	1.646	1.976	2.401	2.968	3.762*	6.015	6.367	6.746	7.163	7.628	8.163	

STEP 4. AT 1100.00DEG., AND 1.00ATM.

DELTA-H= 21.60269 KCAL, DELTA-S= 11.76119 CAL/DEG, DELTA-G= 8.66538 KCAL

H₂S IS THE BASE REACTANT FOR THIS REACTION

0.08570 H ₂ S	1.000*	10.669	11.965	13.586	15.669	18.448	22.337*	12.019	12.372	12.766	13.211	13.724	14.329	
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TABLE 11
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THE ZINC SULFUR PROCESS
TEMPERATURE SCHEDULE 1.

				DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	501.00 DEG. ---> 1200.00 DEG. 1.00 ATM. ---> 0.50 ATM. 1.00 ZNSO4(S) FROM REACTION 1 ---> 1.00 ZNSO4(S)	IN REACTION 2		26.15064	31.8701	-44.00796
STEP 6	1200.00 DEG. ---> 501.00 DEG. 0.50 ATM. ---> 1.00 ATM. 1.00 ZNO(S) FROM REACTION 2 ---> 1.00 ZNO(S)	IN REACTION 1		-8.66022	-10.7329	15.34778
STEP 7	1200.00 DEG. ---> 298.15 DEG. 0.50 ATM. ---> 1.00 ATM. 0.50 O2 FROM REACTION 2 ---> 0.50 O2	FINAL PRODUCT		-3.55562	-6.0498	25.80154
STEP 8	1200.00 DEG. ---> 1200.00 DEG. 0.50 ATM. ---> 0.50 ATM. 0.14 SO3 FROM REACTION 2 ---> 0.14 SO3	IN REACTION 2		0.0	0.0	0.0
STEP 9	850.00 DEG. ---> 1100.00 DEG. 1.00 ATM. ---> 1.00 ATM. 1.00 H2S FROM REACTION 3 ---> 1.00 H2S	IN REACTION 4		2.70981	2.7897	-15.01075
STEP 10	1100.00 DEG. ---> 298.15 DEG. 1.00 ATM. ---> 1.00 ATM. 1.00 H2 FROM REACTION 4 ---> 1.00 H2	FINAL PRODUCT		-5.67039	-9.1858	29.45902
STEP 11	298.15 DEG. ---> 373.47 DEG. 1.00 ATM. ---> 1.00 ATM. 1.00 H2O(L) RAW MATERIAL ---> 1.00 H2O(L)	IN REACTION 12		1.35771	4.0596	-1.41736
STEP 12	373.47 DEG. ---> 373.47 DEG. 1.00 ATM. ---> 1.00 ATM. 1.00 H2O(L) FROM REACTION 11 ---> 1.00 H2O	IN REACTION 13		9.77287	26.1454	0.00847
STEP 13	373.47 DEG. ---> 850.00 DEG. 1.00 ATM. ---> 1.00 ATM. 1.00 H2O FROM REACTION 12 ---> 1.00 H2O	IN REACTION 3		4.15793	7.1054	-24.24113
STEP 14	501.00 DEG. ---> 880.33 DEG. 1.00 ATM. ---> 1.00 ATM. 0.50 Si(L) FROM REACTION 1 ---> 0.50 Si(L)	IN REACTION 15		1.55349	2.3298	-2.88021
STEP 15	880.33 DEG. ---> 880.33 DEG. 1.00 ATM. ---> 1.00 ATM. 0.50 Si(L) FROM REACTION 14 ---> 0.25 S2	IN REACTION 16		6.40757	7.2792	-0.00050
STEP 16	880.33 DEG. ---> 850.00 DEG. 1.00 ATM. ---> 1.00 ATM. 0.25 S2 FROM REACTION 15 ---> 0.25 S2	IN REACTION 3		-0.06649	-0.0769	0.48081
STEP 17	1200.00 DEG. ---> 501.00 DEG. 0.50 ATM. ---> 1.00 ATM. 1.00 SO2 FROM REACTION 2 ---> 1.00 SO2	IN REACTION 1		-8.75697	-12.1846	51.04986
STEP 18	850.00 DEG. ---> 501.00 DEG. 1.00 ATM. ---> 1.00 ATM. 0.50 SO2 FROM REACTION 3 ---> 0.50 SO2	IN REACTION 1		-2.09790	-3.1597	11.86799
STEP 19	1100.00 DEG. ---> 850.00 DEG. 1.00 ATM. ---> 1.00 ATM. 0.50 S2 FROM REACTION 4 ---> 0.50 S2	IN REACTION 3		-1.10236	-1.1366	8.05463
TOTALS FOR STEPS 1 TO 19				68.31610	38.9954	56.69162

TABLE I
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THE ZINC SULFUR PROCESS

TEMPERATURE SCHEDULE 2.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H₂. EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

EPSI EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM						WORK OF SEPARATION OF GASES (KCAL)							
			EXTENT OF REACTION AS PERCENT OF EPSI EQ.						EXTENT OF REACTION AS PERCENT OF EPSI EQ.							
			100	90	80	70	60	50		100	90	80	70	60	50	
STEP 1. AT 501.00DEG., AND 1.00ATM.																
1.5 SO2 + ZNO(S) --> 0.5 S(L) + ZNSO4(S)																
DELTA-H= -42.71829 KCAL, DELTA-S= -60.94596 CAL/DEG, DELTA-G= -12.18437 KCAL																
ZNO(S) IS THE BASE REACTANT FOR THIS REACTION																
* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.286131E-03																
* THE WORK OF SEPARATION = 0.0																
STEP 2. AT 1300.00DEG., AND 0.50ATM.																
0.143 SO3 + ZNSO4(S) --> ZNO(S) + SO2 + 0.5 O2 + 0.143 SO3																
DELTA-H= 71.41278 KCAL, DELTA-S= 55.28579 CAL/DEG, DELTA-G= -0.45875 KCAL																
ZNSO4(S) IS THE BASE REACTANT FOR THIS REACTION																
1.00000	SO3	0.143*	0.000	0.016	0.036	0.061	0.095	0.143*								
	ZNSO4(S)	1.000*	0.000	0.111	0.250	0.429	0.667	1.000*	3.721	3.953	4.168	4.403	4.676	5.008		
STEP 3. AT 850.00DEG., AND 1.00ATM.																
0.75 S2 + H2O --> H2S + 0.5 SO2																
DELTA-H= -5.70502 KCAL, DELTA-S= -7.37816 CAL/DEG, DELTA-G= 0.56642 KCAL																
H2O IS THE BASE REACTANT FOR THIS REACTION																
0.42000	S2	0.750*	1.036	1.234	1.482	1.801	2.226	2.821*								
	H2O	1.000*	1.381	1.646	1.976	2.401	2.968	3.762*	6.015	6.367	6.746	7.163	7.628	8.163		
STEP 4. AT 1200.00DEG., AND 1.00ATM.																
H2S --> H2 + 0.5 S2																
DELTA-H= 21.64293 KCAL, DELTA-S= 11.79632 CAL/DEG, DELTA-G= 7.48735 KCAL																
H2S IS THE BASE REACTANT FOR THIS REACTION																
0.14350	H2S	1.000*	5.969	6.743	7.711	8.955	10.614	12.937*	11.209	11.601	12.037	12.529	13.094	13.760		

TABLE II
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THE ZINC SULFUR PROCESS
TEMPERATURE SCHEDULE 2.

				DELTA-H (KCAL)	DELTA-S (KCAL/DEG)	DELTA-G (KCAL)
STEP 5	501.00 DEG. --> 1300.00 DEG. 1.00 ATM. --> 0.50 ATM.					
1.00 ZNSO4(S)	FROM REACTION 1 --> 1.00 ZNSO4(S)	IN REACTION 2	30.74826	35.5484	-51.94484	
STEP 6	1300.00 DEG. --> 501.00 DEG. 0.50 ATM. --> 1.00 ATM.					
1.00 ZNO(S)	FROM REACTION 2 --> 1.00 ZNO(S)	IN REACTION 1	-9.96905	-11.7804	18.06609	
STEP 7	1300.00 DEG. --> 298.15 DEG. 0.50 ATM. --> 1.00 ATM.					
0.50 O2	FROM REACTION 2 --> 0.50 O2	FINAL PRODUCT	-3.98273	-6.3916	28.87404	
STEP 8	1300.00 DEG. --> 1300.00 DEG. 0.50 ATM. --> 0.50 ATM.					
0.14 SO3	FROM REACTION 2 --> 0.14 SO3	IN REACTION 2	0.0	0.0	0.0	
STEP 9	850.00 DEG. --> 1200.00 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H2S	FROM REACTION 3 --> 1.00 H2S	IN REACTION 4	3.85088	3.7824	-21.20062	
STEP 10	1200.00 DEG. --> 298.15 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H2	FROM REACTION 4 --> 1.00 H2	FINAL PRODUCT	-6.40783	-9.8274	33.53096	
STEP 11	298.15 DEG. --> 373.47 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H2O(L)	RAW MATERIAL --> 1.00 H2O(L)	IN REACTION 12	1.35771	4.0596	-1.41736	
STEP 12	373.47 DEG. --> 373.47 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H2O(L)	FROM REACTION 11 --> 1.00 H2O	IN REACTION 13	9.77287	26.1454	0.00847	
STEP 13	373.47 DEG. --> 850.00 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H2O	FROM REACTION 12 --> 1.00 H2O	IN REACTION 3	4.15793	7.1054	-24.24113	
STEP 14	501.00 DEG. --> 880.33 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 Si(L)	FROM REACTION 1 --> 0.50 Si(L)	IN REACTION 15	1.55349	2.3298	-2.88021	
STEP 15	880.33 DEG. --> 880.33 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 Si(L)	FROM REACTION 14 --> 0.25 S2	IN REACTION 16	6.40757	7.2792	-0.00050	
STEP 16	880.33 DEG. --> 850.00 DEG. 1.00 ATM. --> 1.00 ATM.					
0.25 S2	FROM REACTION 15 --> 0.25 S2	IN REACTION 3	-0.06649	-0.0769	0.48081	
STEP 17	1300.00 DEG. --> 501.00 DEG. 0.50 ATM. --> 1.00 ATM.					
1.00 SO2	FROM REACTION 2 --> 1.00 SO2	IN REACTION 1	-10.09277	-13.2538	58.78667	
STEP 18	850.00 DEG. --> 501.00 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 SO2	FROM REACTION 3 --> 0.50 SO2	IN REACTION 1	-2.09790	-3.1597	11.86799	
STEP 19	1200.00 DEG. --> 850.00 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 S2	FROM REACTION 4 --> 0.50 S2	IN REACTION 3	-1.54623	-1.5228	11.35057	
TOTALS FOR STEPS 1 TO 19			68.31810	38.9954	56.69162	

TABLE I
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THE ZINC SULFUR PROCESS

TEMPERATURE SCHEDULE 3.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H₂. EPS1 EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE.

EPS1 EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM						WORK OF SEPARATION OF GASES (KCAL)					
			EXTENT OF REACTION AS PERCENT OF EPS1 EQ.						EXTENT OF REACTION AS PERCENT OF EPS1 EQ.					
			100	90	80	70	60	50	100	90	80	70	60	50
STEP 1. AT 501.00DEG., AND 1.00ATM.														
1.5 SO ₂ + ZNO(S) → 0.5 S(L) + ZNSO ₄ (S)														
DELTA-H= -42.71829 KCAL, DELTA-S= -60.94596 CAL/DEG, DELTA-G= -12.18437 KCAL														
ZNO(S) IS THE BASE REACTANT FOR THIS REACTION														
* THE EQUILIBRIUM PRESSURE FOR THIS REACTION = 0.286131E-03														
* THE WORK OF SEPARATION = 0.0														
STEP 2. AT 1300.00DEG., AND 0.50ATM.														
0.143 SO ₃ + ZNSO ₄ (S) → ZNO(S) + SO ₂ + 0.5 O ₂ + 0.143 SO ₃														
DELTA-H= 71.41278 KCAL, DELTA-S= 55.28579 CAL/DEG, DELTA-G= -0.45875 KCAL														
ZNSO ₄ (S) IS THE BASE REACTANT FOR THIS REACTION														
1.00000 SO ₃	0.143*	0.000	0.016	0.036	0.061	0.095	0.143*							
ZNSO ₄ (S)	1.000*	0.000	0.111	0.250	0.429	0.667	1.000*	3.721	3.953	4.168	4.403	4.676	5.008	
STEP 3. AT 850.00DEG., AND 1.00ATM.														
0.75 S ₂ + H ₂ O → H ₂ S + 0.5 SO ₂														
DELTA-H= -5.70502 KCAL, DELTA-S= -7.37816 CAL/DEG, DELTA-G= 0.56642 KCAL														
H ₂ O IS THE BASE REACTANT FOR THIS REACTION														
0.42000 S ₂	0.750*	1.036	1.234	1.482	1.801	2.226	2.821*							
H ₂ O	1.000*	1.381	1.646	1.976	2.401	2.968	3.762*	6.015	6.367	6.746	7.163	7.628	8.163	
STEP 4. AT 1300.00DEG., AND 1.00ATM.														
H ₂ S → H ₂ + 0.5 S ₂														
DELTA-H= 21.66681 KCAL, DELTA-S= 11.81551 CAL/DEG, DELTA-G= 6.30665 KCAL														
H ₂ S IS THE BASE REACTANT FOR THIS REACTION														
0.21790 H ₂ S	1.000*	3.589	4.099	4.737	5.556	6.649	8.179*	10.438	10.873	11.355	11.897	12.519	13.249	

TABLE 11
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THE ZINC SULFUR PROCESS
TEMPERATURE SCHEDULE 3.

				DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	501.00 DEG. --> 1300.00 DEG. 1.00 ATM. --> 0.50 ATM.					
1.00 ZNSO ₄ (S)	FROM REACTION 1 --> 1.00 ZNSO ₄ (S)	IN REACTION 2	30.74826	35.5484	-51.94484	
STEP 6	1300.00 DEG. --> 501.00 DEG. 0.50 ATM. --> 1.00 ATM.					
1.00 ZNO(S)	FROM REACTION 2 --> 1.00 ZNO(S)	IN REACTION 1	-9.96905	-11.7804	18.06609	
STEP 7	1300.00 DEG. --> 298.15 DEG. 0.50 ATM. --> 1.00 ATM.					
0.50 O ₂	FROM REACTION 2 --> 0.50 O ₂	FINAL PRODUCT	-3.98273	-6.3916	28.87404	
STEP 8	1300.00 DEG. --> 1300.00 DEG. 0.50 ATM. --> 0.50 ATM.					
0.14 SO ₃	FROM REACTION 2 --> 0.14 SO ₃	IN REACTION 2	0.0	0.0	0.0	
STEP 9	850.00 DEG. --> 1300.00 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H ₂ S	FROM REACTION 3 --> 1.00 H ₂ S	IN REACTION 4	5.01973	4.7178	-27.46683	
STEP 10	1300.00 DEG. --> 298.15 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H ₂	FROM REACTION 4 --> 1.00 H ₂	FINAL PRODUCT	-7.15545	-10.4258	37.66487	
STEP 11	298.15 DEG. --> 373.47 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H ₂ O(L)	RAW MATERIAL --> 1.00 H ₂ O(L)	IN REACTION 12	1.35771	4.0596	-1.41736	
STEP 12	373.47 DEG. --> 373.47 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H ₂ O(L)	FROM REACTION 11 --> 1.00 H ₂ O	IN REACTION 13	9.77287	26.1454	0.00847	
STEP 13	373.47 DEG. --> 850.00 DEG. 1.00 ATM. --> 1.00 ATM.					
1.00 H ₂ O	FROM REACTION 12 --> 1.00 H ₂ O	IN REACTION 3	4.15793	7.1054	-24.24113	
STEP 14	501.00 DEG. --> 880.33 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 Si(L)	FROM REACTION 1 --> 0.50 Si(L)	IN REACTION 15	1.58349	2.3298	-2.88021	
STEP 15	880.33 DEG. --> 880.33 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 Si(L)	FROM REACTION 14 --> 0.25 S ₂	IN REACTION 16	6.40757	7.2792	-0.00650	
STEP 16	880.33 DEG. --> 850.00 DEG. 1.00 ATM. --> 1.00 ATM.					
0.25 S ₂	FROM REACTION 15 --> 0.25 S ₂	IN REACTION 3	-0.06649	-0.0769	0.48081	
STEP 17	1300.00 DEG. --> 501.00 DEG. 0.50 ATM. --> 1.00 ATM.					
1.00 SO ₂	FROM REACTION 2 --> 1.00 SO ₂	IN REACTION 1	-10.09277	-13.2538	58.76667	
STEP 18	850.00 DEG. --> 501.00 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 SO ₂	FROM REACTION 3 --> 0.50 SO ₂	IN REACTION 1	-2.09790	-3.1597	11.66799	
STEP 19	1300.00 DEG. --> 850.00 DEG. 1.00 ATM. --> 1.00 ATM.					
0.50 S ₂	FROM REACTION 4 --> 0.50 S ₂	IN REACTION 3	-1.99135	-1.8791	14.68358	
TOTALS FOR STEPS 1 TO 19			68.31810	38.9954	56.69162	

THE ZINC SULFUR PROCESS
COMPARISON OF EXOTHERMIC AND ENDOTHERMIC STEPS

TEMPERATURE SCHEDULE 1					TEMPERATURE SCHEDULE 2				
STEP	TEMPERATURES (K)		HEAT (KCAL)		*STEP*	TEMPERATURES (K)		HEAT (KCAL)	
	REACTANTS	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*		*REACTANTS*	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*
* 1 *	501.00	501.00	-42.7183		* 1 *	501.00	501.00	-42.7183	
* 2 *	1200.00	1200.00		72.9387	* 2 *	1300.00	1300.00		71.4128
* 3 *	850.00	850.00	-5.7050		* 3 *	850.00	850.00	-5.7050	
* 4 *	1100.00	1100.00		21.6027	* 4 *	1200.00	1200.00		21.6429
* 5 *	501.00	1200.00		28.1506	* 5 *	501.00	1300.00		30.7463
* 6 *	1200.00	501.00	-8.6602		* 6 *	1300.00	501.00	-9.9690	
* 7 *	1200.00	298.15	-3.5556		* 7 *	1300.00	298.15	-3.9827	
* 8 *	1200.00	1200.00	0.0		* 8 *	1300.00	1300.00	0.0	
* 9 *	850.00	1100.00		2.7098	* 9 *	850.00	1200.00		3.8509
* 10 *	1100.00	298.15	-5.6704		* 10 *	1200.00	298.15	-6.4078	
* 11 *	298.15	373.47		1.3577	* 11 *	298.15	373.47		1.3577
* 12 *	373.47	373.47		9.7729	* 12 *	373.47	373.47		9.7729
* 13 *	373.47	850.00		4.1579	* 13 *	373.47	850.00		4.1579
* 14 *	501.00	880.33		1.5535	* 14 *	501.00	880.33		1.5535
* 15 *	880.33	880.33		6.4076	* 15 *	880.33	880.33		6.4076
* 16 *	880.33	850.00	-0.0665		* 16 *	880.33	850.00	-0.0665	
* 17 *	1200.00	501.00	-8.7570		* 17 *	1300.00	501.00	-10.0928	
* 18 *	850.00	501.00	-2.0979		* 18 *	850.00	501.00	-2.0979	
* 19 *	1100.00	850.00	-1.1024		* 19 *	1200.00	850.00	-1.5462	
TOTALS			-78.3331	146.6511				-82.5861	150.9041

THE ZINC SULFUR PROCESS
COMPARISON OF EXOTHERMIC AND ENDOTHERMIC STEPS

TEMPERATURE SCHEDULE 3					TEMPERATURE SCHEDULE 4				
STEP	TEMPERATURES (K)		HEAT (KCAL)		*STEP*	TEMPERATURES (K)		HEAT (KCAL)	
	REACTANTS	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*		*REACTANTS*	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*
* 1 *	501.00	501.00	-42.7183		* 1 *				
* 2 *	1300.00	1300.00		71.4128	* 2 *				
* 3 *	850.00	850.00	-5.7050		* 3 *				
* 4 *	1300.00	1300.00		21.6668	* 4 *				
* 5 *	501.00	1300.00		30.7463	* 5 *				
* 6 *	1300.00	501.00	-9.9690		* 6 *				
* 7 *	1300.00	298.15	-3.9827		* 7 *				
* 8 *	1300.00	1300.00	0.0		* 8 *				
* 9 *	850.00	1300.00		5.0197	* 9 *				
* 10 *	1300.00	298.15	-7.1555		* 10 *				
* 11 *	298.15	373.47		1.3577	* 11 *				
* 12 *	373.47	373.47		9.7729	* 12 *				
* 13 *	373.47	850.00		4.1579	* 13 *				
* 14 *	501.00	880.33		1.5535	* 14 *				
* 15 *	880.33	880.33		6.4076	* 15 *				
* 16 *	880.33	850.00	-0.0665		* 16 *				
* 17 *	1300.00	501.00	-10.0928		* 17 *				
* 18 *	850.00	501.00	-2.0979		* 18 *				
* 19 *	1300.00	850.00	-1.9913		* 19 *				
TOTALS			-83.7789	152.0969					

THE ZINC SULFUR PROCESS
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 1

HEAT		STREAM SUPPLYING HEAT					STREAM ABSORBING HEAT				
EXCHANGED (KCAL)	STEP	TEMPERATURES		AMOUNT OF HEAT			STEP	TEMPERATURES		AMOUNT OF HEAT	
		INITIAL	FINAL	INITIALLY	REMAINING	INITIAL		FINAL	INITIALLY	REMAINING	
				AVAILABLE					NEEDED		
9.773	1	501.00	501.00	-42.718	-32.945	12	373.47	373.47	9.773	0.0	
1.358	1	501.00	501.00	-32.945	-31.588	11	298.15	373.47	1.358	0.0	
1.005	1	501.00	501.00	-31.588	-30.533	13	373.47	501.00	4.158	3.103	
2.098	16	850.00	501.00	-2.098	0.0	13	501.00	741.17	3.103	1.005	
1.005	3	850.00	850.00	-5.705	-4.700	13	741.17	850.00	1.005	0.0	
4.700	3	850.00	850.00	-4.700	0.0	5	501.00	646.32	26.151	21.451	
0.000	10	880.33	850.00	-0.066	0.0	14	501.00	880.33	1.553	1.487	
1.586	10	1100.00	880.33	-5.670	-4.085	15	880.33	880.33	6.408	4.822	
1.054	10	880.33	646.32	-4.085	-2.430	5	646.32	694.83	21.451	19.796	
0.600	10	646.32	559.97	-2.430	-1.824	14	501.00	646.32	1.487	0.881	
0.969	19	1100.00	880.33	-1.102	-0.133	15	880.33	880.33	4.822	3.852	
0.133	19	880.33	850.00	-0.133	0.0	14	646.32	880.33	0.881	0.748	
1.293	6	1200.00	1100.00	-8.660	-7.367	4	1100.00	1100.00	21.603	20.309	
2.712	6	1100.00	880.33	-7.367	-4.585	15	880.33	880.33	3.852	1.071	
2.285	6	880.33	694.83	-4.585	-2.300	5	694.83	759.84	19.796	17.511	
0.164	6	694.83	661.34	-2.300	-2.136	14	646.32	694.83	0.748	0.584	
0.423	7	1200.00	1100.00	-3.556	-3.132	4	1100.00	1100.00	20.309	19.886	
0.913	7	1100.00	880.33	-3.132	-2.219	15	880.33	880.33	1.071	0.157	
0.488	7	880.33	759.84	-2.219	-1.731	5	759.84	773.44	17.511	17.024	
0.211	7	759.84	706.65	-1.731	-1.520	14	694.83	759.84	0.584	0.373	
1.523	17	1200.00	1100.00	-8.757	-7.434	4	1100.00	1100.00	19.886	18.563	
0.157	17	1100.00	1080.05	-7.434	-7.276	15	880.33	880.33	0.157	0.0	
4.043	17	1080.05	173.44	-7.276	-3.234	5	773.44	862.78	17.024	12.961	
0.043	17	773.44	769.98	-3.234	-3.191	14	759.84	773.44	0.373	0.330	

W-INDICATES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.
THE DELTA-T VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES.

THE ZINC SULFUR PROCESS
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 1

HEAT AVAILABLE				HEAT REQUIRED			
STEP	TEMPERATURE	HEAT		STEP	TEMPERATURE	HEAT	
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED
1	501.00	501.00	-30.533	2	1200.00	1200.00	72.939
				4	1100.00	1100.00	18.563
				5	882.78	1200.00	12.981
6	681.34	501.00	-2.136				
7	706.65	298.15	-1.520				
10	559.97	298.15	-1.824	9	850.00	1100.00	2.710
17	769.98	501.00	-3.191	14	773.44	880.33	0.330
TOTALS			-39.204				107.522

THE ZINC SULFUR PROCESS
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 2

HEAT		STREAM SUPPLYING HEAT						STREAM ABSORBING HEAT					
EXCHANGED (KCAL)	STEP	TEMPERATURES		AMOUNT OF HEAT		STEP	TEMPERATURES		AMOUNT OF HEAT				
		INITIAL	FINAL	INITIALLY AVAILABLE	REMAINING		INITIAL	FINAL	INITIALLY NEEDED	REMAINING			
9.773	1	501.00	501.00	-42.718	-32.945	12	373.47	373.47	9.773	0.0			
1.358	1	501.00	501.00	-32.945	-31.588	11	298.15	373.47	1.358	0.0			
1.055	1	501.00	501.00	-31.588	-30.533	13	373.47	501.00	4.152	3.103			
2.095	18	850.00	501.00	-2.098	0.0	13	501.00	741.17	3.103	1.005			
1.005	3	850.00	850.00	-5.705	-4.700	13	741.17	850.00	1.005	0.0			
4.700	5	850.00	850.00	-4.700	0.0	5	501.00	646.32	30.748	26.048			
0.066	16	880.33	850.00	-0.066	0.0	14	501.00	880.33	1.553	1.487			
2.323	10	1200.00	880.33	-6.408	-4.085	15	880.33	880.33	6.408	4.084			
1.054	10	880.33	646.32	-4.085	-2.430	5	646.32	694.83	26.048	24.394			
0.066	10	646.32	559.97	-2.430	-1.825	14	501.00	646.32	1.487	0.881			
1.413	19	1200.00	880.33	-1.546	-0.133	15	880.33	880.33	4.084	2.671			
0.133	19	880.33	850.00	-0.133	0.0	14	646.32	880.33	0.881	0.748			
1.309	6	1300.00	1200.00	-9.969	-8.660	4	1200.00	1200.00	21.643	20.334			
2.671	6	1200.00	992.17	-8.660	-5.989	15	880.33	880.33	2.671	0.0			
5.089	6	992.17	694.83	-5.989	-2.300	5	694.83	798.74	24.394	20.705			
0.104	6	694.83	681.34	-2.300	-2.136	14	646.32	694.83	0.748	0.584			
0.427	7	1300.00	1200.00	-3.983	-3.556	4	1200.00	1200.00	20.334	19.907			
1.008	7	1200.00	798.74	-3.556	-1.888	5	798.74	844.01	20.705	19.037			
0.334	7	798.74	715.20	-1.888	-1.554	14	694.83	798.74	0.584	0.251			
1.330	17	1300.00	1200.00	-10.093	-8.757	4	1200.00	1200.00	19.907	18.571			
4.037	17	1200.00	844.01	-8.757	-4.120	5	844.01	964.90	19.037	14.400			
0.140	17	844.01	832.90	-4.120	-3.900	14	798.74	844.01	0.251	0.111			

W-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.
(THE DELTA-T VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES)

THE ZINC SULFUR PROCESS
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 2

HEAT AVAILABLE				HEAT REQUIRED			
STEP	TEMPERATURE		HEAT	STEP	TEMPERATURE		HEAT
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED
1	501.00	501.00	-30.533	2	1300.00	1300.00	71.413
				4	1200.00	1200.00	18.571
				5	964.90	1300.00	14.400
6	681.34	501.00	-2.136				
7	715.20	298.15	-1.554				
				9	850.00	1200.00	3.851
10	559.97	298.15	-1.825				
				14	644.01	880.33	0.111
17	832.95	501.00	-3.980				
TOTALS			-40.028				108.346

THE ZINC SULFUR PROCESS
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 3

HEAT	STREAM SUPPLYING HEAT						STREAM ABSORBING HEAT					
EXCHANGED	STEP	TEMPERATURES		AMOUNT OF HEAT		STEP	TEMPERATURES		AMOUNT OF HEAT			
(KCAL)		INITIAL	FINAL	INITIALLY	REMAINING		INITIAL	FINAL	INITIALLY	REMAINING		
				AVAILABLE					NEEDED			
9.173	1	501.00	501.00	-42.718	-32.945	12	373.47	373.47	9.773	0.0		
1.358	1	501.00	501.00	-32.945	-31.588	11	298.15	373.47	1.358	0.0		
1.055	1	501.00	501.00	-31.588	-30.533	13	373.47	501.00	4.158	3.103		
2.096	18	850.00	501.00	-2.098	0.0	13	501.00	741.17	3.103	1.005		
1.005	3	850.00	850.00	-5.705	-4.700	15	741.17	850.00	1.005	0.0		
4.700	3	850.00	850.00	-4.700	0.0	5	501.00	646.32	30.748	26.048		
0.066	18	880.33	850.00	-0.066	0.0	14	501.00	880.33	1.553	1.487		
5.354	6	1300.00	880.33	-9.969	-4.585	15	880.33	880.33	6.408	1.024		
1.338	6	880.33	501.00	-4.585	-3.247	14	501.00	839.01	1.487	0.149		
2.034	6	880.33	646.32	-3.247	-1.213	5	646.32	705.78	26.048	24.014		
1.024	7	1300.00	1058.71	-3.983	-2.959	15	880.33	880.33	1.024	0.0		
1.442	7	1058.71	705.78	-2.959	-1.517	5	705.78	746.85	24.014	22.572		
4.016	10	1300.00	746.85	-7.155	-3.138	5	746.85	856.93	22.572	18.554		
5.209	17	1300.00	856.93	-10.093	-4.284	5	856.93	1006.44	18.554	12.745		
0.072	17	856.93	851.26	-4.284	-4.212	9	850.00	856.93	5.020	4.948		
0.044	17	851.26	847.77	-4.212	-4.168	14	839.01	851.26	0.149	0.105		
1.303	19	1300.00	1006.44	-1.991	-0.688	5	1006.44	1038.65	12.745	11.442		
0.056	19	1006.44	856.93	-0.688	-0.030	9	856.93	919.47	4.948	4.290		
0.020	19	856.93	852.27	-0.030	0.0	14	851.26	856.93	0.105	0.084		

M-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.
(THE DELTA-T VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES)

THE ZINC SULFUR PROCESS
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 3

STEP	HEAT AVAILABLE			STEP	HEAT REQUIRED		
	TEMPERATURE		HEAT		TEMPERATURE		HEAT
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED
1	501.00	501.00	-30.533	2	1300.00	1300.00	71.413
				4	1300.00	1300.00	21.667
				5	1038.65	1300.00	11.442
6	646.32	501.00	-1.213				
7	705.78	298.15	-1.517				
				9	919.47	1300.00	4.290
10	746.85	298.15	-3.138				
				14	856.93	880.33	0.084
17	847.77	501.00	-4.166				
TOTALS			-40.568				108.896

THE ZINC SULFUR PROCESS
FIGURES OF MERIT

TEMP.	WORK OF	WORK	TOTAL	FIGURES OF MERIT				
SCHEDULE	SEPARATION	GENERATED	HEAT	1ST ESTIMATE	2ND ESTIMATE			
	MIN	MAX	REQUIRED	MIN	MAX	MIN	MAX	
1	23.166*	27.624*	8.390*	107.522*	0.4259*	0.4694*	0.2591*	0.2920
2	20.946*	26.931*	8.816*	108.346*	0.4322*	0.4946*	0.2643*	0.3125
3	20.175*	26.420*	9.094*	108.896*	0.4369*	0.5039*	0.2682*	0.3206

ALL HEAT ABOVE 500 K WHICH IS STILL AVAILABLE AFTER STREAM MATCHING, IS TURNED INTO WORK GENERATED USING A 30% EFFICIENCY AND SUBTRACTED FROM THE WORK OF SEPARATION NEEDED. THE FIRST ESTIMATE FOR A FIGURE OF MERIT ASSUMES PERFECT HEAT REGENERATION AND 100% EFFICIENCY IN THE WORK OF SEPARATION. THE SECOND ESTIMATE USES THE HEAT REQUIRED AFTER STREAM MATCHING AS THE TOTAL HEAT REQUIRED AND ASSUMES ONLY A 50% EFFICIENCY FOR THE WORK OF SEPARATION. ALL WORK REQUIRED IS ASSUMED TO BE GENERATED FROM HEAT AT A 30% EFFICIENCY.

PROPERTIES OF THE BASE REACTIONS AT 298 K FOR
THE ZINC SULFUR PROCESS

STEP 1. AT 298.15DEG., AND 1.00ATM.			
$1.5 \text{ SO}_2 + \text{ZNO(S)} \rightarrow 0.5 \text{ S(S)} + \text{ZNSO}_4\text{(S)}$			
DELTA-H=	-44.28889 KCAL	DELTA-S=	-64.94528 CAL/DEG, DELTA-G= -24.92546 KCAL
STEP 2. AT 298.15DEG., AND 1.00ATM.			
$0.143 \text{ SO}_3 + \text{ZNSO}_4\text{(S)} \rightarrow \text{ZNO(S)} + \text{SO}_2 + 0.5 \text{ O}_2 + 0.143 \text{ SO}_3$			
DELTA-H=	79.76288 KCAL	DELTA-S=	63.61403 CAL/DEG, DELTA-G= 60.79641 KCAL
STEP 3. AT 298.15DEG., AND 1.00ATM.			
$0.75 \text{ S(S)} + \text{H}_2\text{O(L)} \rightarrow \text{H}_2\text{S} + 0.5 \text{ SO}_2$			
DELTA-H=	27.96222 KCAL	DELTA-S=	56.36014 CAL/DEG, DELTA-G= 11.15845 KCAL
STEP 4. AT 298.15DEG., AND 1.00ATM.			
$\text{H}_2\text{S} \rightarrow \text{H}_2 + 0.5 \text{ S(S)}$			
DELTA-H=	4.88305 KCAL	DELTA-S=	-14.12658 CAL/DEG, DELTA-G= 9.09489 KCAL
TOTALS	DELTA-H= 68.31925 KCAL	DELTA-S=	40.90231 CAL/DEG, DELTA-G= 56.12429 KCAL

PROCESS SUMMARY
THE ZINC SULFUR PROCESS
TEMPERATURE SCHEDULE 1

STAGE	1	2	3	4	SUM
(1) H298, HEAT OF REACTION AT 298K (KCAL)	-44.29	79.76	27.96	4.88	68.32
(2) HT, HEAT OF REACTION AT TEMP T (KCAL)	-42.72	72.94	-5.71	21.60	
(3) T, TEMP. OF REACTION (K)	501.	1200.	850.	1100.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	0.0	5.13	6.02	12.02	23.17
(5) THEO. WORK OF SEPARATION ((	0.0	0.22	0.26	0.52	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	7.09	1.20	0.0	0.10	8.39
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) $QS=(2WS-WG)/0.30$	-23.64	30.23	40.10	79.78	126.47
(8) Q, HEAT REQUIREMENT (KCAL)	6.66	79.43	1.52	19.92	107.52
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	-16.98	109.66	41.62	99.70	234.00
(10) WEIGHING FACTOR (9)/SUM(9)	-0.073	0.469	0.178	0.426	
(11) QREJ, HEAT REJECTED (KCAL)	-33.20	-4.18	0.0	-1.82	-39.20
(12) NUJ, INDIVIDUAL FIGURES OF MERIT	2.608	0.727	0.672	0.049	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)x(12), SUM(13)=OVERALL FIG. MERIT	-0.189	0.341	0.119	0.021	0.292
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	0.140	0.504	0.587	1.195	2.426

PROCESS SUMMARY
THE ZINC SULFUR PROCESS
TEMPERATURE SCHEDULE 2

STAGE	1	2	3	4	SUM
(1) H ₂ 98, HEAT OF REACTION AT 298K (KCAL)	-44.29	79.76	27.96	4.88	68.32
(2) HT, HEAT OF REACTION AT TEMP T (KCAL)	-42.72	71.41	-5.71	21.64	
(3) T, TEMP. OF REACTION (K)	501.	1300.	850.	1200.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	0.0	3.72	6.02	11.21	20.95
(5) THEO. WORK OF SEPARATION ((	0.0	0.18	0.29	0.54	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	7.30	1.42	0.0	0.10	8.82
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) QS=(2WS-WG)/0.30	-24.32	20.09	40.10	74.39	110.25
(8) Q, HEAT REQUIREMENT (KCAL)	7.26	78.61	1.98	20.50	108.35
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	-17.07	98.70	42.08	94.88	218.60
(10) WEIGHING FACTOR (9)/SUM(9)	-0.078	0.452	0.193	0.434	
(11) QREJ, HEAT REJECTED (KCAL)	-33.59	-4.61	0.0	-1.82	-40.03
(12) NUJ, INDIVIDUAL FIGURES OF MERIT	2.595	0.808	0.664	0.051	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)X(12), SUM(13)=OVERALL FIG. MERIT	-0.203	0.365	0.128	0.022	0.313
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	0.136	0.362	0.587	1.116	2.200

PROCESS SUMMARY
THE ZINC SULFUR PROCESS
TEMPERATURE SCHEDULE 3

STAGE	1	2	3	4	SUM
(1) H ₂₉₈ , HEAT OF REACTION AT 298K (KCAL)	-44.29	79.76	27.96	4.88	68.32
(2) H _T , HEAT OF REACTION AT TEMP T (KCAL)	-42.72	71.41	-5.71	21.67	
(3) T, TEMP. OF REACTION (K)	501.	1300.	850.	1300.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	0.0	3.72	6.02	10.44	20.17
(5) THEO. WORK OF SEPARATION (I)	0.0	0.18	0.30	0.52	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	7.19	1.29	0.0	0.62	9.09
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) QS=(2WS-WG)/0.30	-23.96	20.51	40.10	67.53	104.18
(8) Q, HEAT REQUIREMENT (KCAL)	5.76	77.13	2.19	23.81	108.90
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	-18.19	97.65	42.29	91.34	213.08
(10) WEIGHING FACTOR (9)/SUM(9)	-0.085	0.458	0.198	0.429	
(11) QREJ, HEAT REJECTED (KCAL)	-33.22	-4.21	0.0	-3.14	-40.57
(12) NUJ, INDIVIDUAL FIGURES OF MERIT	2.434	0.817	0.661	0.053	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)x(12), SUM(13)=OVERALL FIG. MERIT	-0.208	0.374	0.131	0.023	0.321
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	0.136	0.362	0.587	1.035	2.119

Sample Problem 3. The Mark IX Process

For the following process:

Run reaction (1) at 923 K, stoichiometric composition, and an extent of reaction = 0.30732 with H_2O as the base reactant.

Run reaction (2) at 497 K, stoichiometric composition, and an extent of reaction = 0.51814 with Fe_3O_4 as the base reactant. Fe_2O_3 has been omitted as a product of this reaction in the calculation of the extent of reaction.

Run reaction (3) at 673 K with an extent of reaction = 0.02537.

Run reaction (4) at 605 K (there is no work of separation since this is a dummy reaction to vaporize $\text{FeCl}_3(\text{l})$.)

Input Data Cards for Sample Problem 3

THE MARK 9 PROCESS
NOTES

1 4DUMMY REACTION

2 2FE2O3 WAS OMITTED AS A PRODUCT , CEC72 SAYS OTHERWISE

CHEMICAL REACTIONS

1 REACTANT H 2. O 1.	G4.	B4.
2 REACTANT FE3. O 4.	S1.	B1.
2 REACTANT H 1. CL 1.	G6.	6.
2 REACTANT CL 2.	G1.5	1.5
1 REACTANT FE1. CL2.	S 3.	3.
1 PRODUCT FE3. O 4.	S1.	
1 PRODUCT H 1. CL 1.	G6.	
1 PRODUCT H 2.	G1.	
2 PRODUCT FE1. CL3.	S3.	577.
2 PRODUCT H 2. O 1.	G3.	
2 PRODUCT O 2.	G 0.5	
3 PRODUCT FE1. CL2.	S3.	
3 PRODUCT CL2.	G1.5	
4 REACTANT FE1. CL3.	L3.	B3.
3 REAC FE2. CL 6.	G1.5	B 1.5
4 PROD FE2. CL6.	G1.5	

NAMELISTS

&NAM1 PRES=1,STEP=1,DRAW=T,T=923,EP=.30732	&END
&NAM1 PRES=1,STEP=2,T=497,EP=.951814	&END
&NAM1 PRES=1,STEP=3,T=673,EP=.02537	&END
&NAM1 PRES=1,STEP=4,T=605	&END

END

BEGINNING OF INPUT DATA FOR THE MARK 9 PROCESS

NOTES

1 DUMMY REACTION

2 ZFEZ03 WAS OMITTED AS A PRODUCT, CEC72 SAYS OTHERWISE

U G

CHEMICAL REACTIONS

1REACTANT	H	2.0	1.	0.	0.0	4.000008	4.000	0.0	0.0	0.0
2REACTANT	FE	3.0	4.	0.	0.0	1.000008	1.000	0.0	0.0	0.0
3REACTANT	H	1.0	1.	0.	0.0	6.0000	6.000	0.0	0.0	0.0
4REACTANT	CL	2.	0.	0.	0.0	1.5000	1.500	0.0	0.0	0.0
1PRODUCT	FE	1.0	2.	0.	0.0	3.0000	3.000	0.0	0.0	0.0
1PRODUCT	FE	3.0	4.	0.	0.0	1.0000	0.0	0.0	0.0	0.0
1PRODUCT	H	1.0	1.	0.	0.0	6.0000	0.0	0.0	0.0	0.0
1PRODUCT	H	2.	0.	0.	0.0	1.0000	0.0	0.0	0.0	0.0
2PRODUCT	FE	1.0	3.	0.	0.0	3.0000	577.000	0.0	0.0	0.0
2PRODUCT	H	2.0	1.	0.	0.0	3.0000	0.0	0.0	0.0	0.0
2PRODUCT	U	2.	0.	0.	0.0	0.5000	0.0	0.0	0.0	0.0
3PRODUCT	FE	1.0	2.	0.	0.0	3.0000	0.0	0.0	0.0	0.0
3PRODUCT	CL	2.	0.	0.	0.0	1.5000	0.0	0.0	0.0	0.0
4REACTANT	FE	1.0	3.	0.	0.0	3.000008	3.000	0.0	0.0	0.0
3REAC	FE	2.0	0.	0.	0.0	1.500008	1.500	0.0	0.0	0.0
4PROD	FE	2.0	0.	0.	0.0	1.5000	0.0	0.0	0.0	0.0
U	U	0.	0.	0.	0.0	0.0	0.0	0.0	0.0	0.0

NAMELISTS

NAME1

STEP=	1,T=	923.00000	0.0	0.0	0.0	0.0	0.0	0.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

NAME1, SAME=F, H298=T, EFF= 0.29999995

NAME1

STEP=	2,T=	497.00000	0.0	0.0	0.0	0.0	0.0	0.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

NAME1, SAME=F, H298=T, EFF= 0.29999995

NAME1

STEP=	3,T=	673.00000	0.0	0.0	0.0	0.0	0.0	0.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

NAME1, SAME=F, H298=T, EFF= 0.29999995

NAME1

STEP=	4,T=	805.00000	0.0	0.0	0.0	0.0	0.0	0.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

NAME1, SAME=F, H298=T, EFF= 0.29999995

NAME1

STEP=	4,T=	805.00000	0.0	0.0	0.0	0.0	0.0	0.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0	U.0
1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000

NAME1, SAME=F, H298=T, EFF= 0.29999995

NAME1

THEIRMO DATA FOUND ON TAPE 4

300.000 1000.000 5000.000

```

1 CL2 J 9/65CL 2. 0. 0. 0.6 300.000 5000.000
  0.43077812D 01 0.31182799D-03-0.15310803D-06 0.44511908D-10-0.43057734D-14
  -0.13458250D 04 0.20666676D 01 0.31316881D 01 0.48997849D-02-0.69411462D-05
  0.44785615D-08-0.10621851D-11-0.10979695D 04 0.77833424D 01
2 FECL2(S) J12/70FE 1.CL 2. 0. 0.5 300.000 950.000
  0.0 0.0 0.0 0.0 0.0
  0.0 0.0 0.71122265D 01 0.11086952D-01-0.17072729D-04
  0.13515816D-07-0.41365028D-11-0.43600984D 05-0.28994049D 02
3 FECL2(L) J12/70FE 1.CL 2. 0. 0.1 950.000 5000.000
  0.12288862D 02 0.0 0.0 0.0 0.0
  -0.41109820D 05-0.53193054D 02 0.12288862D 02 0.0 0.0
  0.0 0.0 -0.41109820D 05-0.53193054D 02
4 FECL2 J12/70FE 1.CL 2. 0. 0.6 300.000 5000.000
  0.69492598D 01 0.53371629D-03-0.70221176D-07-0.61475477D-10 0.67933127D-14
  -0.19045828D 05-0.37726698D 01 0.54557505D 01 0.79632923D-02-0.12593963D-04
  0.69976702D-08-0.23242363D-11-0.16844297D 05 0.30096855D 01
5 FECL3(S) J 6/65FE 1.CL 3. 0. 0.5 300.000 577.000
  0.0 0.0 0.0 0.0 0.0
  0.0 0.0 0.11806993D 02 0.18280681D-01-0.19156683D-03
  0.57778459D-06-0.49460636D-09-0.51600496D 05-0.51237244D 02
6 FECL3(L) J 6/65FE 1.CL 3. 0. 0.1 577.000 1500.000
  0.16102570D 02 0.0 0.0 0.0 0.0
  -0.48435531D 05-0.67614578D 02 0.16102570D 02 0.0 0.0
  0.0 0.0 -0.48435531D 05-0.67614578D 02
7 FECL3 J 6/65FE 1.CL 3. 0. 0.6 300.000 5000.000
  0.97771101D 01 0.24421350D-03-0.10313994D-06 0.19207413D-10-0.13179297D-14
  -0.33439566D 05-0.14562301D 02 0.75614872D 01 0.97338222D-02-0.15543294D-04
  0.11186366D-07-0.30022998D-11-0.33013621D 05-0.39989862D 01
8 FE2CL6 BARIN FE 2.CL 6. 0. 0.6 298.150 2000.000
  0.21629181D 02 0.24905079D-03 0.13936284D-06-0.16621871D-09 0.38959135D-13
  -0.85271938D 05-0.58990036D 02 0.18693268D 02 0.99504255D-02-0.84215762D-05
  -0.11545420D-08 0.28227941D-11-0.84642750D 05-0.44496857D 02
9 FE3CL4(S) J 6/65FE 3.0 4. 0. 0.5 300.000 5000.000
  0.24133713D 02 0.41592226D-04-0.26331492D-07 0.66035085D-11-0.56924680D-15
  -0.14121050D 06-0.12006412D 03 0.36198135D 02-0.17437971D 00 0.52475650D-03
  -0.54238217D-06 0.17996202D-09-0.14136725D 06-0.15556682D 03
10 HCL J 9/64H 1.CL 1. 0. 0.6 300.000 5000.000
  0.27665882D 01 0.14381881D-02-0.46992994D-06 0.73499401D-10-0.43731091D-14
  -0.11917465D 05 0.64583540D 01 0.35248165D 01 0.29984862D-04-0.86221688D-06
  0.20979720D-08-0.98658148D-12-0.12150508D 05 0.23957710D 01
11 H2 J 3/61H 2. 0. 0. 0.6 300.000 5000.000
  0.31001892D 01 0.51119458D-03-0.52644207D-07-0.34909964D-10 0.36945341D-14
  -0.87138037D 03-0.19629412D 01 0.30574446D 01 0.26765198D-02-0.58099158D-05
  0.55210378D-08-0.18122734D-11-0.98890454D 03-0.22997055D 01
12 H2O(S) L11/65H 2.0 1. 0. 0.5 200.000 273.150

```

```

  0.0 0.0 0.0 0.0 0.0
  0.0 0.0 -0.39269328D-01 0.16920418D-01 0.0
  0.0 0.0 -0.35949578D 05 0.56933779D 00
13 H2O(L) L11/65H 2.0 1. 0. 0.1 273.150 1000.000
  0.0 0.0 0.0 0.0 0.0
  0.0 0.0 0.12712782D 02-0.17662790D-01-0.22556647D-04
  0.20820903D-06-0.24078606D-09-0.37483199D 05-0.59115341D 02
14 H2O J 3/61H 2.0 1. 0. 0.6 300.000 5000.000
  0.27167625D 01 0.29451572D-02-0.80224373D-06 0.10226681D-09-0.48472138D-14
  -0.29905824D 05 0.66305866D 01 0.40701275D 01-0.11084499D-02 0.41521180D-05
  -0.29637404D-08 0.80702101D-12-0.30279719D 05-0.32270044D 00
15 O2 J 9/65U 2. 0. 0. 0.6 300.000 5000.000
  0.36219530D 01 0.73616256D-03-0.19652225D-06 0.36201556D-10-0.28945625D-14
  -0.12019824D 04 0.36150951D 01 0.36255980D 01-0.18782183D-02 0.70554543D-05
  -0.67635106D-08 0.21555986D-11-0.10475225D 04 0.43052769D 01

```

END OF INPUT DATA FOR THE MARK 9 PROCESS

TEMPERATURE SCHEDULE 1.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOL OF H₂. EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

```

EPSI EQ.    REACTANT    RATIO*    MOLES OF REACTANT IN RECYCLE STREAM    *    WORK OF SEPARATION OF GASES (KCAL)
*
*
* EXTENT OF REACTION AS PERCENT OF EPSI EQ.    *    EXTENT OF REACTION AS PERCENT OF EPSI EQ.
* 100    90    80    70    60    50    * 100    90    80    70    60    50
*-----*-----*
STEP 1.  AT 923.00DEG., AND 1.00ATM.
4 H2O + 3 FECL2(S) --> FE3O4(S) + 6 HCL + H2
DELTA-H= 79.57018 KCAL, DELTA-S= 73.54687 CAL/DEG, DELTA-G= 11.68642 KCAL
H2O IS THE BASE REACTANT FOR THIS REACTION
*-----*-----*
0.30732 H2O    4.000*  9.016  10.462  12.270  14.594  17.693  22.032*
FECL2(S)      3.000*  6.762   7.846   9.202  10.945  13.270  16.524* 25.394 26.832 28.425 30.216 32.268 34.678
*-----*-----*
STEP 2.  AT 497.00DEG., AND 1.00ATM.
FE3O4(S) + 6 HCL + 1.5 CL2 --> 3 FECL3(S) + 3 H2O + 0.5 O2
DELTA-H= -57.88239 KCAL, DELTA-S= -116.13970 CAL/DEG, DELTA-G= -0.16096 KCAL
FE2O3 WAS OMITTED AS A PRODUCT , CEC72 SAYS OTHERWISE
FE3O4(S) IS THE BASE REACTANT FOR THIS REACTION
**ERROR** THE MOLE FRACTION OF ONE OF THE REACTANTS IN THE FINAL REACTION MIXTURE IS NEGATIVE FOR RATIO SET 1
CHECK THE EPSILON FOR THIS SET OF RATIOS.
STEP 3.  AT 673.00DEG., AND 1.00ATM.
1.5 FE2CL6 --> 3 FECL2(S) + 1.5 CL2
DELTA-H= -7.92498 KCAL, DELTA-S= -22.63284 CAL/DEG, DELTA-G= 7.30692 KCAL
FE2CL6 IS THE BASE REACTANT FOR THIS REACTION
*-----*-----*
0.02557 FE2CL6    1.500*  57.625  64.194  72.406  82.964  97.042 116.750* 9.351 9.565 9.804 10.074 10.386 10.754
*-----*-----*
STEP 4.  AT 605.00DEG., AND 1.00ATM.
3 FECL3(L) --> 1.5 FE2CL6
DELTA-H= 15.67912 KCAL, DELTA-S= 25.85424 CAL/DEG, DELTA-G= 0.03731 KCAL
DUMMY REACTION

```


TABLE 11
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THE MARK 9 PROCESS
TEMPERATURE SCHEDULE 1.

					DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	923.00 DEG. ---> 497.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.00 FE3O4(S)	FROM REACTION 1 ---> 1.00 FE3O4(S)	IN REACTION 2			-23.10655	-33.3436	31.25666
STEP 6	923.00 DEG. ---> 497.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
6.00 HCL	FROM REACTION 1 ---> 6.00 HCL	IN REACTION 2			-18.38997	-26.6368	129.41258
STEP 7	923.00 DEG. ---> 298.15 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.00 H2	FROM REACTION 1 ---> 1.00 H2	FINAL PRODUCT			-4.36961	-7.9168	22.41657
STEP 8	497.00 DEG. ---> 577.01 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
3.00 FECL3(S)	FROM REACTION 2 ---> 3.00 FECL3(S)	IN REACTION 9			6.99304	13.0415	-11.78467
STEP 9	577.01 DEG. ---> 577.01 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
3.00 FECL3(S)	FROM REACTION 8 ---> 3.00 FECL3(L)	IN REACTION 10			30.89853	53.5502	-0.00023
STEP 10	577.01 DEG. ---> 605.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
3.00 FECL3(L)	FROM REACTION 9 ---> 3.00 FECL3(L)	IN REACTION 4			2.68733	4.5479	-5.86574
STEP 11	497.00 DEG. ---> 298.15 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
0.50 O2	FROM REACTION 2 ---> 0.50 O2	FINAL PRODUCT			-0.71647	-1.8367	5.06866
STEP 12	673.00 DEG. ---> 923.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
3.00 FECL2(S)	FROM REACTION 5 ---> 3.00 FECL2(S)	IN REACTION 1			15.51450	19.3348	-35.43196
STEP 13	673.00 DEG. ---> 497.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.50 CL2	FROM REACTION 3 ---> 1.50 CL2	IN REACTION 2			-2.30387	-3.9662	15.56426
STEP 14	605.00 DEG. ---> 673.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.50 FE2CL6	FROM REACTION 4 ---> 1.50 FE2CL6	IN REACTION 3			4.41478	6.9153	-16.39690
STEP 15	497.00 DEG. ---> 923.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
3.00 H2O	FROM REACTION 2 ---> 3.00 H2O	IN REACTION 1			11.49194	16.5836	-66.79671
STEP 16	298.15 DEG. ---> 373.47 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.00 H2O(L)	RAW MATERIAL ---> 1.00 H2O(L)	IN REACTION 17			1.35771	4.0596	-1.41736
STEP 17	373.47 DEG. ---> 373.47 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.00 H2O(L)	FROM REACTION 16 ---> 1.00 H2O	IN REACTION 18			9.77287	26.1454	0.00847
STEP 18	373.47 DEG. ---> 923.00 DEG.						
	1.00 ATM. ---> 1.00 ATM.						
1.00 H2O	FROM REACTION 17 ---> 1.00 H2O	IN REACTION 1			4.85195	7.8886	-28.21392
TOTALS FOR STEPS 1 TO 18					68.31810	38.9954	56.69162

THE MARK 9 PROCESS
COMPARISON OF EXOTHERMIC AND ENDOTHERMIC STEPS

TEMPERATURE SCHEDULE 1					TEMPERATURE SCHEDULE 2				
STEP	TEMPERATURES (K)		HEAT (KCAL)		*STEP*	TEMPERATURES (K)		HEAT (KCAL)	
	REACTANTS	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*		*REACTANTS*	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*
* 1 *	923.00	923.00		79.5702	* *				
* 2 *	497.00	497.00	-57.8824		* *				
* 3 *	673.00	673.00	-7.9250		* *				
* 4 *	605.00	605.00		15.6791	* *				
* 5 *	923.00	497.00	-23.1065		* *				
* 6 *	923.00	497.00	-18.3900		* *				
* 7 *	923.00	298.15	-4.3896		* *				
* 8 *	497.00	577.01		6.9930	* *				
* 9 *	577.01	577.01		30.8985	* *				
* 10 *	577.01	605.00		2.6873	* *				
* 11 *	497.00	298.15	-0.7165		* *				
* 12 *	673.00	923.00		15.3145	* *				
* 13 *	673.00	497.00	-2.3039		* *				
* 14 *	605.00	673.00		4.4148	* *				
* 15 *	497.00	923.00		11.4919	* *				
* 16 *	298.15	373.47		1.3577	* *				
* 17 *	373.47	373.47		9.7729	* *				
* 18 *	373.47	923.00		4.8519	* *				
TOTALS			-114.7136	183.0315					

THE MARK 9 PROCESS
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 1

HEAT EXCHANGED (KCAL)	STEP	STREAM SUPPLYING HEAT				STEP	STREAM ABSORBING HEAT			
		TEMPERATURES		AMOUNT OF HEAT			TEMPERATURES		AMOUNT OF HEAT	
		INITIAL	FINAL	INITIALLY	REMAINING		INITIAL	FINAL	INITIALLY	REMAINING
				AVAILABLE					NEEDED	
0.450	11	497.00	373.47	-0.716	-0.267	17	373.47	373.47	9.773	9.323
0.267	11	373.47	298.15	-0.267	0.0	16	298.15	312.97	1.358	1.091
9.323	2	497.00	497.00	-57.882	-48.559	17	373.47	373.47	9.323	0.0
1.091	2	497.00	497.00	-48.559	-47.468	16	312.97	373.47	1.091	0.0
1.021	2	497.00	497.00	-47.468	-46.447	18	373.47	497.00	4.852	3.631
0.396	13	673.00	605.00	-2.304	-1.408	4	605.00	605.00	15.679	14.783
0.367	13	605.00	577.01	-1.408	-1.041	9	577.01	577.01	30.899	30.532
1.041	13	577.01	497.00	-1.041	0.0	8	497.00	509.13	6.993	5.952
7.925	3	673.00	673.00	-7.925	0.0	4	605.00	605.00	14.783	6.858
6.858	5	923.00	798.35	-23.107	-16.246	4	605.00	605.00	6.858	0.0
12.300	5	798.35	577.01	-16.248	-3.948	9	577.01	577.01	30.532	18.232
3.948	5	577.01	509.13	-3.948	-0.572	8	509.13	547.78	5.952	2.576
0.276	5	509.13	497.00	-0.572	-0.297	15	497.00	507.91	11.492	11.216
0.092	5	509.13	497.00	-0.297	-0.205	18	497.00	507.91	3.831	3.739
18.017	6	923.00	577.01	-18.390	-3.373	9	577.01	577.01	18.232	3.214
1.235	6	577.01	547.78	-3.373	-2.138	8	547.78	561.78	2.576	1.341
1.014	6	547.78	523.71	-2.138	-1.123	15	507.91	547.78	11.216	10.202
0.133	6	523.71	520.54	-1.123	-0.990	18	507.91	523.71	3.739	3.605
2.440	7	923.00	577.01	-4.390	-1.944	9	577.01	577.01	3.214	0.769
0.167	7	577.01	561.78	-1.944	-1.837	8	561.78	563.00	1.341	1.234
0.098	7	561.78	547.78	-1.837	-1.739	15	547.78	551.61	10.202	10.104
0.169	7	547.78	523.71	-1.739	-1.571	18	523.71	543.54	3.605	3.437

W-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.
(THE DELTA-T VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES)

THE MARK 9 PROCESS
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 1

HEAT AVAILABLE				HEAT REQUIRED			
STEP	TEMPERATURE		HEAT	STEP	TEMPERATURE		HEAT
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED
2	497.00	497.00	-46.447	1	923.00	923.00	79.570
5	509.13	497.00	-0.205				
6	520.54	497.00	-0.990				
7	523.71	298.15	-1.571				
				8	563.00	577.01	1.234
				9	577.01	577.01	0.769
				10	577.01	605.00	2.687
				12	673.00	923.00	15.314
				14	605.00	673.00	4.415
				15	551.61	923.00	10.104
				18	543.54	923.00	3.437
TOTALS			-49.212				117.530

THE MARK 9 PROCESS

FIGURES OF MERIT

TEMP.	WORK OF	WORK	TOTAL	FIGURES OF MERIT			
SCHEDULE	SEPARATION	GENERATED	HEAT	1ST ESTIMATE	2ND ESTIMATE		
	MIN	MAX	REQUIRED	MIN	MAX	MIN	MAX
1	34.745*	45.432*	0.255*	117.530*	0.3109*	0.3710*	0.1628* 0.1961

ALL HEAT ABOVE 500 K WHICH IS STILL AVAILABLE AFTER STREAM MATCHING, IS TURNED INTO WORK GENERATED USING A 30% EFFICIENCY AND SUBTRACTED FROM THE WORK OF SEPARATION NEEDED. THE FIRST ESTIMATE FOR A FIGURE OF MERIT ASSUMES PERFECT HEAT REGENERATION AND 100% EFFICIENCY IN THE WORK OF SEPARATION. THE SECOND ESTIMATE USES THE HEAT REQUIRED AFTER STREAM MATCHING AS THE TOTAL HEAT REQUIRED AND ASSUMES ONLY A 50% EFFICIENCY FOR THE WORK OF SEPARATION. ALL WORK REQUIRED IS ASSUMED TO BE GENERATED FROM HEAT AT A 30% EFFICIENCY.

PROPERTIES OF THE BASE REACTIONS AT 298 K FOR
THE MARK 9 PROCESS

STEP 1. AT 298.15DEG., AND 1.00ATM.
 $4 \text{ H}_2\text{O}(\text{L}) + 3 \text{ FeCl}_2(\text{S}) \longrightarrow \text{Fe}_3\text{O}_4(\text{S}) + 6 \text{ HCl} + \text{H}_2$
 DELTA-H= 118.33538 KCAL, DELTA-S= 182.55151 CAL/DEG, DELTA-G= 63.90766 KCAL

STEP 2. AT 298.15DEG., AND 1.00ATM.
 $\text{Fe}_3\text{O}_4(\text{S}) + 6 \text{ HCl} + 1.5 \text{ CL}_2 \longrightarrow 3 \text{ FeCl}_3(\text{S}) + 3 \text{ H}_2\text{O}(\text{L}) + 0.5 \text{ O}_2$
 DELTA-H= -91.37969 KCAL, DELTA-S= -206.13509 CAL/DEG, DELTA-G= -29.92055 KCAL

STEP 3. AT 298.15DEG., AND 1.00ATM.
 $1.5 \text{ Fe}_2\text{Cl}_6 \longrightarrow 3 \text{ FeCl}_2(\text{S}) + 1.5 \text{ CL}_2$
 DELTA-H= -10.50582 KCAL, DELTA-S= -28.04376 CAL/DEG, DELTA-G= -2.14457 KCAL

STEP 4. AT 298.15DEG., AND 1.00ATM.
 $3 \text{ FeCl}_3(\text{S}) \longrightarrow 1.5 \text{ Fe}_2\text{Cl}_6$
 DELTA-H= 51.86824 KCAL, DELTA-S= 90.62276 CAL/DEG, DELTA-G= 24.84907 KCAL

TOTALS DELTA-H= 68.31806 KCAL, DELTA-S= 38.99542 CAL/DEG, DELTA-G= 56.69162 KCAL

PROCESS SUMMARY
THE MARK 9 PROCESS
TEMPERATURE SCHEDULE 1

STAGE	1	2	3	4	SUM
(1) H298, HEAT OF REACTION AT 298K (KCAL)	118.34	-91.38	-10.51	51.87	68.32
(2) HT, HEAT OF REACTION AT TEMP T (KCAL)	79.57	-57.88	-7.92	15.68	
(3) T, TEMP. OF REACTION (K)	923.	497.	673.	605.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	25.39	0.0	9.35	0.0	34.74
(5) THEO. WORK OF SEPARATION ((1))	0.73	0.0	0.27	0.0	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	0.15	0.11	0.0	0.0	0.25
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) QS=(2WS-WG)/0.30	168.81	-0.36	62.34	0.0	230.78
(8) Q, HEAT REQUIREMENT (KCAL)	95.72	7.40	9.86	4.55	117.53
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	264.52	7.03	72.20	4.55	348.31
(10) WEIGHING FACTOR (9)/SUM(9)	0.759	0.020	0.207	0.013	
(11) QREJ, HEAT REJECTED (KCAL)	-2.17	-47.04	0.0	0.0	-49.21
(12) NUJ, INDIVIDUAL FIGURES OF MERIT	0.447	-12.994	-0.146	11.393	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)x(12), SUM(13)=OVERALL FIG. MERIT	0.340	-0.262	-0.030	0.149	0.196
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	2.503	0.683	0.913	0.0	4.099

Sample Problem 4. Dummy Version of the IGT Cycle B-1

This is a Dummy Version of the IGT Cycle B-1 that has been modified to provide a check of the HYDRGN program. The results of this problem are useful in checking the operation of the program and are otherwise useless. These results should not be used in comparing this cycle to other cycles as they have been considerably modified.

For the following process:

Run reaction (1) at 1025 K for stoichiometric composition with the extent of reaction being 0.45 and 0.223 at 1 and 25 atmospheres.

Run reaction (2) at 580 K for stoichiometric composition with the extent of reaction of 0.346 at 1 atmosphere.

Run reaction (3) at 700 K with an extent of reaction of 1.0 at 30 atmospheres for stoichiometric composition.

Run reaction (4) at 1200 K for stoichiometric composition with the extent of reaction of 0.713 and 0.32 at 1.0 and 33 atmospheres.

Input Data Cards for Sample Problem 4

THIS IS A DUMMY VERSION OF THE IGT CYCLE B-1, USED TO CHECK THE PROGRAM
CHEMICAL REACTIONS

1REACTANTFE	1CL	2	L	3.	
1REACTANTH	2O	1	G	4.	B
2REACTANTH	1CL	1	G	8.	B
2REACTANTFE	3O	4	S	1.	
3REACTANTFE	1CL	3	G	2.	B
4REACTANTCL	2		G	1.	
4REACTANTH	2O	1	G	1.	B
1PRODUCT H	1CL	1	G	6.	
1PRODUCT FE	3O	4	S	1.	
1PRODUCT H	2		G	1.	
2PRODUCT FE	1CL	3	L	2.	
2PRODUCT FE	1CL	2	S	1.	
2PRODUCT H	2O	1	G	4.	
3PRODUCT FE	1CL	2	S	2.	
4PRODUCT H	1CL	1	G	2.	
3PRODUCT CL	2		G	1.	
4PRODUCT C	2		G	.5	

NAMELISTS

```

&NAM1 STEP=3,T=700,700,PRES=30,30,8*0,EP(1,1)=1.,EP(2,1)=1.,EFF=.42 &END
&NAM1 STEP=1,T=1025.,1025.,PRES=1,25,EFF=.42,EP(1,1)=.45,EP(2,1)=.223 &END
&NAM1 STEP=2,T=580,580,PRES=1,1,EP(1,1)=.346,EP(2,1)=.346,DRAW=T &END
&NAM1 STEP=4,T=1200,1200,PRES=1,33,EP(1,1)=.713,EP(2,1)=.32 &END

```

END

CINETIC REACTIONS

NAMELISTS

```

STEP=      3,T= 700.000000      , 700.000000      , 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      , 1.00000000      , 1.00000000      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , PRES= 30.000000      , 30.000000      ,
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0

```

6564

```

STEP=      1,T= 1025.00000      , 1025.00000      , 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      , EP= 0.44999999      , 0.22299999      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0      , 0.0
0.0      , 0.0      , 0.0      , 0.0      , 0.0      , PRES= 1.00000000      , 25.000000      ,
1.0000000      , 1.00000000      , 1.00000000      , 1.00000000      , 1.00000000      , 1.00000000      , 1.00000000

```

DRAW-
ABLE

[illegible]

END

```

      4,T= 1200.0000 , 1200.0000 , 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 , 0.713000C30 , 0.319999999 , 0.0

```

$\Delta A_n = 1, -AM_c = 1, n \angle 90 = 1, c \neq 1 = 0.41999796$

4410

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THERMO DATA FOUND ON TAPE 4
 300.000 1000.000 5000.000
 1 LL2 J 9/65CL 2. 0. 0. 0.6 300.000 5000.000
 0.43077812D 01 0.311827990-03-0.153108030-06 0.445119080-10-0.430577340-14
 -0.154582500 04 0.200600760 01 0.313168010 01 0.489978490-02-0.094114020-05
 0.441850150-06-0.100216510-11-0.109796950 04 0.778334240 01
 2 FECL2(S) J12/70FE 1.CL 2. 0. 0.5 300.000 950.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.711222650 01 0.110869520-01-0.170727290-04
 0.135158160-07-0.413650260-11-0.430009840 05-0.289940490 02
 3 FECL2(L) J12/70FE 1.CL 2. 0. 0.1 950.000 5000.000
 0.122888620 02 0.0 0.0 0.0
 -0.411098200 05-0.531930540 02 0.122888620 02 0.0
 0.0 0.0 -0.411098200 05-0.531930540 02
 4 FECL2 J12/70FE 1.CL 2. 0. 0.6 300.000 5000.000
 0.694925950 01 0.553716290-03 0.702211760-07-0.614754770-10 0.679331270-14
 -0.190458280 05-0.377266980 01 0.545575050 01 0.796329230-02-0.125939630-04
 0.699767020-06-0.232423630-11-0.168442970 05 0.300968550 01
 5 FECL3(S) J 6/65FE 1.CL 3. 0. 0.5 300.000 577.600
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.118069930 02 0.182806810-01-0.191566830-03
 0.577784590-06-0.494600360-09-0.516004960 05-0.512372440 02
 6 FECL3(L) J 6/65FE 1.CL 3. 0. 0.1 577.000 1500.000
 0.161025700 02 0.0 0.0 0.0
 -0.464355310 05-0.676145780 02 0.161025700 02 0.0
 0.0 0.0 -0.464355310 05-0.676145780 02
 7 FECL3 J 6/65FE 1.CL 3. 0. 0.6 300.000 5000.000
 0.977711010 01 0.244213500-03-0.103139940-06 0.192074130-10-0.131792970-14
 -0.334395000 05-0.145023010 02 0.750148720 01 0.973382220-02-0.155432940-04
 0.111603060-07-0.300229980-11-0.330136210 05-0.399898620 01
 8 FE304(S) J 6/65FE 3.0 4. 0. 0.5 300.000 5000.000
 0.241337130 02 0.415922200-04-0.263314920-07 0.660350850-11-0.569246800-15
 -0.141210500 06-0.120064120 03 0.361981350 02-0.174379710 00 0.524756500-03
 -0.542302170-06 0.179902020-09-0.141387250 06-0.155566820 03
 9 HCL J 9/64H 1.CL 1. 0. 0.6 300.000 5000.000
 0.270658820 01 0.143818810-02-0.469929940-06 0.734994010-10-0.437310910-14
 -0.119174050 05 0.645835400 01 0.352481650 01 0.299848620-04-0.062218880-06
 0.209797200-08-0.980551480-12-0.121505080 05 0.239577100 01
 10 H2 J 3/61H 2. 0. 0. 0.6 300.000 5000.000
 0.310018920 01 0.511194580-03 0.526442070-07-0.349099640-10 0.369453410-14
 -0.8711580370 03-0.190294120 01 0.305744460 01 0.267651980-02-0.580991580-05
 0.552103760-08-0.181227340-11-0.988904540 03-0.229970550 01
 11 H2U(S) L11/65H 2.0 1. 0. 0.5 200.000 273.150
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.392693280-01 0.169204180-01 0.0
 0.0 0.0 -0.359495780 05 0.569337790 00
 12 H2U(L) L11/65H 2.0 1. 0. 0.1 273.150 1000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.127127820 02-0.176627960-01-0.225566470-04
 0.205209030-06-0.240786060-09-0.374831990 05-0.591153410 02
 13 H2L J 3/61H 2.0 1. 0. 0.6 300.000 5000.000
 0.271676250 01 0.294513720-02-0.602243730-06 0.102266810-09-0.484721380-14
 -0.299058240 05 0.663050000 01 0.407012750 01-0.110844990-02 0.415211800-05
 -0.290574040-08 0.807021010-12-0.502797190 05-0.322700440 00
 14 U2 J 9/65U 2. 0. 0. 0.6 300.000 5000.000
 0.302195500 01 0.736162560-03-0.196522250-06 0.362015560-10-0.289456250-14
 -0.120198240 04 0.361509510 01 0.362559800 01-0.187821830-02 0.705545430-05
 -0.070351000-08 0.215559060-11-0.104752250 04 0.430527690 01

END OF INPUT DATA FOR THIS IS A DUMMY VERSION OF THE IGT CYCLE U-1, USED TO CHECK THE PROGRAM
 FOR TEMP. SCHEDULE 1 AND REACTION 7 THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR
 FOR TEMP. SCHEDULE 1 AND REACTION 8 THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR
 FOR TEMP. SCHEDULE 2 AND REACTION 7 THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR
 FOR TEMP. SCHEDULE 2 AND REACTION 8 THE TEMP. IS MORE THAN 10 DEG. OUTSIDE THE RANGE OF THE DATA FOR

FECL3(L)
 FECL3(L)
 FECL3(L)
 FECL3(L)

TABLE I
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THIS IS A DUMMY VERSION OF THE 1GT CYCLE 8-1, USED TO CHECK THE PROGRAM
TEMPERATURE SCHEDULE 1.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H₂. EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

EPSI EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM						WORK OF SEPARATION OF GASES (KCAL)					
			EXTENT OF REACTION AS PERCENT OF EPSI EQ.						EXTENT OF REACTION AS PERCENT OF EPSI EQ.					
			100	90	80	70	60	50	100	90	80	70	60	50
STEP 1. AT 1025.00DEG., AND 1.00ATM.														
3 FeCl ₂ (L) + 4 H ₂ O → 6 HCl + Fe ₃ O ₄ (S) + H ₂														
DELTA-H= 47.98339 KCAL, DELTA-S= 40.33356 CAL/DEG, DELTA-G= 6.64149 KCAL														
H ₂ O IS THE BASE REACTANT FOR THIS REACTION														
0.45000	FeCl ₂ (L)	3.000*	3.667	4.407	5.333	6.524	8.111	10.333*						
	H ₂ O	4.000*	4.889	5.877	7.111	8.698	10.815	13.778*	22.249	23.927	25.769	27.823	30.161	32.889
STEP 2. AT 580.00DEG., AND 1.00ATM.														
6 HCl + Fe ₃ O ₄ (S) → 2 FeCl ₃ (L) + FeCl ₂ (S) + 4 H ₂ O														
DELTA-H= -37.27475 KCAL, DELTA-S= -75.56099 CAL/DEG, DELTA-G= 6.55063 KCAL														
HCl IS THE BASE REACTANT FOR THIS REACTION														
0.34000	HCl	8.000*	15.121	17.690	20.902	25.031	30.536	38.243*						
	Fe ₃ O ₄ (S)	1.000*	1.890	2.211	2.613	3.129	3.817	4.780*	11.303	11.950	12.649	13.415	14.271	15.252
STEP 3. AT 700.00DEG., AND 30.00ATM.														
2 FeCl ₃ → 2 FeCl ₂ (S) + Cl ₂														
DELTA-H= -38.85465 KCAL, DELTA-S= -40.65124 CAL/DEG, DELTA-G= -10.39879 KCAL														
FeCl ₃ IS THE BASE REACTANT FOR THIS REACTION														
1.00000	FeCl ₃	2.000*	0.000	0.222	0.500	0.857	1.333	2.000*	0.000	0.806	1.328	1.783	2.217	2.656
STEP 4. AT 1200.00DEG., AND 1.00ATM.														
Cl ₂ + H ₂ O → 2 HCl + 0.5 O ₂														
DELTA-H= 14.21134 KCAL, DELTA-S= 16.35138 CAL/DEG, DELTA-G= -5.41032 KCAL														
H ₂ O IS THE BASE REACTANT FOR THIS REACTION														
0.71300	Cl ₂	1.000*	0.403	0.558	0.753	1.004	1.338	1.805*						
	H ₂ O	1.000*	0.403	0.558	0.753	1.004	1.338	1.805*	7.359	8.314	9.308	10.369	11.530	12.841

TABLE 11
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THIS IS A DUMMY VERSION OF THE 161 CYCLE D-1, USED TO CHECK THE PROGRAM
TEMPERATURE SCHEDULE 1.

					DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	1025.00 DEG. ---> 580.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 FE3O4(S)	FROM REACTION 1 ---> 1.00 FE3O4(S)	IN REACTION 2			-24.07879	-30.9394	35.86805
STEP 6	1025.00 DEG. ---> 298.15 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 H2	FROM REACTION 1 ---> 1.00 H2	FINAL PRODUCT			-5.12408	-8.6714	26.44850
STEP 7	580.00 DEG. ---> 1555.17 DEG. 1.00 ATM. ---> 30.00 ATM.						
2.00 FECL3(L)	FROM REACTION 2 ---> 2.00 FECL3(L)	IN REACTION 8			62.40778	63.1209	-170.80846
STEP 8	1555.17 DEG. ---> 1555.17 DEG. 30.00 ATM. ---> 30.00 ATM.						
2.00 FECL3(L)	FROM REACTION 7 ---> 2.00 FECL3	IN REACTION 9			21.26468	13.6731	0.00075
STEP 9	1555.17 DEG. ---> 700.00 DEG. 30.00 ATM. ---> 30.00 ATM.						
2.00 FECL3	FROM REACTION 8 ---> 2.00 FECL3	IN REACTION 3			-33.78004	-31.5123	172.38404
STEP 10	580.00 DEG. ---> 1025.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
4.00 H2O	FROM REACTION 2 ---> 4.00 H2O	IN REACTION 1			16.48409	20.9518	-95.05166
STEP 11	700.00 DEG. ---> 1200.00 DEG. 30.00 ATM. ---> 1.00 ATM.						
1.00 CL2	FROM REACTION 3 ---> 1.00 CL2	IN REACTION 4			4.46435	11.5671	-36.31800
STEP 12	1200.00 DEG. ---> 298.15 DEG. 1.00 ATM. ---> 1.00 ATM.						
0.50 O2	FROM REACTION 4 ---> 0.50 O2	FINAL PRODUCT			-3.55562	-5.3611	24.97510
STEP 13	298.15 DEG. ---> 373.47 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 H2O(L)	RAW MATERIAL ---> 1.00 H2O(L)	IN REACTION 14			1.35771	4.0596	-1.41736
STEP 14	373.47 DEG. ---> 373.47 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 H2O(L)	FROM REACTION 13 ---> 1.00 H2O	IN REACTION 15			9.77287	26.1454	0.00847
STEP 15	373.47 DEG. ---> 1200.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 H2L	FROM REACTION 14 ---> 1.00 H2O	IN REACTION 4			7.63353	10.5192	-43.77127
STEP 16	1025.00 DEG. ---> 580.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
6.00 HCL	FROM REACTION 1 ---> 6.00 HCL	IN REACTION 2			-19.49570	-24.8578	137.59312
STEP 17	580.00 DEG. ---> 950.19 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 FECL2(S)	FROM REACTION 2 ---> 1.00 FECL2(S)	IN REACTION 16			7.52490	10.0146	-17.13166
STEP 18	950.19 DEG. ---> 950.19 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 FECL2(S)	FROM REACTION 17 ---> 1.00 FECL2(L)	IN REACTION 19			10.28066	10.8218	-0.00205
STEP 19	950.19 DEG. ---> 1025.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
1.00 FECL2(L)	FROM REACTION 18 ---> 1.00 FECL2(L)	IN REACTION 1			1.82684	1.8507	-4.68856
STEP 20	700.00 DEG. ---> 950.19 DEG. 30.00 ATM. ---> 1.00 ATM.						
2.00 FECL2(S)	FROM REACTION 3 ---> 2.00 FECL2(S)	IN REACTION 21			10.25083	12.5109	-23.98346
STEP 21	950.19 DEG. ---> 950.19 DEG. 1.00 ATM. ---> 1.00 ATM.						
2.00 FECL2(S)	FROM REACTION 20 ---> 2.00 FECL2(L)	IN REACTION 22			20.56137	21.6435	-0.00409
STEP 22	950.19 DEG. ---> 1025.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
2.00 FECL2(L)	FROM REACTION 21 ---> 2.00 FECL2(L)	IN REACTION 1			3.65369	3.7014	-9.37712
STEP 23	1200.00 DEG. ---> 580.00 DEG. 1.00 ATM. ---> 1.00 ATM.						
2.00 HCL	FROM REACTION 4 ---> 2.00 HCL	IN REACTION 2			-9.19631	-10.7150	64.78310
TOTALS FOR STEPS 1 TO 23					68.51810	36.9954	56.69102

TABLE I
ANALYSIS OF THE CHEMICAL REACTION STEPS IN
THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
TEMPERATURE SCHEDULE 2.

TEMPERATURES ARE IN DEGREES KELVIN AND ALL VALUES ARE BASED ON THE PRODUCTION OF ONE GRAM MOLE OF H₂. EPSI EQ. IS THE FRACTION OF THE BASE REACTANT WHICH IS CONVERTED AT EQUILIBRIUM. CALCULATIONS ARE MADE FOR THE FRACTION CONVERTED AT 100, 90, ETC. PERCENT OF THIS EQUILIBRIUM VALUE

EPSI EQ.	REACTANT	RATIO*	MOLES OF REACTANT IN RECYCLE STREAM						WORK OF SEPARATION OF GASES (KCAL)					
			* EXTENT OF REACTION AS PERCENT OF EPSI EQ.						* EXTENT OF REACTION AS PERCENT OF EPSI EQ.					
			100	90	80	70	60	50	100	90	80	70	60	50
STEP 1. AT 1025.00DEG., AND 25.00ATM.														
3 FeCl ₂ (L) + 4 H ₂ O → 6 HCl + Fe ₃ O ₄ (S) + H ₂														
DELTA-H= 47.98339 KCAL, DELTA-S= 21.14425 CAL/DEG, DELTA-G= 26.31053 KCAL														
H ₂ O IS THE BASE REACTANT FOR THIS REACTION														
0.45000	FeCl ₂ (L)	3.000*	3.667	4.407	5.333	6.524	8.111	10.333*						
	H ₂ O	4.000*	4.889	5.877	7.111	8.698	10.815	13.778*	22.249	23.927	25.769	27.823	30.161	32.889
STEP 2. AT 580.00DEG., AND 1.00ATM.														
6 HCl + Fe ₃ O ₄ (S) → 2 FeCl ₃ (L) + FeCl ₂ (S) + 4 H ₂ O														
DELTA-H= -37.27475 KCAL, DELTA-S= -75.56099 CAL/DEG, DELTA-G= 6.55063 KCAL														
HCl IS THE BASE REACTANT FOR THIS REACTION														
0.34800	HCl	8.000*	15.121	17.690	20.902	25.031	30.536	38.243*						
	Fe ₃ O ₄ (S)	1.000*	1.890	2.211	2.613	3.129	3.817	4.780*	11.303	11.950	12.649	13.415	14.271	15.252
STEP 3. AT 700.00DEG., AND 30.00ATM.														
2 FeCl ₃ → 2 FeCl ₂ (S) + Cl ₂														
DELTA-H= -38.85465 KCAL, DELTA-S= -40.65124 CAL/DEG, DELTA-G= -10.39879 KCAL														
FeCl ₃ IS THE BASE REACTANT FOR THIS REACTION														
1.00000	FeCl ₃	2.000*	0.000	0.222	0.500	0.857	1.333	2.000*	0.000	0.806	1.328	1.783	2.217	2.656
STEP 4. AT 1200.00DEG., AND 33.00ATM.														
Cl ₂ + H ₂ O → 2 HCl + 0.5 O ₂														
DELTA-H= 14.21134 KCAL, DELTA-S= 12.87731 CAL/DEG, DELTA-G= -1.24144 KCAL														
H ₂ O IS THE BASE REACTANT FOR THIS REACTION														
0.71300	Cl ₂	1.000*	0.403	0.558	0.753	1.004	1.338	1.805*						
	H ₂ O	1.000*	0.403	0.558	0.753	1.004	1.338	1.805*	7.359	8.314	9.308	10.369	11.530	12.841

TABLE 11
ANALYSIS OF THE HEATING AND COOLING STEPS IN
THIS IS A DUMMY VERSION OF THE 101 CYCLE D-1, USED TO CHECK THE PROGRAM
TEMPERATURE SCHEDULE 2.

					DELTA-H (KCAL)	DELTA-S (CAL/DEG)	DELTA-G (KCAL)
STEP 5	1025.00 DEG. ---> 580.00 DEG. 25.00 ATM. ---> 1.00 ATM.						
1.00 FE3O4(S)	FROM REACTION 1 --->	1.00 FE3O4(S)	IN REACTION 2		-24.07879	-30.9394	35.66865
STEP 6	1025.00 DEG. ---> 298.15 DEG. 25.00 ATM. ---> 1.00 ATM.						
1.00 H2	FROM REACTION 1 --->	1.00 H2	FINAL PRODUCT		-5.12408	-2.2750	19.89215
STEP 7	580.00 DEG. ---> 1555.17 DEG. 1.00 ATM. ---> 30.00 ATM.						
2.00 FECL3(L)	FROM REACTION 2 --->	2.00 FECL3(L)	IN REACTION 8		62.40778	63.1209	-170.80846
STEP 8	1555.17 DEG. ---> 1555.17 DEG. 30.00 ATM. ---> 30.00 ATM.						
2.00 FECL3(L)	FROM REACTION 7 --->	2.00 FECL3	IN REACTION 9		21.26468	13.6731	0.00073
STEP 9	1555.17 DEG. ---> 700.00 DEG. 30.00 ATM. ---> 30.00 ATM.						
2.00 FECL3	FROM REACTION 8 --->	2.00 FECL3	IN REACTION 3		-33.76004	-31.5123	172.38404
STEP 10	580.00 DEG. ---> 1025.00 DEG. 1.00 ATM. ---> 25.00 ATM.						
4.00 H2O	FROM REACTION 2 --->	4.00 H2O	IN REACTION 1		16.48409	-4.6339	-68.82628
STEP 11	700.00 DEG. ---> 1200.00 DEG. 30.00 ATM. ---> 33.00 ATM.						
1.00 CL2	FROM REACTION 3 --->	1.00 CL2	IN REACTION 4		4.46435	4.6189	-27.98024
STEP 12	1200.00 DEG. ---> 298.15 DEG. 33.00 ATM. ---> 1.00 ATM.						
0.50 O2	FROM REACTION 4 --->	0.50 O2	FINAL PRODUCT		-3.55562	-1.8870	20.80622
STEP 13	298.15 DEG. ---> 522.96 DEG. 1.00 ATM. ---> 33.00 ATM.						
1.00 H2O(L)	RAW MATERIAL --->	1.00 H2O(L)	IN REACTION 14		4.10022	10.2354	-5.01031
STEP 14	522.96 DEG. ---> 522.96 DEG. 33.00 ATM. ---> 33.00 ATM.						
1.00 H2O(L)	FROM REACTION 13 --->	1.00 H2O	IN REACTION 15		8.27068	15.8117	0.00164
STEP 15	522.96 DEG. ---> 1200.00 DEG. 33.00 ATM. ---> 33.00 ATM.						
1.00 H2O	FROM REACTION 14 --->	1.00 H2O	IN REACTION 4		6.39320	7.7289	-31.83392
STEP 16	1025.00 DEG. ---> 580.00 DEG. 25.00 ATM. ---> 1.00 ATM.						
6.00 HCL	FROM REACTION 1 --->	6.00 HCL	IN REACTION 2		-19.49570	13.5208	98.25504
STEP 17	580.00 DEG. ---> 950.19 DEG. 1.00 ATM. ---> 25.00 ATM.						
1.00 FECL2(S)	FROM REACTION 2 --->	1.00 FECL2(S)	IN REACTION 18		7.52490	10.0146	-17.13166
STEP 18	950.19 DEG. ---> 950.19 DEG. 25.00 ATM. ---> 25.00 ATM.						
1.00 FECL2(S)	FROM REACTION 17 --->	1.00 FECL2(L)	IN REACTION 19		10.28068	10.8218	-0.00205
STEP 19	950.19 DEG. ---> 1025.00 DEG. 25.00 ATM. ---> 25.00 ATM.						
1.00 FECL2(L)	FROM REACTION 18 --->	1.00 FECL2(L)	IN REACTION 1		1.82684	1.8507	-4.68856
STEP 20	700.00 DEG. ---> 950.19 DEG. 30.00 ATM. ---> 25.00 ATM.						
2.00 FECL2(S)	FROM REACTION 3 --->	2.00 FECL2(S)	IN REACTION 21		10.25083	12.5109	-23.98346
STEP 21	950.19 DEG. ---> 950.19 DEG. 25.00 ATM. ---> 25.00 ATM.						
2.00 FECL2(S)	FROM REACTION 20 --->	2.00 FECL2(L)	IN REACTION 22		20.56137	21.6435	-0.00409
STEP 22	950.19 DEG. ---> 1025.00 DEG. 25.00 ATM. ---> 25.00 ATM.						
2.00 FECL2(L)	FROM REACTION 21 --->	2.00 FECL2(L)	IN REACTION 1		3.65369	3.7014	-9.37712
STEP 23	1200.00 DEG. ---> 580.00 DEG. 33.00 ATM. ---> 1.00 ATM.						
2.00 HCL	FROM REACTION 4 --->	2.00 HCL	IN REACTION 2		-9.19631	3.1813	48.10817
TOTALS FOR STEPS 1 TO 23					68.31810	38.9954	56.69102

THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 1

HEAT		STREAM SUPPLYING HEAT						STREAM ABSORBING HEAT					
EXCHANGED	STEP	TEMPERATURES		AMOUNT OF HEAT		STEP	TEMPERATURES		AMOUNT OF HEAT				
(KCAL)		INITIAL	FINAL	INITIALLY	REMAINING		INITIAL	FINAL	INITIALLY	REMAINING			
				AVAILABLE					NEEDED				
9.773	2	580.00	580.00	-37.275	-27.502	14	373.47	373.47	9.773	0.0			
1.358	2	580.00	580.00	-27.502	-26.144	13	298.15	373.47	1.358	0.0			
1.728	2	580.00	580.00	-26.144	-24.416	15	373.47	580.00	7.634	5.906			
7.680	3	700.00	700.00	-38.855	-31.175	7	580.00	700.00	62.408	54.728			
4.216	3	700.00	700.00	-31.175	-26.959	10	580.00	700.00	16.484	12.268			
1.054	3	700.00	700.00	-26.959	-25.905	15	580.00	700.00	5.906	4.852			
2.400	3	700.00	700.00	-25.905	-23.505	17	580.00	700.00	7.525	5.125			
3.068	5	1025.00	950.19	-24.079	-20.411	18	950.19	950.19	10.281	6.613			
W 13.864	5	950.19	700.00	-20.411	-6.547	7	700.00	916.63	54.728	40.865			
0.539	6	1025.00	950.19	-5.124	-4.585	18	950.19	950.19	6.613	6.073			
W 0.241	6	950.19	916.63	-4.585	-4.344	7	916.63	920.39	40.865	40.624			
1.536	6	916.63	700.00	-4.344	-2.808	10	700.00	742.60	12.268	10.731			
3.386	16	1025.00	950.19	-19.496	-16.110	18	950.19	950.19	6.073	2.688			
W 1.336	16	950.19	920.39	-16.110	-14.774	7	920.39	941.27	40.624	39.266			
W 0.044	16	920.39	769.69	-14.774	-8.130	10	742.60	920.39	10.731	4.087			
W 0.616	16	769.69	755.50	-8.130	-7.513	11	700.00	769.69	4.464	3.848			
W 0.501	16	755.50	743.93	-7.513	-7.012	15	700.00	755.50	4.852	4.350			
W 0.889	16	743.93	723.37	-7.012	-6.123	17	700.00	743.93	5.125	4.237			
W 0.944	16	723.37	701.45	-6.123	-5.179	20	700.00	723.37	10.251	9.307			
0.738	12	1200.00	1025.00	-3.556	-2.616	1	1025.00	1025.00	47.983	47.246			
0.311	12	1025.00	950.19	-2.616	-2.507	18	950.19	950.19	2.688	2.376			
W 0.037	12	950.19	941.27	-2.507	-2.470	7	941.27	941.85	39.288	39.251			
W 0.086	12	941.27	920.39	-2.470	-2.384	10	920.39	922.63	4.087	4.001			
0.613	12	920.39	769.69	-2.384	-1.771	11	769.69	838.72	3.848	3.235			
W 0.057	12	769.69	755.50	-1.771	-1.714	15	755.50	761.72	4.350	4.294			
W 0.046	12	755.50	743.93	-1.714	-1.668	17	743.93	746.21	4.237	4.191			
W 0.082	12	743.93	723.37	-1.668	-1.586	20	723.37	725.39	9.307	9.225			
2.696	23	1200.00	1025.00	-9.196	-6.499	1	1025.00	1025.00	47.246	44.548			
1.129	23	1025.00	950.19	-6.499	-5.370	18	950.19	950.19	2.376	1.248			
W 0.125	23	950.19	941.85	-5.370	-5.245	7	941.85	943.80	39.251	39.126			
W 0.287	23	941.85	922.63	-5.245	-4.958	10	922.63	930.08	4.001	3.714			
W 0.748	23	922.63	872.25	-4.958	-4.210	11	838.72	922.63	3.235	2.487			
W 1.028	23	872.25	802.21	-4.210	-3.183	15	761.72	872.25	4.294	3.266			
W 0.812	23	802.21	746.21	-3.183	-2.370	17	746.21	786.15	4.191	3.378			
W 0.300	23	746.21	725.39	-2.370	-2.070	20	725.39	732.80	9.225	8.925			
20.920	9	1555.17	1025.00	-33.780	-12.800	1	1025.00	1025.00	44.548	23.568			
1.248	9	1025.00	993.40	-12.800	-11.552	18	950.19	950.19	1.248	0.0			
1.705	9	993.40	950.19	-11.552	-9.846	21	950.19	950.19	20.561	18.856			
W 0.252	9	950.19	943.80	-9.846	-9.594	7	943.80	947.74	39.126	38.874			
W 0.530	9	943.80	930.36	-9.594	-9.064	10	930.08	943.80	3.714	3.184			
W 0.069	9	930.36	928.61	-9.064	-8.995	11	922.63	930.36	2.487	2.418			
W 0.538	9	928.61	914.96	-8.995	-8.457	15	872.25	928.61	3.266	2.728			
W 2.647	9	914.96	847.77	-8.457	-5.810	17	786.15	914.96	3.378	0.731			
W 4.522	9	847.77	732.80	-5.810	-1.288	20	732.80	843.63	8.925	4.403			

W-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.

(THE DELTA-T VERSUS TEMPERATURE CURVES FOR THE TWO STREAMS EITHER CROSS OR APPROACH EACH OTHER WITHIN FIVE DEGREES)

THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 1

HEAT AVAILABLE				*	HEAT REQUIRED			
STEP	TEMPERATURE		HEAT	STEP	TEMPERATURE		HEAT	
	INITIAL	FINAL	AVAILABLE		INITIAL	FINAL	REQUIRED	
2	580.00	580.00	-24.416	1	1025.00	1025.00	23.568	
3	700.00	700.00	-23.505	4	1200.00	1200.00	14.211	
5	700.00	580.00	-6.547	7	947.74	1555.17	38.874	
6	700.00	298.15	-2.808	8	1555.17	1555.17	21.265	
9	732.80	700.00	-1.288	10	943.80	1025.00	3.184	
12	723.37	298.15	-1.586	11	930.36	1200.00	2.418	
16	701.45	580.00	-5.179	15	928.61	1200.00	2.728	
				17	914.96	950.19	0.731	
				19	950.19	1025.00	1.827	
				20	843.63	950.19	4.403	
				21	950.19	950.19	18.856	
				22	950.19	1025.00	3.654	
23	725.39	580.00	-2.070					
TOTALS			-67.400				135.718	

THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
MATCHING OF STREAMS FOR HEAT EXCHANGE FOR TEMPERATURE SCHEDULE 2

HEAT		STREAM SUPPLYING HEAT						STREAM ABSORBING HEAT					
EXCHANGED	STEP	TEMPERATURES		AMOUNT OF HEAT		STEP	TEMPERATURES		AMOUNT OF HEAT				
(KCAL)		INITIAL	FINAL	INITIALLY*	REMAINING*		INITIAL	FINAL	INITIALLY*	REMAINING			
				AVAILABLE*					NEEDED				
8.271	2	580.00	580.00	-37.275	-29.004	14	522.96	522.96	8.271	0.0			
4.100	2	580.00	580.00	-29.004	-24.904	13	298.15	522.96	4.100	0.0			
0.487	2	580.00	580.00	-24.904	-24.417	15	522.96	580.00	6.393	5.906			
7.680	3	700.00	700.00	-38.855	-31.175	7	580.00	700.00	62.408	54.728			
4.216	3	700.00	700.00	-31.175	-26.959	10	580.00	700.00	16.484	12.268			
1.054	3	700.00	700.00	-26.959	-25.905	15	580.00	700.00	5.906	4.852			
2.400	3	700.00	700.00	-25.905	-23.505	17	580.00	700.00	7.525	5.125			
3.668	5	1025.00	950.19	-24.079	-20.411	18	950.19	950.19	10.281	6.613			
W 13.864	5	950.19	700.00	-20.411	-6.547	7	700.00	916.63	54.728	40.865			
0.539	6	1025.00	950.19	-5.124	-4.585	18	950.19	950.19	6.613	6.073			
W 0.241	6	950.19	916.63	-4.585	-4.344	7	916.63	920.39	40.865	40.624			
1.536	6	916.63	700.00	-4.344	-2.808	10	700.00	742.60	12.268	10.731			
3.366	16	1025.00	950.19	-19.496	-16.110	18	950.19	950.19	6.073	2.686			
W 1.336	16	950.19	920.39	-16.110	-14.774	7	920.39	941.27	40.624	39.268			
W 6.644	16	920.39	769.69	-14.774	-8.120	10	742.60	920.39	10.731	4.087			
W 0.616	16	769.69	755.50	-8.120	-7.513	11	700.00	769.69	4.464	3.848			
W 0.501	16	755.50	743.93	-7.513	-7.012	15	700.00	755.50	4.852	4.350			
W 0.889	16	743.93	723.37	-7.012	-6.123	17	700.00	743.93	5.125	4.237			
W 0.944	16	723.37	701.45	-6.123	-5.179	20	700.00	723.37	10.251	9.307			
0.738	12	1200.00	1025.00	-3.556	-2.818	1	1025.00	1025.00	47.983	47.246			
0.311	12	1025.00	950.19	-2.818	-2.507	18	950.19	950.19	2.688	2.376			
W 0.037	12	950.19	941.27	-2.507	-2.470	7	941.27	941.85	39.288	39.251			
W 0.060	12	941.27	920.39	-2.470	-2.384	10	920.39	922.63	4.087	4.001			
0.613	12	920.39	769.69	-2.384	-1.771	11	769.69	838.72	3.848	3.235			
W 0.057	12	769.69	755.50	-1.771	-1.714	15	755.50	761.72	4.350	4.294			
W 0.046	12	755.50	743.93	-1.714	-1.668	17	743.93	746.21	4.237	4.191			
W 0.062	12	743.93	723.37	-1.668	-1.566	20	723.37	725.39	9.307	9.225			
2.698	23	1200.00	1025.00	-9.196	-6.499	1	1025.00	1025.00	47.246	44.548			
1.129	23	1025.00	950.19	-6.499	-5.370	18	950.19	950.19	2.376	1.248			
W 0.125	23	950.19	941.85	-5.370	-5.245	7	941.85	943.80	39.251	39.126			
W 0.287	23	941.85	922.63	-5.245	-4.958	10	922.63	930.08	4.001	3.714			
W 0.746	23	922.63	872.25	-4.958	-4.210	11	838.72	922.63	3.235	2.487			
W 1.028	23	872.25	802.21	-4.210	-3.183	15	761.72	872.25	4.294	3.266			
W 0.812	23	802.21	746.21	-3.183	-2.370	17	746.21	786.15	4.191	3.376			
W 0.300	23	746.21	725.39	-2.370	-2.070	20	725.39	732.80	9.225	8.925			
20.980	9	1555.17	1025.00	-33.780	-12.800	1	1025.00	1025.00	44.548	23.568			
1.248	9	1025.00	993.40	-12.800	-11.552	18	950.19	950.19	1.248	0.0			
1.705	9	993.40	950.19	-11.552	-9.846	21	950.19	950.19	20.561	18.856			
W 0.252	9	950.19	943.80	-9.846	-9.594	7	943.80	947.74	39.126	38.874			
W 0.530	9	943.80	930.36	-9.594	-9.064	10	930.08	943.80	3.714	3.184			
W 0.069	9	930.36	928.61	-9.064	-8.995	11	922.63	930.36	2.487	2.418			
W 0.538	9	928.61	914.96	-8.995	-8.457	15	872.25	928.61	3.266	2.728			
W 2.647	9	914.96	847.77	-8.457	-5.810	17	786.15	914.96	3.378	0.731			
W 4.522	9	847.77	732.80	-5.810	-1.288	20	732.80	843.63	8.925	4.403			

W-DENOTES THAT A POSSIBLE SECOND LAW VIOLATION HAS OCCURRED FOR THIS MATCH.

THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
SUMMARY OF REQUIRED AND AVAILABLE HEAT AFTER MATCHING
FOR TEMPERATURE SCHEDULE 2

HEAT AVAILABLE				*	HEAT REQUIRED			
STEP	TEMPERATURE		HEAT	*	STEP	TEMPERATURE		HEAT
	INITIAL	FINAL	AVAILABLE	*		INITIAL	FINAL	REQUIRED
2	580.00	580.00	-24.417		1	1025.00	1025.00	23.568
3	700.00	700.00	-23.505		4	1200.00	1200.00	14.211
5	700.00	580.00	-6.547		7	947.74	1555.17	38.874
6	700.00	298.15	-2.808		8	1555.17	1555.17	21.265
9	732.80	700.00	-1.288		10	943.80	1025.00	3.184
12	723.37	298.15	-1.586		11	930.36	1200.00	2.418
16	701.45	580.00	-5.179		15	928.61	1200.00	2.728
					17	914.96	950.19	0.731
					19	950.19	1025.00	1.827
					20	843.63	950.19	4.403
					21	950.19	950.19	18.856
					22	950.19	1025.00	3.654
23	725.39	580.00	-2.070					
TOTALS			-67.400					135.718

THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
COMPARISON OF EXOTHERMIC AND ENDOTHERMIC STEPS

TEMPERATURE SCHEDULE 1					TEMPERATURE SCHEDULE 2				
STEP	TEMPERATURES (K)		HEAT (KCAL)		*STEP*	TEMPERATURES (K)		HEAT (KCAL)	
	REACTANTS	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*		*REACTANTS*	*PRODUCTS*	*EXOTHERMIC*	*ENDOTHERMIC*
* 1 *	1025.00	1025.00		47.9834	* 1 *	1025.00	1025.00		47.9834
* 2 *	580.00	580.00	-37.2748		* 2 *	580.00	580.00	-37.2748	
* 3 *	700.00	700.00	-38.8547		* 3 *	700.00	700.00	-38.8547	
* 4 *	1200.00	1200.00		14.2113	* 4 *	1200.00	1200.00		14.2113
* 5 *	1025.00	580.00	-24.0788		* 5 *	1025.00	580.00	-24.0788	
* 6 *	1025.00	298.15	-5.1241		* 6 *	1025.00	298.15	-5.1241	
* 7 *	580.00	1555.17		62.4078	* 7 *	580.00	1555.17		62.4078
* 8 *	1555.17	1555.17		21.2647	* 8 *	1555.17	1555.17		21.2647
* 9 *	1555.17	700.00	-33.7800		* 9 *	1555.17	700.00	-33.7800	
* 10 *	580.00	1025.00		16.4841	* 10 *	580.00	1025.00		16.4841
* 11 *	700.00	1200.00		4.4644	* 11 *	700.00	1200.00		4.4644
* 12 *	1200.00	298.15	-3.5556		* 12 *	1200.00	298.15	-3.5556	
* 13 *	298.15	373.47		1.3577	* 13 *	298.15	522.96		4.1002
* 14 *	373.47	373.47		9.7729	* 14 *	522.96	522.96		8.2707
* 15 *	373.47	1200.00		7.6335	* 15 *	522.96	1200.00		6.3932
* 16 *	1025.00	580.00	-19.4957		* 16 *	1025.00	580.00	-19.4957	
* 17 *	580.00	950.19		7.5249	* 17 *	580.00	950.19		7.5249
* 18 *	950.19	950.19		10.2807	* 18 *	950.19	950.19		10.2807
* 19 *	950.19	1025.00		1.8268	* 19 *	950.19	1025.00		1.8268
* 20 *	700.00	950.19		10.2508	* 20 *	700.00	950.19		10.2508
* 21 *	950.19	950.19		20.5614	* 21 *	950.19	950.19		20.5614
* 22 *	950.19	1025.00		3.6537	* 22 *	950.19	1025.00		3.6537
* 23 *	1200.00	580.00	-9.1963		* 23 *	1200.00	580.00	-9.1963	
TOTALS			-171.3597	239.6776				-171.3597	239.6776

THIS IS A DUMMY VERSION OF THE 1GT CYCLE B-1, USED TO CHECK THE PROGRAM
FIGURES OF MERIT

TEMP. SCHEDULE	WORK OF		WORK GENERATED	TOTAL HEAT REQUIRED	FIGURES OF MERIT			
	SEPARATION				1ST ESTIMATE		2ND ESTIMATE	
	MIN	MAX			MIN	MAX	MIN	MAX
1	40.910	63.637	24.177	135.718	0.3108	0.4122	0.1792	0.2503
2	40.910	63.637	24.177	135.718	0.3108	0.4122	0.1792	0.2503

ALL HEAT ABOVE 500 K WHICH IS STILL AVAILABLE AFTER STREAM MATCHING, IS TURNED INTO WORK GENERATED USING A 30% EFFICIENCY AND SUBTRACTED FROM THE WORK OF SEPARATION NEEDED. THE FIRST ESTIMATE FOR A FIGURE OF MERIT ASSUMES PERFECT HEAT REGENERATION AND 100% EFFICIENCY IN THE WORK OF SEPARATION. THE SECOND ESTIMATE USES THE HEAT REQUIRED AFTER STREAM MATCHING AS THE TOTAL HEAT REQUIRED AND ASSUMES ONLY A 50% EFFICIENCY FOR THE WORK OF SEPARATION. ALL WORK REQUIRED IS ASSUMED TO BE GENERATED FROM HEAT AT A 42% EFFICIENCY.

PROPERTIES OF THE BASE REACTIONS AT 298 K FOR
THIS IS A DUMMY VERSION OF THE IGT CYCLE B-1, USED TO CHECK THE PROGRAM

STEP 1. AT 298.15DEG., AND 1.00ATM.

DELTA-H= 118.33538 KCAL, DELTA-S= 182.55151 CAL/DEG, DELTA-G= 63.90766 KCAL

STEP 2. AT 298.15DEG., AND 1.00ATM.

DELTA-H= -101.78475 KCAL, DELTA-S= -229.06050 CAL/DEG, DELTA-G= -33.49041 KCAL

STEP 3. AT 298.15DEG., AND 1.00ATM.

DELTA-H= 27.57495 KCAL, DELTA-S= 41.71933 CAL/DEG, DELTA-G= 15.13634 KCAL

STEP 4. AT 298.15DEG., AND 1.00ATM.

DELTA-H= 24.19254 KCAL, DELTA-S= 43.78508 CAL/DEG, DELTA-G= 11.13802 KCAL

TOTALS DELTA-H= 68.31506 KCAL, DELTA-S= 38.99542 CAL/DEG, DELTA-G= 56.69162 KCAL

PROCESS SUMMARY

THIS IS A DUMMY VERSION OF THE IGT CYCLE B-1, USED TO CHECK THE PROGRAM
TEMPERATURE SCHEDULE 1

STAGE	1	2	3	4	SUM
(1) H298, HEAT OF REACTION AT 298K (KCAL)	118.34	-101.78	27.57	24.19	68.32
(2) HT, HEAT OF REACTION AT TEMP T (KCAL)	47.98	-37.27	-38.85	14.21	
(3) T, TEMP. OF REACTION (K)	1025.	580.	700.	1200.	
(4) WS, THEO. WORK OF SEPARATION (KCAL)	22.25	11.30	0.00	7.36	40.91
(5) THEO. WORK OF SEPARATION (I)	0.54	0.28	0.00	0.18	
(6) WG, WORK GENERATED INTERNALLY (KCAL)	2.67	10.46	10.36	0.69	24.18
(7) HEAT REQUIRED TO GENERATE WORK (KCAL) QS=(2WS-WG)/0.42	99.60	28.91	-24.66	33.40	137.25
(8) Q, HEAT REQUIREMENT (KCAL)	39.89	32.94	44.73	18.15	135.72
(9) QT, TOTAL HEAT REQ. (7)+(8) (KCAL)	139.49	61.85	20.07	51.55	272.97
(10) WEIGHING FACTOR (9)/SUM(9)	0.511	0.227	0.074	0.189	
(11) QREJ, HEAT REJECTED (KCAL)	-8.67	-31.96	-24.15	-2.62	-67.40
(12) NOJ, INDIVIDUAL FIGURES OF MERIT	0.848	-1.646	1.374	0.469	
(13) WEIGHING FACTOR TIMES FIGURE OF MERIT (10)x(12), SUM(13)=OVERALL FIG. MERIT	0.434	-0.373	0.101	0.089	0.250
(14) LOSS COEFFICIENT, ((7)+(11))/68.3	1.585	0.891	-0.008	0.527	2.996

TABLE I

Chemical Reaction Cards

Contents	Format	Card Columns
REACTANT Cards - one card per reactant for each reaction		
1) Reaction number	I2	1-2
2) The word 'REACTANT'	2A4	3-10
3) Atomic symbols and formula numbers (Maximum of 4 sets)	4(A2,F3.0)	11-30
4) Phase: S, L or G for solid, liquid or Gas	A1	31
5) Stoichiometric coefficient	F9.4	32-40
6) The code 'B' if the 'base' reactant or blank otherwise	A1	41
7) Relative number of moles entering reactor, L_i (Maximum of 4 values)	4F8.3	42-73
PRODUCT Cards - one card per product for each reaction		
1) Reaction number	I2	1-2
2) The word 'PRODUCT'	2A4	3-9
3) Atomic symbols and formula numbers	4(A2,F3.0)	11-30
4) Phase: S, L or G	A1	31
5) Stoichiometric coefficient	F9.4	32-40
6) Temperatures of phase changes (Max. of 4) in ascending order	4F8.3	42-73

TABLE II

NAMELIST (NAM1) Variables

Variable	Dimension	Type	Comments
STEP	1	I	the number of the chemical reaction
T	10	R	temperature of the reaction in each temperature schedule (degrees Kelvin)
EP	10,4	R	extent of reaction at equilibrium for each temperature (first subscript) and each set of ratios of reactants (second subscript)
PRES	1	R	Pressure (atmospheres)
DRAW	1	L	DRAW = T causes heating and cooling steps to be set up. Default value is FALSE
SAME	1	L	SAME = T means that the compounds used are the same as those of the preceeding cycle and no new Thermo Data is needed. Default value is FALSE
H298	1	L	H298 = T calls for ΔH° , ΔS° , and ΔG° to be calculated at 298°K for all chemical reactions. Default value is FALSE
EFF	1	R	The efficiency for conversion of heat to work if other than 0.3.

TABLE III

NOTES Cards

Maximum number of cards for each reaction is five

Variable	Format	Columns
Number of Comment Card for this Reaction (Max. if 5)	I2	1-2
Reaction Number	I2	3-4
Comments	19A4	5-80

TABLE IV

Order and Format of THERMO Data Cards

Card Order	Contents	Format	Card Column
1	Temperature ranges for 2 sets of coefficients: lowest temperature (300K), common temperature (1000K), and highest temperature (5000K)	3F10.3	1 to 30
2	Species name	3A4	1 to 12
	Date and Reference Source	2A3	19 to 24
	Atomic symbols and formula	4(A2,F3.0)	25 to 44
	Phase of species (S, L, or G for solid, liquid or gas, respectively)	A1	45
	Temperature range of original source	2F10.3	46 to 65
	Integer 1	I15	80
3	Coefficients a_i ($i = 1$ to 5) in equations 32 to 35 (for upper temperature range)	5(E15.8)	1 to 75
	Integer 2	I5	80
4	Coefficients in equations 32 to 35 (a_6, a_7 for upper temperature interval and a_1, a_2, a_3 for lower)	5(E15.8)	1 to 75
	Integer 3	I5	80
5	Coefficients in equations 32 to 35 (a_4, a_5, a_6, a_7 for lower temperature interval)	4(E15.8)	1 to 60
	Integer 4	I20	80
(a)	Repeat cards numbered 1 to 4 in CC80 for each species		
(Final Card)	END	3A4	1 to 3

(a) The data sets for the different phases of the same species must be adjacent with the condensed phases, in ascending order of their temperature ranges, coming first and the gas phase being last.

The data are written on the tape with the same formats as the above cards except that the card numbers in column 80 are omitted.

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