CALCULATED CHEMICAL REACTION EQUILIBRIUM FOR THE CLAUS PROCESS

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Dedicated to my Father

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PREFACE

Calculating chemical reaction equilibrium by the free energy minimization method is convenient especially for multi-component multi-reaction systems. A computer program based on this method was obtained, tested, and modified. The program was used to study the thermodynamic, equilibrium and efficiency of the Claus process which is commonly used for converting hydrogen sulfide in acid gases to sulfur. The study considered all possible reaction products including the eight sulfur polymers that were generally neglected in previous studies. Several variables that might influence sulfur recovery in a Claus plant were examined. In addition to considering sulfur recovery the concentrations of sulfur containing components in the plant tail gas were determined.

I am gratefully indebted to my adviser, Dr. R. N. Maddox, for his help and guidance during the course of my doctoral program. I am also thankful to the members of my Advisory Committee, Dr. J. H. Erbar, Dr. G. J. Mains, and Dr. J. R. Norton, for their suggestions and help. The help provided by all faculty and staff of the School of Chemical Engineering is also acknowledged.

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NOMENCLATURE

English Letters

a_{ij} - stoichiometric coefficients, g-atoms of element i per g-mole of species j, $(\text{g-atom})_i/(\text{g-mole})_j$

$a_{i(i=1\text{ to }7)}$ - least square coefficients

B_i - g-atoms of element i in the mixture

B_i^o - assigned g-atoms of element i in total reactant

b_i - g-atoms of element i per gram of mixture

b_i^o - assigned g-atoms of element i per gram of total reactant

$(C_p^o)_j$ - standard state constant pressure specific heat for species or reactant j, cal/g-mole ^oK

%F - percent of total fuel in total reactant by weight (or mass)

$\hat{f}_j$ - fugacity of species j in mixture, atm

f_j^o - standard state fugacity of species j, atm

$\bar{f}$ - composition, temperature and Lagrange multiplier vector function

G - Gibbs free energy of mixture, cal/g

G^t - total Gibbs free energy of mixture, cal

ΔG^o - standard Gibbs free energy change, cal/g-mole

ΔG^{o}_{fj} - standard Gibbs free energy of formation for species j, cal/g-mole

$(H^{o}_{T})_{j}$ - standard state enthalpy for species j, cal/g-mole

$(\Delta H^{o}_{f})_{T}$ - heat of formation at temperature T, cal/g-mole

h - enthalpy of mixture, cal/g

h_{o} - enthalpy of total reactants, cal/g

$J(\overline{X})$ - Jacobian matrix $(\frac{\partial \overline{f}}{\partial \overline{X}})$

K - chemical reaction equilibrium constant

M - molecular weight of mixture, g/g-mole

M_{j} - molecular weight of species j, g/g-mole

N_{j} - g-moles of species j in mixture

n - g-moles per gram of mixture, g-mole/g

n_{j} - g-moles of species j per gram of mixture, g-mole/g

o/f - oxidant to fuel weight (or mass) ratio

P - pressure, atm

P_{j} - partial pressure of species j, atm

R - universal gas constant, 1.987 cal/g-mole ^{o}K

S_{j} - entropy of species j, cal/g-mole ^{o}K

$(S^{o}_{T})_{j}$ - standard state entropy for species j, cal/g-mole ^{o}K

T - temperature, ^{o}K

V - volume, cm^{3}/g-mole

$\overline{X}$ - composition, temperature and Lagrange multiplier vector variable

y_{j} - mole fraction of species j in a gas phase

Greek Letters

∂ - partial derivative

Δ - finite difference, final-initial value

λ_i - Lagrangian multiplier for chemical element i, cal/g-atom

μ_j - chemical potential of species j, cal/g-mole

μ_j^o - standard state chemical potential for species j, cal/g-mole

π_i - Lagrangian multiplier of chemical element i, λ_i/RT, g-mole/g-atom

ρ - density, g/cm^3

$\hat{\phi}_j$ - fugacity coefficient of species j = $\hat{f}_j/y_j$

Subscripts

i - chemical element

j - chemical species

k - iteration K

o - an assigned or initial condition

Indices

ℓ - number of chemical elements

m - number of possible gaseous species

n - number of possible species, gases and condensed

CHAPTER I

INTRODUCTION

Whenever a chemical reaction is allowed to take place, whether on paper or in a full-scale plant, chemists and chemical engineers desire to know the composition of the product that is expected at thermodynamic equilibrium. The equilibrium yield represents the maximum yield obtainable under specified reaction conditions of temperature and pressure. Knowledge of the yield can help process designers and plant operators adjust reaction conditions or use catalysts to maximize production of desired products and eliminate or reduce undesired side reactions.

To many persons chemical equilibrium is characterized by a single equilibrium constant which allows equilibrium compositions to be easily calculated. A simple example is the reaction between molecular and atomic hydrogen,

$$\frac{1}{2} H_2 \rightleftharpoons H \quad . \tag{1-1}$$

The reaction equilibrium constant is related to thermodynamic data and partial pressures by the following equation:

$$K = e^{-\Delta G^{o}/RT} = \frac{P_H}{\left(P_{H_2}\right)^{1/2}} \tag{1-2}$$

From Equation (1-2) and the ideal gas law the composition of the gas can easily be determined at any temperature and pressure. In some cases two or three reactions proceed simultaneously and two or three non-linear equations similar to Equation (1-2) have to be solved simultaneously for product composition.

The need for accurate composition data, therefore solution of many simultaneous reaction equations, became apparent as people began to study chemical processes at extreme temperatures and pressures and as environmental regulations became more strict. In combustion problems such as the Claus process furnace, where the hydrogen sulfide rich gas is burned with air, more than twenty-five reactions can take place simultaneously involving as many as fifty chemical species. Nearly all of these reactions have to be considered for accurate composition data because we are not only interested in the concentrations of the dominant species but also in the minor species present in the ppm range as well. Clearly a digital computer is necessary to carry out the calculations for such large systems.

There are basically two methods for calculating chemical equilibrium compositions for multi-reaction systems. The first is the equilibrium constant method, and the second is the free energy minimization method. Both methods are based on the same principle for the condition of chemical equilibrium; that is, minimum free energy. The principle can be expressed mathematically as:

$$\left(dG^t\right)_{T,P} = 0 \qquad (1\text{-}3)$$

The meaning of Equation (1-3) is that the equilibrium state of a closed system at constant temperature and pressure is that state for which the total Gibbs free energy is a minimum with respect to all possible variations in composition. Depending on the details of how Equation (1-3) is developed, the end result will be either the equilibrium constant method or the free energy minimization method (41).

The equilibrium constant method has been in use for many years and is the one usually described in thermodynamic textbooks (4, 36). In this method selected independent overall reactions are written and their equilibrium constants determined. The chemical species involved in these reactions are usually called key components in order to distinguish them from other species which are present in the reaction system, but neglected. Expressions such as Equation (1-2) are written for these key reactions, and are solved simultaneously by algebraic reduction or some other numerical technique (41). The equilibrium reaction equations are usually non-linear and their number and complexity increases as the number of species in a reaction increases.

The disadvantages of a generalized equilibrium constant method are (25): a lot of bookkeeping; difficulties with component selection; numerical difficulties with compositions that become extremely small; difficulties in testing for the presence of some condensed species; difficulties in extending the generalized method to non-ideal equations of state.

The above difficulties are less found in the free energy minimization method. According to Gibbs (10) at equilibrium the free energy of any system is at a minimum. This concept is illustrated in Figure 1 where the free energy of the mixture of H_2 and H in reaction (1-1) at 3000^oK and 1 atm is plotted against the partial pressure of H_2. The minimum free energy occurs at $P_{H_2} = 0.855$ which is exactly the value obtained by the equilibrium constant method, Equation (1-2). However, this example is trivial and the picture becomes more complicated as the number of reactions increases. Here the free energy minimization method becomes very helpful. With this method individual equilibria are not considered, as such. Rather, the possible product species are indicated and the distribution of these species is determined using a completely general mathematical technique to give a minimum free energy for the system. The mathematical procedure usually requires no prior knowledge of the chemistry of the system nor does it require accurate initial guesses. What it requires is a specification of the reaction conditions (say temperature and pressure), the initial elemental composition, and the product species. From this information the equilibrium composition can be calculated.

A versatile computer program was developed by NASA (14) to calculate complex chemical equilibrium compositions by the free energy minimization method. The program contains its own thermodynamic data file.

One of the objectives of this work is to examine and test the free energy minimization technique with several simple reactions and compare the results against those obtained by the equilibrium con-

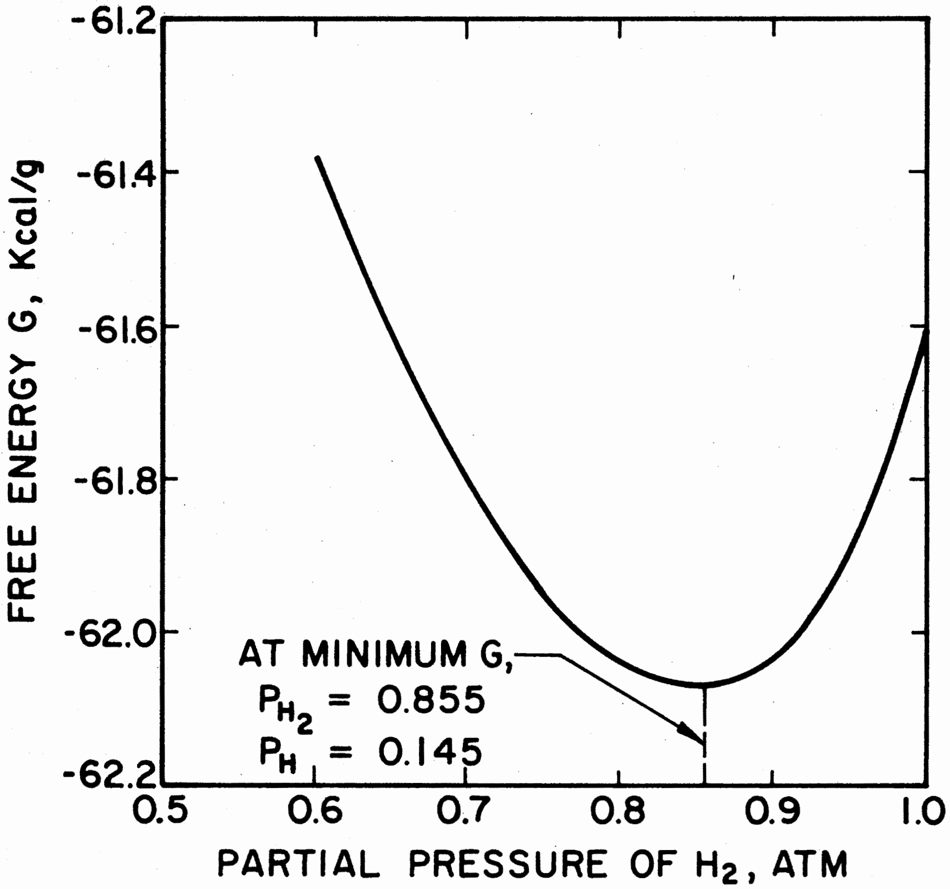

Figure 1. Example of Minimum Free Energy as Criterion for Equilibrium; Mixture of H_2 and H at T = 3000°K and P=1 Atmosphere (25)

stant method or reported in the literature. The NASA computer program was obtained and modified for this purpose. Once the results of the program were satisfactory, it was used to study the Claus process. This process is very widely used for the conversion of hydrogen sulfide in natural gas streams to sulfur. The Claus process is important economically for the production of sulfur and environmentally for the reduction of the concentrations of air polluting sulfur compounds in effluent gases released to the atmosphere. Due mostly to the latter, efforts are continuously being made to improve the efficiency of the process. However almost all of the published research is based on old thermodynamic data and on selected reactions. Also, some of the assumptions usually made with regard to the sulfur vapor composition are not quite accurate.

The objective here is to examine calculationally the equilibrium and the efficiency of the Claus process using the latest published thermodynamic properties of the sulfur compounds. The effects of impurities in the acid gases, such as carbon dioxide, water, hydrocarbons, and ammonia, on the efficiency of hydrogen sulfide conversion and recovery and on the tail gas composition is to be studied. Several other Claus process parameters are to be examined. These studies would have been extremely difficult to conduct without the powerful free energy minimization technique.

CHAPTER II

LITERATURE REVIEW

Computation of Chemical Equilibrium by Free Energy Minimization

Prior to 1958 all chemical equilibrium calculations were carried out using the equilibrium constant procedure. Key components and reactions in the system were usually selected and their non-linear governing equations were solved simultaneously in closed forms or using numerical approximation. In 1958 White, Johnson, and Dantzig (40) suggested that equilibrium compositions be calculated by the free energy minimization technique. Soon their method attracted many of the people making thermodynamic calculations, especially calculations for multi-reaction systems. The development of large core digital computers and their availability to do the tedious numerical calculations was the main factor behind the success of the free energy minimization method. The method became the modern way of calculating equilibrium compositions. Oliver et al. (32) reviewed the classical equilibrium constant solution and explained the free energy minimization technique with a methane water reaction example taken from Dodge (6). They indicated that the equilibrium constant method relies on experience to reduce the number of reactions to a managable one to be solved by trial and error, simultaneous equations, etc. Thus the solution is not general and each reaction system will require reexamination and reevaluation. Erroneous results can occur if any of the important species or reactions are not included in the calculations.

Oliver et al. stated the advantages of the energy minimization method over the equilibrium constant method. These advantages include: capability to consider all possible product species without having to worry about individual reactions; generality of mathematical procedures; no necessary prior knowledge of the chemistry of the system.

An excellent review of the calculation of complex chemical equilibria was provided by Zeleznik and Gordon (41). They reviewed some of the pertinent thermodynamic principles and derived the equations that are used in the computation of chemical equilibria. They briefly discussed some of the calculating techniques that are available for solving the non-linear chemical equilibrium equations. The authors stated that, compared with other methods, the descent Newton method is the best method for calculating equilibrium composition and thermodynamic derivatives. The two methods for calculating chemical equilibrium compositions, free energy minimization method and equilibrium constant method, were compared in the article and some applications were discussed.

The book by Van Zeggeren and Storey (39) is considered a major contribution to the literature of the thermodyanmics of complex chemical equilibria because it provides a critical survey of the analytical techniques developed in many countries over the past quarter century.

Several computer programs have been written to calculate chemical equilibrium compositions utilizing the free energy minimization technique. Ma et al. (27) developed a computer program to compute complex equilibria compositions given fixed temperature, pressure, the amounts of the chemical elements, and the chemical potentials of possible chemical species at the pressure and temperature specified. A preliminary estimate of the compositions and the amounts of the various phases is obtained by direct minimization of Gibbs' function using a modified Naphtali (39) method. This estimate is then used to obtain an exact solution by application of the Newton-Raphson method (15) to the set of non-linear equations describing the equilibrium condition. The author states that the latter procedure was necessary because all of the direct minimization methods produce a truncation error which is intolerable.

Boyd et al. (2) developed a computer program to calculate equilibrium compositions in multicomponent, multiphase mixtures. The program converts the Gibbs free energy of the mixture into an unconstrained form, then minimizes using the Powell method. The program can handle up to three multicomponent phases and fifteen components, and it can handle adiabatic calculations.

The NASA program (14) was developed in 1967 and has undergone several improvements and modifications since then. It calculates equilibrium composition by minimizing free energy, and has been used to solve hundreds of problems. The program is developed for ideal gases but can handle condensed species up to several percent by weight.

In this case condensed species are assumed to occupy a negligible volume and exert a negligible pressure compared to the gaseous species. Detailed description of the program will be found in Chapter III and reference (14). This program contains its own thermodynamic data file and is able to calculate the various thermodynamic properties of the chemical species. In this work, the computer program was modified and tested by several examples. Also, the data file was expanded. Then it was used to study the equilibrium and efficiency of the Claus process for converting hydrogen sulfide in natural gas streams to sulfur.

Thermodynamic Fundamentals

The condition for equilibrium may be stated in terms of any of several thermodynamic functions such as the minimization of the Gibbs free energy or Helmholtz free energy or the maximization of entropy. If temperature and pressure are used to characterize a thermodynamic state then the Gibbs free energy is most easily minimized because temperature and pressure are its natural variables.

The total Gibbs free energy of a single phase (gas phase) for a mixture of n chemical species at a specified temperature and pressure is given by:

$$G^t = \sum_{j=1}^{n} N_j \mu_j \qquad (2\text{-}1)$$

The above function is to be minimized with respect to the number of moles of each species in the mixture (N_j) at constant temperature and pressure. This minimization is usually subject to certain constraints imposed by material balances which will be discussed later in this section. The chemical potential μ_j is given by:

$$\mu_j = \mu_j^o + RT \ln(\hat{f}_j/f_j^o) \tag{2-2}$$

and the fugacity $\hat{f}_j$ is related to the fugacity coefficient $\hat{\phi}_j$ by

$$\hat{f}_j = y_j\hat{\phi}_j P \tag{2-3}$$

The standard state for gas is taken as the hypothetical ideal-gas state of the pure gas at 1 (atm) pressure. If the system pressure is expressed in atmospheres then.

$$f_j^o = 1 \tag{2-4}$$

Also if μ_j^o is arbitrarily set equal to zero for all elements in their standard states, then for compounds

$$\mu_j^o = \Delta G_{fj}^o \ . \tag{2-5}$$

where ΔG_{fj}^o is the Gibbs free energy change for the standard formation reaction of species j.

Combination of the above five equations after rearrangement gives

$$\begin{aligned} G^t = \sum_{j=1}^{n} N_j \Delta G_{fj}^o + \left(\sum_j^n N_j\right) RT \ln P + RT\sum_j^n N_j \ln N_j \\ - RT\sum_j^n N_j \ln\left(\sum_j^n N_j\right) + RT\sum_j^n N_j \ln \hat{\phi}_j \end{aligned} \tag{2-6}$$

The y_j have been eliminated in favor of the mole numbers N_j. The problem now is to find the set (N_j) which minimizes G^t at constant T and P subject to the constraints of the material balances. The standard solution to this problem is through the method of Lagrange's undetermined multipliers. Constraints imposed by the mass balances should be incorporated in the expression for G^t.

In a chemically reacting system the molecular species are not conserved but the mass is. Let B_i^o be the number of atomic weights of the ith element present in the system as determined by the initial composition of the mixture. Let a_{ij} be the number of atoms of the ith element present in each molecule of chemical species j. Then for each element i,

$$\sum_{j=1}^{n} N_j a_{ij} = B_i^o \tag{2-7}$$

or

$$B_i - B_i^o = 0$$

where

$$B_i = \sum_{j=1}^{n} N_j a_{ij} \qquad i = 1, \ldots, \ell$$

Equation (2-7) is multiplied by an undetermined Lagrangian constant λ_i and the equation is then summed over all i giving:

$$\sum_{i=1}^{\ell} \lambda_i (B_i - B_i^o) = 0 \tag{2-8}$$

The above quantity is zero and can be added to Equation (2-6) to yield

$$G^t = \sum_{j=1}^{n} N_j \, \Delta G^o_{fj} + \sum_{j=1}^{n} N_j \quad RT\ell nP + RT \sum_{j=1}^{n} N_j \ell n \, N_j$$

$$- RT \sum_{j=1}^{n} N_j \ell n \sum_{j=1}^{n} N_j + RT \sum_{j=1}^{n} N_j \ell n \hat{\phi}_j + \sum_{i=1}^{\ell} \lambda_i (B_i - B_i^o) = 0 \qquad (2\text{-}9)$$

Differentiating the above equation and setting the derivative equal to zero to meet the equilibrium criterion

$$\left(\frac{\partial G^t}{\partial N_j}\right)_{T,P,N_{i \neq j}} = 0$$

we obtain

$$\Delta G^o_{fj} + RT\ell nP + RT\ell n y_j + RT\ell n\hat{\phi}_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} = 0 \qquad (2\text{-}10)$$

$$j = 1,\ldots,n$$

There are n such equations. In addition there are ℓ material balance equations of the form

$$\sum_{j=1}^{n} y_j a_{ij} = B_i^o / \sum_{j=1}^{n} N_j \qquad i,\ldots,\ell \qquad (2\text{-}11)$$

where ℓ is the number of elements present in the species which make up the system. Also, the y_j must satisfy

$$\sum_{j=1}^{n} y_j = 1 \quad . \qquad (2\text{-}12)$$

This provides a total of $n + \ell + 1$ equations. The unknowns in these equations are the y_j of which there are n, the λ_i of which there are

ℓ and the term $\sum_{j}^{n} N_j$ giving a total of $n + \ell + 1$ unknowns. Therefore, Equations (2-10), (2-11) and (2-12) can be solved for all the unknowns.

Equation (2-10) was derived assuming that all the $\hat{\phi}_j$'s are known. If the phase is an ideal gas, then each $\hat{\phi}_j$ is equal to unity and Equation (2-10) reduces to:

$$\Delta G^{o}_{fj} + RT\ell nP + RT\ell ny_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} = 0 \tag{2-13}$$

For real gases each $\hat{\phi}_j$ is a function of the various y_j which are to be calculated. Thus an iterative procedure is required which is initiated by setting the $\hat{\phi}_j$ equal to unity. Solution of the equations then provides a preliminary set of y_j. For cases of low pressures or high temperatures this result is usually adequate. When it is not, an equation of state is used together with the calculated y_j to give a new and more nearly correct set of $\hat{\phi}_j$ for use in Equation (2-10), and a new set of y_j is calculated. The process is repeated until successive iterations produce no significant change in the values of y_j.

As can be seen from the above derivation, with the energy minimization method, the question of what chemical reactions took place never enters directly into any of the equations. All we need do is specify the product species. The numerical solution of the above equations is discussed in detail in Chapter III.

The Claus Process

Process Features

The Claus process is commonly used for converting hydrogen sulfide in acid gases to sulfur and recovering the pure sulfur as a liquid. The basic reactions are:

$$H_2S + \frac{3}{2} O_2 \rightleftharpoons SO_2 + H_2O + \text{Heat} \qquad (2\text{-}14)$$

$$2H_2S + SO_2 \rightleftharpoons 3S + 2H_2O + \text{Heat} \qquad (2\text{-}15)$$

The process works well for gas streams containing greater than about 20% hydrogen sulfide. The feed acid gases are usually produced from gas sweetening plants which separate the hydrogen sulfide along with carbon dioxide from natural gas streams (11). The original Claus process was reported by Chance and Claus in 1885 (9). Since that time, it has undergone extensive investigation and major modification so there is little resemblance between the original process flow scheme and what is being used in industry today. Gamson and Elkins (8) presented an excellent review of the process history and development. They also reviewed in detail its thermodynamics, equilibrium and efficiency. More recent investigations and reviews of the Claus process are available in the literature (1,3,11,19-24,33).

Presently, variations of the process are used depending upon the H_2S content of the acid gas feed, investment cost, and other factors (34,38). The primary difference between these variations or designs is the manner in which heat balance is maintained in the process. Although the many design variations will not be discussed here, two basic flow schemes will be briefly described.

Figure 2 shows a typical "once-through" Claus plant flow scheme. This scheme is used when the H_2S concentration of the acid gas is high enough to produce a stable flame in the combustion zone of the furnace. The acid gas feed enters the reaction furnace and is burned with sufficient air that the H_2S/SO_2 ratio in the tail gas is 2 to 1. This is the theoretically optimum ratio for maximum sulfur conversion. The hot combustion products flow from the furnace to the waste heat boiler and the first condenser where they are cooled to about 422^oK. The heat is used to generate high and low pressure steam in the waste heat boiler and the condenser respectively. Condensed sulfur is withdrawn from the bottom of the first condenser. Most of the sulfur recovered in the Claus plant is formed in the combustion step. The cooled gases coming out of the first condenser are reheated before entering the first catalytic reactor. Reheating is necessary in order to keep the temperature in the reactor above the sulfur dew point because liquid sulfur will cause plugging and catalyst deactivation. In the reactor, H_2S and SO_2 react on a bauxite catalyst to form sulfur and water. The products of the reaction are cooled in the second condenser and liquid sulfur is removed. Cooled gases are then reheated and fed to the second reactor. Further conversion of H_2S to sulfur takes place in the second reactor and liquid sulfur is removed in the third condenser. In some cases there is a third or a fourth reactor but that is determined by process economics and type of tail gas clean-up process. The temperature of the liquid sulfur in the condensers must be maintained below 433^oK because the viscosity increases very rapidly above that temperature, and the sulfur becomes so thick and viscous that it is very difficult to remove (30).

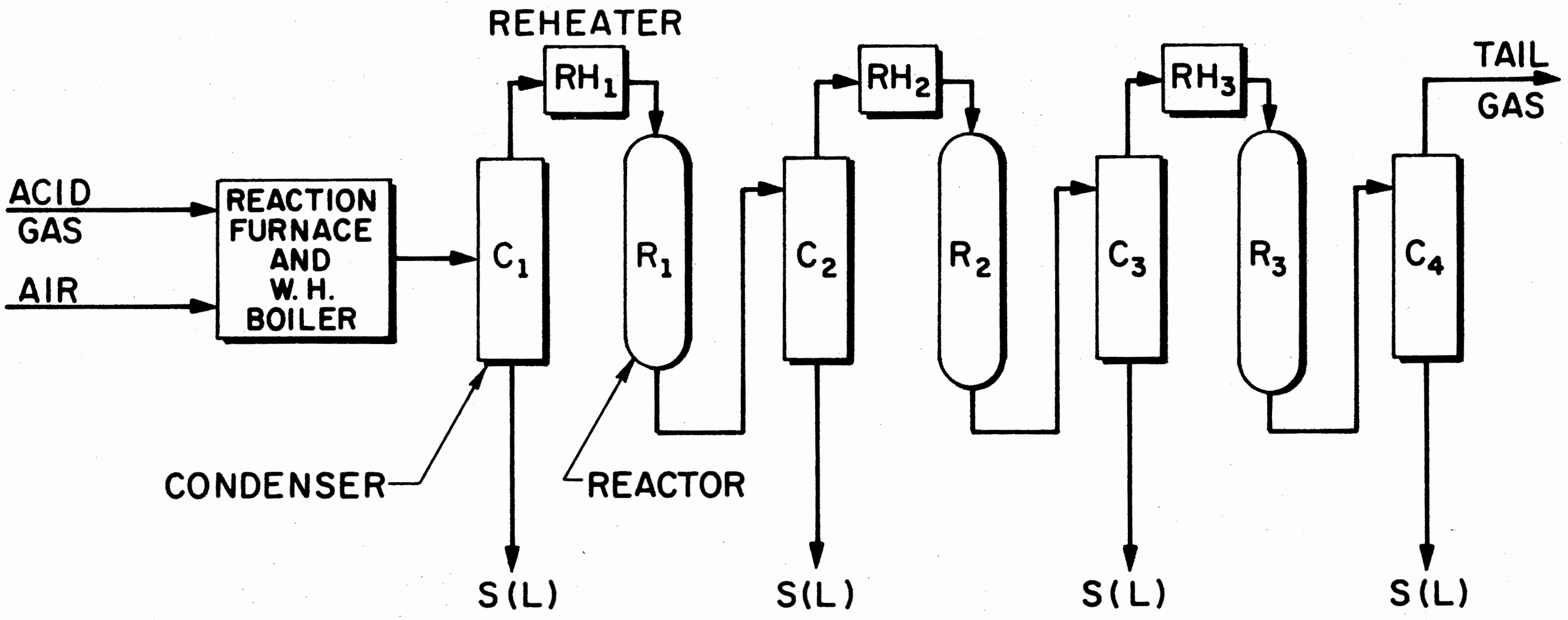

Figure 2. Claus "Once Through" Process Flow Scheme

If the acid gas entering the Claus plant is low in H_2S (below approximately 25%) then the "Split Flow" scheme shown in Figure 3 is employed. The reason for this arrangement is that there is not sufficient heat of reaction to raise the entire acid gas stream to satisfacotry temperature levels. Therefore, only about one third to two thirds of the acid gas enters the furnace for combustion. The combustion products, which usually contain little hydrogen sulfide, flow through the waste heat boiler as in the previous scheme. After that they are combined with the unburned portion of the acid gas feed to form a single stream with an H_2S/SO_2 content ratio of 2 to 1. This stream flows to the first catalytic reactor. The rest of the flow scheme in the "Split Flow" arrangement is similar to that of the "once through" process.

The preheating before the reactors is usually done by one of the following methods:

1. Hot gas by-pass, where a portion of partially cooled waste heat boiler effluent is diverted to mix with and heat the condenser outlet before entering the first reactor.
2. Auxiliary in-line burners, which burn a small side stream of acid gas with air to produce hot gases that are then mixed with the condenser effluent.
3. Gas-to-gas exchangers, where the condenser effluent is heated by exchanging heat in a heat exchanger with the outlet stream from the next reactor.
4. Indirect heat exchange with combustion product gases in the waste heat boiler.
5. Indirect heaters, using either fuel firing or steam heating.

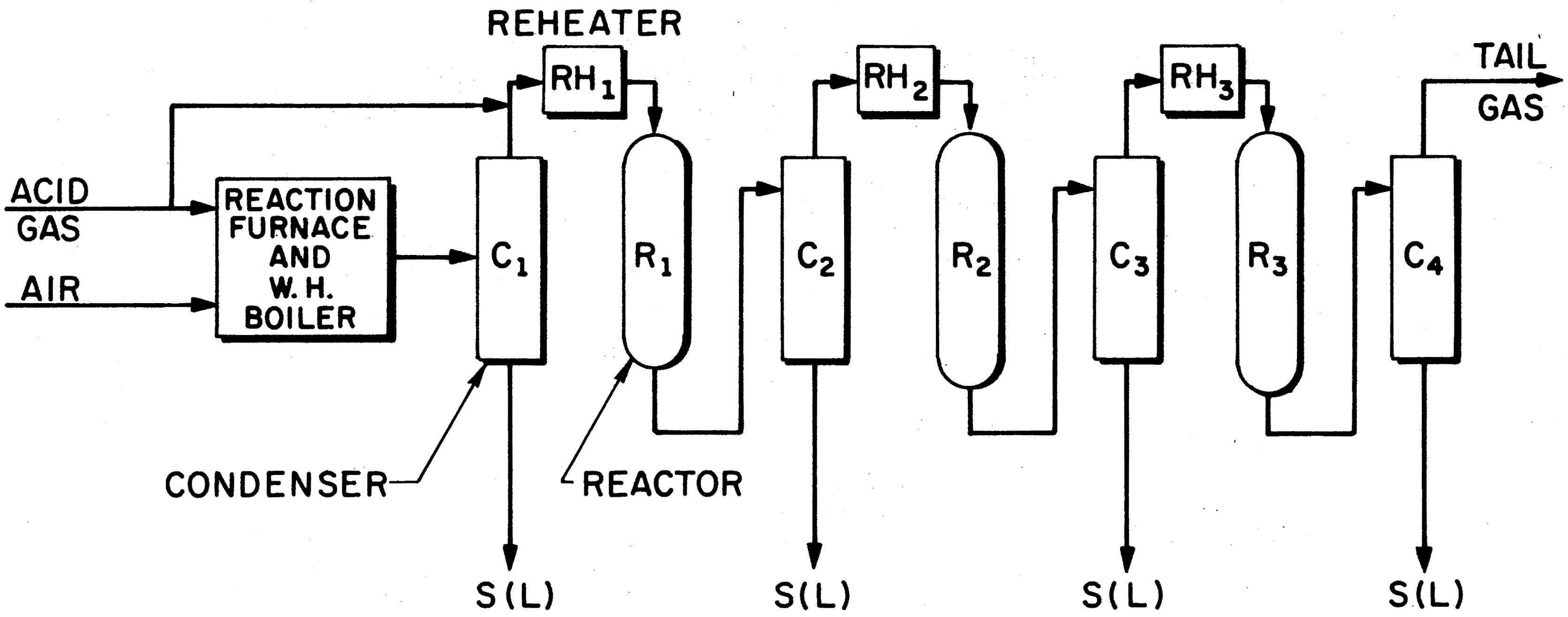

Figure 3. Claus "Split Flow" Process Flow Scheme

The above preheating methods are listed in general order of increasing cost and in general order of increasing overall sulfur conversion efficiency (12).

There are many design and operating considerations for the Claus process discussed in the literature (34,38). Goar (12) listed the major variables and criteria to be considered as:

1. Composition of acid-gas feed.
2. Combustion of acid gas.
3. For a once-through scheme, retention time of combustion gases at elevated temperatures.
4. Catalytic-reactors feed-gas temperature.
5. Optimum reheat scheme(s)
6. Space velocity in reactors.
7. Sulfur condensing temperatures.
8. Coalescing and separation of entrained sulfur from condenser effluent gases.
9. Turndown of plant throughput.

The three major process control variables in a Claus plant are (11):

1. H_2S to SO_2 ratio which must be maintained at 2 to 1.
2. Catalytic reactors inlet temperatures to avoid either excess or low temperatures in the reactors.
3. Sulfur condenser outlet temperatures to maintain low viscosity of liquid sulfur.

Claus Reactions

The Claus reaction is deceptively simple (28). The overall reaction is:

$$3H_2S + \frac{3}{2} O_2 \rightleftharpoons 3S + 3H_2O. \qquad (2\text{-}16)$$

Reaction (2-16) is normally written to take place in two steps. First a portion of the hydrogen sulfide is burned with a limiting supply of air in the Claus furnace to produce sulfur dioxide and water

$$H_2S + \frac{3}{2} O_2 \rightleftharpoons SO_2 + H_2O + \text{Heat}. \qquad (2\text{-}14)$$

The second step is a combination of the sulfur dioxide and hydrogen sulfide in the catalytic reactor to produce sulfur

$$2H_2S + SO_2 \rightleftharpoons 3S + 2H_2O + \text{Heat}. \qquad (2\text{-}15)$$

The heat given off by reactions (2-14) and (2-15) is -124 kcal/gmole H_2S and -35 kcal/gmole SO_2, respectively yielding a total of -159 kcal/g mole H_2S for reaction (2-16), (7).

If reactions (2-14) and (2-15) were the only reactions taking place, the Claus process would be a simple one from which to predict yields and/or sulfur production. There are, however, many side reactions that can occur. Hyne (16) has listed some of the possible reactions that might occur in the combustion zone of a Claus sulfur process. His suggested reactions are summarized in Table I.

The presence of impurities in the acid gas multiplies the number of possible reactions that can occur. Some possible side reactions involving hydrocarbons and carbon dioxide are shown in Table II.

In addition to the multiplicity of chemical reactions that may occur in the Claus process, there is a variety of forms in which sulfur vapor or liquid can exist. The reactions for formation of these different sulfur species, based on S_2, are:

TABLE I

SOME FURNACE REACTIONS

$$H_2S + O_2 \longrightarrow HO_2 + HS$$

$$H_2S \longrightarrow HS + H$$

$$H + H_2S \longrightarrow HS + H_2$$

$$HS + O_2 \longrightarrow SO + OH$$

$$OH + H_2S \longrightarrow H_2O + HS$$

$$OH + HO_2 \longrightarrow H_2O + O_2$$

$$SO + O_2 \longrightarrow SO_2 + O$$

$$O + H_2S \longrightarrow OH + SH$$

$$SO + O \longrightarrow SO_2^* \longrightarrow SO_2 + h\nu$$

$$SO + SO \longrightarrow S_2O_2$$

$$HS + HS \longrightarrow H_2 + S_2$$

$$HS + HO \longrightarrow H_2O + S$$

$$S + O \longrightarrow SO$$

$$S + S \longrightarrow S_2$$

$$SO_2 + O + M \longrightarrow SO_3 + M$$

$$SO + O_2 + M \longrightarrow SO_3 + M$$

$$SO_3 + H_2 \longrightarrow SO_2 + H_2O$$

TABLE II

SOME POSSIBLE SIDE REACTIONS IN THE CLAUS FURNACE AND REACTORS

$$\text{Hydrocarbons} \longrightarrow CO_2,\ CO,\ H_2O,\ H_2$$

$$CO_2 + H_2S \rightleftharpoons COS + H_2O$$

$$CH_4 + SO_2 \rightleftharpoons COS + H_2O + H_2$$

$$CO_2 + SO_2 \rightleftharpoons COS + \frac{3}{2}O_2$$

$$CO + S \rightleftharpoons COS$$

$$CH_4 + 2S_2 \rightleftharpoons CS_2 + 2H_2S$$

$$2CO + S_2 \rightleftharpoons CS_2 + CO_2$$

$$\frac{3}{2} S_2 \rightleftharpoons S_3 \qquad (2\text{-}17)$$

$$2 S_2 \rightleftharpoons S_4 \qquad (2\text{-}18)$$

$$\frac{5}{2} S_2 \rightleftharpoons S_5 \qquad (2\text{-}19)$$

$$3 S_2 \rightleftharpoons S_6 \qquad (2\text{-}20)$$

$$\frac{7}{2} S_2 \rightleftharpoons S_7 \qquad (2\text{-}21)$$

$$4 S_2 \rightleftharpoons S_8 \qquad (2\text{-}22)$$

All of the foregoing greatly complicates the procedure for estimating sulfur recoveries from Claus sulfur plants. Originally hand or desk calculations considered only reactions (2-14) and (2-15) in combination with sulfur species S_2, S_6, and S_8. Gamson and Elkins (8) presented a scheme for calculating the equilibrium composition based on the equilibrium constants for these reactions.

Other, more recent, investigators (1,7,33) used the computer to calculate equilibrium compostions but their calculations were based on selected reactions and did not include all species known to be present at equilibrium. Reasonably accurate predictions of sulfur recovery can be made by such procedures. However, major variations in tail gas composition frequently result.

Carbonyl sulfide and carbon disulfide, whose formation reactions are shown in Table II, are of particular importance to Claus plant operators and designers. These compounds seem not to be affected by present Claus catalysts and wind up either depositing on the catalyst surface and reducing its activity or passing through the process unchanged and adding to the total sulfur values in the tail gas.

Goar (13) used a proprietary computer program to study the affects of impurities in the feed acid gases on the Claus process efficiency and tail gas composition. However, his calculations were also based on selected reactions and did not include all species present in the furnace or the reactors. His general conclusions were that the presence of impurities reduced the conversion, raised the operating and equipment costs for Claus plants, and increased the costs for the tail gas desulfurization plants.

CHAPTER III

THE FREE ENERGY MINIMIZATION PROGRAM

The free energy minimization computer program used in this study was developed by NASA (14). Program equations and numerical techniques as well as tests and modifications that were made during this work will be examined in this chapter.

Equations Describing Chemical Equilibrium

Fundamental Equations

All gases are assumed to be ideal and interactions between phases are assumed to be negligible. The equation of state for the mixture is

$$\left.\begin{aligned} PV &= nRT \\ &\text{or} \\ \frac{P}{\rho} &= nRT \end{aligned}\right\} \tag{3-1}$$

The above equation is assumed to be correct even when small amounts of condensed species (up to several percent by weight) are present. In this case, the condensed species are assumed to occupy negligible volume and exert negligible pressure compared to the gaseous species. In Equation (3-1) the volume and moles refer to gases only while the mass is for the entire mixture including condensed species. The term "mixture" will be used in this chapter to refer to mixtures of species as distinguished from mixtures of reactants which will be referred to as "total reactants."

The molecular weight of the mixture is defined as:

$$M = \frac{\sum_{j=1}^{n} n_j M_j}{\sum_{j=1}^{m} n_j} = \frac{1}{n} \qquad (3\text{-}2)$$

where:

$$n = \sum_{j=1}^{m} n_j \qquad (3\text{-}3)$$

Among the n possible species which may be considered in a mixture, gases are indexed from 1 to m and condensed species from m+1 to n.

Based on the above assumptions, the chemical potential can be written as:

$$\mu_j = \begin{cases} \mu_j^o + RT\,\ell n\left(\frac{n_j}{n}\right) + RT\,\ell n\,P_{atm} & j=1,\ldots,m \\ \mu_j^o & j=m+1,\ldots,n \end{cases} \qquad (3\text{-}4)$$

where μ_j^o is the chemical potential of species j in the standard state. For a gas, the standard state is the ideal gas at unit fugacity. For a pure liquid or solid, the standard state is the substance in the condensed phase under a pressure of one atmosphere. Generally, the numerical values of μ_j^o found in the literature (17) depend partly on a term involving units of atmospheres. Therefore, to be consistent, pressure P_{atm} in Equation (3-4) must be in units of atmospheres.

The necessary equations for calculating equilibrium compositions by free energy minimization were derived in Chapter II. They are Equations (2-10), (2-11), and (2-12). Rewriting the first two equations to be per unit weight of mixture, we obtain:

$$\mu_j + \sum_{i=1}^{\ell} \lambda_i a_{ij} = 0 \qquad j=1,\ldots,n \tag{3-5}$$

$$\sum_{j=1}^{n} n_j a_{ij} - b_i^o = 0 \qquad i=1,\ldots,\ell \tag{3-6}$$

If the thermodynamic state of the mixture is specified by an assigned temperature and pressure, then we have the additional pair of trivial equations

$$T = T_o \tag{3-7}$$

$$P = P_o \quad . \tag{3-8}$$

The above four equations permit determination of the equilibrium composition.

For the case of constant pressure combustion the thermodynamic state is specified by Equation (3-8) and by

$$h = h_o \tag{3-9}$$

instead of Equation (3-7). Here, h is the enthalpy of the mixture and h_o is a constant equal to the enthalpy of the total reactants. The expression for h is

$$h = \sum_{j=1}^{n} n_j (H_T^o)_j \tag{3-10}$$

The equations required to obtain equilibrium compositions are not all linear in the composition variables and, therefore, an iteration procedure is generally required. The iteration technique and the Gibbs iteration equations will be discussed next.

Iteration Technique

The Newton-Raphson method is probably the most popular (and is certainly the best known) method of finding numerical roots for a set of non-linear equations. In this method the finite-difference approximation to the total differential serves as the basis for the iteration procedure. The method will be illustrated by a simple example before going to the free energy equations.

Let f_1 and f_2 be two non-linear functions of x and y such that

$$\left.\begin{aligned} f_1 &= f_1(x,y) = 0 \\ f_2 &= f_2(x,y) = 0 \end{aligned}\right\} \tag{3-11}$$

and let their simultaneous solution be x_o and y_o. For any other values of x and y, say x_K and y_K

$$\left.\begin{aligned} f_1(x_K,y_K) &\neq f_1(x_o,y_o) \\ f_2(x_K,y_K) &\neq f_2(x_o,y_o) \end{aligned}\right\} \tag{3-12}$$

or

$$\begin{aligned} \Delta f_1 &= f_1(x_o,y_o) - f_1(x_K,y_K) \\ \Delta f_2 &= f_2(x_o,y_o) - f_2(x_K,y_K) \end{aligned} \qquad (3\text{-}13)$$

Assuming that f_1 and f_2 are differentiable, the total differentials of (3-11) are

$$\begin{aligned} df_1 &= \frac{\partial f_1}{\partial x}\, dx + \frac{\partial f_1}{\partial y}\, dy \\ df_2 &= \frac{\partial f_2}{\partial x}\, dx + \frac{\partial f_2}{\partial y}\, dy \end{aligned} \qquad (3\text{-}14)$$

The finite difference forms of these equations are:

$$\begin{aligned} \Delta f_1 &= \left(\frac{\partial f_1}{\partial x}\right)\Delta x + \left(\frac{\partial f_1}{\partial y}\right)\Delta y \\ \Delta f_2 &= \left(\frac{\partial f_2}{\partial x}\right)\Delta x + \left(\frac{\partial f_2}{\partial y}\right)\Delta y \end{aligned} \qquad (3\text{-}15)$$

If the difference terms Δf_1 and Δf_2 and the analytic expression for the partial derivatives are evaluated numerically at the point x_K, y_K, the correction variables Δx and Δy can be determined, since Equation (3-15) is a simultaneous linear set of equations in the correction variables. Equation (3-15) is not exact, therefore:

$$\begin{aligned} x_{K+1} &= (x_K + \Delta x) \neq x_o \\ y_{K+1} &= (y_K + \Delta y) \neq y_o \end{aligned} \qquad (3\text{-}16)$$

But x_{K+1} and y_{K+1} will in general be a better approximation to x_o and y_o than x_K and y_K. The process of solving for corrections Δx and Δy is repeated until Δx and Δy (or Δf_1 and Δf_2) are sufficiently small.

The general Newton-Raphson iteration formula is

$$\bar{x}_{K+1} = \bar{x}_K - J^{-1}(\bar{x}_K)\bar{f}(\bar{x}_K) \tag{3-17}$$

The iteration is performed by truncating the Taylor expansion of $\bar{f}(x)$ after the first derivative.

Gibbs Iteration Equations

The Newton-Raphson method is used to solve for corrections to initial estimates of compositions n_j, Lagrange multipliers λ_i, moles n, and (when required) temperature T. The correction variables are $\Delta \ell n\ n_j (j=1,\ldots,m)$, $\Delta n_j\ (j=m+1,\ldots,n)$, $\Delta \ell n\ n$, $\pi_i = -\lambda_i/RT$ and $\Delta \ell n\ T$.

After making dimensionless those equations containing thermodynamic functions, the Newton-Raphson equations obtained from Equations (3-5), (3-6), (3-3), and (3-9) are:

$$\Delta \ell n\ n_j - \sum_{i=1}^{\ell} a_{ij}\pi_i - \Delta \ell n\ n - \left[\frac{(H_T^o)_j}{RT}\right]\Delta \ell n T = \frac{-\mu_j}{RT} \qquad j=1,\ldots,m \tag{3-18}$$

$$-\sum_{i=1}^{\ell} a_{ij}\pi_i - \left[\frac{(H_T^o)_j}{RT}\right]\Delta \ell n T = \frac{-\mu_j}{RT} \qquad j=m+1,\ldots,n \tag{3-19}$$

$$\sum_{j=1}^{m} a_{kj}\, n_j\, \Delta \ell n\, n_j + \sum_{j=m+1}^{n} a_{kj}\, \Delta n_j = b_k^o - b_k \qquad k=1,\ldots,\ell \tag{3-20}$$

$$\sum_{j=1}^{m} n_j\, \Delta \ell n\, n_j - n\, \Delta \ell n\, n = n - \sum_{j=1}^{m} n_j \tag{3-21}$$

$$\sum_{j=1}^{m} \left[\frac{n_j (H_T^o)_j}{RT} \right] \Delta \ell n\, n_j + \sum_{j=m+1}^{n} \left[\frac{(H_T^o)_j}{RT} \right] \Delta n_j + \left[\sum_{j=1}^{n} \frac{n_j (C_P^o)_j}{R} \right] \Delta \ell n T = \frac{h_o - h}{RT} \tag{3-22}$$

Equations (3-18) to (3-21) are used to obtain corrections to the estimates for problems with assigned thermodynamic state (T, P). Likewise Equations (3-18) to (3-22) are used with assigned thermodynamic state (H, P).

If a chemical system contains many species, then we would have to solve a large number of simultaneous equations. However, by a simple algebraic substitution this large number of equations can be greatly reduced. If we substitute the expression for $\Delta \ell n_j$ obtained from Equation (3-18) into Equations (3-20) to (3-21), and if Equation (3-19) is written with signs reversed, the resulting reduced equations are:

$$\sum_{i=1}^{\ell}\sum_{j=1}^{m} a_{kj}a_{ij}n_j\pi_i + \sum_{j=m+1}^{n} a_{kj}\Delta n_j + \sum_{j=1}^{m} a_{kj}n_j \, \Delta\ell n \; n \; +$$

(3-23)

$$\left[\sum_{j=1}^{m} \frac{a_{kj}n_j(H_T^o)_j}{RT}\right]\Delta\ell nT = (b_k^o - b_k) + \sum_{j=1}^{m}\frac{a_{kj}n_j\mu_j}{RT} \qquad (k=1,\ldots,\ell)$$

$$\sum_{i=1}^{\ell} a_{ij}\pi_i + \left[\frac{(H_T^o)_j}{RT}\right]\Delta\ell nT = \frac{\mu_j}{RT} \qquad (j=m+1,\ldots,n) \qquad (3\text{-}24)$$

$$\sum_{i=1}^{\ell}\sum_{j=1}^{m} a_{ij}n_j\pi_i + \left(\sum_{j=1}^{m} n_j - n\right)\Delta\ell n \; n + \left[\sum_{j=1}^{m}\frac{n_j(H_T^o)_j}{RT}\right]\Delta\ell nT =$$

$$n - \sum_{j=1}^{m} n_j + \sum_{j=1}^{m}\frac{n_j\mu_j}{RT} \qquad (3\text{-}25)$$

$$\sum_{i=1}^{\ell}\left[\sum_{j=1}^{m}\frac{a_{ij}n_j(H_T^o)_j}{RT}\right]\pi_i + \sum_{j=m+1}^{n}\left[\frac{(H_T^o)_j}{RT}\right]\Delta n_j \; +$$

$$\left[\sum_{j=1}^{m}\frac{n_j(H_T^o)_j}{RT}\right]\Delta\ell n \; n + \left[\sum_{j=1}^{n}\frac{n_j(C_P^o)_j}{R} + \sum_{j=1}^{m}\frac{n_j(H_T^o)_j^2}{R^2T^2}\right]\Delta\ell nT =$$

$$\frac{h_o - h}{RT} + \sum_{j=1}^{m}\frac{n_j(H_T^o)_j\mu_j}{R^2T^2} \qquad (3\text{-}26)$$

The above equations and others are listed in tabular form in reference (14).

A summary of the correction equations required for the two types of constant pressure problems of concern here are as follows (i=1 to ℓ, j=m+1 to n):

Type of Problem	Equations Required	Correction Variables
Assigned temperature and pressure (TP)	(3-23), (3-24), (3-25)	π_i, Δn_j, $\Delta \ell n\ n$
Assigned enthalpy and pressure (HP)	(3-23), (3-24), (3-25) (3-26)	π_i, Δn_j, $\Delta \ell n\ n$ $\Delta \ell n T$

After obtaining the above correction variables, the corrections for gaseous species $\Delta \ell n\ n_j$ (j=1,...,m) are obtained from Equation (3-18). In order to achieve convergence the size of the corrections must be controlled before they are applied. For convergence discussion, initial estimates procedures, and condensed phases problems the reader is referred to the literature (14).

Computer Program Description

Original Version

A computer program (Fortran IV) was developed by NASA to calculate complex chemical equilibrium compositions by the free energy minimization method. The program is based on the equations and assumptions that have been discussed in the previous section. It also contains a thermodynamic data file. A detailed description of the program and its use is provided by Gordon and McBride (14). Only a brief description will be given here.

The computer program is composed of a main program and sixteen subroutines. A subroutine tree diagram is shown in Figure 4. The program can be divided into five modules.

General Input Module. This module is controlled by the main program. The module sets up input required by all application modules. Input data include the following:

1. THERMO data. The main program reads the thermodynamic data cards for all species and writes the data on disk or tape. Subroutine SEARCH pulls the data for the appropriate species for a specified chemical system from disk or tape and stores the data in core.
2. REACTANTS cards. These cards are read and processed by subroutine REACT. There is one card for each reactant. The reactant card must give the chemical formula and the relative amount of the reactant in terms of moles, mole fraction, mass or mass fraction. For HP problems, an assigned enthalpy is required for any reactant that is not in THERMO data file and is totally consumed in the reaction.
3. INPT2 namelist data. The main program initializes the variables, reads and writes the problem designation and data such as T, P, o/f, and converts some of the data to the form required by the remainder of the program.
4. BLOCK DATA. These data are set and remain for the entire computer run. Data such as atomic weights of the chemical elements are stored here.
5. Composition Estimates. These estimates and associated variables are set for the first iteration for the first point only.

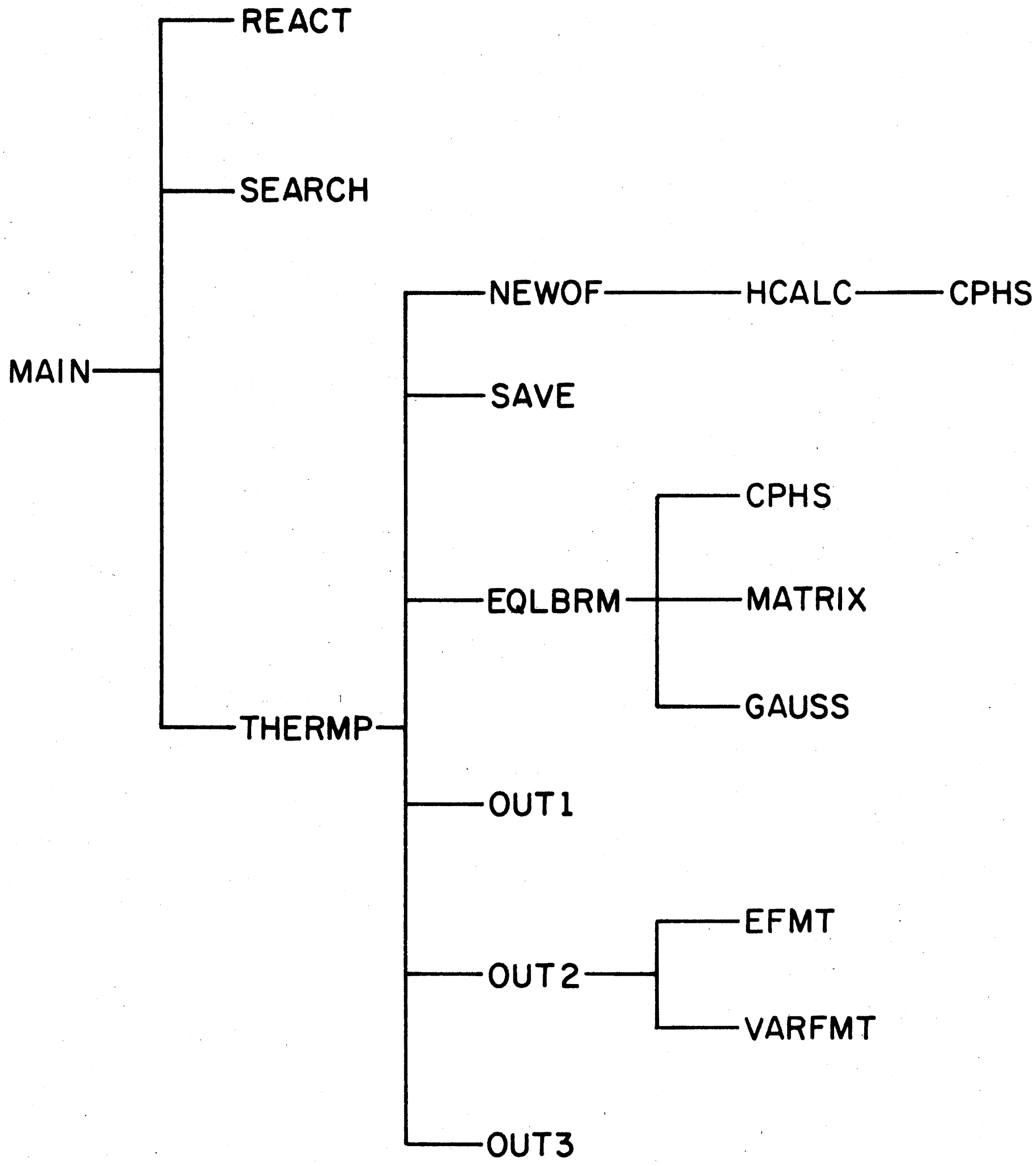

Figure 4. Subroutine Tree Diagram

Application Module. The application module is called from the main program according to the type of problem designated in namelist INPT2. Subroutine THERMP is the application module for TP and HP problems of interest in this study. The module controls the flow of the program until the problem is completed. Control is then returned to the main program where the next code card is read. The module is responsible for:

1. Reading any additional input for the particular problem.
2. Doing any calculation peculiar to the problem.
3. Calling routines in the additional input processing module as required.
4. Setting a point number NPT and setting certain variables required for the assigned thermodynamic states for that point if they have not already been set in the main program.
5. Calling the equilibrium module (subroutine EQLBRM).
6. Printing special output for the problem and calling the output module to print general output.

Equilibrium Module. The equilibrium module calculates thermodynamic properties and compositions at a given point NPT. This module is controlled by subroutine EQLBRM. Subroutine EQLBRM calls three subroutines:

1. CPHS to calculate thermodynamic functions of the individual species such as specific heat, enthalpy and entropy at a specified temperature and pressure.
2. MATRIX to set up the matrix according to the Gibbs iteration equations discussed earlier.
3. GAUSS to solve the set of simultaneous linear iteration

equations constructed by subroutine MATRIX. The solution is accomplished by performing a Gauss reduction using a modified pivot technique. In this modified pivot technique only rows are interchanged. The row to be used for the elimination of a variable is selected on the basis that the largest of its elements, after division by the leading element, must be smaller than the largest element of the other rows after division by their leading elements.

Additional Input Processing Module. This module consists of routines which are called for several purposes:

1. NEWOF is called by an application module to adjust values of b_i^o, ρ_o, and h_o/R for each oxidant to fuel ratio (o/f).
2. SAVE is called to save or move composition data from one point to another. The purpose is to use the calculated results from a previous point as initial estimates for the current point.
3. HCALC is called from NEWOF to calculate enthalpies for reactants if the enthalpy values are not indicated on the reactant cards.
4. CPHS is called by HCALC to calculate thermodynamic functions for an individual reactant using the THERMO data.

Output Module. The output module consists of the three subroutines VARFMT, EFMT, and OUT1 with two entries OUT2 and OUT3. OUT1 lists data given on the REACTANTS cards as well as o/f, %F, and ρ_o. OUT2 lists the properties P_{atm}, T, ρ(g/cc), h(cal/g), S(cal/(g)(k)), $(\partial \ell nV/\partial \ell nP)_T$, $(\partial \ell nV/\partial \ell nT)_p$, C_p(cal/(g)(k)). There is an option for listing these values in SI units. OUT3 lists equilibrium mole fractions of the reaction species. Subroutines VARFMT and EFMT are called from OUT2 and OUT3. VARFMT adjusts the number of decimal places in a variable format according to the size of the numbers. EFMT sets up a special E-type format for printing density and mole fractions.

Modified Version

The NASA computer program was written to calculate equilibrium composition for certain reactants at a thermodynamic state specified by constant temperature and pressure, constant enthalpy and pressure, constant entropy and pressure, constant temperature and volume, or constant entropy and volume. The program did not have any continuation capabilities, that is, it could not do a series of calculations based on the original reactants or feed. In order to conduct the Claus sulfur process studies, the program was modified to do all the process equilibrium calculations in one run. Starting with the acid gas and air feed to the furnace, the program calculates the adiabatic temperature and equilibrium composition then uses these compositions as the feed to the first condenser. It calculates the equilibrium composition in the condenser at a specified temperature and pressure. Also, the amount of liquid sulfur recovered in the condenser is calculated and removed from the gas stream before entering the first reheater. The reheater equilibrium composition is calculated at a specified temperature and pressure. The reheated gas then enters the first reactor which is assumed to operate adiabatically and at constant pressure. The reactor product equilibrium composition and temperature are determined. The program continues to repeat the calculations for any specified number of condensers, reheaters, and reactors. All possible product species with thermodynamic data in THERMO data file are considered in each stage.

However, the user has the option of omitting from consideration, putting as inert or as active any chemical species in the stream. The meaning of these and other code words that were added to the program are:

MOD OMIT - The listed species are omitted from consideration as product species.

MOD INERT - The listed species are not allowed to react, but are considered in all material and energy balance calculations.

MOD ACTIVE - The listed species are allowed to react after being treated as inert in the previous calculation point.

MOD REMOVE - The amounts of the listed species are to be removed from stream (remove liquid sulfur from gas stream).

Other modifications included changing some variable dimensions. The number of reactants and the total number of elements were increased to 25 each. The number of elements was increased in order to accomodate the MOD INERT features. The program can handle up to 150 species of which 15 can be declared inert.

The process feed composition indicated on the reactants cards can be in weight fraction or mole fraction. A sample listing of Input Cards for a Claus process calculation is given in Appendix A.

Although the modified program was mainly used for the Claus process study, it is completely general and can be used for studying any other process. A flow diagram of the new main program is shown in Figure 5.

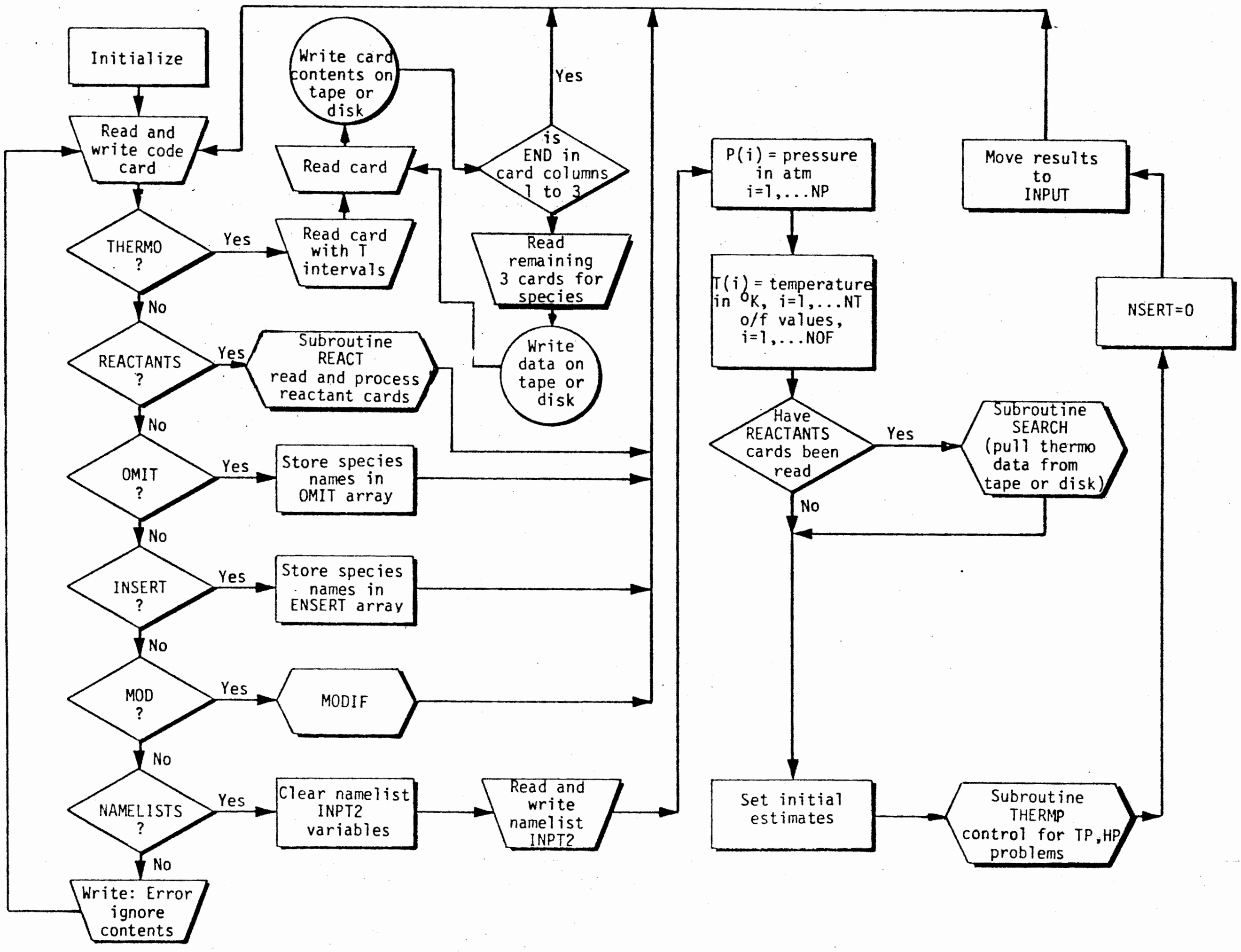

Figure 5. Flow Diagram for Main Program

Thermodynamic Data File

The library of thermodynamic (THERMO) data used in this study contains data for over 100 reaction species (solid, liquid, and gas phases of a species are counted as a separate species). Most of the data are taken from the JANAF tables (17) and from reference (14). The data literature source is indicated in file for each species. Literature sources of some species of interest in this study, such as the sulfur compounds, are indicated in Table III.

Least Squares Coefficients

For each reaction species, the specific heat, enthalpy, and entropy as functions of temperature are given in the form of least squares coefficients as follows:

$$\frac{C_P^o}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \tag{3-27}$$

$$\frac{H_T^o}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \tag{3-28}$$

$$\frac{S_T^o}{R} = a_1 \ell nT + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7 \tag{3-29}$$

For each species, two sets of coefficients are included in THERMO data file for two adjacent temperature intervals, 300^oK to 1000^oK and 1000^oK to 5000^oK. The data have been constrained to be equal at 1000^oK. Most of the coefficients a_1 to a_7 are taken directly from NASA literature (14). For the species listed in Table III, the thermodynamic functions are taken from the indicated references for reduction

TABLE III

THERMODYNAMIC PROPERTIES LITERATURE SOURCES

Chemical Species	Literature Sources
CH_2	17
CN_2	17
COS	17
C_2H_6	17
C_3H_8	37
$C_4H_{10}(n)$	37
$C_4H_{10}(i)$	37
$C_5H_{12}(n)$	37
$C_5H_{12}(i)$	37
HCO	17
HNCO	17
HNO	17
HNO_2	17
HNO_3	17
H_2S (liquid)	17
H_2S_2	29
HCO	17
NH	17
NO_3	17
OH	17
S	17
SO	17
S_2O	17
S_2	17,18
S_3	18,5
S_4	18,5
S_5	18,5
S_6	18,5
S_7	18,5
S_8	18,5

to coefficient form. The format and listing of coefficient data are given in THERMO data file Appendix F.

Assigned Enthalpies

For each species, heats of formation (and when applicable heats of transition) were combined with sensible heats to give assigned enthalpies H_T^o. By definition,

$$H_T^o = H_{298.15}^o + (H_T^o - H_{298.15}^o). \tag{3-30}$$

We have arbitrarily assumed that $H_{298.15}^o = (\Delta H_f^o)_{298.15}$. Equation (3-30) then becomes

$$H_T^o = (\Delta H_f^o)_{298.15} + (H_T^o - H_{298.15}^o). \tag{3-31}$$

In general, $H_T^o \neq (\Delta H_f^o)_T$ for $T \neq 298.15^oK$. For reference elements $(\Delta H_f^o)_{298.15} = H_{298.15}^o = 0$.

Assigned enthalpies of reactants are required for constant enthalpy and pressure problems. If the values are not indicated on the individual reactant cards, the program will automatically calculate them from THERMO data file at the inlet conditions using equation (3-28).

Program Evaluation

We have not been able to find in the literature any direct comparisons between chemical equilibrium compositions calculated by the free energy minimization method and those calculated by the equilibrium constant method or obtained by other techniques. Such comparisons are necessary to assess the accuracy and reliability of the free energy minimization basic equations and numerical computation. Several test cases were used for this purpose, and four of them are given here starting from a simple reaction system to a much more complex one.

Case 1.

Consider the water-gas shift reaction

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad (3\text{-}32)$$

Let the feed stream contain:

Component	Moles
CO	3
H_2O	1
CO_2	2
H_2	1

This is a non-equilibrium composition. Calculate the equilibrium composition at $T = 1000^{o}K$ and $P = 1$ atm assuming that the gases are ideal and no other species are formed.

The equilibrium composition calculated by the equilibrium constant method is reported in Perry's handbook (35). Table IV contains the literature composition and that calculated by the free energy minimization program. The free energy minimization results are very close to those reported in the literature. The slight differences are most probably due to minor differences in the thermodynamic data used.

TABLE IV

COMPARISON OF EQUILIBRIUM COMPOSITION FOR CASE 1

Species	Literature (35)	Computer Program	$\|\Delta y\|\%$
CO	0.391	0.39004	0.25
H_2O	0.106	0.10433	1.58
CO_2	0.323	0.32424	0.38
H_2	0.180	0.18139	0.77

Case 2

Assume that chemical equilibrium is established at one atmosphere and $1000^{o}K$ in a system containing CH_4, H_2O, CO, CO_2, and H_2. The initial charge is 2 moles of CH_4 and 3 moles of H_2O. What is the equilibrium composition?

The equilibrium composition determined by the free energy minimization program and that calculated by Smith and Van Ness (36) are compared in Table V. The agreement is satisfactory.

Case 3

Lees and Ryan (26) calculated the equilibrium composition variation with temperature for a sulfur plant feed using a free energy minimization procedure. No liquid sulfur was removed from the system. The equilibrium conversion of H_2S to sulfur vapor was calculated. The feed gas composition is:

Component	Mole Fraction
CH_4	0.032
CO_2	0.050
H_2S	0.232
N_2	0.507
O_2	0.179

Their results are shown as the solid lines in Figures 6 and 7. Figure 7 is an expanded scale showing the concentrations of the minor species.

TABLE V

COMPARISON OF EQUILIBRIUM COMPOSITION FOR CASE 2

Species	Literature (36)	Computer Program	$\|\Delta y\|\%$
CH_4	0.0199	0.0205	3.00
H_2O	0.0995	0.0991	0.40
CO	0.1753	0.1737	0.91
CO_2	0.0359	0.0371	3.34
H_2	0.6694	0.6696	0.03

The present free energy minimization program was used to calculate the composition and the conversion for this case, and the results are shown as points on the figures. Except for small differences in the S_8 and S_6 concentrations (Maximum about 5% at 300°F) the agreement

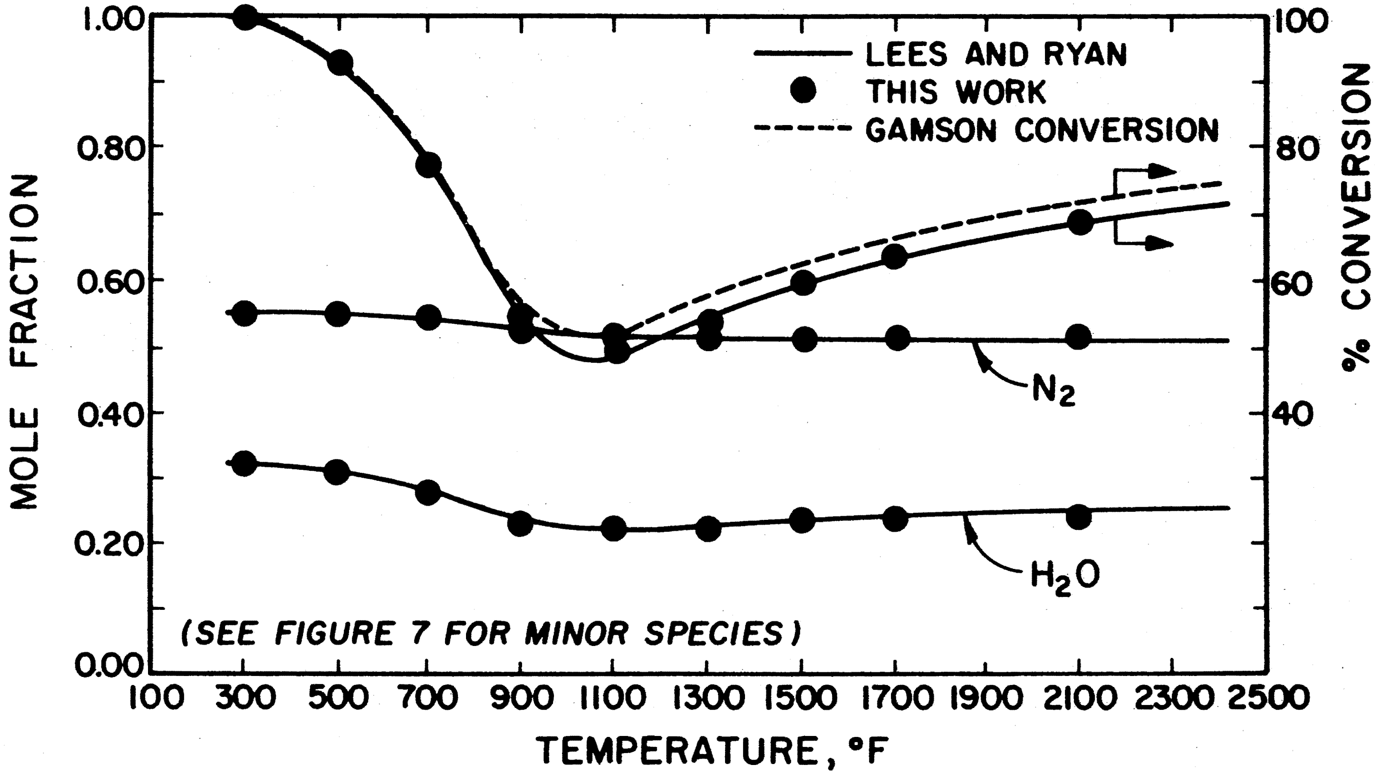

Figure 6. Equilibrium Composition and Conversion Variation with Temperature for Case 3

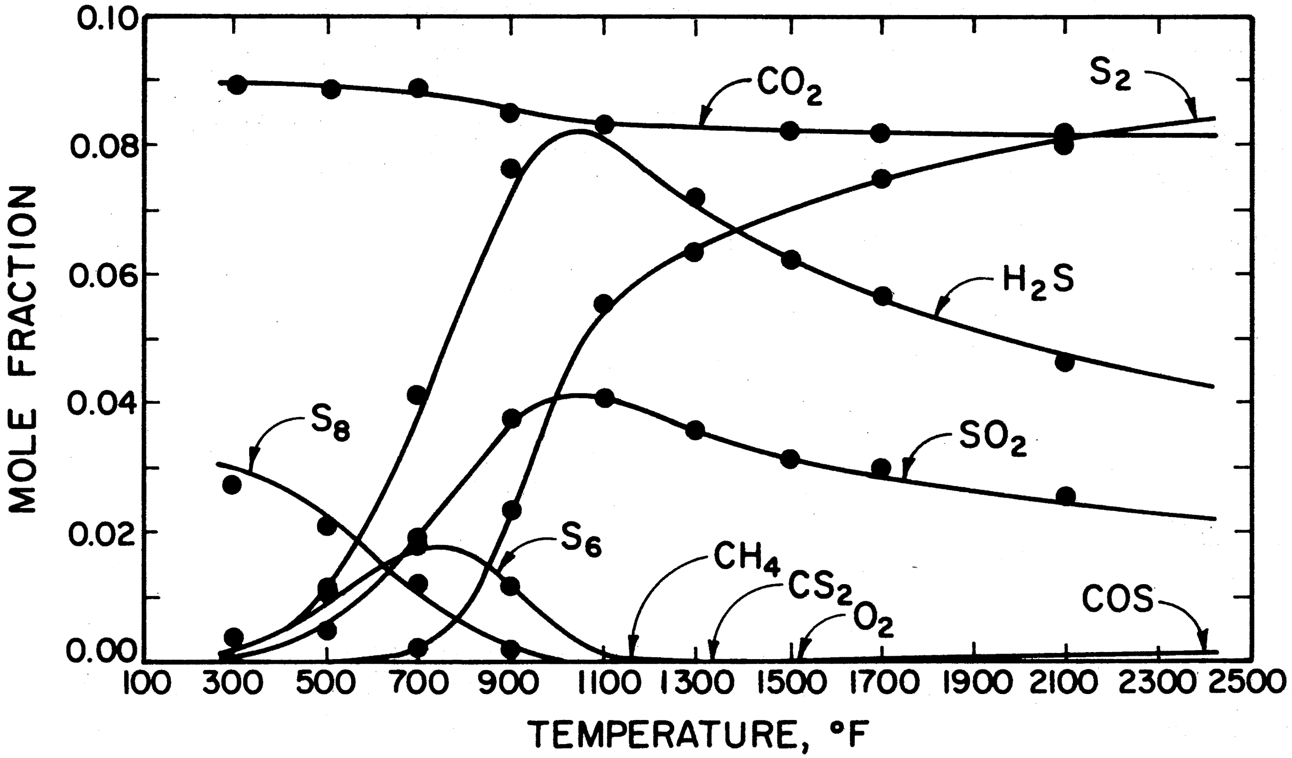

Figure 7. Equilibrium Composition Variation with Temperature for Case 3 (Expanded Scale)

is excellent. The differences in S_8 and S_6 concentrations could be due to the more recent thermodynamic data for the sulfur species that are used in this study.

Case 4.

Meisen and Bennett (31) studied the reactions taking place in a Claus process furnace considering all possible product species. Their numerical calculations were based on the equilibrium constant method. The feed to the Claus furnace was assumed to contain 85% H_2S and 15% CO_2 and was oxidized with a stoichiometric amount of air (79% N_2 and 21% O_2). The total system pressure was 1 atm, and all gases were assumed ideal. They calculated the partial pressure variation with temperature and found that 30 compounds had partial pressures exceeding 10^{-7} atm for at least some temperatures between 600^o and 2000^oK. Their composition data were presented graphically in four figures.

In an attempt to check their results, the current free energy minimization program was used to calculate the equilibrium composition for this system. Since the gases are ideal, the partial pressures are equal to the mole fractions. The computed mole fractions are presented in Table VI. Species with concentrations less than 0.1 ppmv are not included. The data agree satisfactorily with what is reported by Meisen and Bennett; there are, indeed, 30 species with mole fractions exceeding 10^{-7} in the 600^o to 2000^oK temperature range.

From the results of the above four test cases and others, we conclude that the present free energy minimization method and program are giving satisfactory results. The accuracy of the results will

TABLE VI

EQUILIBRIUM COMPOSITION VARIATION WITH TEMPERATURE FOR CASE 4

Species	Temperature, °K							
	600	800	1000	1200	1400	1600	1800	2000
CO	--	0.0000113	0.0002945	0.0023357	0.0083847	0.0173245	0.0257728	0.0320659
COS	0.0000071	0.0001615	0.0003888	0.0005333	0.0005516	0.0004458	0.0003164	0.0002147
CO_2	0.0547178	0.0518253	0.0499258	0.0473696	0.0408619	0.0315117	0.0226644	0.0159317
CS_2	--	0.0000001	0.0000007	0.0000137	0.0000169	0.0000142	0.0000010	0.0000006
CS	--	--	--	--	--	0.0000002	0.0000005	0.0000011
H	--	--	--	--	0.0000007	0.0000107	0.0000865	0.0004545
H_2	0.0000063	0.0001943	0.0017914	0.0079545	0.0209001	0.0388688	0.0588852	0.0788868
H_2O	0.2833610	0.2095320	0.2101590	0.2198730	0.2192700	0.2104350	0.1956020	0.1772970
H_2S	0.0264231	0.0831720	0.0739097	0.0564085	0.0416471	0.0293338	0.0204794	0.0144537
H_2S_2	0.0002918	0.0017340	0.0009018	0.0004028	0.0002010	0.0001010	0.0000497	0.0000228
NH_3	--	--	--	--	0.0000002	0.0000003	0.0000003	0.0000003
NO	--	--	--	--	--	0.0000001	0.0000014	0.0000093
N_2	0.5832540	0.5541940	0.5393960	0.5354540	0.5307640	0.5252610	0.5196270	0.5138540
O	--	--	--	--	--	--	--	0.0000004
OH	--	--	--	--	0.0000001	0.0000022	0.0001858	0.0001003
O_2	--	--	--	--	--	--	--	0.0000004

TABLE VI (Continued)

Species	Temperature, ^{o}K							
	600	800	1000	1200	1400	1600	1800	2000
S	--	--	--	0.000002	0.0000037	0.0000381	0.0002309	0.0009562
SH	--	0.0000001	0.0000055	0.0000602	0.0003140	0.0010095	0.0023722	0.0045036
SN	--	--	--	--	--	0.0000004	0.0000018	0.0000067
SO	--	0.0000002	0.0000072	0.0000449	0.0004606	0.0018476	0.0055069	0.0129550
SO_2	0.0133461	0.0419871	0.0377177	0.0328809	0.0347682	0.0413995	0.0496101	0.0565732
SO_3	--	--	--	--	--	--	--	0.0000002
S_2O	0.0000363	0.0012991	0.0018477	0.0018283	0.0018486	0.0019399	0.0019983	0.0019646
S_2	0.0005549	0.0408612	0.0819562	0.0942319	0.0997442	0.1003190	0.0966885	0.0896959
S_3	0.000751	0.0028925	0.0015530	0.0005777	0.0002769	0.001501	0.0000872	0.0000526
S_4	0.0000411	0.0006545	0.0000833	0.0000100	0.0000021	0.0000006	0.0000002	--
S_5	0.0014941	0.0031309	0.0000485	0.0000012	--	--	--	--
S_6	0.108850	0.0048922	0.0000124	--	--	--	--	--
S_7	0.0086844	0.0024568	0.0000019	--	--	--	--	--
S_8	0.0168220	0.0010027	0.0000001	--	--	--	--	--

undoubtedly always depend on the accuracy of the thermodynamic data used. Certainly, the program is efficient and very convenient.

CHAPTER IV

CLAUS PROCESS RESULTS AND ANALYSIS OF RESULTS

Sulfur Vapor Composition

Sulfur vapors are very complex in composition; molecules from S_1 to S_8 are known to exist in equilibrium. However, due to the lack of reliable thermodynamic data for the sulfur polymers S_3, S_4, S_5, and S_7 they usually have been neglected. Almost all previous Claus process investigators have assumed that the sulfur vapor is represented by S_2, S_6, and S_8 (8,12,26).

Detry et al. (5) presented new thermodynamic data for all the sulfur polymers based on mass spectrometric measurements. These data are probably the best in the open literature. Kellog (18) used the data provided by Detry et al. and deduced a series of free energy equations for the interconversions of the various sulfur molecules as shown in Table VII.

Based on these recent data, equilibrium calculations were made to predict the composition that would exist at a given temperature considering all possible sulfur species. The results of these calculations are presented in Figure 8. The concentration of S_5, and certainly S_7, is sufficiently high to raise a question as to whether or not these species should be included in the Claus sulfur process calculations.

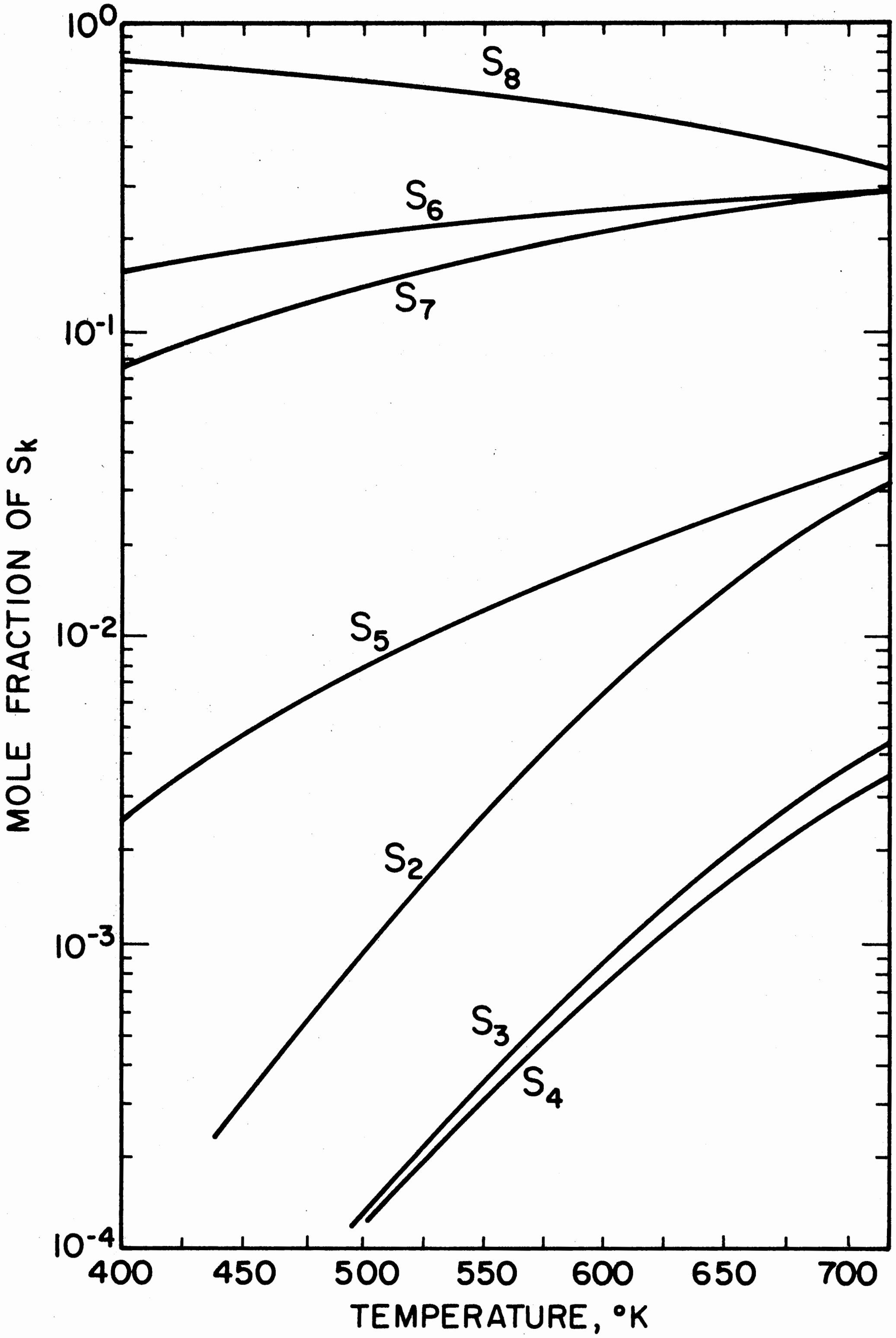

Figure 8. Equilibrium Distribution of Sulfur Polymers in the Saturated Vapor

TABLE VII

SULFUR VAPOR EQUILIBRIA

Equilibrium	ΔG^o vs T (400^o to 700^oK)
$2S(L) = S_2$	$32458 + 8.20T\ell nT - 92.380T$
$3/2S_2 = S_3$	$-13687 - 0.50T\ell nT + 22.843T$
$2S_2 = S_4$	$-29053 - 1.80T\ell nT + 50.031T$
$5/2S_2 = S_5$	$-50351 - 3.80T\ell nT + 84.905T$
$3S_2 = S_6$	$-69463 - 6.00T\ell nT + 118.510T$
$7/2S_2 = S_7$	$-82750 - 7.20T\ell nT + 141.601T$
$4S_2 = S_8$	$-100980 - 8.00T\ell nT + 168.242T$

Least squares coefficients in THERMO data file for the sulfur polymers in the temperature range 400^o to 1000^oK are based on Kellogg's data. For temperatures higher than 1000^oK, the coefficients for S_2, S_6, and S_8 are obtained from the JANAF Tables (17) while for the species S_3, S_4, S_5, and S_7 the coefficients derived from Kellogg's equations were used. The concentrations of these latter species are extremely small, therefore the use of Kellogg's data in the high temperature range is not introducing major errors in the calculations. Actually for the Claus process study the important temperature range, where all sulfur species are present in significant quantities, is 400^o to 700^oK. At high temperatures the sulfur vapor is almost totally S_2.

Guidelines for Free Energy Minimization

With the powerful energy minimization technique and the capability of considering all chemical species, certain assumptions and guidelines had to be developed for conducting the Claus process calculations. The basis for all calculations reported in this thesis is a simple three reactor "once-through" Claus sulfur conversion process as shown in Figure 2. The reheat before each reactor is by indirect heat from the combustion zone or some other source. Typical Claus plant operating conditions are assumed. The assumptions used throughout this work are summarized below:

1. All gases are assumed to be ideal.
2. Thermodynamic equilibrium is achieved at the furnace and the catalytic reactors.
3. Heat losses from the furnace and the reactors are assumed to be negligible.
4. Acid gases are burned with sufficient air that the H_2S/SO_2 ratio in the tail gas is 2 to 1.
5. Streams entering the catalytic reactors are preheated to temperatures equal to the dew point temperatures of the product streams. This insures that no sulfur condensation will take place in the reactors.
6. All condensers are assumed to operate at $417^{o}K$ where liquid sulfur flows readily (30).
7. Acid gases entering the Claus process are assumed to be saturated with water at $311^{o}K$ and 1.429 atm.
8. Air entering the furnace is assumed to be 50% saturated

with water at 297.22^{o}K.

9. The furnace pressure was assumed to be 1.429 atm (21 psia). The pressure then gradually decreases to 1 atm in the fourth condenser. The assumed pressure profile throughout the process is indicated in the results tables.

The necessity for some guidelines is clearly illustrated in Table VIII in which the results of calculations using various options in the free energy minimization technique are presented. The gas considered in the calculations reported in Table VIII had a high concentration of H_2S. The exact composition is:

Component	Mole %
H_2S	89.72
CO_2	4.98
CH_4	0.80
H_2O	4.50

The first case considers only the combustion furnace followed by one condenser. All species present in the natural gas or formed in the furnace were allowed to reach their equilibrium composition at condenser conditions. The sulfur recovery of 99.39% clearly does not in any way resemble the actual production from the first condenser of a Claus unit, even with high H_2S concentration gas feed. This means that some modifications must be made in the free energy minimization procedure if the results are to reasonably predict Claus process sulfur recoveries.

The second case used the same acid gas composition. In the combustion chamber and the reactor bed all species present were

TABLE VIII

OPTIONS IN THE FREE ENERGY MINIMIZATION CALCULATIONS

Case	1	2	3	4
Condition	Thermodynamic Equilibrium, All Species Considered	CO, COS, CO_2, H_2, H_2O, H_2S, and SO_2 Were Not Allowed to React in Condensers and Reheaters	H_2S and SO_2 Were Not Allowed to React in Condensers and Reheaters	As in Case 3 Plus No Mass or Heat Considerations in Condensers and Reheaters
Furnace				
1st Condenser Recovery %	99.39	71.17	47.80	48.44
Reactor #1				
T_{in} (^{o}K)		502	529	529
T_{out}		637	620	624
% Recovery		13.79	37.44	37.49
Reactor #2				
T_{in}		490	490	490
T_{out}		524	523	527
% Recovery		10.62	10.44	10.07
Reactor #3				
T_{in}		458	457	457
T_{out}		467	466	466
% Recovery		2.65	2.61	2.37
Total Sulfur % Recovery	99.39	98.23	98.29	98.37

allowed to react to their equilibrium composition. However, in the condenser carbon monoxide, carbonyl sulfide, carbon dioxide, hydrogen, water, hydrogen sulfide and sulfur dioxide were considered to be inert and incapable of reaction at condenser temperature. The difference in sulfur recovery in the first condenser is very striking.

The third case treated H_2S and SO_2 as non-reactants in the condenser. The results here are primarily different by shifting a considerable amount of the sulfur conversion duty from the first condenser to the first reactor chamber.

In cases two and three the species treated as being inert were still included in the heat and material balances. In case four the H_2S and SO_2 not only were not allowed to react but were completely withdrawn from the reaction mixture. The higher sulfur recovery in both the first condenser and the first reactor are caused by the higher concentration resulting from omitting the H_2S and SO_2 from the gas analysis.

Case two above probably most closely represents the reaction behavior in a real Claus unit. Reaction rates for reactions involving the compounds listed as inert are slow at typical sulfur condenser or reheater temperatures (8,20). Therefore, in our investigations of the Claus process, all species will be allowed to react and reach their equilibrium composition in the furnace and the reactors.
In the condensers and the reheaters carbon monoxide, carbonyl sulfide, carbon dioxide, hydrogen, water, hydrogen sulfide, and sulfur dioxide will be treated as inert. Other species, including the sulfur polymers, will be allowed to react to reach equilibrium.

Effect of Considering All Sulfur Polymers

As mentioned earlier most investigators have neglected in their Claus process calculations the sulfur polymers S_3, S_4, S_5 and S_7. By examining the sulfur vapor equilibrium composition presented in Figure 8, we realize that S_5 and S_7 are present in high enough concentration that they should be included in any accurate equilibrium and yield calculations. To check their affect, a series of calculations was carried out using the modified free energy minimization approach (CO, COS, CO_2, H_2, H_2O, H_2S, SO_2 inerts in condensers and reheaters). One case considered all forms of sulfur while the other considered only S_2, S_6 and S_8. Two types of acid gases were used. The results of the calculations are summarized in Table IX.

The typical acid gas contained 73.0% H_2S and 20.0% CO_2. The sulfur recoveries at each stage of the Claus process are close for the two cases. After the first condenser and two reactors sulfur recovery is 94.93% considering all forms of sulfur and 94.45% considering only S_2, S_6 and S_8. After three reactors the total recovery is even closer 98.01% and 97.88% respectively.

The same comparison was made for sulfur recovery from pure H_2S gas burned with air. The sulfur recovery from the first condenser and two reactors is 96.11% considering all forms of sulfur and 95.63% considering only S_2, S_6 and S_8. After three reactors the total recovery is 98.43% and 98.26% respectively.

From the standpoint of predicted sulfur yield there appears to be little difference in sulfur recovery whether all sulfur species are considered or only the traditional S_2, S_6 and S_8 species are

TABLE IX

COMPARISON OF SULFUR RECOVERY WHEN ALL OR SOME OF THE SULFUR POLYMERS ARE CONSIDERED IN CLAUS PROCESS CALCULATIONS

Feed Type	Typical Acid Gas*		Pure H_2S Gas	
Case	All Sulfur Species Considered	Only S_2, S_6, S_8 Considered	All Sulfur Species Considered	Only S_2, S_6, S_8 Considered
Sulfur Recovery %				
Condenser #1	68.54	68.54	73.49	73.48
Condenser #2	13.27	12.37	13.28	12.39
Condenser #3	13.12	13.54	9.34	9.76
Condenser #4	3.08	3.43	2.32	2.63

* Typical Acid Gas Composition

Component	Mole %
H_2S	73.0
CO_2	20.0
H_2O	3.8
CH_4	2.5
C_2H_6	0.4
C_3H_8	0.1
C_4H_{10}	0.2

considered. The maximum difference is about 0.48% for two reactors while the minimum is about 0.13% for three reactors process.

Table X shows the three reactor process tail gas composition which results from the comparative calculations on sulfur species. The tail gas compositions shown are for a typical acid gas and for pure H_2S gas. The only significant difference is in the concentration of H_2S and SO_2 in the tail gases. These are slightly higher if only S_2, S_6, and S_8 are considered than they would be for all forms of sulfur. For a typical acid gas with all forms of sulfur considered the H_2S plus SO_2 concentration in the tail gas is 3914 ppmv while with only S_2, S_6, and S_8 considered the H_2S plus SO_2 concentration is 4415 ppmv. This is a 12.8% increase in sulfur tail gas concentration between the two cases. For pure H_2S the increase is 15.6% from 4220 to 4879 ppmv. These differences can be significant for tail gas cleanup processes and for environmental considerations. With the availability of thermodynamic data for all the sulfur species, and with the convenience of the free energy minimization program, all sulfur species should be taken into consideration when conducting accurate Claus process calculations.

Effect of Impurities in the Acid Gas Feed

Acid gases derived from natural gas streams usually contain measurable quantities of one or more impurities. These impurities can be hydrocarbons, carbon dioxide, water, and possibly ammonia or amine. The impurities can reduce the efficiency of the Claus process and create costly problems affecting design, maintenance and operation. In the combustion zone they can produce materials that participate in side reactions and/or compete for the sulfur molecules formed. Some

TABLE X

COMPARISON OF TAIL GAS COMPOSITIONS WHEN ALL OR SOME OF THE SULFUR POLYMERS ARE CONSIDERED IN CLAUS PROCESS CALCULATIONS (Mole Fractions)

Feed Type	Typical Acid Gas		Pure H_2S Gas	
Case / Species	All Sulfur Species Considered	Only S_2, S_6, S_8 Considered	All Sulfur Species Considered	Only S_2, S_6, S_8 Considered
CO_2	0.086977	0.086964	--	--
H_2O	0.309511	0.309128	0.343751	0.343239
H_2S	0.002609	0.002943	0.002813	0.003252
H_2S_2	0.000006	0.000008	0.000007	0.000009
N_2	0.599432	0.599339	0.651862	0.651727
SO_2	0.001305	0.001472	0.001407	0.001627
S_5	0.000001	--	0.000001	--
S_6	0.000027	0.000027	0.000027	0.000027
S_7	0.000014	--	0.000014	--
S_8	0.000120	0.000120	0.000120	0.000120

of the products of these reactions, such as carbonyl sulfide (COS) and carbon disulfide (CS_2), seem not to be affected by present Claus catalysts and either deposit on the catalyst surface reducing its activity or pass through the process unchanged and add to the total sulfur values in the tail gas.

The affects and the fate of the various impurities in the acid gases were studied utilizing the modified free energy minimization program. The base case for comparison is a relatively clean, high H_2S concentration gas that contains approximately 90% H_2S, 5% CO_2, 5% water, and a trace of hydrocarbons. Results of the Claus process calculations for this feed are presented in Table XI. Included in the table are the pressure and temperature profiles across the process, the concentration profiles for all species present at equilibrium (with concentrations higher than 1 ppmv), and the sulfur yield at each condenser. Complete results for the base case are given as a computer program sample output in Appendix B.

Carbon Dioxide

Two cases were run to demonstrate the affect of feeding excessive amounts of CO_2 to a Claus sulfur process. In cases 2 and 3 in Table XII, the CO_2 concentration was elevated at the expense of H_2S concentration with hydrocarbon and water content remaining essentially constant. The affect of higher CO_2 concentration in the acid gas feed on the furnace temperature is shown in Figure 9. The furnace temperature decreases dramatically as the CO_2 concentration increases. The complete Claus process temperature and concentration profiles for cases 2 and 3 are given in Appendix C. Figure 10 shows the affect

TABLE XI

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR THE BASE CASE

	Furnace	Condenser #1	Reheater #1	Reactor #1	Condenser #2	Reheater #2
Pressure (atm)	1.429	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^oK)	1524	417	502	637	417	490
Chemical Species Mole Fractions:						
CO	0.004695	0.004277	0.005211	--	--	--
COS	0.000197	0.000179	0.000218	0.000004	0.000004	0.000004
CO_2	0.012931	0.011778	0.014349	0.020188	0.019484	0.020333
CS_2	0.000001	--	--	--	--	--
H	0.000003	--	--	--	--	--
H_2	0.031865	0.029022	0.035360	0.000014	0.000014	0.000015
H_2O	0.233758	0.212906	0.259399	0.315856	0.304847	0.318121
H_2S	0.039644	0.036107	0.043992	0.030214	0.029161	0.030431
H_2S_2	0.000181	0.000471	0.000574	0.000326	0.000315	0.000329
N_2	0.539200	0.419110	0.598345	0.610839	0.589550	0.615221
OH	0.000001	--	--	--	--	--
S	0.000014	--	--	--	--	--
S(L)	--	0.179424	--	--	0.041748	--
SH	0.000666	--	--	--	--	--
SO	0.001005	--	--	--	--	--
SO_2	0.036964	0.033667	0.041019	0.015249	0.014718	0.015358
SO_3	--	0.000873	0.000893	--	0.000009	--
S_2O	0.001979	0.000099	0.000634	0.000054	0.000025	0.000054
S_2	0.096684	--	0.000001	0.000841	--	0.000001
S_3	0.000211	--	--	0.000083	--	--
S_4	0.000001	--	--	0.000031	--	--
S_5	--	--	0.000001	0.000587	0.000001	0.000004
S_6	--	0.000016	0.000003	0.002500	0.000021	0.000047
S_7	--	0.000008	0.000001	0.001507	0.000011	0.000021
S_8	--	0.000072	0.000001	0.001708	0.000094	0.000061
Stage Sulfur Recovery %		71.17	--	--	13.79	--
Total Sulfur Recovery %		71.17	--	--	84.96	--

TABLE XI (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^{o}K)	524	417	458	467	417	417
Chemical Species Mole Fractions:						
CO	--	--	--	--	--	--
COS	--	--	--	--	--	--
CO_2	0.020469	0.019891	0.020565	0.020600	0.020450	0.020624
CS_2	--	--	--	--	--	--
H	--	--	--	--	--	--
H_2	0.000001	0.000001	0.000001	--	--	--
H_2O	0.342578	0.332894	0.344186	0.350471	0.347915	0.350873
H_2S	0.008552	0.008310	0.008592	0.002943	0.002921	0.002946
H_2S_2	0.000043	0.000042	0.000043	0.000007	0.000007	0.000007
N_2	0.619238	0.601732	0.622144	0.623202	0.618656	0.623916
OH	--	--	--	--	--	--
S	--	--	--	--	--	--
S(L)	--	0.032815	--	--	0.008430	--
SH	--	--	--	--	--	--
SO	--	--	--	--	--	--
SO_2	0.004293	0.004172	0.004313	0.001471	0.001461	0.001473
SO_3	--	--	--	--	--	--
S_2O	0.000002	0.000002	0.00002	--	--	--
S_2	0.000017	--	--	0.000001	--	--
S_3	0.000002	--	--	--	--	--
S_4	0.000001	--	--	--	--	--
S_5	0.000102	0.000001	0.000002	0.000013	0.000001	0.000001
S_6	0.001222	0.000024	0.000041	0.000262	0.000026	0.000027
S_7	0.000842	0.000012	0.000020	0.000165	0.000014	0.000014
S_8	0.002638	0.000106	0.000090	0.000865	0.000119	0.000120
Stage Sulfur Recovery %		10.62	--	--	2.65	--
Total Sulfur Recovery %		95.58	--	--	98.23	--

of feed gas CO_2 impurity on furnace effluent composition (expressed as moles/mole acid gas feed). In all cases, the concentrations of NH_3, NO, NO_2, SN and HCN are smaller than 1 ppmv and are considered negligible. Interestingly, the CO concentration (and amount) is a maximum with approximately 35% CO_2. This undoubtedly is caused by the fact that the combustion zone temperature drops sharply when the CO_2 concentration goes to 75%. Although the concentration of COS continues to increase as the CO_2 content in the acid gas increases, the amount of effluent seems to have a maximum with approximately 55% CO_2 in the feed. Also, the amount and concentration of CS_2 have a maximum at approximately 45% CO_2. In all cases, the equilibrium concentrations of COS and CS_2 are much lower than plant data indicate (19). This fact will be discussed in a later section after the various impure acid gases are considered.

TABLE XII

CLAUS PROCESS ACID GAS FEEDS WITH CARBON DIOXIDE IMPURITY

Case Component	1 Base Case Mole %	2 Mole %	3 Mole %
H_2S	89.72	49.84	20.00
CO_2	4.98	45.22	75.32
CH_4	0.80	0.44	0.18
H_2O	4.50	4.50	4.50
Total	100.00	100.00	100.00

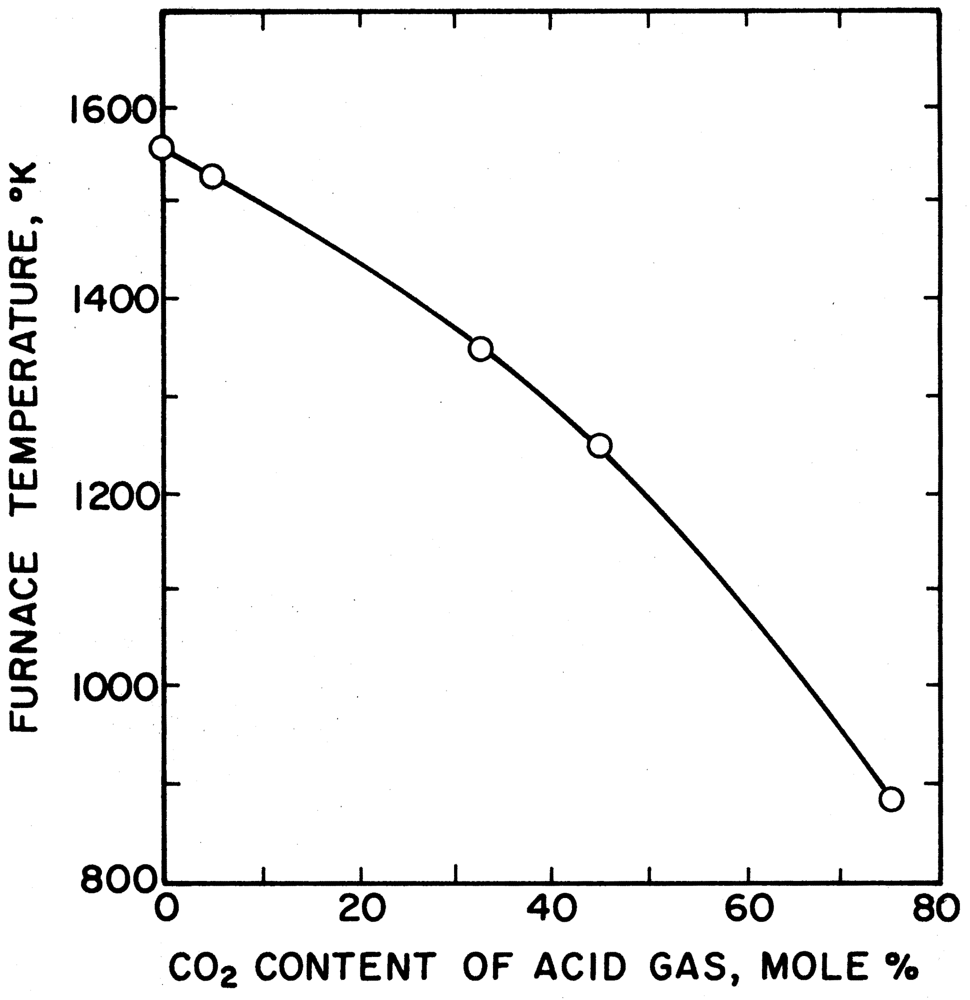

Figure 9. Affect of Feed Gas Carbon Dioxide Impurity on Furnace Temperature

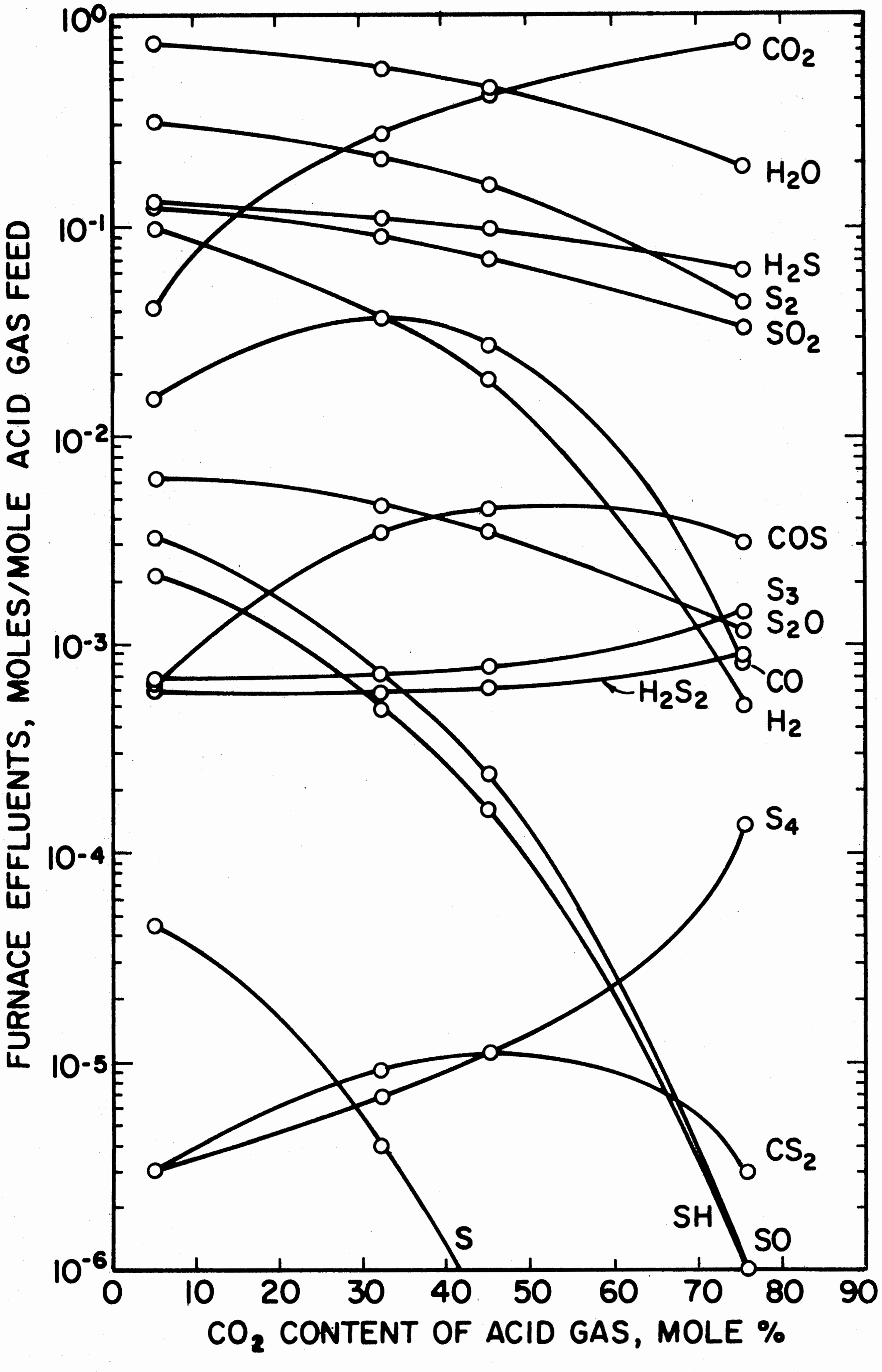

Figure 10. Affect of Feed Gas Carbon Dioxide Impurity on Furnace Effluent Composition

Claus process sulfur recovery results for the high CO_2 concentration feed gases are compared against the base case in Table XIII. Due to changes in feed composition, the reactor inlet temperatures (which are equal to reactor product gases dewpoint temperatures) in cases 2 and 3 are generally lower than those in the base case. This has the effect of slightly increasing the sulfur recovery and compensating for some of the impurity affects as illustrated in Table XIII. If reactor inlet temperatures for cases 2 and 3 were assumed to be the same as those in the base case, then we would observe a decrease in the overall conversion as CO_2 impurity increases. Otherwise the presence of CO_2 seems to merely shift a considerable amount of the sulfur conversion duty from the first condenser to the second with no affect on the overall sulfur recovery.

TABLE XIII

AFFECT OF FEED GAS CARBON DIOXIDE IMPURITY ON SULFUR RECOVERY

Case	1	2		3	
Reactor Inlet Temperature	Base Case	As in Case 1	Recalculated for this case	As in case 1	Recalculated for this case
Sulfur Recovery %					
Condenser #1	71.17	64.68	64.68	47.88	47.88
Condenser #2	13.79	21.75	21.48	42.11	41.43
Condenser #3	10.62	9.50	10.03	5.95	7.61
Condenser #4	2.65	2.21	2.14	1.67	1.31
Total Recovery %	98.23	98.14	98.33	97.61	98.23

The tail gases for the three cases, each case with its own calculated reactor inlet temperatures, are compared in Table XIV. The concentrations of COS and CS_2 in the tail gases are less than 0.1 ppmv indicating that these compounds almost totally react in the reactors. The change in total sulfur emissions for cases 2 and 3 is smaller than might be expected in a real Claus plant because of the low furnace temperature and small combustion air requirement.

In summary, carbon dioxide in the acid gases acts mainly as an inert diluent. It lowers the effective partial pressure of hydrogen sulfide, but it does not require additional quantities of combustion air and does not seem to cause major side reactions.

Hydrocarbons

In this comparison study the hydrocarbon concentration was increased from 0.8% in the base case to 5% and 15% with corresponding decrease in H_2S concentration. The hydrocarbon was assumed to be totally methane. Compositions for the new cases are given in Table XV.

Excessive hydrocarbon content in the acid gas feed increases combustion air requirement, furnace temperature, and due to production of additional inerts the Claus process gas flow increases. This generally results in a larger plant size and lower conversion of H_2S to sulfur. Hydrocarbons may also enter some of the side reactions listed in Table II which lead to formation of COS and CS_2. These two compounds do not seem to react well on present Claus reactors catalyst and might either deposit on the catalyst surface and reduce

TABLE XIV

AFFECT OF FEED GAS CARBON DIOXIDE IMPURITY ON PROCESS TAIL GAS FLOW

Case	1 Base Case	2	3
Effluent Gases	(moles/mole acid gas feed for each case)		
CO_2	0.057763	0.456555	0.754864
H_2O	0.982727	0.566666	0.254655
H_2S	0.008251	0.003881	0.001223
H_2S_2	0.000019	0.000008	0.000002
N_2	1.747466	0.970845	0.389587
SO_2	0.004126	0.001937	0.000612
S_5	0.000003	0.000002	0.000001
S_6	0.000076	0.000053	0.000037
S_7	0.000039	0.000028	0.000020
S_8	0.000336	0.000239	0.000168
Total Flow	2.80804	2.000213	1.401169
Total "S" equivalent to atmosphere:			
(atoms/mole acid gas feed)	0.015847	0.008270	0.003550
(atoms/mole H_2S feed)	0.017663	0.016592	0.017748
Change in sulfur emissions %	0.0	-6.06	0.48

TABLE XV

CLAUS PROCESS ACID GAS FEEDS WITH HYDROCARBON IMPURITY

Case	1 Base Case	2	3
Component	Mole %	Mole %	Mole %
H_2S	89.72	85.74	76.27
CO_2	4.98	4.76	4.23
CH_4	0.80	5.00	15.00
H_2O	4.50	4.50	4.50
Total	100.00	100.00	100.00

its activity or pass through the process unchanged and add to the total sulfur values in the tail gas.

The results of equilibrium calculations for cases 2 and 3 are presented in Appendix D. The affect of feed gas hydrocarbon impurity on furnace effluent composition is shown in Figure 11. The amount of CO_2 and CO produced in the combustion zone increases as the hydrocarbon content of the acid gas increases. COS and CS_2 are only slightly increased. The affect of feed gas hydrocarbon impurity on Claus process sulfur recovery is presented in Table XVI. The total sulfur recovery decreases from 98.23% for the clean or base case to 98.00% and 97.4% for cases 2 and 3 respectively.

The tail gases for the three cases are compared in Table XVII. The major affects of hydrocarbon impurities on tail gas flow and composition and on sulfur emissions to the atmosphere or to the tail gas clean-up processes are apparent. Increasing the hydrocarbon content in the acid gas feed from 0.8% to 5%, as in case 2, results in an increase of about 12% in the tail gas flow and of about 13% in total sulfur emissions. If the hydrocarbon content in the feed gas is increased to 15%, as in case 3, the resulting increase in tail gas flow and in total sulfur emissions is about 40% and 47.4% respectively.

In order to insure high efficiency of the Claus process, the hydrocarbon content of the acid gas feed must be extremely small. Some corrective measures in the design of acid gas sweetening plants need to be taken to achieve this. For "physical solvent" sweetening processes that have excessive heavy hydrocarbons in the acid gas, a charcoal adsorption unit should be considered for treating the acid gas prior to sending it to the Claus plant (13).

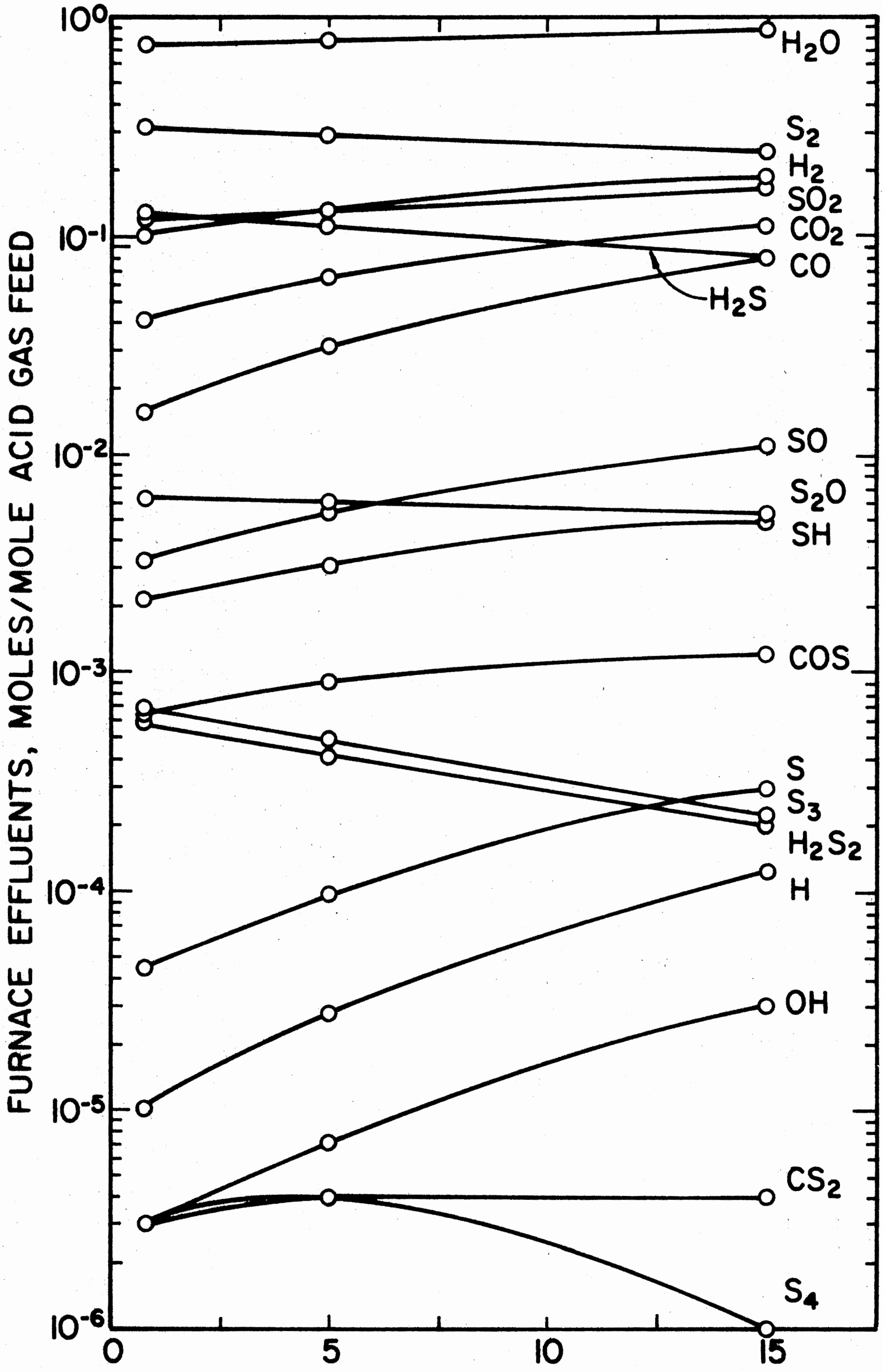

Figure 11. Affect of Feed Gas Hydrocarbon Impurity on Furnace Effluent Composition

TABLE XVI

AFFECT OF FEED GAS HYDROCARBON IMPURITY ON SULFUR RECOVERY

Case	1	2		3	
Reactor Inlet Temperature	Base Case	As in Case 1	Recalculated for this case	As in Case 1	Recalculated for this case
Sulfur Recovery %					
Condenser #1	71.17	70.09	70.09	65.07	65.07
Condenser #2	13.79	11.79	12.45	8.55	10.39
Condenser #3	10.62	13.01	12.37	19.47	17.88
Condenser #4	2.65	3.10	3.09	4.28	4.06
Total Recovery %	98.23	97.99	98.00	97.37	97.40

TABLE XVII

AFFECT OF FEED GAS HYDROCARBON IMPURITY ON PROCESS TAIL GAS FLOW

Case	1 Base Case	2	3
Effluent Gases	(moles/mole acid gas feed for each case)		
CO_2	0.057763	0.097594	0.192332
H_2O	0.982727	1.030963	1.145825
H_2S	0.008251	0.008829	0.010018
H_2S_2	0.000019	0.000022	0.000024
N_2	1.747466	1.988979	2.563153
SO_2	0.004126	0.004415	0.005008
S_5	0.000003	0.000003	0.000004
S_6	0.000076	0.000083	0.000104
S_7	0.000039	0.000049	0.000055
S_8	0.000336	0.000375	0.000469
Total Flow	2.800804	3.131304	3.916990
Total "S" equivalent to atmosphere:			
(atoms/mole acid gas feed)	0.015847	0.017108	0.019855
(atoms/mole H_2S feed)	0.017663	0.019953	0.026034
Increase in sulfur emissions %	0.0	12.97	47.39

Ammonia and Water

Impurities in acid gas feeds to Claus plants can include ammonia from gas treatment plants or refineries and water vapor. In our comparative study, one case was run with the addition of ammonia and another with increased water concentration. The compositions for the two cases as well as for the clean or base case are listed in Table XVIII. The calculation results including pressure, temperature, and concentration profiles across the Claus process for these two cases are given in Appendix E.

TABLE XVIII

CLAUS PROCESS ACID GAS FEEDS WITH AMMONIA AND WATER IMPURITIES

Case Number	1	2	3
Impurity	Base Case	NH_3	H_2O
Component	Mole %	Mole %	Mole %
H_2S	89.72	75.63	70.46
CO_2	4.98	4.20	3.91
CH_4	0.80	0.67	0.63
H_2O	4.50	4.50	25.00
NH_3	--	15.00	--
Total	100.00	100.00	100.00

The affect of ammonia and water impurities on the furnace products is shown in Table XIX. The addition of ammonia had little affect on CO production while water actually suppressed its formation. The presence of ammonia and the additional water seem to slightly suppress the formation of COS. Some possible reactions of ammonia in Claus plants are (3):

$$2NH_3 \rightleftharpoons N_2 + 3H_2 \qquad (4\text{-}1)$$

$$2NH_3 + \frac{3}{2} O_2 \longrightarrow N_2 + 3H_2O \qquad (4\text{-}2)$$

$$2NH_3 + \frac{5}{2} O_2 \longrightarrow 2NO + 3H_2O \qquad (4\text{-}3)$$

Reaction (4-1) is simply the thermal decomposition of ammonia. Reaction (4-2) is the complete oxidation of the hydrogen in ammonia which most likely occurs with oxidizing conditions in the furnace. The oxidation of both nitrogen and hydrogen in ammonia is represented by reaction (4-3).

The combustion condition for case 2 in this study was probably an oxidizing condition. Almost all of the ammonia reacted to form nitrogen. The equilibrium concentration of NO in the combustion zone was only about 0.14 ppmv which means that reaction (4-3) is not important at the furnace temperature ($1607^{\circ}K$). Equilibrium concentration of NH_3 in the combustion zone was about 0.4 ppmv.

The combustion products (nitrogen and water) tend to depress the Claus reaction, reaction (2-15). Nitrogen acts as an inert diluent while water is a Claus reaction product in addition to being an inert.

The affect of ammonia and water in the feed gases on the sulfur recovery is presented in Table XX. The presence of ammonia in case

TABLE XIX

AFFECT OF FEED GAS AMMONIA AND WATER IMPURITIES ON FURNACE EFFLUENT COMPOSITION

Case	1	2	3
Impurity	Base Case	Ammonia in Feed Gas	Water in Feed Gas
Species	(moles/mole acid gas feed)	(moles/mole acid gas feed)	(moles/mole acid gas feed)
CO	0.015216	0.015884	0.007197
COS	0.000638	0.000403	0.000410
CO_2	0.041908	0.031032	0.032256
CS_2	0.000003	0.000001	0.000001
H	0.000010	0.000034	0.000003
H_2	0.103271	0.136879	0.066153
H_2O	0.757584	0.804163	0.691586
H_2S	0.128482	0.101482	0.113372
H_2S_2	0.000587	0.000349	0.000551
NH_3	---	0.000001	---
N_2	1.747489	1.904661	1.205562
OH	0.000003	0.000008	---
S	0.000045	0.000099	0.000012
SH	0.002158	0.003041	0.000973
SN	---	0.000001	---
SO	0.003257	0.005152	0.001388
SO_2	0.119796	0.123055	0.091194
S_2O	0.006414	0.005250	0.005378
S_2	0.313342	0.244489	0.200054
S_3	0.000684	0.000363	0.000521
S_4	0.00003	0.000001	0.000004
Total Flow	3.240892	3.386348	2.750339
Furnace Temperature, ^{o}K	1524	1607	1444

TABLE XX

AFFECT OF FEED GAS AMMONIA AND WATER IMPURITIES ON SULFUR RECOVERY

Case	1	2		3	
Impurity		Ammonia		Water	
Reactor Inlet Temperature	Base Case	As in Case 1	Recal-culated for this case	As in Case 1	Recal-culated for this case
Sulfur Recovery %					
Condenser #1	71.17	67.92	67.92	65.85	65.85
Condenser #2	13.79	12.60	13.44	17.51	17.33
Condenser #3	10.62	13.78	13.09	11.41	11.50
Condenser #4	2.65	3.42	3.28	3.11	3.11
Total Recovery %	98.23	97.72	97.73	97.88	97.79

2 decreased the overall recovery by 0.5% while additional water in case 3 caused a reduction of 0.44%.

The tail gas flow for the two cases is compared against the base case in Table XXI. The increase in sulfur emissions for the ammonia case is 23.39% while for the additional water case the increase is 25.84%. Goar (13) presented similar results for a Claus process with two reactors and hot gas bypasses. Although the two results cannot be directly compared due to different reaction conditions and assumptions, they indicate the necessity for removing or reducing the impurities before entering the Claus plants.

Production of CS_2 and COS in the Claus Furnace

The equilibrium concentrations of CS_2 and COS calculated in this study and presented in Figures 10 and 11 are much below observed plant data. This has been observed and reported by Kerr (19) who found from collected plant data that CS_2 concentration in the furnace effluent is directly proportional to the hydrocarbon content of the acid gas feed. For example, when the total carbon from hydrocarbons in an acid gas is 0.8 mole % the CS_2 concentration in the furnace effluent is about 0.8 mole %. The observed high concentration is probably due to kinetic limitations - rapid CS_2 formation from hydrocarbon impurities. This can be supported by the experimental observation that sulfur reacts with hydrocarbons at rates orders of magnitude greater than oxygen with hydrocarbons (20). Figure 10 indicates that CS_2 is also formed from CO reacting with S_2, though

TABLE XXI

AFFECT OF FEED GAS AMMONIA AND WATER IMPURITIES ON PROCESS TAIL GAS FLOW

Case	1	2	3
Impurity	Base Case	Ammonia	Water
Effluent Gases	(moles/mole acid gas feed for each case)		
CO_2	0.057763	0.046869	0.045388
H_2O	0.982727	1.025959	0.984533
H_2S	0.008251	0.008534	0.008449
H_2S_2	0.000019	0.000021	0.000022
N_2	1.747466	1.896507	1.372612
SO_2	0.004126	0.004267	0.004223
S_5	0.000003	0.000003	0.000002
S_6	0.000076	0.000079	0.000064
S_7	0.000039	0.000042	0.000034
S_8	0.000336	0.000357	0.000289
Total Flow	2.800804	2.982638	2.415617
Total "S" equivalent to atmosphere:			
(atoms/mole acid gas feed)	0.015847	0.016483	0.015662
(atoms/mole H_2S feed)	0.017663	0.021795	0.022228
Increase in sulfur emissions %	0.0	23.39	25.84

this reaction is governed by overall system equilibrium. Some possible reactions involving CS_2 and COS are given in Table II (page 23).

The production of COS in a Claus process furnace appears to be related to equilibrium production of CO. According to Kerr neither COS nor CO exhibit any meaningful trend, individually, for various plant feeds as a function of hydrocarbon or hydrogen sulfide. But he observed that their sum exhibits the same trend as predicted by thermodynamic equilibrium at the adiabatic flame temperature. He concluded that COS is probably formed from CO reacting with sulfur:

$$CO + S \rightleftharpoons COS \qquad (4\text{-}4)$$

Kerr presented a chart similar to that shown in Figure 12 comparing plant test data with the results of his equilibrium calculations. The results of the acid gases studied with impurities in this work are summarized in Table XXII and shown in Figure 12. The agreement with the data of Kerr is good and the curve through the present data appears to have the same shape. Therefore, the higher than thermodynamic equilibrium concentration of COS in the Claus furnace could be due to rapid formation of COS from CO and sulfur vapor.

Sulfur Recovery After a Fourth Reactor

The sulfur recovery after a fourth reactor in a Claus process was calculated for rich and lean acid gases (cases 1 and 2 in Table XII). The results are presented in Table XXIII. For the rich acid gas feed, the fourth reactor increased the overall sulfur recovery by 0.69%. For the lean acid gas feed, the overall sulfur

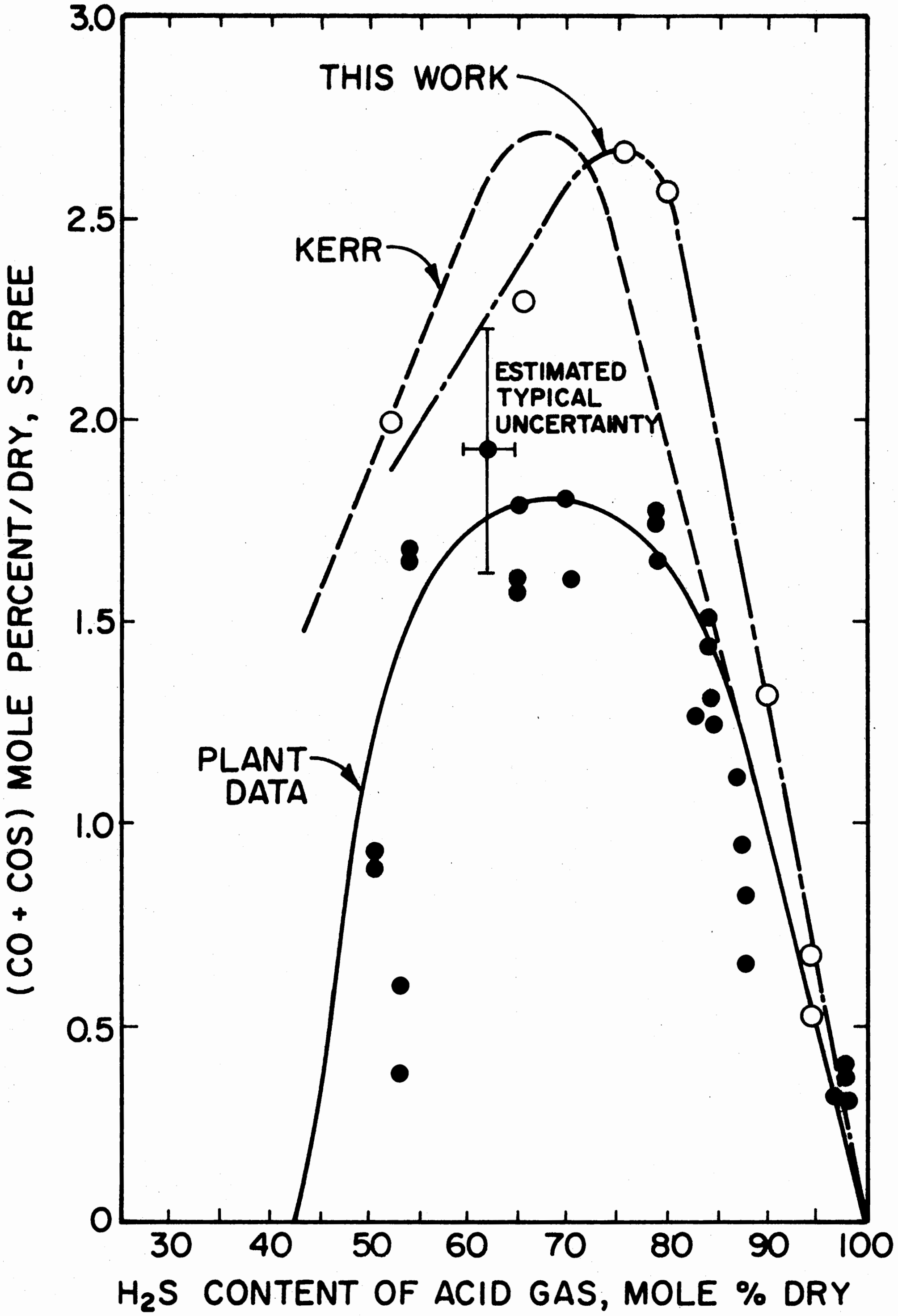

Figure 12. Thermodynamic Equilibrium (CO + COS) at Adiabatic Flame Temperature

recovery was increased by only 0.51%. These increases in sulfur recovery probably do not justify the cost of adding a fourth reactor to a Claus plant especially if a tail gas cleanup unit is included. Only for very large plants, with high levels of sulfur emissions, would a fourth reactor be considered.

TABLE XXII

EQUILIBRIUM CONCENTRATIONS OF (CO + COS) IN CLAUS FURNACE

H_2S in Acid Gas Mole % Dry	(CO + COS) Mole % Dry, S-Free
93.95	0.73
93.95	0.50
89.78	1.31
79.86	2.55
75.90	2.66
66.00	2.29
52.20	1.98

TABLE XXIII

SULFUR RECOVERY AFTER FOUR CLAUS REACTORS

Acid Gas Feed	Stage					Total Recovery %
	Furnace	Reactor #1	Reactor #2	Reactor #3	Reactor #4	
H_2S-Rich	71.17	13.79	10.62	2.65	0.69	98.92
H_2S-Lean	64.68	21.48	10.03	2.14	0.51	98.84

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

The free energy minimization method for calculating chemical equilibrium is convenient especially for handling multi-component multi-reaction systems. With this method individual equilibria are not considered, as such. Rather, the possible product species are indicated and the distribution of these species is determined using a completely general mathematical technique to give the minimum free energy for the system. The mathematical procedure requires no prior knowledge of the chemistry of the system nor does it require accurate initial guesses.

A computer program which calculates chemical equilibrium by the free energy minimization method was obtained and tested by several examples. The results of the program agree with equilibrium data in the literature.

The program was modified to enable the user to make process equilibrium calculations at constant temperature and pressure or constant enthalpy and pressure. The thermodynamic data file was expanded. The program was made more flexible in that any species could be included or excluded, declared inert or active at any stage in the process calculations. Condensed species could be removed from the reaction mixture.

The modified free energy minimization program was convenient to use, and proved to be successful in conducting the Claus process study.

From the Claus process investigation, the following conclusions can be drawn:

1. About thirty compounds produced in the Claus process have concentrations exceeding 0.1 ppmv and should be included in any accurate Claus process calculations.
2. All sulfur polymers should be considered in Claus process calculations. Their neglect can cause up to 16% difference in total sulfur concentration in the tail gas.
3. Certain guidelines need to be drawn to take care of kinetic limitations to the reactions of some compounds. Kinetic limitations to CO, COS, CO_2, H_2, H_2O, H_2S and SO_2 reactions in condensers and preheaters can be accommodated by treating them as inert.
4. Equilibrium concentrations of COS and CS_2 in the furnace product gas are much below observed plant data which mean that kinetic limitations are important.
5. The presence of impurities in the acid gas feed causes a reduction in furnace sulfur conversion, a reduction in overall plant sulfur recovery, and an increase in sulfur emissions in the tail gas. Impurities generally increase the volume of process gas leading to a larger Claus plant size.
6. Acid gas ammonia impurity seems to totally burn to nitrogen. The equilibrium concentrations of catalyst poisonous

compounds HCN, NH_3 and NO_x in the furnace product gas are less than 1 ppmv.

7. A fourth reactor in the Claus process can increase the overall sulfur recovery by about 0.69%. This might not be enough to justify the cost of adding it.

Recommendations

The Modified free energy minimization computer program is a general purpose program. It can be further improved and modified to do any particular process calculations. Before using the program the thermodynamic data file will have to be checked to see if it includes all possible reaction species. If it does not, then the thermodynamic data will have to be obtained first. Without any doubt the present thermodynamic data file needs to be expanded.

Currently the program assumes that gases are ideal and that interactions between phases are negligible. A major improvement to the program would be to use an equation of state to allow for non-ideal conditions. Accommodation of phase interactions in free energy minimization techniques needs to be studied.

From the Claus process study the following recommendations for further work are made:

1. The computer program should be used to study an operating Claus plant. The program equilibrium results should be compared against plant data and the stages that do not seem to operate at equilibrium should be identified. The reasons for not reaching equilibrium should be examined. The

computer program should be modified if it is to be used for plant simulation.

2. The kinetics of COS and CS_2 reactions in the Claus furnace need to be studied. A method, theoretical or empirical, to simulate COS and CS_2 production in the furnace need to be developed and incorporated in the program.
3. The present computer program needs to be modified to handle different Claus process flow schemes. The program can be expanded to conduct equipment design calculations.
4. The possible use of the computer program in Claus plants optimization and/or monitoring should be explored.

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APPENDIX A

COMPUTER PROGRAM INPUT FOR THE BASE CASE

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          **********  EQUILIBRIUM CALCULATIONS FOR THE CLAUS PROCESS  **********
          ***************************  FURNACE  ******************************
REACTANTS
H    2. S      1.                  00       0.90710          G311.0   F
C    1. O      2.                  00       0.06500          G311.0   F
C    1. H      4.                  00       0.0C380          G311.0   F
H    2. C      1.                  00       0.02410          G311.0   F
O    2.                            00       0.23C78          G297.22  G
N    2.                            00       0.76004          G297.22  C
H    2. O      1.                  00       0.00918          G297.22  O

CMIT          C4H10(I)       H2O2           C2H7NO(L)      C5H12(I)
CMIT          CH             C3O2           N              O3
OMIT          CN2            C2H            C2N            HO2
CMIT          NH             NH2            N3             C2O
CMIT          CH2            CH2O           CN             H2S(L)
OMIT          C4H11NO2(L)    H2O(L)         HCO            HNO
OMIT          NCO            N2O            H2O(S)         NO3
OMIT          N2O4           N2O5           C5H12(N)       N2O
OMIT          HNCO           N2H4           H2O2           HNO2
CMIT          C(S)           C              C2             C3
OMIT          C4             C5             CNN            S(S)
NAMELISTS
 &INPT2 HP=T,P=1.429,CF=T,MIX=1.910920,OFNEXT=1.910920,
 TRACE=1.E-15 &END
          ***************************  CCNDENSER # 1  ***************************
MOD INERT     COS            CO2            H2
MOD INERT     H2C            H2S            SO2
MOD OMIT      CH4            CH3
INSERT        S(L)
NAMELISTS
 &INPT2 TP=T,P=1.3609,T=417,
 TRACE=1.E-15 &END
          ***************************  REHEATER # 1  ****************************
MOD REMOVE    S(L)
NAMELISTS
 &INPT2 TP=T,P=1.3269,T=502,
 TRACE=1.E-15 &END
          ***************************  REACTOR # 1  *****************************
MCD ACTIVE    COS            CO2            H2
MCD ACTIVE    H2C            H2S            SO2
NAMELISTS
 &INPT2 HP=T,P=1.2929,
 TRACE=1.E-15 &END
          ***************************  CONDENSER # 2  ***************************
MOD INERT     COS            CO2            H2
MOD INERT     H2C            H2S            SO2
NAMELISTS
 &INPT2 TP=T,P=1.2248,T=417,
 TRACE=1.E-15 &END
```

```
            ***************************  REHEATER # 2  ***************************
MOD REMOVE     S(L)
NAMELISTS
 &INPT2 TP=T,P=1.1908,T=490,
 TRACE=1.E-15 &END
            ***************************  REACTOR # 2  ****************************
MOD ACTIVE     COS            CO2            H2
MOD ACTIVE     H2O            H2S            SO2
NAMELISTS
 &INPT2 HP=T,P=1.1568,
 TRACE=1.E-15 &END
            ***************************  CONDENSER # 3  **************************
MOD INERT      COS            CO2            H2
MOD INERT      H2O            H2S            SO2
NAMELISTS
 &INPT2 TP=T,P=1.0887,T=417,
 TRACE=1.E-15 &END
            ***************************  REHEATER # 3  ***************************
MOD OMIT       C2H6           C3H8           C4H10(N)
MOD OMIT       C2H2           C2H4           C2N2           HCN
MOD OMIT                      CS2            CS             SN
MOD OMIT       CC
MOD REMOVE     S(L)
NAMELISTS
 &INPT2 TP=T,P=1.0551,T=458,
 TRACE=1.E-15 &END
            ***************************  REACTOR # 3  ****************************
MOD ACTIVE     H2O            H2S            SO2
MOD ACTIVE     COS            CO2            H2
NAMELISTS
 &INPT2 HP=T,P=1.0207,
 TRACE=1.E-15 &END
            ***************************  CONDENSER # 4  **************************
MOD INERT      COS            CO2            H2
MOD INERT      H2O            H2S            SO2
NAMELISTS
 &INPT2 TP=T,P=1.0000,T=417,
 TRACE=1.E-15 &END
            ***************************    TAIL GAS    ***************************
MOD REMOVE     S(L)
NAMELISTS
 &INPT2 TP=T,P=1.0000,T=417,
 TRACE=1.E-15&END
******************  END OF CALCULATIONS - ALI G. MAADAH   *********************
```

APPENDIX B

COMPUTER PROGRAM OUTPUT FOR THE BASE CASE

```
          **********  EQUILIBRIUM CALCULATIONS FOR THE CLAUS PROCESS  **********

          **************************   FURNACE   ******************************

REACTANTS
H    2.0000  S    1.0000      0.0          0.0      00  0.0       0.907100          0.0   G    311.000     F     0.0
C    1.0000  O    2.0000      0.0          0.0      00  0.0       0.065000          0.0   G    311.000     F     0.0
C    1.0000  H    4.0000      0.0          0.0      00  0.0       0.003800          0.0   G    311.000     F     0.0
H    2.0000  O    1.0000      0.0          0.0      00  0.0       0.024100          0.0   G    311.000     F     0.0
O    2.0000       0.0         0.0          0.0      00  0.0       0.230780          0.0   G    297.220     O     0.0
N    2.0000       0.0         0.0          0.0      00  0.0       0.760040          0.0   G    297.220     O     0.0
H    2.0000  O    1.0000      0.0          0.0      00  0.0       0.009180          0.0   G    297.220     O     0.0
OMIT              C4H10(I)         H2O2            C2H7NO(L)          C5H12(I)
OMIT              CH               C3O2            N                  O3
OMIT              CN2              C2H             C2N                HO2
OMIT              NH               NH2             N3                 C2O
OMIT              CH2              CH2O            CN                 H2S(L)
OMIT              C4H11NO2(L)      H2O(L)          HCO                HNO
OMIT              NCO              N2O             H2O(S)             NO3
OMIT              N2O4             N2O5            C5H12(N)           N2O
OMIT              HNCO             N2H4            H2O2               HNO2
OMIT              C(S)             C               C2                 C3
OMIT              C4               C5              CNN                S(S)
NAMELISTS

SPECIES BEING CONSIDERED IN THIS SYSTEM
    J 6/69  CH3                J 3/61  CH4               J 9/65  CO               J 3/61  COS              J 9/65  CO2
    J 6/61  CS2                J12/62  CS                J 3/61  C2H2             J 9/65  C2H4             L 5/72  C2H6
    J 3/61  C2N2               AGM001  C3H8              AGM001  C4H10(N)         J 9/65  H                L12/69  HCN
    J 6/63  HNO3               J 3/61  H2                J 3/61  H2O              J12/65  H2S              J12/65  H2S2
    J 9/65  NH3                J 6/63  NO                J 9/64  NO2              J 9/65  N2               J 6/62  O
    J12/70  OH                 J 9/65  O2                J12/65  S(L)             J 6/71  S                J 6/67  SH
    J 6/61  SN                 J 6/71  SO                J 6/61  SO2              J 9/65  SO3              J12/65  S2O
    J12/65  S2                 AGM002  S3                AGM002  S4               AGM002  S5               AGM002  S6
    AGM002  S7                 J 6/64  S8

CF =    1.910920
                          EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                      HPP(2)                   HPP(1)                  HSUBO
(KG-MOL)(DEG K)/KG       -0.17472676E+03         -0.14935472E+02         -0.69829193E+02

KG-ATOMS/KG                  BOP(I,2)                 BOP(I,1)                  BO(I)
      H                   0.568566190-01           0.101913130-02           0.202012060-01
      S                   0.266168350-01           0.0                      0.914378740-02
      C                   0.171380180-02           0.0                      0.588749170-03
      O                   0.429162640-02           0.149338600-01           0.112778910-01
      N                   0.0                      0.542626080-01           0.356215580-01

PT       H         S         C         O         N
 1    -10.862   -11.360   -15.742   -24.783   -13.154    16.000
```

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                                   THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

                                                    PRESSURES

                                                                          WT FRACTION   ENERGY    STATE    TEMP     DENSITY
          CHEMICAL FORMULA                                                (SEE NOTE)    CAL/MOL            DEG K     G/CC
FUEL     H  2.00000   S  1.00000                                           0.90710    -4774.699    G      311.00   0.0
FUEL     C  1.00000   O  2.00000                                           0.06500   -93933.312    G      311.00   0.0
FUEL     C  1.00000   H  4.00000                                           0.00380   -17785.781    G      311.00   0.0
FUEL     H  2.00000   O  1.00000                                           0.02410   -57692.078    G      311.00   0.0
OXIDANT O  2.00000                                                         0.23078       -6.614    G      297.22   0.0
OXIDANT N  2.00000                                                         0.76004       -6.536    G      297.22   0.0
OXIDANT H  2.00000    O  1.00000                                           0.00918   -57802.723    G      297.22   0.0

        O/F=  1.9109    PERCENT FUEL=  34.3534    EQUIVALENCE RATIO= 2.6216    PHI=2.9313    REACTANT DENSITY=  0.0


THERMODYNAMIC PROPERTIES


P, ATM              1.4290
T, DEG K              1524
RHO, G/CC       3.45943-4
H, CAL/G            -138.8
S, CAL/(G)(K)       2.0564

M, MOL WT           30.274
(DLV/DLP)T        -1.00480
(DLV/DLT)P          1.0718
CP, CAL/(G)(K)      0.4029
TOTAL MOLES       0.033032


MOLE FRACTIONS


CH3             1.1445-14
CH4             4.3004-12
CO              4.69535-3
COS             1.56654-4
CO2             1.29310-2
CS2             6.73294-7
CS              3.89476-8
H               3.47463-6
HCN             2.1624-10
H2              3.18649-2
H2O             2.33758-1
H2S             3.96436-2
H2S2            1.81484-4
NH3             3.46795-7
NO              4.25367-8
NO2             8.3756-15
N2              5.39200-1
O               7.3599-11
OH              7.67168-7
C2              2.5203-10
```

```
S              1.38543-5
SH             6.65859-4
SN             1.64331-7
SO             1.00493-3
SO2            3.69639-2
SO3            2.33887-8
S2O            1.97895-3
S2             9.66839-2
S3             2.10995-4
S4             1.28522-6
S5             3.52798-8
S6             5.3364-10
S7             1.5802-11
S8             5.3063-14

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS

C2H2          C2H4          C2H6          C2N2          C3H8          C4H10(N)     HNO3          S(L)

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS
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```
          **********  EQUILIBRIUM CALCULATIONS FOR THE CLAUS PROCESS  **********

          ***************************  CONDENSER # 1  ***************************

MOD INSERT      COS              CO2              H2
MOD INSERT      H2O              H2S              SO2
MOD OMIT        CH4              CH3
INSERT          S(L)
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

OF =    0.0
                        EFFECTIVE FUEL         EFFECTIVE OXIDANT           MIXTURE
ENTHALPY                    HPP(2)                  HPP(1)                   HSUB0
(KG-MOL)(DEG K)/KG     -0.69829239E+02         0.0                      -0.69829239E+02

KG-ATOMS/KG                 BOP(I,2)                BOP(I,1)                  BO(I)
       H               0.34158545D-04          0.0                       0.34158545D-04
       S               0.66068042D-02          0.0                       0.66068042D-02
       C               0.15511960D-03          0.0                       0.15511960D-03
       O               0.25368790D-03          0.0                       0.25368790D-03
       N               0.35621558D-01          0.0                       0.35621558D-01
       COS             0.64958532D-05          0.0                       0.64958532D-05
       CO2             0.42713371D-03          0.0                       0.42713371D-03
       H2              0.10525554D-02          0.0                       0.10525554D-02
       H2O             0.77214672D-02          0.0                       0.77214672D-02
       H2S             0.13095012D-02          0.0                       0.13095012D-02
       SO2             0.12209862D-02          0.0                       0.12209862D-02

PT       H         S         C         O         N        COS      CO2       H2       H2O       H2S      SO2
 1    -13.543   -4.037   -11.483   -49.279   -11.708   -76.141 -143.369  -18.914   -93.689   -33.648 -118.588    20.000
```

```
                    THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                              TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES


P, ATM            1.3609
T, DEG K             417
RHO, G/CC     1.33644-3
H, CAL/G          -552.0
S, CAL/(G)(K)     1.5623

M, MOL WT         33.602
(DLV/DLP)T     -1.00017
(DLV/DLT)P        1.0045
CP, CAL/(G)(K)    0.2854
TOTAL MOLES     0.036267


MOLE FRACTIONS


CO              4.27715-3
COS             1.79112-4
CO2             1.17775-2
CS2             1.4676-11
H2              2.90224-2
H2O             2.12906-1
H2S             3.61072-2
H2S2            4.70795-4
NH3             9.05772-8
N2              4.91101-1
S(L)            1.79424-1
SO              4.8051-13
SO2             3.36666-2
SO3             8.73020-4
S2O             9.87888-5
S2              1.29074-8
S3              1.52665-9
S4              1.17139-9
S5              4.65248-7
S6              1.59845-5
S7              8.46168-6
S8              7.21895-5
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


CS           C2H2         C2H4         C2H6         C2N2         C3H8         C4H10(N)     H            HCN          HNO3
NO           NO2          O            OH           O2           S            SH           SN
```

```
          **********  ECUILIBRIUM CALCULATICNS FOR THE CLAUS PROCESS  **********

          **************************  REHEATER # 1  **************************

MCC REMCVE     S(L)

S(L)         REMOVEC:  0.6507172D-02 KG-MOL/KG (  0.2086459D+00 KG/KG) OF CRIGINAL PROCESS FEED.
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =    C.C
                           EFFECTIVE FUEL         EFFECTIVE OXIDANT           MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                   HSUB0
(KG-MCL)(DEG K)/KG        -0.51605347E+03          0.0                    -C.51605347E+03

KG-ATCMS/KG                   BOP(I,2)                BOP(I,1)                 BO(I)
      H                    0.43164679D-04          0.0                     0.43164679D-04
      S                    0.12590141D-03          0.0                     0.12590141D-03
      C                    C.19601795D-03          0.0                     0.19601795D-03
      C                    0.32057445D-03          0.0                     C.32057445D-03
      N                    0.45013425D-01          0.0                     0.45013425D-01
      CCS                  0.82085293D-05          0.0                     0.82085293C-05
      CC2                  0.53975044D-03          0.0                     0.53975044D-03
      H2                   0.133CC688D-C2          0.0                     C.13300688D-02
      H20                  0.97572848D-02          0.0                     0.97572848D-02
      H2S                  0.16547601D-02          0.0                     C.16547601D-02
      SC2                  0.15429076D-02          0.0                     0.15429076D-02

PT       H          S        C         O         N        COS      CO2       H2       H20       H2S      SO2
 1    -12.756    -5.357  -13.008   -42.609   -11.834   -69.756 -124.491  -19.165   -82.170   -32.950 -104.449    20.000
```

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                                      THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                                 TEMPERATURE AND PRESSURE


THERMODYNAMIC PROPERTIES


P, ATM              1.3269
T, DEG K               502
RHO, G/CC       8.56377-4
H, CAL/G            -683.1
S, CAL/(G)(K)       1.9396

M, MOL WT           26.585
(DLV/DLP)T        -1.00001
(DLV/DLT)P          1.0004
CP, CAL/(G)(K)      0.2917
TOTAL MOLES       0.037615


MOLE FRACTIONS


CO              5.21117-3
COS             2.18225-4
CO2             1.43494-2
CS2             1.2630-10
H2              3.53601-2
H2O             2.59399-1
H2S             4.39921-2
H2S2            5.73544-4
NH3             1.51024-7
N2              5.98345-1
SH              2.2502-13
SO              2.0468-10
SO2             4.10185-2
SO3             8.92516-4
S2O             6.33809-4
S2              8.16017-7
S3              4.38688-8
S4              1.16978-8
S5              5.12852-7
S6              3.09762-6
S7              8.63423-7
S8              1.36073-6
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS

CS            C2H2          C2H4          C2H6          C2N2          C3H8          C4H10(N)      H             HCN           HNO3
NO            NO2           C             OH            O2            S(L)          S             SN
```

```
          **********  EQUILIBRIUM CALCULATICNS FOR THE CLAUS PROCESS  **********

          *****************************  REACTOR # 1  *****************************

MOC ACTIVE      COS              CO2              H2
MCD ACTIVE      H2O              H2S              SO2
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =    C.C
                              EFFECTIVE FUEL          EFFECTIVE OXIDANT              MIXTURE
ENTHALPY                        HPP(2)                    HPP(1)                      HSUBO
(KG-MOL)(DEG K)/KG          -0.34373730E+03           0.0                       -0.34373730E+03

KG-ATOMS/KG                     BOP(I,2)                  BOP(I,1)                     BO(I)
      H                       0.255273920-01            0.0                        0.255273920-01
      S                       C.333177760-C2            0.0                        0.333177760-02
      C                       0.743976920-C3            0.0                        C.743976920-03
      O                       0.142513840-01            0.0                        C.142513840-01
      N                       0.450134250-01            0.0                        C.450134250-01

PT        H          S          C          O          N
 1     -13.695     -5.414   -19.177    -42.773    -12.035     24.000
```

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                    THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

                                             PRESSURES

THERMODYNAMIC PROPERTIES


P, ATM             1.2929
T, DEG K              637
RHO, G/CC      6.70926-4
H, CAL/G           -683.1
S, CAL/(G)(K)      1.9751

M, MOL WT          27.140
(DLV/DLP)T      -1.00182
(DLV/DLT)P         1.0538
CP, CAL/(G)(K)     0.4194
TOTAL MOLES      0.036846


MOLE FRACTIONS


CO             5.11788-8
COS            4.02246-6
CO2            2.01877-2
CS2            1.8484-10
H2             1.44509-5
H2O            3.15856-1
H2S            3.02139-2
H2S2           3.26480-4
NH3            1.25860-9
N2             6.10839-1
SH             2.0735-10
SO             3.3272-10
SO2            1.52491-2
SO3            2.1136-12
S2O            5.35619-5
S2             8.41450-4
S3             8.25818-5
S4             3.09536-5
S5             5.86735-4
S6             2.49982-3
S7             1.50669-3
S8             1.70807-3

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


CS          C2H2        C2H4        C2H6        C2N2        C3H8        C4H10(N)    H           HCN         HNO3
NO          NO2         C           OH          O2          S(L)        S           SN
```

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          **********  ECUILIBRIUM CALCULATICNS FOR THE CLAUS PROCESS  **********

          ***************************  CCNDENSER # 2  ***************************

MOD INERT       COS             CO2             H2
MOC INERT       H2O             H2S             SO2
NAMELISTS

NC INFT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

OF =    C.C
                            EFFECTIVE FUEL           EFFECTIVE OXIDANT             MIXTURE
ENTHALPY                        HPP(2)                    HPP(1)                   HSUBO
(KG-MOL)(DEG K)/KG         -0.34373730E+03            0.0                    -0.34373730E+03

KG-ATCMS/KG                     BOP(I,2)                 BOP(I,1)                  BO(I)
      H                     0.24058685D-04            0.0                     C.24058685D-04
      S                     0.16565193D-02            0.0                     0.16565193D-02
      C                     0.18857108D-08            0.0                     C.18857108D-08
      O                     0.19754054D-05            0.0                     0.19754054D-05
      N                     0.45013425D-01            0.0                     0.45013425D-01
      CCS                   0.14820971D-06            0.0                     C.14820971D-06
      CC2                   0.74382682D-03            0.0                     0.74382682D-03
      H2                    0.53245136D-06            0.0                     0.53245136D-06
      H2O                   0.11637885D-01            0.0                     C.11637885D-01
      H2S                   0.11132494D-02            0.0                     C.11132494D-02
      SC2                   0.56186078D-03            0.0                     0.56186078D-03

PT       H         S         C         O         N        COS       CO2        H2       H2O       H2S       SO2
 1    -14.366    -3.548   -21.010   -51.387   -11.749   -80.239  -143.132   -26.821   -93.596   -34.128  -119.682     30.000
ADC S(L)
 1    -13.874    -4.037   -21.493   -50.899   -11.746   -80.233  -143.126   -26.815   -93.591   -34.122  -119.676      6.000
```

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                         THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                     TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES


P, ATM               1.2248
T, DEG K                417
RHO, G/CC       9.78473-4
H, CAL/G           -753.2
S, CAL/(G)(K)      1.8437

M, MOL WT          27.336
(DLV/DLP)T       -1.00014
(DLV/DLT)P         1.0035
CP, CAL/(G)(K)     0.2956
TOTAL MOLES      0.038176


MOLE FRACTIONS


CO              4.93950-8
COS             3.88226-6
CO2             1.94841-2
H2              1.39472-5
H2O             3.04847-1
H2S             2.91609-2
H2S2            3.15038-4
NH3             4.18667-8
N2              5.89550-1
S(L)            4.17482-2
SO             1.2337-13
SO2             1.47176-2
SO3             8.77687-6
S2O             2.53645-5
S2              1.67479-8
S3              1.98089-9
S4              1.51993-9
S5              6.03679-7
S6              2.07406-5
S7              1.09794-5
S8              9.36689-5

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


CS2          CS           C2H2         C2H4         C2H6         C2N2         C3H8         C4H10(N)     H            HCN
HNO3         NO           NO2          O            OH           O2           S            SH           SN
```

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          **********  ECUILIBRIUM CALCULATIONS FOR THE CLAUS PROCESS  **********

          ***************************  REHEATER # 2  ***************************

MOD REMCVE      S(L)

S(L)         REMOVED:  0.1261248D-02 KG-MOL/KG (  0.4044065D-01 KG/KG) OF ORIGINAL PROCESS FEED.
                       0.1593785D-02 KG-MOL/KG (  0.5110310D-01 KG/KG) OF CURRENT STREAM.
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =    C.C
                        EFFECTIVE FUEL          EFFECTIVE OXIDANT             MIXTURE
ENTHALPY                   HPP(2)                     HPP(1)                   HSUBO
(KG-MCL)(CEG K)/KG     -0.43317358E+03          0.0                      -0.43317358E+03

KG-ATCMS/KG                BOP(I,2)                BOP(I,1)                  BO(I)
      H                 0.25354373D-04          0.0                       0.25354373D-04
      S                 0.66113313D-04          0.0                       0.66113313D-04
      C                 C.19872663D-C8          0.0                       0.19872663D-08
      C                 0.20817914D-05          0.0                       C.20817914D-05
      N                 0.47437636D-01          0.0                       0.47437636D-01
      CCS               0.15619159D-06          0.0                       0.15619159D-06
      CC2               0.78388582D-03          0.0                       C.78388582D-03
      H2                0.56112667D-06          0.0                       0.56112667D-06
      H2O               0.12264646D-C1          0.0                       C.12264646D-01
      H2S               0.11732037D-02          0.0                       0.11732037D-02
      SC2               0.59211994D-03          0.0                       0.59211994D-03

PT       H        S        C        O        N       COS      CO2       H2       H2O      H2S      SO2
 1    -13.582   -4.794  -21.274  -46.590  -11.857  -74.610 -126.512  -27.035  -83.453  -33.506 -107.231    32.000
```

```
                                  THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                             TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES


P, ATM              1.1908
T, DEG K               490
RHO, G/CC       7.68195-4
H, CAL/G            -774.4
S, CAL/(G)(K)       1.9740

M, MOL WT           25.938
(DLV/DLP)T        -1.00000
(DLV/DLT)P          1.0001
CP, CAL/(G)(K)      0.2962
TOTAL MOLES       0.038553


MOLE FRACTIONS


CO              5.15459-8
COS             4.05131-6
CO2             2.03325-2
CS2             5.3038-14
H2              1.45545-5
H2O             3.18121-1
H2S             3.04307-2
H2S2            3.28796-4
NH3             1.72485-8
N2              6.15221-1
SH              7.9425-14
SO              7.0071-12
SO2             1.53584-2
SO3             1.08518-7
S2O             5.36206-5
S2              1.26456-6
S3              1.11510-7
S4              5.03325-8
S5              4.28426-6
S6              4.74989-5
S7              2.13220-5
S8              6.13971-5
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


CS            C2H2          C2H4          C2H6          C2N2          C3H8          C4H10(N)     H             HCN           HNO3
NO            NO2           C             OH            O2            S(L)          S            SN
```

```
          **********  EGUILIBRIUM CALCULATICNS FOR THE CLAUS PRCCESS  **********

          ***************************  REACTOR # 2  ****************************

MOC ACTIVE     COS            CO2            H2
MCC ACTIVE     H2C            H2S            SO2
NAMELISTS

NC INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =   C.C
                         EFFECTIVE FUEL           EFFECTIVE OXIDANT             MIXTURE
ENTHALPY                     HPP(2)                    HPP(1)                    HSUBO
(KG-MCL)(CEG K)/KG      -0.38971777E+03            0.0                     -C.38971777E+03

KG-ATCMS/KG                 BOP(I,2)                  BOP(I,1)                  BO(I)
      H                  0.26902177D-01            0.0                        C.26902177D-01
      S                  0.18315932D-02            0.0                        0.18315932D-02
      C                  0.78404400D-03            0.0                        0.78404400D-03
      O                  0.15018896D-01            0.0                        C.15018896D-01
      N                  0.47437636D-01            0.0                        C.47437636D-01

PT      H        S        C        O        N
 1    -14.996   -4.605  -21.051  -49.663  -11.917   25.000
```

```
                                   THERMODYNAMIC EQUILIBRIUM COMBUSTICN PRCPERTIES AT ASSIGNED

                                                          PRESSURES

THERMCDYNAMIC PROPERTIES


P, ATM              1.1568
T, CEG K               524
RHC, G/CC       7.02177-4
H, CAL/G           -774.4
S, CAL/(G)(K)      1.9793

M, MCL WT          26.107
(CLV/CLP)T       -1.C0055
(CLV/CLT)P         1.0204
CP, CAL/(G)(K)     0.3579
TOTAL MCLES      0.038303


MOLE FRACTICNS


CC              5.7789-1C
COS             2.61C92-7
CO2             2.04691-2
CS2             7.6396-13
H2              8.59C71-7
H2C             3.42578-1
H2S             8.55150-3
H2S2            4.30330-5
NH3             1.3162-10
N2              6.19238-1
SH              2.7079-13
SC              4.8438-13
SO2             4.29328-3
SO3             2.8837-14
S2C             1.76933-6
S2              1.67546-5
S3              2.15653-6
S4              1.30470-6
S5              1.02472-4
S6              1.22175-3
S7              8.42009-4
S8              2.63768-3
ACCITICNAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS

CS          C2H2        C2H4        C2H6        C2N2        C3H8        C4H10(N)    H           HCN         HNO3
NO          NO2         O           OH          O2          S(L)        S           SN
```

```
          **********  EQUILIBRIUM CALCULATICNS FOR THE CLAUS PROCESS  **********

          ***************************  CONDENSER # 3  ***************************

MOC INERT      COS            CO2            H2
MOC INERT      H2O            H2S            SO2
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =    0.C
                         EFFECTIVE FUEL          EFFECTIVE OXIDANT            MIXTURE
ENTHALPY                     HPP(2)                   HPP(1)                   HSUBO
(KG-MCL)(CEG K)/KG      -0.38971777E+03           0.0                   -C.38971777E+03

KG-ATCMS/KG                 BOP(I,2)                 BOP(I,1)                 BO(I)
      H                  0.32966079D-05           0.0                    0.32966079D-05
      S                  0.13395863D-02           0.0                    0.13395863D-02
      C                  0.99999998D-17           0.0                    0.99999998D-17
      C                  0.67770975D-07           0.0                    0.67770975D-07
      N                  0.47437636D-01           0.0                    0.47437636D-01
      CCS                0.10000665D-07           0.0                    0.10000665D-07
      CC2                0.78403400D-03           0.0                    C.78403400D-03
      H2                 0.32905191D-07           0.0                    0.32905191D-07
      H2O                0.13121857D-01           0.0                    C.13121857D-01
      H2S                0.32755026D-03           0.0                    C.32755026D-03
      SC2                0.16444659D-03           0.0                    0.16444659D-03

PT      H        S        C        O        N        COS      CO2       H2       H2O      H2S      SO2
 1    -15.394   -3.593  -36.999  -54.611  -11.802  -83.093 -143.237  -29.763  -93.634  -35.509 -121.068   49.000
ADC S(L)
 1    -14.947   -4.037  -37.885  -53.721  -11.8C0  -83.C88 -143.233  -29.758  -93.630  -35.505 -121.064    6.000
```

```
                         THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                    TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES


P, ATM             1.0887
T, DEG K              417
RHO, G/CC      8.34572-4
H, CAL/G           -809.9
S, CAL/(G)(K)      1.9083

M, MOL WT          26.230
(DLV/DLP)T       -1.00015
(DLV/DLT)P         1.0036
CP, CAL/(G)(K)     0.3036
TOTAL MOLES      0.039416


MOLE FRACTIONS


COS            2.53711-7
CO2            1.98905-2
H2             8.34785-7
H2O            3.32894-1
H2S            8.30976-3
H2S2           4.18138-5
NH3            1.80118-9
N2             6.01732-1
S(L)           3.28145-2
SO             8.3322-15
SO2            4.17191-3
SO3            2.09686-9
S2O            1.71302-6
S2             1.90172-8
S3             2.24930-9
S4             1.72588-9
S5             6.85477-7
S6             2.35510-5
S7             1.24671-5
S8             1.06361-4
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


CO            CS2           CS            C2H2          C2H4          C2H6          C2N2          C3H8          C4H10(N)      H
HCN           HNO3          NO            NO2           O             OH            O2            S             SH            SN
```

```
          **********  ECUILIBRIUM CALCULATICNS FOR THE CLAUS PROCESS  **********

          ***************************  REHEATER # 3  ***************************

MOD CMIT        C2H6            C3H8            C4H10(N)
MOC CMIT        C2H2            C2H4            C2N2            HCN
MCD CMIT                        CS2             CS              SN
MOD CMIT        CO
MCC REMCVE      S(L)

S(L)         REMOVED:  0.9712824D-03 KG-MOL/KG (  0.3114319D-01 KG/KG) OF ORIGINAL PROCESS FEED.
                       C.1293468D-02 KG-MOL/KG (  0.4147375D-01 KG/KG) OF CURRENT STREAM.
NAMELISTS

NO INPT2 VALUE GIVEN FOR CF, EQRAT, FA, CR FPCT

CF =    C.C
                          EFFECTIVE FUEL         EFFECTIVE OXIDANT              MIXTURE
ENTHALPY                     HPP(2)                  HPP(1)                       HSUBO
(KG-MCL)(CEG K)/KG       -0.45227246E+03          C.0                      -C.45227246E+03

KG-ATCMS/KG                 BOP(I,2)                BOP(I,1)                      BO(I)
      H                  0.34392464D-05           0.0                       0.34392464D-05
      S                  0.48113929D-04           0.0                       C.48113929D-04
      SC2                0.17156190D-03           0.0                       0.17156190D-03
      C                  0.70703306D-07           0.0                       0.70703306D-07
      N                  0.49490179D-01           0.0                       C.49490179D-01
      CCS                0.10433376D-07           0.0                       0.10433376D-07
      CO2                0.81795777D-03           0.0                       0.81795777D-03
      H2                 0.34328940D-07           0.0                       0.34328940D-07
      H2O                0.13689617D-01           0.0                       0.13689617D-01
      H2S                0.34172278D-03           0.0                       0.34172278C-03

PT       H         S        SO2        O         N        COS       CO2        H2        H2O       H2S
 1    -14.784    -4.476 -113.583  -51.580   -11.868   -79.705 -133.247   -29.894   -87.540   -35.135    22.000
```

```
                    THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                              TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES

P, ATM             1.0551
T, DEG K              458
RHO, G/CC       7.05864-4
H, CAL/G           -834.3
S, CAL/(G)(K)      2.0066

M, MOL WT          25.142
(DLV/DLP)T       -1.00000
(DLV/DLT)P         1.0001
CP, CAL/(G)(K)     0.3016
TOTAL MOLES      0.039774

MOLE FRACTIONS

COS             2.62317-7
CO2             2.05652-2
H2              8.63103-7
H2O             3.44186-1
H2S             8.59163-3
H2S2            4.32334-5
NH3             1.02419-9
N2              6.22144-1
SH             2.8099-15
SO             6.1881-14
SO2             4.31343-3
SO3            3.9637-11
S2O             1.77763-6
S2              2.66258-7
S3              2.66237-8
S4              1.49594-8
S5              2.36915-6
S6              4.14926-5
S7              2.00405-5
S8              8.97383-5
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS

H            HNO3         NO           NO2          O            OH           O2           S(L)         S
```

```
          **********  EQUILIBRIUM CALCULATIONS FOR THE CLAUS PROCESS  **********

          ***************************  REACTOR # 3  ****************************

MOC ACTIVE     H2O           H2S            SO2
MCC ACTIVE     COS           CO2            H2
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =    C.C
                         EFFECTIVE FUEL        EFFECTIVE OXIDANT           MIXTURE
ENTHALPY                     HPP(2)                HPP(1)                   HSUBO
(KG-MCL)(DEG K)/KG     -0.41983984E+03         0.0                    -0.41983984E+03

KG-ATCMS/KG                 BOP(I,2)              BOP(I,1)                  BO(I)
      H                0.28066187D-01          0.0                    C.28066187D-01
      S                0.56140905D-03          0.0                    0.56140905D-03
      C                0.81796820D-03          0.0                    C.81796820D-03
      C                0.15668737D-01          0.0                    C.15668737D-01
      N                C.49490179D-01          0.0                    C.49490179D-01

PT       H         S         C         O         N
 1    -15.542    -4.281   -22.374   -54.468   -11.896    22.000
```

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                              THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED
                                                    PRESSURES

THERMODYNAMIC PROPERTIES


P, ATM             1.0207
T, DEG K              467
RHO, G/CC      6.70754-4
H, CAL/G           -834.3
S, CAL/(G)(K)      2.0098

M, MOL WT          25.185
(DLV/DLP)T       -1.00018
(DLV/DLT)P         1.0077
CP, CAL/(G)(K)     0.3284
TOTAL MOLES      0.039706


MOLE FRACTIONS


COS              3.37432-8
CO2              2.06004-2
H2               1.24867-7
H2O              3.50471-1
H2S              2.94291-3
H2S2             7.27925-6
NH3              2.6085-11
N2               6.23202-1
SH               2.3808-15
SO               4.5575-15
SO2              1.47143-3
SO3              1.2026-15
S2O              1.18026-7
S2               8.07331-7
S3               1.03808-7
S4               7.29430-8
S5               1.28201-5
S6               2.61565-4
S7               1.64978-4
S8               8.64912-4

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS

H            HNO3           NO            NO2           O             OH            O2            S(L)          S
```

```
          **********  ECUILIBRIUM CALCULATIONS FOR THE CLAUS PROCESS  **********

          ***************************  CCNDENSER # 4  ***************************

MOD INERT       COS              CO2              H2
MOC INERT       H2O              H2S              SC2
NAMELISTS

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

CF =    C.C
                           EFFECTIVE FUEL          EFFECTIVE OXIDANT               MIXTURE
ENTHALPY                       HPP(2)                   HPP(1)                      HSUBO
(KG-MCL)(CEG K)/KG        -0.41983960E+03           0.0                      -0.41983960E+03

KG-ATCMS/KG                   BOP(I,2)                 BOP(I,1)                     BO(I)
      H                    0.57806512D-06           0.0                       C.578C6512D-06
      S                    0.38613050D-03           0.0                       0.38613050D-03
      H2S                  0.11685214D-03           0.0                       C.11685214D-03
      C                    0.46863823D-08           0.0                       0.46863823D-08
      N                    0.4949C179D-01           0.0                       0.49490179D-01
      SC2                  0.58425064D-04           0.0                       0.58425064D-04
      CCS                  0.13398216D-08           0.0                       0.13398216D-08
      CC2                  0.81796686D-03           0.0                       0.81796686D-03
      H2                   0.49580126D-08           0.0                       0.49580126D-08
      H2O                  0.13915947D-01           0.0                       0.13915947D-01

PT       H          S        H2S        O          N        SO2       COS       CO2       H2       H2O
 1    -16.150    -3.768   -36.661   -57.053   -11.841  -122.224   -85.224  -143.316   -31.776   -93.697     24.000
ADD S(L)
 1    -15.880    -4.C37   -36.660   -56.514   -11.841  -122.223   -85.223  -143.315   -31.775   -93.696      5.000
```

```
                              THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                         TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES


P, ATM              1.0000
T, DEG K               417
RHO, G/CC       7.36871-4
H, CAL/G            -850.3
S, CAL/(G)(K)       1.9752

M, MOL WT           25.214
(DLV/DLP)T        -1.00016
(DLV/DLT)P          1.0039
CP, CAL/(G)(K)      0.3079
TOTAL MOLES       0.039998


MOLE FRACTIONS


COS              3.34971-8
CO2              2.04501-2
H2               1.23956-7
H2O              3.47915-1
H2S              2.92144-3
H2S2             7.22598-6
NH3              1.1755-10
N2               6.18656-1
S(L)             8.43030-3
SO2              1.46069-3
SO3              5.3856-13
S2O              1.17165-7
S2               2.12260-8
S3               2.51055-9
S4               1.92634-9
S5               7.65094-7
S6               2.62863-5
S7               1.39151-5
S8               1.18715-4

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


H            HNO3          NO           NO2          C            OH           O2           S            SH           SO
```

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          **********  ECUILIBRIUM CALCULATICNS FOR THE CLAUS PROCESS  **********

          ***************************     TAIL GAS     ***************************

MOD REMCVE     S(L)

S(L)          REMOVED:  0.2427039D-03 KG-MOL/KG (  0.7782057D-02 KG/KG) OF ORIGINAL PROCESS FEED.
                        C.3371964D-C3 KG-MCL/KG (  0.1081186D-01 KG/KG) OF CURRENT STREAM.
NAMELISTS

NO INPT2 VALUE GIVEN FOR CF, EQRAT, FA, OR FPCT

OF =    C.C
                         EFFECTIVE FUEL          EFFECTIVE OXIDANT           MIXTURE
ENTHALPY                    HPP(2)                    HPP(1)                  HSUBO
(KG-MCL)(CEG K)/KG      -0.43940039E+C3           0.0                    -0.43940039E+03

KG-ATCMS/KG                BOP(I,2)                  BOP(I,1)                 BO(I)
      H                  0.58438339D-06           0.0                     C.58438339C-06
      S                  0.49468980D-04           0.0                     0.49468980D-04
      H2S                0.11812934D-03           0.0                     C.11812934D-03
      O                  0.47376046D-08           0.0                     0.47376046D-08
      N                  C.50031108D-01           0.0                     C.50031108D-01
      SC2                0.59063652D-04           0.0                     C.59063652D-04
      CCS                0.13544659D-C8           0.0                     0.13544659D-08
      CC2                0.82690727D-03           0.0                     0.82690727D-03
      H2                 0.50122039D-08           0.0                     0.50122039D-08
      H2O                0.14C68049D-01           0.0                     0.14068049D-01

PT       H          S        H2S        O          N        SO2       COS       CO2       H2       H2O
 1    -15.880    -4.C37   -36.660   -56.514   -11.841  -122.223   -85.223 -143.315  -31.775   -93.696    24.000
```

```
                     THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                 TEMPERATURE AND PRESSURE

THERMODYNAMIC PROPERTIES


P, ATM             1.0000
T, DEG K              417
RHO, G/CC      7.28905-4
H, CAL/G           -860.0
S, CAL/(G)(K)      1.9931

M, MOL WT          24.941
(DLV/DLP)T       -1.00000
(DLV/DLT)P         1.0001
CP, CAL/(G)(K)     0.3011
TOTAL MOLES      0.040094


MOLE FRACTIONS


COS            3.37819-8
CO2            2.06240-2
H2             1.25010-7
H2O            3.50873-1
H2S            2.94628-3
H2S2           7.28741-6
NH3            1.1855-10
N2             6.23916-1
SO2            1.47311-3
SO3            5.4317-13
S2O            1.18163-7
S2             2.14065-8
S3             2.53190-9
S4             1.94271-9
S5             7.71599-7
S6             2.65098-5
S7             1.40334-5
S8             1.19724-4

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.10000E-14 FOR ALL ASSIGNED CONDITIONS


H            HNO3        NO          NO2         O           OH          O2          S(L)        S           SH
SO
```

APPENDIX C

CLAUS PROCESS RESULTS FOR ACID GAS FEEDS WITH CARBON DIOXIDE IMPURITY

TABLE XXIV

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR AN ACID GAS FEED WITH CARBON DIOXIDE IMPURITY (CASE 2)

	Furnace	Condenser #1	Reheater #1	Reactor #1	Condenser #2	Reheater #2
Pressure (atm)	1.4290	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^oK)	1252	417	505	613	417	483
Chemical Species Mole Fractions						
CO	0.012350	0.011522	0.013313	--	--	--
COS	0.002008	0.001873	0.002164	0.000030	0.000029	0.000030
CO_2	0.190166	0.177348	0.204911	0.224124	0.214571	0.225940
CS_2	0.000005	--	--	--	--	--
H_2	0.008486	0.007914	0.009144	0.000007	0.000007	0.000007
H_2O	0.204172	0.190411	0.220004	0.258393	0.247380	0.260487
H_2S	0.042624	0.039751	0.045929	0.021513	0.020596	0.021687
H_2S_2	0.000279	0.000296	0.00341	0.000211	0.000202	0.000213
N_2	0.434922	0.405608	0.468646	0.476655	0.456338	0.480517
S(L)	--	0.134704	--	--	0.050332	--
SH	0.000075	--	--	--	--	--
SO	0.000109	--	--	--	--	--
SO_2	0.032057	0.029896	0.034543	0.010863	0.010400	0.010951
SO_3	--	0.000491	0.000402	--	0.000003	--
S_2O	0.001565	0.000084	0.000594	0.000029	0.000018	0.000029
S_2	0.070823	--	0.000001	0.000438	--	0.000001
S_3	0.000354	--	--	0.000047	--	--
S_4	0.000005	--	--	0.000020	--	--
S_5	--	--	0.000001	0.000519	0.000001	0.000004
S_6	--	0.000017	0.000005	0.002786	0.000021	0.000046
S_7	--	0.000009	0.000002	0.001798	0.000011	0.000021
S_8	--	0.000076	0.000003	0.002569	0.000093	0.000067
Stage Sulfur Recovery %		64.68	--	--	21.48	--
Total Sulfur Recovery %		64.68	--	--	86.16	--

TABLE XXIV (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^{o}K)	507	417	450	455	417	417
Chemical Species Mole Fractions						
CO	--	--	--	--	--	--
COS	0.000002	0.000002	0.000002	--	--	--
CO_2	0.227067	0.222295	0.227842	0.228090	0.227041	0.228253
CS_2	--	--	--	--	--	--
H_2	--	--	--	--	--	--
H_2O	0.278243	0.272396	0.279193	0.283100	0.281799	0.283303
H_2S	0.005500	0.005384	0.005518	0.001939	0.001930	0.001940
H_2S_2	0.000023	0.000022	0.000023	0.000004	0.000004	0.000004
N_2	0.482851	0.472705	0.484500	0.485024	0.482795	0.485371
S(L)	--	0.024350	--	--	0.005308	--
SH	--	--	--	--	--	--
SO	--	--	--	--	--	--
SO_2	0.002758	0.002700	0.002768	0.000968	0.000963	0.000969
SO_3	--	--	--	--	--	--
S_2O	0.000001	0.000001	0.000001	--	--	--
S_2	0.000007	--	--	--	--	--
S_3	0.000001	--	--	--	--	--
S_4	0.000001	--	--	--	--	--
S_5	0.000059	0.000001	0.000002	0.000007	0.000001	0.000001
S_6	0.000832	0.000024	0.000038	0.000167	0.000026	0.000027
S_7	0.000568	0.000013	0.000019	0.000102	0.000014	0.000014
S_8	0.002088	0.000107	0.000094	0.000599	0.000119	0.000120
Stage Sulfur Recovery %		10.03	--	--	2.14	--
Total Sulfur Recovery %		96.19	--	--	98.33	--

TABLE XXV

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR AN ACID GAS FEED WITH CARBON DIOXIDE IMPURITY (CASE 3)

	Furnace	**Condenser #1**	**Reheater #1**	**Reactor #1**	**Condenser #1**	**Reheater #1**
Pressure (atm)	1.4290	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^oK)	883	417	509	561	417	465
Chemical Species Mole Fractions						
CO	0.000539	0.000524	0.000559	--	--	--
COS	0.002160	0.002091	0.002230	0.000025	0.000023	0.000025
CO_2	0.506832	0.490564	0.523201	0.531991	0.506595	0.536424
CS_2	0.000002	--	--	--	--	--
H_2	0.000348	0.000337	0.000359	0.000002	0.000015	0.000015
H_2O	0.12889	0.124753	0.133053	0.171027	0.162862	0.172452
H_2S	0.042882	0.041505	0.044267	0.009245	0.008803	0.009321
H_2S_2	0.000600	0.000580	0.000169	0.000067	0.000064	0.000067
N_2	0.262971	0.254531	0.271464	0.274574	0.261466	0.276862
S(L)	--	0.062565	--	--	0.055613	--
SO	0.000001	--	--	--	--	--
SO_2	0.022875	0.022141	0.023614	0.004665	0.006662	0.004706
SO_3	--	0.000229	0.000098	--	--	--
S_2O	0.000782	0.000069	0.000510	0.000006	0.000005	0.000005
S_2	0.029786	--	0.000002	0.000078	--	--
S_3	0.000782	--	--	0.000010	--	--
S_4	0.000097	--	--	0.000005	--	--
S_5	0.000148	0.000001	0.000002	0.000271	0.000001	0.000003
S_6	0.000085	0.000018	0.000012	0.002387	0.000020	0.000040
S_7	0.000021	0.000010	0.000004	0.001694	0.000011	0.000018
S_8	0.000003	0.000082	0.000007	0.003956	0.000092	0.000076
Stage Sulfur Recovery %		47.88	--	--	41.43	--
Total Sulfur Recovery %		47.88	--	--	89.31	--

TABLE XXV (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^{o}K)	475	417	434	436	417	417
Chemical Species Mole Fractions						
CO	--	--	--	--	--	--
COS	0.000001	0.000001	0.000001	--	--	--
CO_2	0.537606	0.532614	0.538392	0.538605	0.537735	0.538739
CS_2	--	--	--	--	--	--
H_2	--	--	--	--	--	--
H_2O	0.180060	0.178387	0.180323	0.181700	0.181406	0.181765
H_2S	0.002170	0.002149	0.002173	0.000872	0.000871	0.000873
H_2S_2	0.000006	0.000006	0.000006	0.000001	0.000001	0.000001
N_2	0.277460	0.274884	0.277867	0.277975	0.277526	0.278044
S(L)	--	0.010734	--	--	0.001864	--
SO	--	--	--	--	--	--
SO_2	0.001087	0.001077	0.001089	0.000436	0.00435	0.000436
SO_3	--	--	--	--	--	--
S_2O	--	--	--	--	--	--
S_2	0.000001	--	--	--	--	--
S_3	--	--	--	--	--	--
S_4	--	--	--	--	--	--
S_5	0.000017	--	0.000001	0.000002	0.000001	0.000001
S_6	0.000327	0.000024	0.000031	0.000071	0.000026	0.000026
S_7	0.000212	0.000012	0.000016	0.000041	0.000014	0.000014
S_8	0.001051	0.000108	0.000102	0.000294	0.000120	0.000120
Stage Sulfur Recovery %		7.61	--	--	1.31	--
Total Sulfur Recovery %		96.92	--	--	98.23	--

APPENDIX D

CLAUS PROCESS RESULTS FOR ACID GAS FEEDS WITH HYDROCARBON IMPURITY

TABLE XXVI

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR AN ACID GAS FEED WITH HYDROCARBON IMPURITY (CASE 2)

	Furnace	**Condenser #1**	**Reheater #1**	**Reactor #1**	**Condenser #2**	**Reheater #2**
Pressure (atm)	1.4290	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^oK)	1592	417	494	646	417	492
Chemical Species Mole Fractions						
CO	0.008867	0.008185	0.009691	--	--	--
COS	0.000256	0.000236	0.000280	0.000007	0.000007	0.000007
CO_2	0.018233	0.016830	0.019925	0.030549	0.029728	0.030728
CS_2	0.000001	--	--	--	--	--
H	0.000008	--	--	--	--	--
H_2	0.036825	0.033992	0.040243	0.000017	0.000016	0.000017
H_2O	0.222896	0.205750	0.243585	0.295214	0.287287	0.296940
H_2S	0.031196	0.028795	0.034091	0.030003	0.029198	0.030179
H_2S_2	0.000118	0.000513	0.000607	0.000325	0.000316	0.000326
N_2	0.557536	0.514648	0.609285	0.622736	0.606014	0.626377
OH	0.000002	--	--	--	--	--
S	0.000027	--	--	--	--	--
S(L)	--	0.155513	--	--	0.032534	--
SH	0.000865	--	--	--	--	--
SO	0.001458	--	--	--	--	--
SO_2	0.037247	0.034381	0.040706	0.015143	0.014736	0.015232
SO_3	--	0.000950	0.000960	--	0.000010	--
S_2O	0.001741	0.000103	0.000619	0.000059	0.000027	0.000059
S_2	0.082586	--	--	0.000985	--	0.000001
S_3	0.000137	--	--	0.000091	--	--
S_4	0.000001	--	--	0.000032	--	--
S_5	--	--	--	0.000524	--	0.000004
S_6	--	0.000016	0.000005	0.002005	0.000021	0.000048
S_7	--	0.000008	0.000002	0.001460	0.000011	0.000021
S_8	--	0.000074	0.000003	0.001166	0.000095	0.000060
Stage Sulfur Recovery %		70.09	--	--	12.45	--
Total Sulfur Recovery %		70.09	--	--	82.54	--

TABLE XXVI (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^{o}K)	526	417	458	467	417	417
Chemical Species Mole Fractions						
CO	--	--	--	--	--	--
COS	--	--	--	--	--	--
CO_2	0.030934	0.030064	0.031079	0.031132	0.030906	0.031167
CS_2	--	--	--	--	--	--
H	--	--	--	--	--	--
H_2	--	--	--	--	--	--
H_2O	0.321147	0.312110	0.322651	0.328869	0.326481	0.329244
H_2S	0.008398	0.002816	0.008438	0.002816	0.002796	0.002820
H_2S_2	0.000043	0.000042	0.000043	0.000007	0.000007	0.000007
N_2	0.630446	0.612706	0.633397	0.634468	0.629862	0.635192
OH	--	--	--	--	--	--
S	--	--	--	--	--	--
S(L)	--	0.032673	--	--	0.008390	--
SH	--	--	--	--	--	--
SO	--	--	--	--	--	--
SO_2	0.004217	0.004984	0.004237	0.001408	0.001398	0.001410
SO_3	--	--	--	--	--	--
S_2O	0.000002	0.000002	0.000002	--	--	--
S_2	0.000018	--	--	--	--	--
S_3	0.000002	--	--	--	--	--
S_4	0.000001	--	--	--	--	0.000001
S_5	0.000011	--	0.000002	0.000013	--	0.000001
S_6	0.001234	0.000024	0.000041	0.000260	0.000026	0.000027
S_7	0.000848	0.000012	0.000020	0.000164	0.000014	0.000014
S_8	0.002602	0.000106	0.000090	0.000861	0.000119	0.000120
Stage Sulfur Recovery %		12.37	--	--	3.09	--
Total Sulfur Recovery %		94.91	--	--	98.00	--

TABLE XXVII

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR AN ACID GAS FEED WITH HYDROCARBON IMPURITY (CASE 3)

	Furnace	Condenser #1	Reheater #1	Reactor #1	Condenser #2	Reheater #2
Pressure (atm)	1.4290	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^oK)	1712	417	481	667	417	491
Chemical Species Mole Fractions						
CO	0.018574	0.017597	0.019731	--	--	--
COS	0.000278	0.000263	0.000295	0.000015	0.000015	0.000055
CO_2	0.025450	0.024110	0.027033	0.048198	0.047453	0.048398
CS_2	--	--	--	--	--	--
H	0.000029	--	--	--	--	--
H_2	0.043323	0.041042	0.046018	0.000023	0.000023	0.000023
H_2O	0.203626	0.192907	0.216294	0.259374	0.255368	0.260453
H_2S	0.018646	0.017664	0.019806	0.030028	0.029565	0.030153
H_2S_2	0.000048	0.000619	0.000694	0.000327	0.000322	0.000328
N_2	0.590407	0.559328	0.627138	0.642528	0.632604	0.645202
OH	0.000007	--	--	--	--	--
S	0.000069	--	--	--	--	--
S(L)	--	0.108307	--	--	0.019558	--
SH	0.001174	--	--	--	--	--
SO	0.002560	--	--	--	--	--
SO_2	0.038804	0.036760	0.041218	0.015156	0.014922	0.015219
SO_3	--	0.00181	0.001174	--	0.000015	--
S_2O	0.001294	0.000115	0.000580	0.000076	0.000031	0.000075
S_2	0.055653	--	--	0.001411	--	0.000001
S_3	0.000056	--	--	0.000113	--	--
S_4	--	--	--	0.000033	--	--
S_5	--	--	--	0.000406	--	0.000004
S_6	--	0.000017	0.00009	0.001212	0.000021	0.000047
S_7	--	0.000009	0.000003	0.000613	0.000011	0.000021
S_8	--	0.000078	0.000008	0.000487	0.000096	0.000059
Stage Sulfur Recovery %		65.07	--	--	10.39	--
Total Sulfur Recovery %		65.07	--	--	75.46	--

TABLE XXVII (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^{o}K)	526	417	458	466	417	417
Chemical Species Mole Fractions						
CO	--	--	--	--	--	--
COS	--	--	--	--	--	--
CO_2	0.048737	0.047329	0.048972	0.049050	0.048717	0.049102
CS_2	--	--	--	--	--	--
H	--	--	--	--	--	--
H_2	--	--	--	--	--	--
H_2O	0.285085	0.276846	0.286455	0.292216	0.290232	0.292527
H_2S	0.007775	0.007553	0.007815	0.002555	0.002538	0.002558
H_2S_2	0.000040	0.000039	0.000040	0.000006	0.000006	0.000006
N_2	0.649515	0.630744	0.652638	0.653671	0.649233	0.654368
OH	--	--	--	--	--	--
S	--	--	--	--	--	--
S(L)	--	0.033552	--	--	0.007847	--
SH	--	--	--	--	--	--
SO	--	--	--	--	--	--
SO_2	0.003905	0.003792	0.003924	0.001277	0.001269	0.001279
SO_3	--	--	--	--	--	--
S_2O	0.000002	0.000002	0.000002	--	--	--
S_2	0.000018	--	--	--	--	--
S_3	0.000002	--	--	--	--	--
S_4	0.000001	--	--	--	--	--
S_5	0.000107	--	0.000002	0.000012	0.000001	0.000001
S_6	0.001261	0.000024	0.000041	0.000247	0.000026	0.000027
S_7	0.000869	0.000012	0.000020	0.000155	0.000014	0.000014
S_8	0.002679	0.000106	0.000090	0.000811	0.000119	0.000120
Stage Sulfur Recivery %		17.88	--	--	4.06	--
Total Sulfur Recovery %		93.34	--	--	97.40	--

APPENDIX E

CLAUS PROCESS RESULTS FOR ACID GAS FEEDS WITH AMMONIA OR WATER IMPURITY

TABLE XXVIII

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR AN ACID GAS FEED WITH AMMONIA IMPURITY

	Furnace	Condenser #1	Reheater #1	Reactor #1	Condenser #2	Reheater #2
Pressure (atm)	1.4290	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^{o}K)	1607	417	493	637	417	490
Chemical Species Mole Fractions						
CO	0.004690	0.004373	0.005068	--	--	--
COS	0.000119	0.0001107	0.000128	0.000003	0.000003	0.000003
CO_2	0.009164	0.0085428	0.009900	0.015421	0.015019	0.015505
CS_2	--	--	--	--	--	--
H	0.000009	--	--	--	--	--
H_2	0.040421	0.037682	0.043672	0.000014	0.000014	0.000014
H_2O	0.237472	0.221384	0.256574	0.311556	0.303447	0.313258
H_2S	0.029968	0.027938	0.032379	0.028574	0.027830	0.028730
H_2S_2	0.000103	0.000521	0.000604	0.000295	0.000287	0.000297
N_2	0.565406	0.527103	0.610887	0.624107	0.607861	0.627515
OH	0.000002	--	--	--	--	--
S	0.000029	--	--	--	--	--
S(L)	--	0.137341	--	--	0.031339	--
SH	0.000898	--	--	--	--	--
SO	0.001521	--	--	--	--	--
SO_2	0.036339	0.033877	0.039262	0.014415	0.014040	0.014494
SO_3	--	0.000921	0.000903	--	0.000008	--
S_2O	0.001550	0.000104	0.000612	0.000048	0.000024	0.000048
S_2	0.072199	--	--	0.00764	--	0.000001
S_3	0.000107	--	--	0.000072	--	--
S_4	--	--	--	0.000026	--	--
S_5	--	--	0.000001	0.000470	0.000001	0.000004
S_6	--	0.000017	0.000005	0.001921	0.000021	0.000048
S_7	--	0.000009	0.000002	0.001086	0.000011	0.000021
S_8	--	0.000076	0.000003	0.002060	0.000095	0.000062
Stage Sulfur Recovery %		67.92	--	--	13.44	--
Total Sulfur Recovery %		67.92	--	--	81.36	--

TABLE XXVIII (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^oK)	522	417	458	467	417	417
Chemical Species Mole Fractions						
CO	--	--	--	--	--	--
COS	--	--	--	--	--	--
CO_2	0.015603	0.015188	0.015672	0.015697	0.015589	0.015714
CS_2	--	--	--	--	--	--
H	--	--	--	--	--	--
H_2	0.000001	0.000001	0.00001	--	--	--
H_2O	0.336212	0.327270	0.337692	0.343606	0.341245	0.343977
H_2S	0.008148	0.007932	0.008184	0.002858	0.002839	0.002861
H_2S_2	0.000040	0.000049	0.000040	0.000007	0.000007	0.000007
N_2	0.631368	0.614576	0.634148	0.635164	0.630799	0.635849
OH	--	--	--	--	--	--
S	--	--	--	--	--	--
S(L)	--	0.03869	--	--	0.007944	--
SH	--	--	--	--	--	--
SO	--	--	--	--	--	--
SO_2	0.004090	0.003981	0.004108	0.001429	0.001492	0.001431
SO_3	--	--	--	--	--	--
S_2O	0.000002	0.000002	0.000002	--	--	--
S_2	0.000015	--	--	0.000001	--	--
S_3	0.000002	--	--	--	--	--
S_4	0.000001	--	--	--	--	--
S_5	0.000095	--	0.000002	0.000012	0.000001	0.000001
S_6	0.001146	0.000023	0.000041	0.000250	0.000026	0.000027
S_7	0.000785	0.000025	0.000020	0.000156	0.000014	0.000014
S_8	0.002493	0.000107	0.000090	0.000820	0.000119	0.000120
Stage Sulfur Recovery %		13.09	--	--	3.28	--
Total Sulfur Recovery %		94.45	--	--	97.73	--

TABLE XXIX

SPECIES CONCENTRATIONS AND SULFUR RECOVERY ACROSS THE CLAUS PROCESS FOR AN ACID GAS FEED WITH WATER IMPURITY

	Furnace	Condenser #1	Reheater #1	Reactor #1	Condenser #2	Reheater #2
Pressure (atm)	1.4290	1.3609	1.3269	1.2929	1.2248	1.1908
Temperature (^oK)	1444	417	504	626	417	491
Chemical Species Mole Fractions						
CO	0.002979	0.002749	0.003255	--	--	--
COS	0.000170	0.000157	0.000185	0.000003	0.000003	0.000003
CO_2	0.013353	0.012318	0.014585	0.018380	0.017646	0.018525
CS_2	--	--	--	--	--	--
H	0.000001	--	--	--	--	--
H_2	0.027386	0.025262	0.029912	0.000013	0.000012	0.000013
H_2O	0.286298	0.264101	0.312705	0.371045	0.356219	0.373964
H_2S	0.046933	0.043294	0.051262	0.030796	0.029566	0.031039
H_2S_2	0.000228	0.000397	0.000470	0.000320	0.000307	0.000323
N_2	0.499070	0.460376	0.545102	0.555918	0.533704	0.560292
OH	--	--	--	--	--	--
S	0.000005	--	--	--	--	--
S(L)	--	0.155625	--	--	0.047471	--
SH	0.000403	--	--	--	--	--
SO	0.000574	--	--	--	--	--
SO_2	0.037752	0.034825	0.041234	0.015539	0.014918	0.015661
SO_3	--	0.000703	0.000662	--	0.000007	--
S_2O	0.001813	0.000094	0.000621	0.000044	0.000023	0.000044
S_2	0.082817	--	0.000001	0.000630	--	0.000001
S_3	0.000216	--	--	0.000065	--	--
S_4	0.000002	--	--	0.000026	--	--
S_5	0.000002	--	--	0.000574	--	0.000004
S_6	--	0.000016	0.000004	0.002743	0.000021	0.000048
S_7	--	0.000009	0.000001	0.001719	0.000011	0.000022
S_8	--	0.000074	0.000002	0.002185	0.000093	0.000062
Stage Sulfur Recovery %		65.85	--	--	17.33	--
Total Sulfur Recovery %		65.85	--	--	83.18	--

TABLE XXIX (Continued)

	Reactor #2	Condenser #3	Reheater #3	Reactor #3	Condenser #4	Tail Gas
Pressure (atm)	1.1568	1.0887	1.0551	1.0207	1.0000	1.0000
Temperature (^{o}K)	524	417	461	471	417	417
Chemical Species Mole Fractions						
CO	--	--	--	--	--	--
COS	--	--	--	--	--	--
CO_2	0.018646	0.01827	0.018733	0.018767	0.018621	0.01870
CS_2	--	--	--	--	--	--
H	--	--	--	--	--	--
H_2	0.000001	0.000001	0.000001	--	--	--
H_2O	0.398434	0.387329	0.400277	0.407072	0.403910	0.407570
H_2S	0.009464	0.009200	0.009508	0.003493	0.003466	0.003498
H_2S_2	0.000048	0.000046	0.000048	0.000001	0.000009	0.000009
N_2	0.563897	0.548180	0.566505	0.567530	0.563121	0.568224
OH	--	--	--	--	--	--
S	--	--	--	--	--	--
S(L)	--	0.032354	--	--	0.008981	--
SH	--	--	--	--	--	--
SO	--	--	--	--	--	--
SO_2	0.004750	0.004618	0.004772	0.001746	0.001733	0.001748
SO_3	--	--	--	--	--	--
S_2O	0.000002	0.000002	0.000002	--	--	--
S_2	0.000017	--	--	--	--	--
S_3	0.000002	--	--	--	--	--
S_4	0.000001	--	--	--	--	--
S_5	0.000102	--	0.000003	0.000015	--	0.000001
S_6	0.001209	0.000024	0.000043	0.000284	0.000026	0.000027
S_7	0.000832	0.000012	0.000021	0.000179	0.000014	0.000014
S_8	0.002595	0.000106	0.000088	0.000904	0.000119	0.000120
Stage Sulfur Recovery %		11.50	--	--	3.11	--
Total Sulfur Recovery %		94.68	--	--	97.79	--

APPENDIX F

LISTING OF THERMO DATA FILE

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FOR EVERY SPECIES:
FIRST CARD CONTAINS: SPECIES NAME,THERMO DATA SOURCE,ATOMIC COMPOSITION,STATE,
 TEMPERATURE RANGE.
THE SEVEN HIGH TEMPERATURE LEAST SQUARE COEFFICIENTS ARE IN CARDS TWO AND THREE
LOW TEMPERATURE COEFFICIENTS ARE IN CARDS THREE AND FOUR.

BEGIN FILE LISTING:

   300.000  1000.000  5000.000
C(S)          J 3/61C  1.                    0S   300.000  5000.000            1
 0.13604942E 01 0.19182237E-02-0.84040389E-06 0.16448707E-09-0.11672670E-13    2
-0.65713870E 03-0.80070207E 01-0.44778053E 00 0.53691002E-02-0.39775571E-06    3
-0.40459298E-08 0.21134939E-11-0.94280688E 02 0.16840791E 01                   4
C             J 3/61C  1.                    0G   300.000  5000.000            1
 0.25810663E 01-0.14696202E-03 0.74388084E-07-0.79481079E-11 0.58900977E-16    2
 0.85216294E 05 0.43128879E 01 0.25328705E 01-0.15887641E-03 0.30682082E-06    3
-0.26770064E-09 0.87488827E-13 0.85240422E 05 0.46062374E 01                   4
C+            L12/66C  1.E -1.               0G   300.000  5000.000            1
 0.25118274E 01-0.17359784E-04 0.95042676E-08-0.22188518E-11 0.18621892E-15    2
 0.21667721E 06 0.42861298E 01 0.25953840E 01-0.40686645E-03 0.68923669E-06    3
-0.52664878E-09 0.15083377E-12 0.21666281E 06 0.38957298E 01                   4
C-            J 9/65C  1.E  1.                G   300.000  5000.000            1
 0.24470591E 01 0.11286428E-03-0.78591462E-07 0.19778614E-10-0.11105555E-14    2
 0.69972969E 05 0.42356992E 01 0.24925640E 01 0.53153068E-04-0.13307994E-06    3
 0.13951379E-09-0.52150992E-13 0.69955757E 05 0.39811657E 01                   4
CH            J12/67C  1.H  1.               0G   300.000  5000.000            1
 0.22673116E 01 0.22043000E-02-0.62250191E-06 0.69689940E-10-0.21274952E-14    2
 0.70838037E 05 0.87889352E 01 0.35632752E 01-0.20031372E-03-0.40129814E-06    3
 0.18226922E-08-0.86768311E-12 0.70405506E 05 0.17628023E 01                   4
CH+           J12/71C  1.H  1.E -1.          0G   300.000  5000.000            1
 0.27466401E+01 0.15496991E-02-0.52858324E-06 0.86132075E-10-0.50909775E-14    2
 0.19483672E+06 0.46994695E+01 0.35601593E+01-0.22478101E-03-0.26341623E-06    3
 0.16716214E-08-0.89478626E-12 0.19460363E+06 0.41570213E+00                   4
CH2           J12/72C  1.H  2.                G   300.0    5000.0              1
 0.27525479E+01 0.39782047E-02-0.14921731E-05 0.25956899E-09-0.17110673E-13    2
 0.45547759E+05 0.66534799E+01 0.35883347E+01 0.21724137E-02-0.13323408E-05    3
 0.19469445E-08-0.89431394E-12 0.45315188E+05 0.22627869E+01                   4
CH3           J 6/69C  1.H  3.                G   300.0    5000.0              1
 0.28400327E 01 0.60869086E-02-0.21740338E-05 0.36042576E-09-0.22725300E-13    2
 0.16449813E 05 0.55056751E 01 0.34666350E 01 0.38301845E-02 0.10116802E-05    3
-0.18859236E-08 0.66803182E-12 0.16313104E 05 0.24172192E 01                   4
CH4           J 3/61C  1.H  4.                G   300.0    5000.0              1
 0.15027072E 01 0.10416798E-01-0.39181522E-05 0.67777899E-09-0.44283706E-13    2
-0.99787078E 04 0.10707143E 02 0.38261932E 01-0.39794581E-02 0.24558340E-04    3
-0.22732926E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00                   4
CH2O          J 3/61C  1.H  2.O  1.           G   300.0    5000.0              1
 0.28364249E 01 0.68605298E-02-0.26882647E-05 0.47971258E-09-0.32118406E-13    2
-0.15236031E 05 0.78531169E 01 0.37963783E 01-0.25701785E-02 0.18548815E-04    3
-0.17869177E-07 0.55504451E-11-0.15088947E 05 0.47548163E 01                   4
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CN              J 6/69C  1.N  1.                   G   300.000  5000.000        1
 0.36036285E 01 0.33644390E-03 0.10028933E-06-0.16318166E-10-0.36286722E-15    2
 0.51159833E 05 0.35454505E 01 0.37386307E 01-0.19239224E-02 0.47035189E-05    3
-0.31113000E-08 0.61675318E-12 0.51270927E 05 0.34490218E 01                   4
CN+             J12/70C  1.N  1.E -1.             0G   300.000  5000.000        1
 0.36522919E+01 0.81427579E-03-0.20853348E-06 0.29071604E-10-0.17865094E-14    2
 0.21560182E+06 0.43916910E+01 0.36175018E+01-0.20179550E-02 0.79359855E-05    3
-0.77300616E-08 0.24798477E-11 0.21578134E+06 0.53579527E+01                   4
CN-             J12/70C  1.N  1.E  1.             0G   300.000  5000.000        1
 0.29471725E+01 0.14988427E-02-0.57579547E-06 0.10177789E-09-0.67478503E-14    2
 0.63644338E+04 0.63743952E+01 0.37034310E+01-0.14896426E-02 0.31864701E-05    3
-0.14831305E-08 0.48121663E-13 0.62335826E+04 0.27722843E+01                   4
CNN             J 6/66C  1.N  2.                   G   300.000  5000.000        1
 0.48209077E 01 0.24790014E-02-0.94644109E-06 0.16548764E-09-0.10899129E-13    2
 0.68685948E 05-0.48484039E 00 0.35077779E 01 0.72023958E-02-0.75574589E-05    3
 0.42979217E-08-0.94257935E-12 0.68994281E 05 0.60234964E 01                   4
CN2             J12/70C  1.N  2.                   G   300.000  5000.000        1
 0.55626268E+01 0.20860606E-02-0.88123724E-06 0.16505783E-09-0.11366697E-13    2
 0.54897907E+05-0.55989355E+01 0.32524003E+01 0.70010737E-02-0.22653599E-05    3
-0.28939808E-08 0.18270077E-11 0.55609085E+05 0.66966778E+01                   4
CO              J 9/65C  1.O  1.                   G   300.0    5000.0          1
 0.29840696E 01 0.14891390E-02-0.57899684E-06 0.10364577E-09-0.69353550E-14    2
-0.14245228E 05 0.63479156E 01 0.37100928E 01-0.16190964E-02 0.36923594E-05    3
-0.20319674E-08 0.23953344E-12-0.14356310E 05 0.29555351E 01                   4
COS             J 3/61C  1.O  1.S  1.              G   300.0    5000.0          1
 0.52392000E 01 0.24100584E-02-0.96064522E-06 0.17778347E-09-0.12235704E-13    2
-0.18480455E 05-0.30910517E 01 0.24625321E 01 0.11947992E-01-0.13794370E-04    3
 0.80707736E-08-0.18327653E-11-0.17803987E 05 0.10792556E 02                   4
CO2             J 9/65C  1.O  2.                   G   300.0    5000.0          1
 0.44608041E 01 0.30981719E-02-0.12392571E-05 0.22741325E-09-0.15525954E-13    2
-0.48961442E 05-0.98635982E 00 0.24007797E 01 0.87350957E-02-0.66070878E-05    3
 0.20021861E-08 0.63274039E-15-0.48377527E 05 0.96951457E 01                   4
CS2             J 6/61C  1.S  2.                   G   300.0    5000.0          1
 0.59867719E 01 0.16394436E-02-0.68384845E-06 0.12836890E-09-0.89167448E-14    2
 0.12043850E 05-0.63998223E 01 0.32144238E 01 0.10443846E-01-0.11062989E-04    3
 0.52967662E-08-0.83022695E-12 0.12745874E 05 0.76185765E 01                   4
CO2-            J12/66C  1.O  2.E -1.              G   300.000  5000.000        1
 0.45454640E 01 0.26054316E-02-0.10928732E-05 0.20454421E-09-0.14184542E-13    2
-0.54761968E 05 0.18317369E 01 0.34743737E 01 0.16913805E-02 0.73533803E-05    3
-0.99554255E-08 0.36846719E-11-0.54249049E 05 0.83834329E 01                   4
CS              J12/62C  1.S  1.                   G   300.0    5000.0          1
 0.36942533E 01 0.89086274E-03-0.36600044E-06 0.68778176E-10-0.47810000E-14    2
 0.26452213E 05 0.38176082E 01 0.33093030E 01 0.28164439E-04 0.44317874E-05    3
-0.55253895E-08 0.20392468E-11 0.26658986E 05 0.62942707E 01                   4
C2              J12/69C  2.                       0G   300.000  5000.000        1
 0.40435359E 01 0.20573654E-03 0.10907575E-06-0.36427874E-10 0.34127865E-14    2
 0.99709486E 05 0.12775158E 01 0.74518140E 01-0.10144686E-01 0.85879735E-05    3
 0.87321100E-09-0.24429792E-11 0.98911989E 05-0.15846678E 02                   4
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C2-          J12/69C  2.E  1.               G   3C0.000  5000.000              1
 0.36926257E 01 0.41576040E-03 0.11654211E-07 0.23755880E-11-0.14585314E-14    2
 0.52118953E 05 0.22470173E 01 0.37342914E 01-0.23034649E-02 0.68417833E-05    3
-0.58120827E-08 0.16604296E-11 0.52281427E 05 0.27860423E 01                   4
C2H          J 3/67C  2.h  1.              OG   300.000  5000.000              1
 0.44207650E 01 0.22119303E-02-0.59294945E-06 0.94195775E-10-0.68527594E-14    2
 0.55835444E 05-0.11588093E 01 0.26499400E 01 0.84919515E-02-0.98165375E-05    3
 0.65373629E-08-0.17356273E-11 0.56275751E 05 0.76898609E 01                   4
C2H2         J 3/61C  2.H  2.              OG   300.000  5000.000              1
 0.45751083E 01 0.51238358E-02-0.17452354E-05 0.28673065E-09-0.17951426E-13    2
 0.25607428E 05-0.35737940E 01 0.14102768E 01 0.19057275E-01-0.24501390E-04    3
 0.16390872E-C7-C.41345447E-11 0.26188208E 05 0.11393827E 02                   4
C2H4         J 9/65C  2.H  4.               G   300.000  5000.000              1
 0.34552152E 01 0.11491803E-01-0.43651750E-05 0.76155095E-09-0.50123200E-13    2
 0.44773119E 04 0.26987959E 01 0.14256821E 01 0.11383140E-01 0.79890006E-05    3
-0.16253679E-07 0.67491256E-11 0.53370755E 04 0.14621819E 02                   4
C2H6         L 5/72C  2.H  6.               G   300.0    1500.0                1
 0.21555281E+01 0.14779861E-01 0.23352804E-05-0.64146428E-08 0.19036925E-11    2
-0.11524517E+05 0.10776316E+02 0.21415788E+01 0.10529720E-01 0.18730274E-04    3
-0.26691187E-07 0.10049332E-10-0.11410486E+05 0.11647757E+02                   4
C2H7NO(L)    AGM003C  2.h  7.N  1.O  1.     L   298.15   400.0                 1
 0.0            0.0            0.0            0.0            0.0               2
 0.0            0.0           +0.15283000E+02 0.0            0.0               3
 0.0            0.0           -0.37571000E+05-0.61000000E+02                   4
C2N          J 3/67C  2.N  1.               G   300.000  5000.000              1
 0.61931308E 01 0.14327539E-02-0.61255161E-06 0.11578707E-09-0.80401339E-14    2
 0.64818372E 05-0.84132298E 01 0.32670394E 01 0.98211307E-02-0.83284733E-05    3
 0.17650559E-08 0.59632768E-12 0.65589057E 05 0.65682304E 01                   4
C2N2         J 3/61C  2.N  2.              OG   3C0.00C  5000.000              1
 0.65968935E 01 0.38694131E-02-0.15516161E-05 0.28141546E-09-0.19069442E-13    2
 0.34883726E 05-C.10001801E 02 0.39141782E 01 0.14011008E-01-0.17404350E-04    3
 0.12012779E-07-0.33565772E-11 0.35514550E 05 0.32384353E 01                   4
C2O          J 9/66C  2.O  1.              OG   300.000  5000.000              1
 0.48990313E 01 C.2843C384E-02-0.10209669E-05 0.16112165E-09-0.95542914E-14    2
 0.32800545E 05-0.91382280E 00 0.35364815E 01 0.69543872E-02-0.53071374E-05    3
 0.17030470E-C8-0.14108072E-13 0.33151572E 05 0.60172370E 01                   4
C3           J12/69C  3.                   OG   3C0.000  5000.000              1
 0.36815361E 01 0.24165236E-02-0.84348112E-06 0.14508198E-09-0.95697300E-14    2
 0.97413955E 05 0.68377802E 01 0.57408464E 01-0.84281238E-02 0.18620198E-04    3
-0.14510529E-07 0.39676977E-11 0.97157524E 05-0.23837376E 01                   4
C3H8         AGM001C  3.H  8.              OG   3C0.000  1000.000              1
 0.0            0.0            0.0            0.0            0.0               2
 0.0            0.0           +0.42271007E+00+0.29225861E-01+0.14891375E-05    3
-0.19134164E-07+0.90500275E-11-0.13892381E+05+0.21426428E+02                   4
C3O2         J 6/68C  3.O  2.              OG   300.000  5000.000              1
 0.81435964E 01 0.54395018E-02-0.22192869E-05 0.40778627E-09-0.27915974E-13    2
-0.14230013E 05-0.15456769E 02 0.37161005E 01 0.19872164E-01-0.20935751E-04    3
 0.11750112E-07-0.26589416E-11-0.13089402E 05 0.69298412E 01                   4
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C4           J12/69C  4.                   0G   3C0.000  5000.000              1
 0.65602101E 01 0.40985234E-02-0.17000471E-05 0.31615228E-09-0.21842144E-13    2
 0.11430434E 06-0.11820311E 02 0.18432021E 01 0.19343592E-01-0.20627502E-04    3
 0.10822626E-07-0.21289203E-11 0.11550276E C6 0.12006898E 02                  4
C4H10(N)     AGM0C1C  4.H 10.              0G   300.000  10C0.000              1
 0.0            0.0            0.0            0.0            0.0               2
 0.0            0.0           +0.13449176E+01+0.34710813E-01+0.78904074E-05    3
-0.25898492E-07+0.13242880E-10-0.17130404E+05+0.19175675E+02                   4
C4H10(I)     AGM001C  4.H 10.              0G   300.00C  1000.000              1
 0.0            0.0            0.0            0.0            0.0               2
 0.0            0.0           -0.32918879E+00+0.45116824E-01-0.15323081E-04    3
-0.59305385E-08+0.38259723E-11-0.17939230E+05+0.24584896E+02                   4
C4H11NO2(L)  AGM003C  4.H 11.N   1.O  2.    L   298.15   500.0                 1
 0.0            0.0             0.0           0.0            0.0               2
 0.0            0.0           +0.28100000E+02 0.0            0.0               3
 0.0            0.0           -0.65038000E+05-0.12800000E+03                   4
C5           J12/69C  5.                    G   300.000  5000.000              1
 0.82067016E 01 0.54889888E-02-0.22694876E-05 0.42073365E-09-0.28981924E-13    2
 0.11463647E 06-0.20246108E 02 0.11012446E 01 0.29513421E-01-0.33754342E-04    3
 0.19056534E-07-0.40989018E-11 0.11637970E 06 0.15360193E 02                  4
C5H12(N)     AGM001C  5.H 12.               G   300.000  1000.000              1
 0.0            0.0            0.0            0.0            0.0               2
 0.0            0.0           +0.14198721E+01+0.44449470E-01+0.62311981E-01    3
-0.34141837E-07+0.15536745E-10-0.20004347E+05+0.20619925E+02                   4
C5H12(I)     AGM001C  5.H 12.               G   300.000  1000.000              1
0.0            0.0            0.0            0.0            0.0                2
C.0            0.0            +0.38677456E+00+0.48882346E-01-0.26422140E-07    3
-0.30114558E-07+0.14652864E-10-0.20811424E+05+0.24786350E+02                   4
H            J 9/65H  1.                    G   3CC.00C  5000.000              1
 0.25C00C00E 01 0.             0.             0.             0.                2
 0.25471627E 05-0.46011763E 00 0.25000000E 01 0.             0.                3
 0.             0.             0.25471627E 05-0.46011762E 00                   4
H+           J 6/66H  1.E -1.               G   300.0    5000.0                1
 0.25000000E 01 0.             0.             0.             0.                2
 0.18403344E 06-0.11538620E 01 0.25000000E 01 0.             0.                3
 0.             0.             0.18403344E 06-0.11538621E 01                   4
H-           J 9/65H  1.E  1.              0G   3C0.000  5000.000              1
 0.25000000E 01 0.             0.             0.             0.                2
 0.15961045E 05-0.11524488E 01 0.25000000E 01 0.             0.                3
 0.             0.             0.15961045E 05-0.11524486E 01                   4
HCL          J 9/64H  1.CL 1.              0G   300.000  5000.000              1
 0.27665884E 01 0.14381883E-02-0.46993000E-06 0.73499408E-10-0.43731106E-14    2
-0.11917468E 05 0.64583540E 01 0.35248171E 01 0.29984862E-04-0.86221891E-06    3
 0.2C979721E-08-0.98658191E-12-0.12150509E 05 0.23957713E 01                  4
HCN          L12/69H  1.C  1.N  1.          G   300.0    5000.0                1
 0.37068121E 01 0.33382803E-02-0.11913320E-05 0.19992917E-09-0.12826452E-13    2
 0.14962636E 05 0.20794904E 01 0.24513556E 01 0.87208371E-02-0.10094203E-04    3
 0.67255698E-08-0.17626959E-11 0.15213002E 05 0.8C830085E 01                  4
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HCO               J12/70H  1.C  1.O  1.            G    3C0.0     5000.0             1
 0.34738348E+01 0.34370227E-02-0.13632664E-05 0.24928645E-09-0.17044331E-13    2
 0.39594005E+04 0.60453340E+01 0.38840192E+01-0.82974448E-03 0.77900809E-05    3
-0.70616962E-08 0.19971730E-11 0.40563860E+04 0.48354133E+01                   4
HCO+              J12/70H  1.C  1.O  1.E -1.       G    300.000  5000.000        1
 0.37411880E+01 0.33441517E-02-0.12397121E-05 0.21189388E-09-0.13704150E-13    2
 0.98884078E+05 0.20654768E+01 0.24739736E+01 0.86715590E-02-0.10031500E-04    3
 0.67170527E-08-0.17872674E-11 0.99146608E+05 0.81625751E+01                   4
HNCO              J12/70H  1.N  1.C  1.O  1.       G    300.0     5000.0         1
 0.51300390E+01 0.43551371E-02-0.16269022E-05 0.28035605E-09-0.18276037E-13    2
-0.14101787E+05-0.22010995E+01 0.23722164E+01 0.13664040E-01-0.13323158E-04    3
 0.64475457E-08-0.10402894E-11-0.13437059E+05 0.11588263E+02                   4
HNO               J 3/63H  1.N  1.C  1.            G    300.000  5000.000        1
 0.35548619E 01 0.32713182E-02-0.12734071E-05 0.22602046E-09-0.15064827E-13    2
 0.10693734E 05 0.51684901E 01 0.37412008E 01-0.2C067061E-03 0.75409300E-05    3
-0.79105713E-08 0.25928389E-11 0.10817845E 05 0.50063473E 01                   4
HNO2              J 6/63H  1.N  1.O  2.            G    300.000  5000.000        1
 0.55144941E+01 0.41394403E-02-0.15878702E-05 0.27977639E-09-0.18584209E-13    2
-0.11276885E+05-0.31425253E+01 0.25098874E+01 0.12171605E-01-0.78618375E-05    3
 0.35351571E-09 0.11540858E-11-0.10450008E+05 0.12399634E+02                   4
HNO3              J 6/63H  1.N  1.O  3.            G    300.000  50C0.000        1
 0.70591100E+01 0.56769446E-02-0.22348863E-05 0.40155529E-09-0.27080510E-13    2
-0.18920009E+05-0.10778285E+02 0.14377135E+01 0.2C903552E-01-0.14574553E-04    3
 0.11972023E-08 0.19117285E-11-0.17385368E+05 0.18246253E+02                   4
HO2               J 3/64H  1.O  2.                 G    3C0.000  5000.000        1
 0.37866280E 01 0.27885404E-02-0.10168708E-05 0.17183946E-09-0.11021852E-13    2
 0.11888500E 04 0.48147611E 01 0.35094850E 01 0.11499670E-02 0.58784259E-05    3
-0.77795519E-08 0.29607883E-11 0.13803331E 04 0.68276325E 01                   4
H2                J 3/61H  2.                      G    3C0.000  5000.000        1
 0.31001901E 01 0.51119464E-03 0.52644210E-07-0.34909973E-10 0.36945345E-14    2
-0.87738042E 03-0.19629421E 01 0.30574451E 01 0.26765200E-02-0.58099162E-05    3
 0.55210391E-08-0.18122739E-11-0.98890474E 03-0.22997056E 01                   4
H2O(S)            L11/65H  2.O  1.                 S    200.000   273.150        1
 0.             0.             0.             0.             0.                2
 0.             0.            -0.39269330E-01 0.16920420E-01 0.                3
 0.             0.            -0.35949581E 05 0.56933784E 00                   4
H2O(L)            L11/65H  2.O  1.                 L    273.15    373.15         1
 0.             0.             0.             0.             0.                2
 0.             0.             0.12712782E 02-0.17662790E-01-0.22556661E-04    3
 0.2C820908E-06-0.24078614E-09-0.37483200E 05-0.59115345E 02                   4
H2O               J 3/61H  2.C  1.             G    300.0     5000.0             1
 0.27167633E 01 0.29451374E-02-0.80224374E-06 0.1C226682E-09-0.48472145E-14    2
-0.29905826E 05 0.66305671E 01 0.40701275E 01-0.11084499E-02 0.41521180E-05    3
-0.29637404E-08 C.80702103E-12-0.30279722E 05-0.32270046E 00                   4
H2O2              L 2/69H  2.O  2.                 G    300.00C  50C0.000        1
 0.45731667E 01 0.43361363E-02-0.14746888E-05 0.23489037E-09-0.14316536E-13    2
-0.18006961E 05 0.50113696E 00 0.33887536E 01 0.65692260E-02-0.14850126E-06    3
-0.46258055E-08 0.24715147E-11-0.17663147E 05 0.67853631E 01                   4
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H2S(L)            AGM003H  2.S  1.          L   298.15   400.0                 1
 0.0            0.0            0.0            0.0            0.0               2
 0.0            0.0            0.53347000E+01 0.0            0.0               3
 0.0            0.0           -0.11799000E+05-0.15750000E+02                   4
H2S               J12/65H  2.S  1.          G   300.0    5000.0                1
 0.28479103E 01 0.38415990E-02-0.14099367E-05 0.24278754E-09-0.15783283E-13    2
-0.34469788E 04 0.74781412E 01 0.38811293E 01-0.13211856E-03 0.36517726E-05    3
-0.21820445E-08 0.28783779E-12-0.36350917E 04 0.25161511E 01                   4
H2S2              J12/65H  2.S  2.          G   300.0    2000.0                1
+0.32513763D+01+0.16261720D-01-0.28512746D-04+0.26093000D-07-0.90376270D-11    2
+0.36344945D+02+0.90196481D+01+0.32513763D+01+0.16261720D-01-0.28512746D-04    3
+0.26093000D-07-0.90376270D-11+0.36344945D+02+0.90196481D+01                   4
N                 J 3/61N  1.               G   300.000  5000.000              1
 0.24502682E 01 0.10661458E-03-0.74653373E-07 0.18796524E-10-0.10259839E-14    2
 0.56116040E 05 0.44487581E 01 0.25030714E 01-0.21800181E-04 0.54205287E-07    3
-0.56475602E-10 0.20999044E-13 0.56098904E 05 0.41675764E 01                   4
NCO               J12/70N  1.C  1.O  1.    0G   300.000  5000.000              1
 0.49964357E+01 0.26250880E-02-0.10928387E-05 0.20309111E-09-0.13915195E-13    2
 0.17379356E+05-0.17325320E+01 0.31092021E+01 0.66201022E-02-0.26070086E-05    3
-0.14966380E-08 0.10922032E-11 0.17977514E+05 0.83561334E+01                   4
NH                J12/71N  1.H  1.          G   300.000  5000.000              1
 0.27789900E+01 0.13266349E-02-0.41101218E-06 0.69414505E-10-0.44536190E-14    2
 0.44567973E+05 0.57593434E+01 0.34938318E+01 0.24529034E-03-0.12578521E-05    3
 0.22011922E-08-0.92288834E-12 0.44326826E+05 0.18451723E+01                   4
NH2               J12/65N  1.H  2.         0G   300.000  5000.000              1
 0.25769524E 01 0.35896090E-02-0.12276328E-05 0.19549576E-09-0.11873401E-13    2
 0.19335912E 05 0.79074890E 01 0.40385791E 01-0.10098163E-02 0.40120903E-05    3
-0.23085312E-08 0.39022887E-12 0.18973010E 05 0.52464285E 00                   4
NH3               J 9/65N  1.H  3.          G   300.000  5000.000              1
 0.24165177E 01 0.61871211E-02-0.21785136E-05 0.37599090E-09-0.24448856E-13    2
-0.64747177E 04 0.77043482E 01 0.35912768E 01 0.49388668E-03 0.83449322E-05    3
-0.83833385E-08 0.27299092E-11-0.66717143E 04 0.22520966E 01                   4
NO                J 6/63N  1.O  1.          G   300.000  5000.000              1
 0.31890000E 01 0.13382281E-02-0.52899318E-06 0.95919332E-10-0.64847932E-14    2
 0.98283290E 04 0.67458126E 01 0.40459521E 01-0.34181783E-02 0.79819190E-05    3
-0.61139316E-08 0.15919076E-11 0.97453934E 04 0.29974988E 01                   4
NO+               J 6/66N  1.O  1.E -1.     G   300.000  5000.000              1
 0.28885488E 01 0.15217119E-02-0.57531241E-06 0.10051081E-09-0.66044294E-14    2
 0.11819245E 06 0.70027197E 01 0.36685056E 01-0.11544580E-02 0.21755608E-05    3
-0.48227472E-09-0.27847906E-12 0.11803369E 06 0.31779324E 01                   4
NO2               J 9/64N  1.O  2.         0G   300.000  5000.000              1
 0.46240771E 01 0.25260332E-02-0.10609498E-05 0.19879239E-09-0.13799384E-13    2
 0.22899900E 04 0.13324138E 01 0.34589236E 01 0.20647064E-02 0.66866067E-05    3
-0.95556725E-08 0.36195881E-11 0.28152265E 04 0.83116983E 01                   4
NO2-              J 6/72N  1.O  2.E -1.    0G   300.000  5000.000              1
 0.50160903E+01 0.21884463E-02-0.94586144E-06 0.17939789E-09-0.12052428E-13    2
-0.26200160E+05-0.12861447E+01 0.29818036E+01 0.49398681E-02 0.28557293E-05    3
-0.78905297E-08 0.35391483E-11-0.25501540E+05 0.99161680E+01                   4
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NO3          J12/64N  1.O  3.                G   300.000  5000.000              1
 0.72033289E+01 0.30908791E-02-0.13329045E-05 0.25461601E-09-0.17939047E-13    2
 0.58244016E+04-0.12608119E+02 0.76867377E+00 0.21181075E-01-0.16980256E-04    3
 0.22963836E-08 0.19321041E-11 0.75292921E+04 0.20406284E+02                   4
N2           J 9/65N  2.                     G   300.000  5000.000              1
 0.28963194E 01 0.15154866E-02-0.57235277E-06 0.99807393E-10-0.65223555E-14    2
-0.90586184E 03 0.61615148E 01 0.36748261E 01-0.12081500E-02 0.23240102E-05    3
-0.63217559E-09-0.22577253E-12-0.10611588E 04 0.23580424E 01                   4
N2H4         J12/65N  2.H  4.               OG   300.000  5000.000              1
 0.50947770E 01 0.93296138E-02-0.33626986E-05 0.56308304E-09-0.35859661E-13    2
 0.92996644E 04-0.35950952E 01 0.79803836E 00 0.21788097E-01-0.13456754E-04    3
-0.12698753E-09 0.25865213E-11 0.10379887E 05 0.18248696E 02                   4
N2O          J12/64N  2.O  1.                G   300.000  5000.000              1
 0.47306679E 01 0.28258267E-02-0.11558115E-05 0.21263683E-09-0.14564087E-13    2
 0.81617682E 04-0.17151073E 01 0.26189196E 01 0.86439616E-02-0.68110624E-05    3
 0.22275877E-08-0.80650330E-13 0.87590123E 04 0.92266952E 01                   4
N2O+         J12/70N  2.O  1.E -1.           G   300.000  5000.000              1
 0.53926946E+01 0.22337196E-02-0.93548832E-06 0.17466166E-09-0.12059043E-13    2
 0.15847633E+06-0.36920186E+01 0.34273064E+01 0.63787690E-02-0.22585149E-05    3
-0.20421800E-08 0.13481477E-11 0.15909237E+06 0.67997616E+01                   4
N2O4         J 9/64N  2.O  4.                G   300.000  5000.000              1
 0.10506637E 02 0.58723267E-02-0.24766296E-05 0.46556024E-09-0.32402082E-13    2
-0.28609096E 04-0.26252230E 02 0.36662865E 01 0.23491748E-01-0.16007297E-04    3
 0.11845939E-08 0.20001618E-11-0.90631797E 03 0.93973337E 01                   4
N2O5         J12/64N  2.O  5.                G   300.000  5000.000              1
 0.14413736E+02 0.40494080E-02-0.17661640E-05 0.33912224E-09-0.23926356E-13    2
-0.38366062E+04-0.43313433E+02 0.32144535E+01 0.37992511E-01-0.36847600E-04    3
 0.12409293E-07 0.24351911E-12-0.98609506E+03 0.13555831E+02                   4
N3           J12/70N  3.                     G   300.000  5000.000              1
 0.51996828E+01 0.24335678E-02-0.10192340E-05 0.19062350E-09-0.13212412E-13    2
 0.47963131E+05-0.35547759E+01 0.30624389E+01 0.73590658E-02-0.38229374E-05    3
-0.71824202E-09 0.91110236E-12 0.48614547E+05 0.77570129E+01                   4
O            J 6/62O  1.                     G   300.000  5000.000              1
 0.25420596E 01-0.27550619E-04-0.31028033E-08 0.45510674E-11-0.43680515E-15    2
 0.29230803E 05 0.49203080E 01 0.29464287E 01-0.16381665E-02 0.24210316E-05    3
-0.16028432E-08 0.38906964E-12 0.29147644E 05 0.29639949E 01                   4
O+           L12/66O  1.E -1.                G   300.000  5000.000              1
 0.25060486E 01-0.14464249E-04 0.12446049E-07-0.46858472E-11 0.65548873E-15    2
 0.18794700E 06 0.43479741E 01 0.24984794E 01 0.11410972E-04-0.29761395E-07    3
 0.32246539E-10-0.12375517E-13 0.18794908E 06 0.43864355E 01                   4
O-           J 6/65O  1.E -1.                G   300.000  5000.000              1
 0.25437173E 01-0.53258700E-04 0.25119617E-07-0.51851466E-11 0.39011542E-15    2
 0.11480516E 05 0.45202538E 01 0.28115796E 01-0.11905697E-02 0.18710553E-05    3
-0.13479178E-08 0.36663554E-12 0.11428431E 05 0.32402855E 01                   4
OH           J12/70O  1.H  1.                G   300.000  5000.000              1
 0.29131230E+01 0.95418248E-03-0.19084325E-06 0.12730795E-10 0.24803941E-15    2
 0.39647060E+04 0.54288735E+01 0.38365518E+01-0.10702014E-02 0.94849757E-06    3
 0.20843575E-09-0.23384265E-12 0.36715807E+04 0.49805456E+00                   4
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OH+               J12/700  1.H  1.E -1.           G   300.000  5000.000        1
 0.27381495E+01 0.14613173E-02-0.46950536E-06 0.73663560E-10-0.41410922E-14    2
 0.15761683E+06 0.61343811E+01 0.35365969E+01-0.47029254E-04-0.62344259E-06    3
 0.17601461E-08-0.82678699E-12 0.15736677E+06 0.18477172E+01                   4
CH-               J12/700  1.H  1.E  1.           G   300.000  5000.000        1
 0.28881148E+01 0.96560229E-03-0.19659254E-06 0.14053802E-10 0.12080617E-15    2
-0.18086455E+05 0.41896259E+01 0.34621427E+01 0.40525802E-03-0.13516992E-05    3
 0.17899459E-08-0.63434810E-12-0.18312355E+05 0.92893220E+00                   4
O2                J 9/650  2.                     G   300.000  5000.000        1
 0.36219535E 01 0.73618264E-03-0.19652228E-06 0.36201558E-10-0.28945627E-14    2
-0.12019825E 04 0.36150960E 01 0.36255985E 01-0.18782184E-02 0.70554544E-05    3
-0.67635137E-08 0.21555993E-11-0.10475226E 04 0.43052778E 01                   4
O2-               J12/660  2.E  1.                G   300.000  5000.000        1
 0.38147234E 01 0.77444546E-03-0.30677649E-06 0.56618118E-10-0.38229492E-14    2
-0.69910087E 04 0.29587995E 01 0.31440525E 01 0.12127972E-02 0.23812161E-05    3
-0.40914092E-08 0.16885304E-11-0.67369752E 04 0.67688687E 01                   4
O3                J 6/610  3.                     G   300.000  5000.000        1
 0.54665239E+01 0.17326031E-02-0.72204889E-06 0.13721660E-09-0.96233828E-14    2
 0.15214096E+05-0.34712616E+01 0.24660617E+01 0.91703209E-02-0.49698480E-05    3
-0.20634230E-08 0.20015595E-11 0.16059556E+05 0.12172130E+02                   4
S(S)              J12/65S  1.                     S   300.000   388.360        1
 0.             0.             0.             0.             0.                2
 0.             0.            -0.50637025E 01 0.28819353E-02-0.21330205E-04    3
 0.84787862E-06-0.17344967E-08 0.71482629E 03 0.28714074E 02                   4
S(L)              J12/65S  1.                     L   388.360  2000.000        1
 0.36036672E 01 0.99033405E-03-0.10114410E-05 0.40536327E-09-0.56679135E-13    2
-0.84538383E 03-0.16344708E 02-0.12706310E 02 0.90725216E-01-0.16951786E-03    3
 0.13070637E-06-0.35276150E-10 0.12346069E 04 0.56210160E 02                   4
S                 J 6/71S  1.                     G   300.000  5000.000        1
 0.29093331E+01-0.55587281E-03 0.27836947E-06-0.50194768E-10 0.31254639E-14    2
 0.32531543E+05 0.37928327E+01 0.29270078E+01 0.21982555E-03-0.23808853E-05    3
 0.29034821E-08-0.10846692E-11 0.32491577E+05 0.35120600E+01                   4
S+                L12/66S  1.E -1.                G   300.000  5000.000        1
 0.24118653E 01 0.22103303E-03-0.18939564E-06 0.61886675E-10-0.53887720E-14    2
 0.15375732E 06 0.58861130E 01 0.25088214E 01-0.62478561E-04 0.15513305E-06    3
-0.16148749E-09 0.60012108E-13 0.15373003E 06 0.53857186E 01                   4
SH                J 6/67S  1.H  1.                G   300.000  5000.000        1
 0.30371382E 01 0.12752466E-02-0.42314345E-06 0.67719668E-10-0.40934312E-14    2
 0.16545437E 05 0.60722981E 01 0.44098953E 01-0.22063747E-02 0.13171081E-05    3
 0.16467179E-08-0.12144787E-11 0.16180734E 05-0.10226129E 01                   4
SN                J 6/61S  1.N  1.                G   300.000  5000.000        1
 0.38493976E 01 0.72756788E-03-0.29370203E-06 0.55013628E-10-0.38123551E-14    2
 0.30459962E 05 0.44179139E 01 0.39422971E 01-0.20035515E-02 0.73534644E-05    3
-0.75168560E-08 0.25591098E-11 0.30563949E 05 0.45669484E 01                   4
SO                J 6/71S  1.O  1.                G   300.000  5000.000        1
 0.40039062E+01 0.29471359E-03 0.63481159E-07-0.28687405E-10 0.25022781E-14    2
-0.72238721E+03 0.35413673E+01 0.31258711E+01 0.13512854E-02 0.21503879E-05    3
-0.39964434E-08 0.17048142E-11-0.41679715E+03 0.84036007E+01                   4
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SO2          J 6/61S  1.0  2.                G   300.000  5000.000              1
 0.52451364E 01 0.19704204E-02-0.80375769E-06 0.15149969E-09-0.10558004E-13    2
-0.37558227E 05-0.10873524E 01 0.32665338E 01 0.53237902E-02 0.68437552E-06    3
-0.52810047E-08 0.25590454E-11-0.36908148E 05 0.96513476E 01                   4
SO3          J 9/65S  1.0  3.                G   300.000  5000.000              1
 0.70757376E 01 0.31763387E-02-0.13535760E-05 0.25630912E-09-0.17936044E-13    2
-0.50211376E 05-0.11200793E 02 0.25780385E 01 0.14556335E-01-0.91764173E-05    3
-0.79203022E-09 0.19709473E-11-0.48931753E 05 0.12251863E 02                   4
S2O          J12/65S  2.0  1.                G   300.0    2500.0                1
+0.47462541E+01+0.39213961E-02-0.27447525E-05+0.86623576E-09-0.10194171E-12    2
-0.83978219E+04+0.39322899E+01+0.36075344E+01+0.63649675E-02-0.83477066E-06    3
-0.59312363E-08+0.34913234E-11-0.81341062E+04+0.97014880E+01                   4
S2           J12/65S  2.                     G   300.000  5000.000              1
 0.42051134E 01 0.35309150E-03-0.13543069E-06 0.25245375E-10-0.17357488E-14    2
 0.14182908E 05 0.32094717E 01 0.41268240D+01 0.0            0.0               3
 0.0            0.0           +0.14278007D+05+0.38842476D+01                   4
S3           AGM002S  3.                     G   400.0    2000.0                1
+0.64418720D+01 0.0            0.0           0.0             0.0               2
+0.14528737D+05-0.52637140D+01+0.64418720D+01 0.0            0.0               3
 0.0            0.0           +0.14528737D+05-0.52637140D+01                   4
S4           AGM002S  4.                     G   400.0    2000.0                1
+0.91595370D+01 0.0            0.0            0.0            0.0               2
+0.13934474D+05-0.16594600D+02+0.91595370D+01 0.0            0.0               3
 0.0            0.0           +0.13934474D+05-0.16594600D+02                   4
S5           AGM002S  5.                     G   400.0    2000.0                1
+0.12229490D+02 0.0            0.0            0.0             0.0              2
+0.10354813D+05-0.30608550D+02+0.12229490D+02 0.0            0.0               3
 0.0            0.0           +0.10354813D+05-0.30608550D+02                   4
S6           AGM002S  6.                     G   300.000  5000.000              1
+0.10946149E+02+0.13162404E-01-0.12816001E-04+0.52824158E-08-0.77054900E-12    2
+0.81282658E+04-0.23197232E+02 0.15400100D+02 0.0            0.0               3
 0.0            0.0           +0.78752894D+04-0.44938467D+02                   4
S7           AGM002S  7.                     G   400.0    2000.0                1
+0.18067438D+02 0.0            0.0             0.0            0.0              2
+0.83273278D+04-0.53878130D+02+0.18067438D+02 0.0            0.0               3
 0.0            0.0           +0.83273278D+04-0.53878130D+02                   4
S8           J 6/64S  8.                     G   300.000  5000.000              1
+0.20988816E+02+0.10719352E-02-0.44901051E-06+0.84142467E-10-0.58548537E-14    2
+0.56884396E+04-0.69101739E+02 0.20533400D+02 0.0            0.0               3
 0.0            0.0           +0.62917230D+04-0.64990000D+02                   4
END
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VITA 2

Ali Ghormullah Maadah

Candidate for the Degree of

Doctor of Philosophy

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Major Field: Chemical Engineering

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