New Jersey Institute of Technology
Digital Commons @ NJIT

6-30-1973

Computer simulation of a split feed Claus sulfur recovery plant

Thomas R. Woolley
New Jersey Institute of Technology

Follow this and additional works at: https://digitalcommons.njit.edu/theses

Part of the Chemical Engineering Commons

Recommended Citation

Woolley, Thomas R., "Computer simulation of a split feed Claus sulfur recovery plant" (1973). *Theses*. 2478.
https://digitalcommons.njit.edu/theses/2478

This Thesis is brought to you for free and open access by the Electronic Theses and Dissertations at Digital Commons @ NJIT. It has been accepted for inclusion in Theses by an authorized administrator of Digital Commons @ NJIT. For more information, please contact digitalcommons@njit.edu.

Copyright Warning & Restrictions

The copyright law of the United States (Title 17, United States Code) governs the making of photocopies or other reproductions of copyrighted material.

Under certain conditions specified in the law, libraries and archives are authorized to furnish a photocopy or other reproduction. One of these specified conditions is that the photocopy or reproduction is not to be "used for any purpose other than private study, scholarship, or research." If a, user makes a request for, or later uses, a photocopy or reproduction for purposes in excess of "fair use" that user may be liable for copyright infringement,

This institution reserves the right to refuse to accept a copying order if, in its judgment, fulfillment of the order would involve violation of copyright law.

Please Note: The author retains the copyright while the New Jersey Institute of Technology reserves the right to distribute this thesis or dissertation

Printing note: If you do not wish to print this page, then select "Pages from: first page # to: last page #" on the print dialog screen

NJIT
New Jersey's Science & Technology University

The Van Houten library has removed some of the personal information and all signatures from the approval page and biographical sketches of theses and dissertations in order to protect the identity of NJIT graduates and faculty.

COMPUTER SIMULATION OF A SPLIT FEED
CLAUS SULFUR RECOVERY PLANT

BY

THOMAS R. WOOLLEY

A THESIS
PRESENTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE
OF
MASTER OF SCIENCE IN CHEMICAL ENGINEERING
AT
NEWARK COLLEGE OF ENGINEERING

This thesis is to be used only with due regard to the rights of the author. Bibliographical references may be noted, but passages must not be copied without permission of the College and without credit being given in subsequent written or published work.

Newark, New Jersey
1973

ABSTRACT

A computer program which calculates a complete heat and material balance around a "split feed" Claus sulfur recovery plant was written in Fortran IV for the RCA Spectra 70 computer. The program provides for up to three catalytic reactors, the hot gas bypass method of reheating, and a feed gas containing hydrogen sulfide, water vapor, hydrogen, and nitrogen. The program user specifies as input data the feed stream composition and temperature, the number of reactors, the combustion air temperature, the conversion in each reactor, the outlet temperature in each condenser, and the fraction of burner exit gas used for reheating the feed gases to each reactor. The program prints out the input data, the adiabatic flame temperature of the burner combustion gases, the cooling load of the waste heat boiler and each condenser, the reheater heating loads, and a complete stream summary.

APPROVAL OF THESIS

COMPUTER SIMULATION OF A SPLIT FEED

CLAUS SULFUR RECOVERY PLANT

BY

THOMAS R. WOOLLEY

FOR

DEPARTMENT OF CHEMICAL ENGINEERING

NEWARK COLLEGE OF ENGINEERING

BY

FACULTY COMMITTEE

APPROVED:

NEWARK, NEW JERSEY

JUNE, 1973

TABLE OF CONTENTS

Page

APPENDIX:

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

The Claus process is essentially a vapor phase oxidation of hydrogen sulfide with air or sulfur dioxide which yields sulfur and water. The reaction takes place as high temperatures (730°C to 1000°C) in the absence of a catalyst and at lower temperatures (<730°C) in the presence of a catalyst. Although there are a wide variety of flow schemes, three basic flow schemes are generally recognized. They are: the split feed, the once through, and the direct oxidation. A typical Claus plant is a series of conversion and condensation steps where the vapors are reheated following each condensation step.

The use of Claus type sulfur recovery plants to recover sulfur from hydrogen sulfide has increased in recent years because of strict state and federal government air pollution standards put into effect, public pressure, and a more responsible attitude by industry toward environmental problems. This has created a need for computer programs which can perform the tedious heat and material balance calculations required to evaluate the design and operation of these plants. A single fairly accurate hand-calculated heat and material balance may require from three to four man weeks and the calculation will have to be made many times to properly evaluate a given problem because of the number of variables and possible flow schemes involved.(11) These programs have been written by Opekar and Goar(11), Boas and Andrade(1) and others, but because of their proprietary nature, only brief descriptions of the capabilities of these programs and their results and not the programs have been published.

The objective of this thesis is to produce a flexible computer program which calculates a heat and material balance around a "split feed" Claus sulfur recovery plant with hot gas bypass reheating, and to verify the results of others. A secondary objective is to provide a thorough study of industrial Claus plants and their operation.

Although this work is of limited scope and duplicates the work of others, it provides a non-proprietary independently written program with which to verify previous results and is also a good basis for future industrial or student work of broader scope. The program, in addition, will provide a quick way of studying the effect of such variables as the number of reactors, the converter operating temperatures, the condenser operating temperatures, and the amount of hot gas bypass reheating on the overall operation of a "split feed" Claus plant. It is limited in scope in that different flow schemes and reheating methods are not considered as they have been in previous work.

The primary source of thermodynamic properties of sulfur and sulfur bearing compounds for both this project and work by others is Kelley(8). Kelley has used the basic vapor density data of Preuner and Schupp(14) in the development of this data. The best single source found on the Claus process is Gamson and Elkins(3).

The author would like to acknowledge Dr. E. C. Roche for his assistance in both the programming and chemical engineering aspects of this thesis.

CHAPTER 2

GENERAL PROCESS DESCRIPTION

Vapor Phase Oxidation Methods

The Claus process is one of the most important methods for the recovery of sulfur from hydrogen sulfide. In this process, hydrogen sulfide is oxidized in the vapor phase with either air or sulfur dioxide according to the overall reaction:

$$H_2S + [O] \rightarrow H_2O + S \qquad \text{(R2-1)}$$

This oxidation is a high temperature reaction which may occur at lower temperatures on surfaces or in solution. Taylor and Wesley showed that the oxidation occurred only by contact catalysis below 730°C. Although numerous catalysts including $A\ell_2O_3$(bauxite), activated carbons, silica gel, silicates of $A\ell^{+++}$ and Fe^{+++} and alkali and alkaline earth metals, metal sulfides, and alkaline compounds can be used for this oxidation, bauxite is the most satisfactory because of its low cost, durability, and high activity.

The conventional Claus plant is a series of sulfur conversion and condensation steps. One of the basic differences in commercial Claus plants is the method of carrying out the initial oxidation step. The three basic methods for doing this are: the direct oxidation, the split feed, and the straight through or once through. The initial oxidation step is then followed by one or more catalytic reactors depending on the conversion requirements of the particular process. Two or more catalytic conversion steps are usually required with present day air pollution standards. Yields of 90 to 95% with two catalytic reactors and 95 to 98% with three are usually attained. Each catalytic reactor is followed by a sulfur condenser to recover the sulfur as a liquid. After each condensation step, the vapors are reheated to prevent the condensation of sulfur in the catalyst bed and subsequent catalyst poisoning.

The earliest commercial method for carrying the vapor phase oxidation of H_2S was the original Claus process or the direct oxidation method, discovered by C. F. Claus in 1890 and from which the other two methods have evolved. This process comprised the oxidation of hydrogen sulfide with air in the stoichiometric proportion over bauxite in a single reactor according to the highly exothermic reaction

$$3H_2S + 3/2\ O_2 \rightarrow 3H_2O + 3/e\ S_e \qquad \text{(R2-2)}$$

$$\Delta H = 145\text{-}173\ \text{Kcal}$$

This value of ΔH gives the heat of reaction over a wide temperature range, thus accounting for its variability. Although the yield increases with decreasing temperature, the reaction must be carried out at a temperature greater than that at which sulfur begins to condense, since liquid sulfur effectively poisons the catalyst. Since radiation was the only provision for removing the large quantities of heat evolved in the process, the temperature was controlled by restricting the space velocity.(1) In order to obtain yields of 80-90%, only two or three volumes of hydrogen sulfide (S.T.P.) could be converted per volume of catalyst per hour. This method is still used today for very low concentration H_2S streams for which it is difficult to sustain combustion with the other two methods. In this case, the air and/or the acid gas is usually preheated and fed to the catalytic reactor. A diagram of a Claus direct oxidation plant is shown in Figure 1.

The split feed process developed by I. G. Farbenindustrie around 1937 was the first significant improvement in the original Claus process. This is a two stage process in which the hydrogen sulfide stream is split, one third being burned completely to sulfur dioxide under a waste heat boiler according to the reaction

$$H_2S + \frac{3}{2} O_2 \rightleftarrows H_2O + SO_2 \qquad \text{(R2-3)}$$

$$\Delta H = 124\text{-}138 \text{ Kcal}$$

---

(1) Space velocity is defined as the volume of feed gas (S.T.P.) per hour per volume of catalyst.

and then reacted with the remaining two thirds of the hydrogen sulfide in a catalytic reactor according to the reaction

$$2H_2S + SO_2 \rightleftarrows 2H_2O + 3/e\ S_e \qquad \text{(R2-4)}$$

$$\Delta H = 21\text{-}35 \text{ Kcal}$$

A diagram of the process is shown in Figure 2. The improvement results from the fact that almost 80% of the total heat of reaction is liberated before the final catalytic conversion. As a result, the space velocity can be increased about one hundred fold while maintaining operating temperatures at sufficiently low levels. Another advantage of this process is that if hydrocarbons and carbon dioxide are present in the feed, the formation of carbonyl sulfide in the high temperature region and the amount of carbon in the resulting sulfur product are minimized.

This process is used for acid gas with low H_2S content (less than 25%) to insure stable operation of the acid gas burner. By bypassing part of the acid gas around the burner, the flame temperature is kept high enough for stable combustion. In case of very low H_2S concentrations, the flame temperature could be boosted by adding supplemental hydrocarbons or by indirectly preheating the air or acid gas before charging to the burner. The direct oxidation process is usually more economical in such cases however.

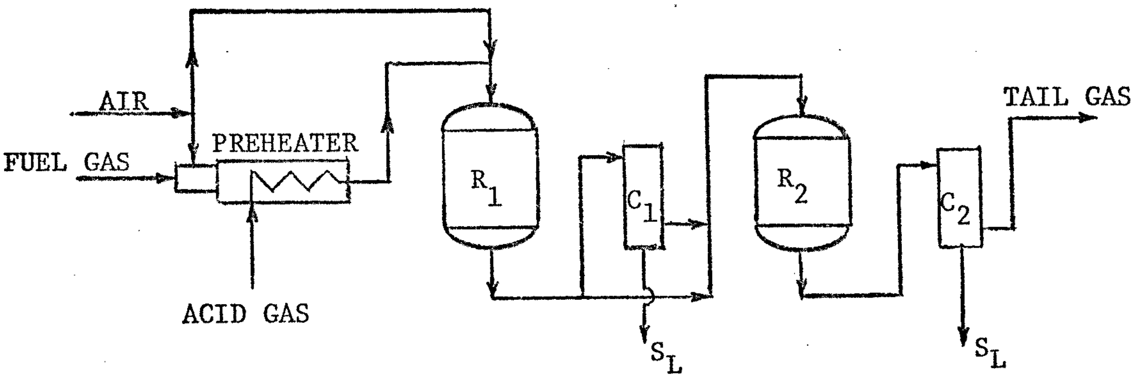


Fig.1. Claus direct oxidation plant.

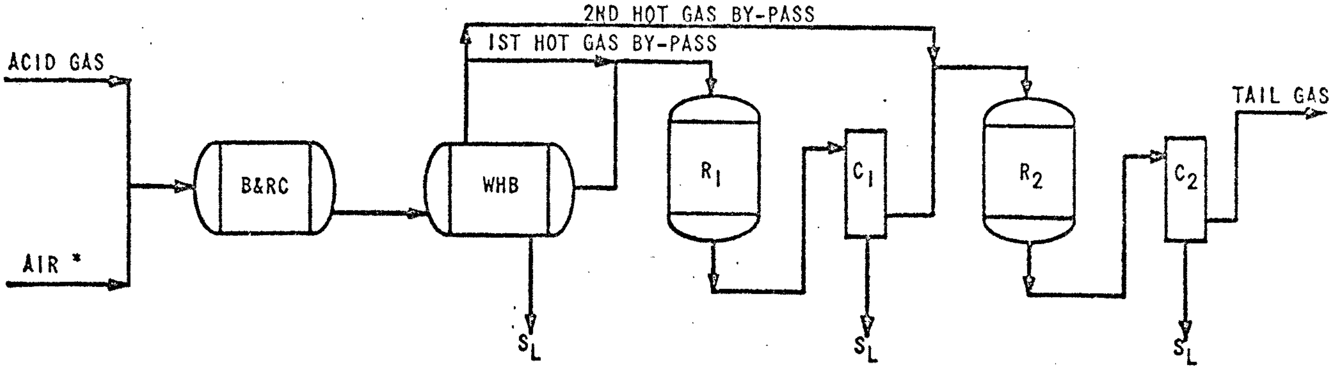


Fig.2. "Once through" scheme with sufficient air to burn ⅓ of total H_2S to SO_2 and all hydrocarbon to CO_2.

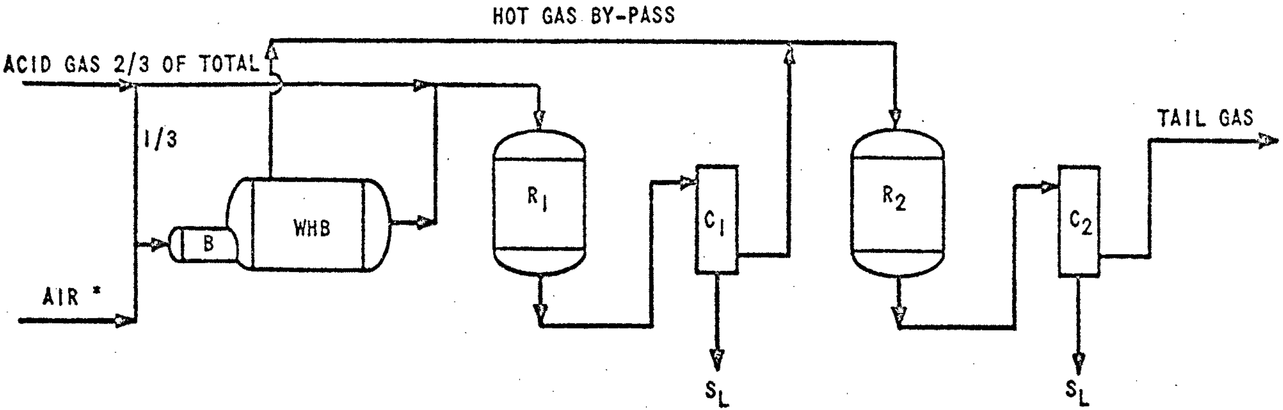


Fig.3. "Split stream" flow with sufficient air to burn all H_2S to SO_2 and all hydrocarbon to CO_2 in ⅓ of acid gas.

A second modification of the Claus process was developed by I. G. Farbenindustrie at about the same time as the first. This process, called the straight through or once through, is a high temperature (up to 1000°C) non-catalytic combustion of the entire hydrogen sulfide stream with air in the required stoichiometric proportion for complete conversion to sulfur. The reaction takes place in a free flame or over an inert mass with yields of approximately 60%. The high temperature combustion is then followed by one or more catalytic conversion steps to recover effectively all of the sulfur. A diagram of a straight through Claus plant is shown in Figure 3.

This process is used for highly concentrated H_2S streams to reduce the load on the catalytic conversion steps both from a kinetic as well as a thermochemical point of view. In the thermal reactor from 90 to 95% of the total heat of reaction is liberated, and about 60% of the total conversion to sulfur is accomplished. This sulfur is normally removed prior to the first catalytic conversion step to lower the dew point of the gas mixture in the first catalytic reactor, and thus increase the maximum theoretical yield attainable. By effecting the complete combustion of hydrocarbons, the free flame combustion also serves to protect the catalyst from deactivation.

Vapor Reheating Methods

In addition to the initial oxidation step, Claus plants also differ in the method of reheating the gas following a condensation step. The four most important methods in commercial use today are:

1. Hot gas bypass
2. In-line burner
3. Gas-to-gas exchanger
4. Indirect fired reheater

These four methods are depicted in Figure 4. In the hot gas bypass method, the cooled gas leaving each condenser is raised to operating temperature of the converter which follows by direct mixing with hot gas extracted from the outlet of one of the passes of a multipass waste heat boiler.

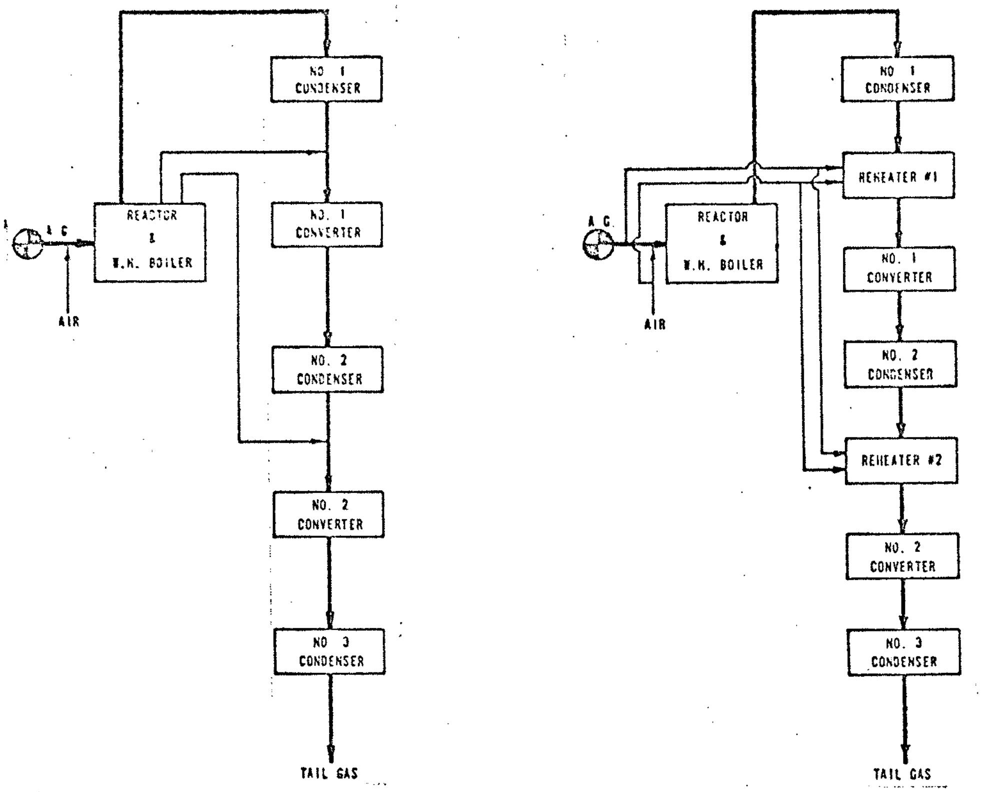
The second method of reheating consists of a direct fired refractory lined furnace in which the products of combustion of a side stream of acid gas furnish the heat to bring the main stream of gas to operating temperature.

The gas-to-gas exchange method utilizes the exothermic heat produced in the converters to reheat the feed gas to the converter by gas-to-gas exchanger. This method is the least flexible in adapting to verying feed rates and compositions.

Converter temperatures become difficult to sustain without some form of auxilliary heat with a decrease in either the acid gas feed rate or H_2S content. With a decrease in feed rate, heat losses become more significant. In the case of reduced H_2S content, the amount of gas to be reheated remains about the same, while the total heat of reaction decreases.

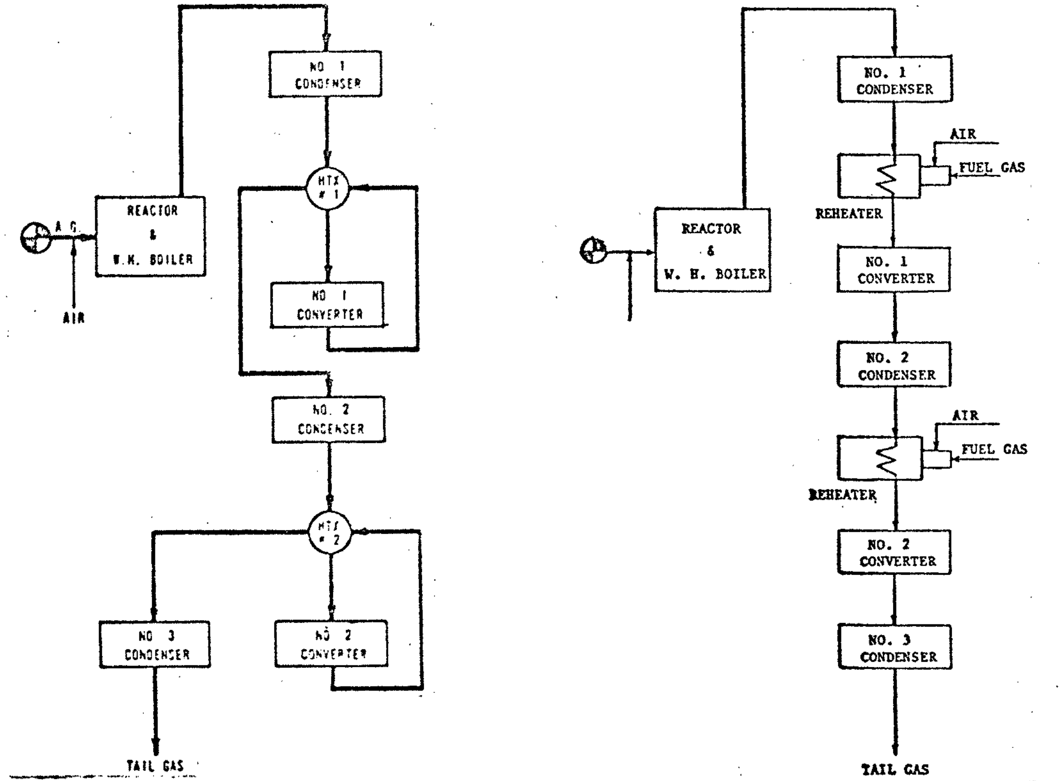
The indirect fired reheaters utilize the heat transfer media of a thin metal wall, refractories, or silica glass to transport heat from the combustion process to the gas stream to be heated.

Both the hot gas bypass and in-line burner methods result in recoveries which are several percent lower than the other two methods because some acid gas feed is bypassed around one or more conversion steps. The indirect fired reheater and the gas-to-gas exchanger methods require the highest capital investment because each uses heat exchangers which have poor heat transfer coefficients and, therefore, require large heat transfer surface areas. Capital investment for Method 2 is also relatively high because each in-line burner requires a ratio control system to maintain the proper air to acid gas ratio. The hot gas bypass method requires the lowest capital cost.



HOT GAS BYPASS

IN-LINE BURNER



GAS-TO-GAS EXCHANGE

INDIRECT FIRED REHEATER

Fig.4. Vapor Reheating Methods.

COS Conversion

One of the major problems encountered in Claus plants where the feed contains carbon dioxide and light hydrocarbons is the formation of carbonyl sulfide during high temperature combustion. The conversion of carbonyl sulfide to sulfur according to the reaction

$$2\ COS + SO_2 \rightarrow 3S + 2\ CO_2 \qquad (R2\text{-}5)$$

is favored at high temperatures, but high conversion can be obtained at low temperatures at space velocities below 200. A graph of COS conversion versus temperature is shown in Figure 5. At space velocities above 200 and at temperatures where the conversion of carbonyl sulfide is complete, the conversion of hydrogen sulfide is incomplete. For this reason, most commercial processes involve two catalytic reactors where COS is present; the first is operated at a temperature level of about 400°C to assure high conversion of carbonyl sulfide, and the second reactor operating at as low a temperature as practicable to maintain high conversion of hydrogen sulfide. At space velocities below 200, high conversion of carbonyl sulfide will occur around 260°C, thus making it possible to obtain conversion over 90% for both carbonyl sulfide and hydrogen sulfide in a single catalytic converter.

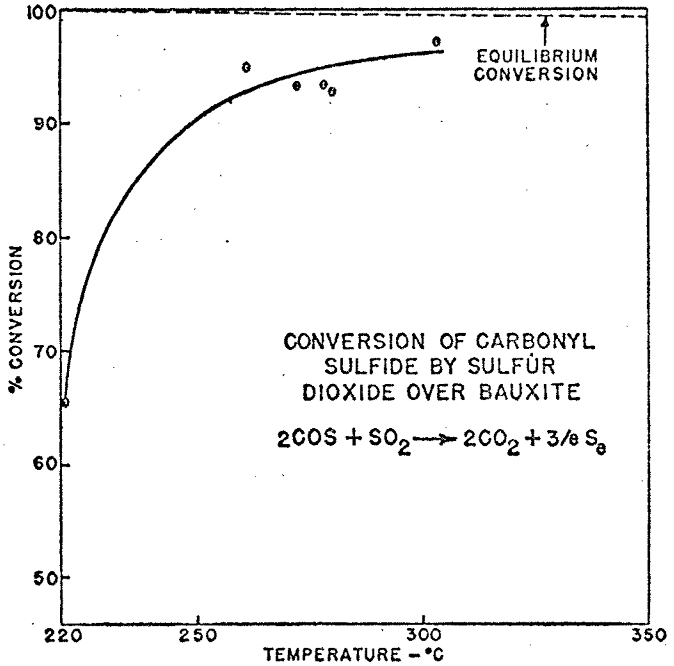


Fig.5. Conversion of carbonyl sulfide by sulfur dioxide over bauxite.

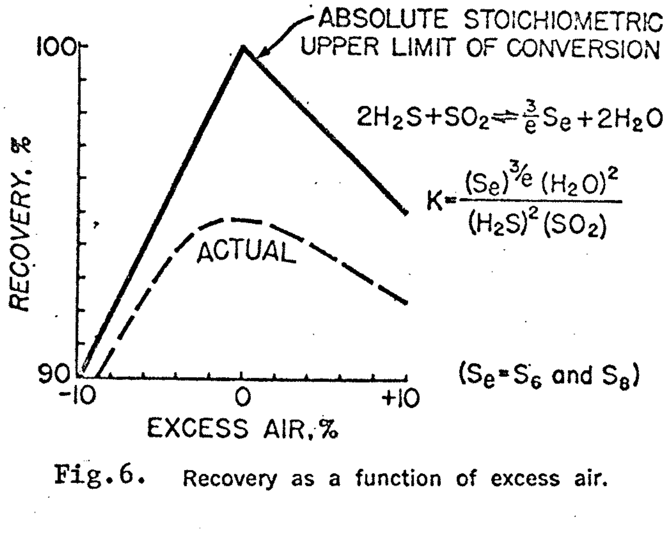


Fig.6. Recovery as a function of excess air.

Ratio of Air to Acid Gas

To anyone studying Claus sulfur recovery processes, a thorough understanding of the effect of the air to acid gas ratio on the overall recovery is essential. For any given feed composition, the air to acid gas ratio that will yield an H_2S to SO_2 ratio in the tail gas of 2.0 must be maintained for optimum sulfur recovery. When recovery is high, the ratio in the tail gas is very sensitive to the ratio of air to acid gas. Since, with ordinary instrumentation, the H_2S to SO_2 ratio cannot be maintained exactly, it is important to be aware of the loss in sulfur yield within the probable control range of 90 to 110% of the correct stoichiometric amount of air. The loss in recovery is greater for a given percent deficiency when compared with the same percent excess. This can be shown by studying the stoichiometry and the equilibrium of the reactions involved. The overall reaction to produce sulfur from hydrogen sulfide is:

$$2H_2S + O_2 \rightleftarrows 2S + 2H_2O \qquad \text{(R2-6)}$$

From the reaction, it can be seen that one mole of oxygen will react to form two atoms of sulfur. An excess of oxygen would convert sulfur already produced to SO_2 by the reaction

$$S + O_2 \rightleftarrows SO_2 \qquad \text{(R2-7)}$$

Looking at the stoichiometry of the two reactions only, the effect on sulfur yield is only half as great for a given percentage excess air as for the same percentage deficiency. The percentage deficiency or excess of air will set an upper stoichiometric limit on the conversion possible. The difference between this upper limit and 100% will be twice as great for a deficiency. For example, the upper limit for a 10% deficiency is 90%, while the upper limit for a 10% excess is 95%. The maximum theoretical yield for each case will be governed by the kinetics of the following reaction:

$$2H_2S + SO_2 \rightleftarrows 3/2\ S_2 + 2H_2O \qquad \text{(R2-8)}$$

The equilibrium expression for this reaction is represented by

$$K = \frac{(S_2)^{3/2}(H_2O)^2}{(H_2S)^2\ (SO_2)} \qquad \text{(E2-1)}$$

From this expression, it can be seen that a higher than normal H_2S concentration (deficiency of air) will have a greater effect on driving the reaction to the right than a higher than normal SO_2 concentration (excess of air). This is because the H_2S concentration is raised to the second power in the equilibrium expression while the SO_2 concentration is raised to the first power. Thus, the theoretical recovery in the case of a deficiency approaches the stoichiometric limit more closely than for the same percent excess, but since the stoichiometric limit is lower than that for an excess, the actual yield is lower. Secondary effects, such as reactor temperature rise and change in gas volume due to the excess or deficiency have a negligible effect. A plot from the literature(4) showing the sulfur recovery as a function of excess air for a once through Claus plant with 100% H_2S feed is shown in Figure 6. The relationship between excess air and sulfur recovery for a given plant is useful in determining the economics of a tail gas analyzer with or without automatic control of the air to acid gas ratio by the analyzer.

Catalytic Reactor

Conversion variables. Various laboratory studies have been made to determine the effect of variables such as temperature, gas velocity, catalyst depth, and percent water in the feed on the conversion in a catalytic reactor. Graphs of variables versus conversion obtained from laboratory studies made at the Matheison Chemical Corporation's McKamie plant are shown in Figures 7 through 10. This particular study represents the conversion of the H_2S in furnace exit gas to elemental sulfur. In Figure 7, the conversion is shown as a function of catalyst temperature. The solid and dotted lines represent furnace feed gas with no methane and 4% methane respectively. For the case of 0% methane, the principal reaction is between hydrogen sulfide and sulfur dioxide. Over

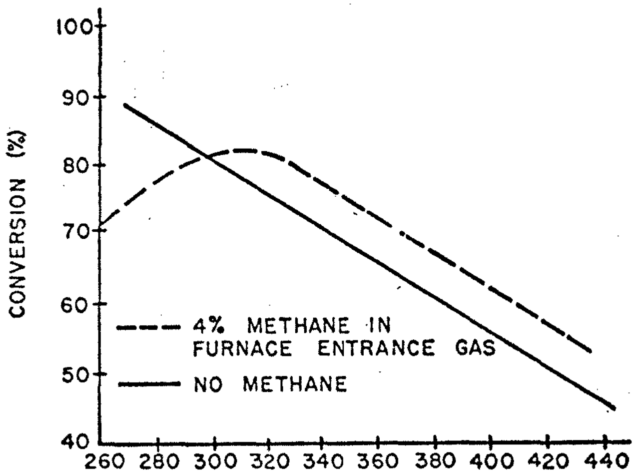


Fig.7. **Catalyst Temperature.**

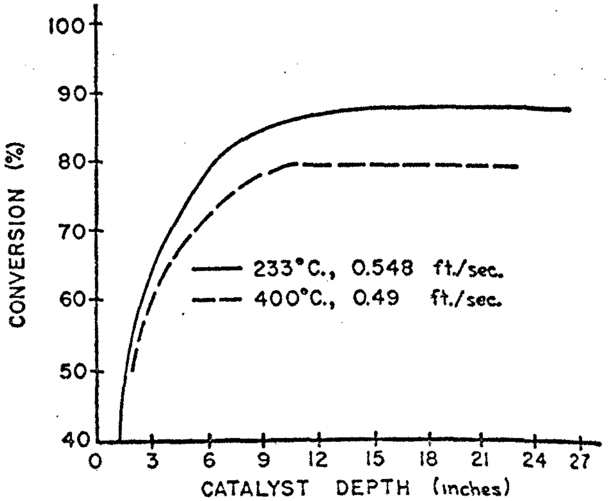


Fig.8. **Catalyst Bed Depth**

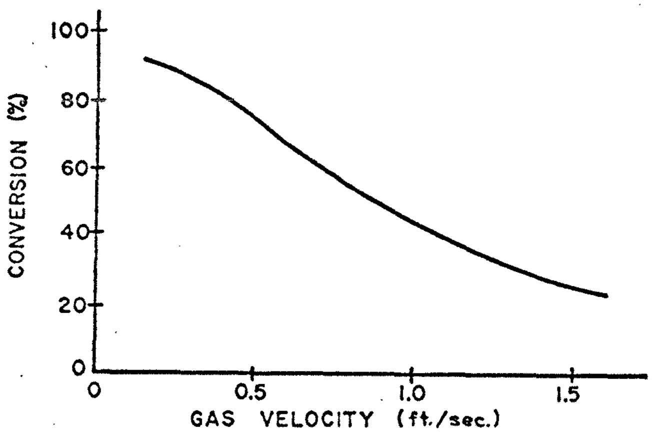


Fig.9. **Linear Gas Velocity**

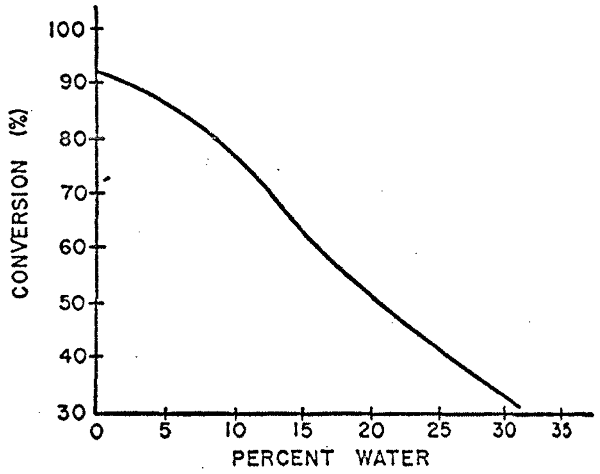


Fig.10. **Water Vapor Concentration**

Effects of Principal Variables on Conversion as Determined in Laboratory Equipment

the entire range studied, the conversion was favored by decreasing temperature. For the case of 4% methane feed, the conversion passes through a maximum at 320°C. The combustion of methane results in the formation of carbonyl sulfide, the conversion of which is favored with increasing temperature. At low temperatures, the carbonyl sulfide passes unchanged through the converter resulting in a low overall conversion even though the hydrogen sulfide-sulfur dioxide reaction is substantially complete. As the temperature increases, more carbonyl sulfide is converted and less sulfur is formed via the hydrogen sulfide-sulfur dioxide reaction. Below 320°C, the increase in conversion due to the conversion of carbonyl sulfide is greater than the decrease due to the reduction in the primary reaction. Above 320°C, the reverse is true.

The effect of the catalyst bed depth on conversion is shown in Figure 8. The shape of the conversion-catalyst bed depth curves depends to a large extent on the gas velocity used, but an optimum catalyst depth generally exists for each set of conditions, above which the addition of catalyst has a negligible effect on the conversion obtained. Thus, for both curves shown in Figure 8, a 9 inch bed depth would be considered optimum. At practical space velocities, the optimum bed depth seldom exceeds 22 inches.

The study of linear gas velocity through the catalyst bed is closely associated with the determination of the optimum depth of the catalyst bed. For a linear velocity of zero, equilibrium conditions would be obtained, and for high velocities, the conversion would approach zero. The useful range of gas velocity for the case of the 4 inch catalyst bed is shown in Figure 9. In this range, the conversion decreases in a linear manner with increasing gas velocity. Although low velocities are desirable for high conversion, the size of the converter required at extremely low velocities becomes impractible. The range generally used is 0.5 to 2.0 feet per second (S.T.P.).

The effect of water vapor in the feed gas on the conversion is shown in Figure 10. The conversion increases with decreasing concentration of water in the feed. The presence of water vapor decreases both the rate of reaction and the equilibrium conversion.

Temperature profile. Typical curves of the temperature profile in a catalytic reactor are shown in Figure 11. The linear temperature profile represented by the circular data points indicates that the reaction, or heat generating rate is essentially constant over the range of the primary reaction. The sharp change in slope of the profile indicates the termination of the primary reaction. For the case of the temperature profile represented by the triangular data points, a secondary reaction is indicated by the continued temperature rise after the change in slope due to the termination of the primary reaction. This secondary reaction is probably a sulfur vapor molecular weight change.

Catalyst bed contamination. To date no limit on the life of bauxite catalyst has been observed, but because the catalyst particles may become coated with carbon deposits, causing increased pressure drop through the bed, the catalyst is changed every three to five years.

If the temperature in the catalyst bed drops below the dew point of the reaction mixture, the sulfur will deposit on and deactivate the catalyst. This is only a temporary poison and full activity can be restored by passing hot gas well above its dew point through the bed until the condensed sulfur is removed. Sulfur removal can be followed by observing the catalyst bed temperature rise. Some sulfur is always present inside an operating catalyst and does not necessarily indicate an activity problem. It is hazardous to pass air over a reactor containing sulfur when the bed temperature is over 300°F. The fire resulting from such a practice has been known to burn a hole in the side of a reactor.

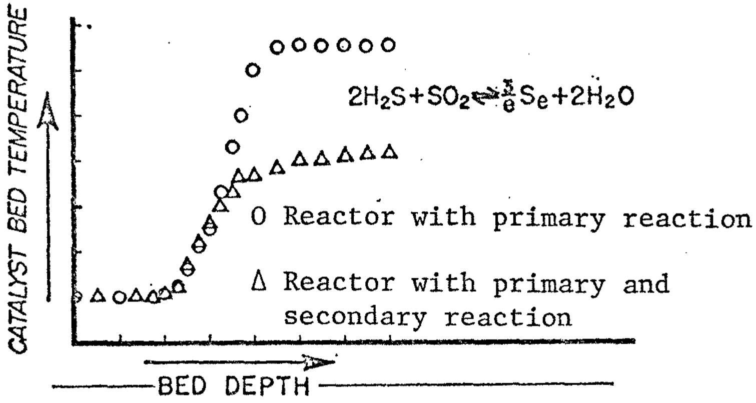


Fig.11. Catalyst bed temperature as a function of bed depth.

CHAPTER 3

THERMODYNAMIC DATA

A study of the vapor density of sulfur by Preuner and Schupp(14) has shown that at temperatures above 1200°K and below 2000°K, the sole stable specie of sulfur is S_2. Below 1200°K and above 300°K, a complicated equilibrium exists between S_2, S_6, and S_8 which is a function of temperature and the total sulfur partial pressure. Preuner and Schupp have made extensive measurements from 573°K to 1123°K and found that the average molecular weight of sulfur vapor in the range of the normal boiling point is between that of S_6 and S_8 and that the observed vapor densities can be explained by a stepwise dissociation of the type $S_8 \rightleftarrows S_6 \rightleftarrows S_2$. Their work seems to rule out the presence of S_4, since the resulting equilibria were not consistent with their findings. Presumably, a four membered ring of sulfur atoms is not sufficiently stable at these temperatures.

Preuner and Schupp measured the total pressure, the volume, temperature, and mass of a system containing sulfur vapor. They assumed that at 573°K and 623°K the concentration of S_2 is so low that it can be neglected, and therefore, the only equilibrium to be considered is:

$$3S_8 \rightleftarrows 4S_6 \qquad \text{(R3-1)}$$

The equilibrium expression for this reaction is

$$K_1 = (S_6)^4/(S_8)^3 \qquad \text{(E3-1)}$$

This system is conditioned by the equations

$$P_T = p_6 + p_8 \qquad \text{(E3-2)}$$

$$P_T\ V = mRT/M32 \qquad \text{(E3-3)}$$

where p_6 = partial pressure of S_6

p_8 = partial pressure of S_8

P_T = total system pressure

V = system volume

m = system mass

M = atoms per molecule

R = gas law constant

T = absolute temperature

Values of p_6 and p_8 were calculated by substituting the experimental data into equations E3-2 and E3-3 and were then used to evaluate K, at 573°K and 623°K from equation E3-1 . From the values of K_1 at 573°K and 623°K, the standard heat of reaction, ΔH°, was calculated using the van't Hoff equation shown below.

$$\ell n\ K_1(T_1)/K_1(T_2) = -\Delta H°/R\ 1/T_1 - 1/T_2 \qquad \text{(E3-4)}$$

By assuming the heat of reaction, ΔH°, is constant, K_1 values at higher temperatures were calculated.

In the temperature range from 623°K to 1123°K, the reactions

$$S_6 \rightleftarrows 3S_2 \qquad \text{(R3-2)}$$

$$S_8 \rightleftarrows 4S_2 \qquad \text{(R3-3)}$$

and their equilibrium expressions

$$K_3 = (S_2)^3/S_6 \qquad \text{(E3-5)}$$

$$K_2 = (S_2)^4/S_8 \qquad \text{(E3-6)}$$

were considered in addition to reaction R3-1. With S_2 present, the system is described by the following three equations:

$$p_2 + p_6 + p_8 = P_T \qquad \text{(E3-7)}$$

$$MP_T = 8p_8 + 6p_6 + 2p_2 \qquad \text{(E3-8)}$$

$$K_1 = (S_6)^4/(S_8)^3 \qquad \text{(E3-9)}$$

Solving equations E3-7, E3-8, and E3-9 simultaneously, the partial pressures of all 3 species were calculated over the temperature range of interest and were then used to calculate the values of K_2 and K_3 from equations E3-5 and E3-6 respectively. Based upon the calculated equilibrium constants, the systematic variations of S_2, S_6, and S_8 have been developed and are shown in Figures 12, 13, and 14. The variation obtained between the various types of sulfur at 1 atmosphere total pressure above the boiling point of sulfur and the saturated vapor pressure below are shown in Figure 15. Klemm and Kilian(17), Braune and Nevelling(2), and others have also studied the vapor density of sulfur. Klemm and Kilian, working with more modern equipment, reported higher molecular weights, but their work was interrupted by World War II and never completed. Although Braune and Nevelling reported the existence of S_4 in addition to S_2, S_6, and S_8, preliminary calculations in the critical temperature regions indicate that the yield of sulfur based on the data of Preuner and Schupp is in fair agreement.

Free Energy Relationships

Kelley(8) has developed thermodynamic relationships for the standard free energy change of reactions R3-1, R3-2, and R3-3 from the equilibrium constant values of Preuner and Schupp. A discussion of Kelley's method of developing these free energy relationships will follow.

ΔF°_T for the reaction $S_8 \rightleftarrows 4S_2$. Since the specific heat of S_8 is unknown and there is no satisfactory method available for calculating this quantity, it was arbitrarily assumed that

Fig.12. Variation of diatomic sulfur with temperature and pressure when the total pressure is due to sulfur.

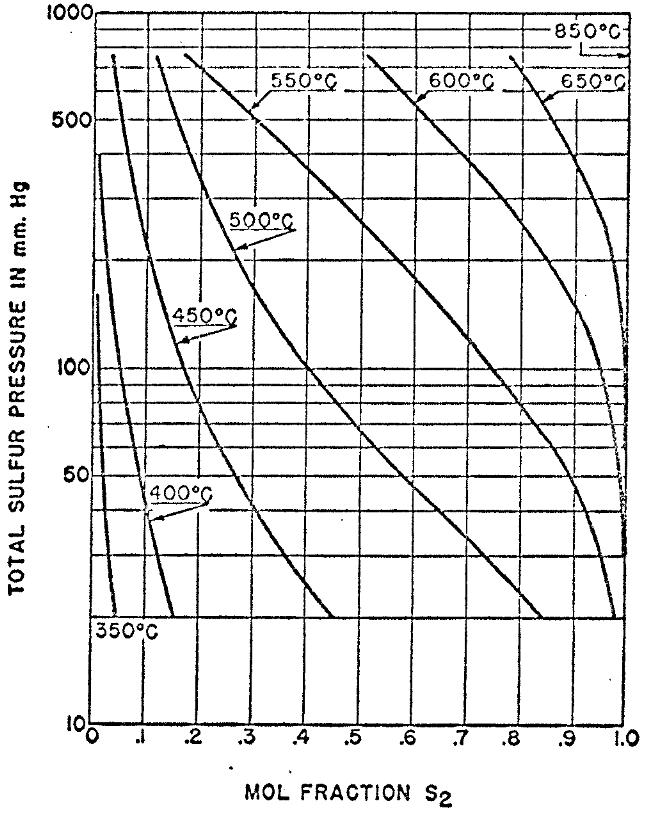
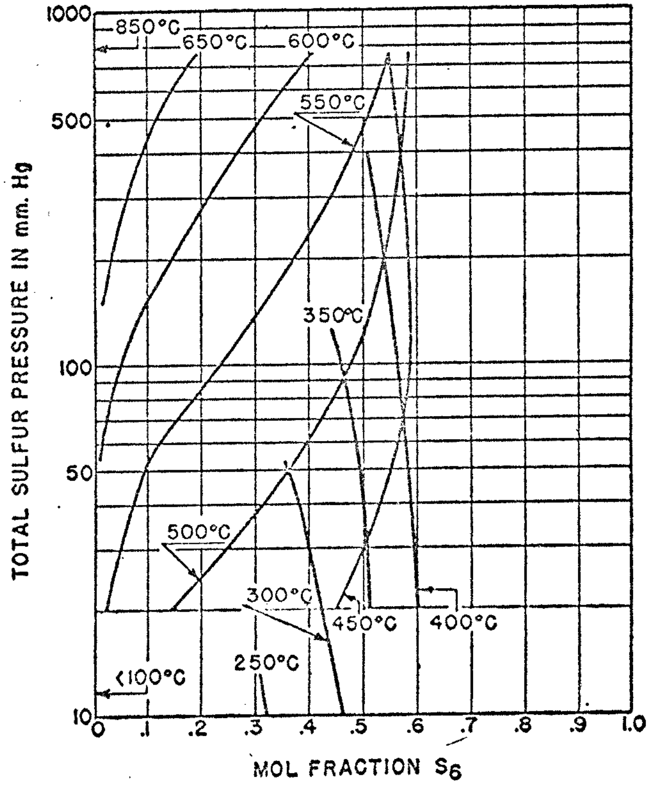


Fig.13. Variation of hexatomic sulfur with temperature and pressure when the total pressure is due to sulfur.



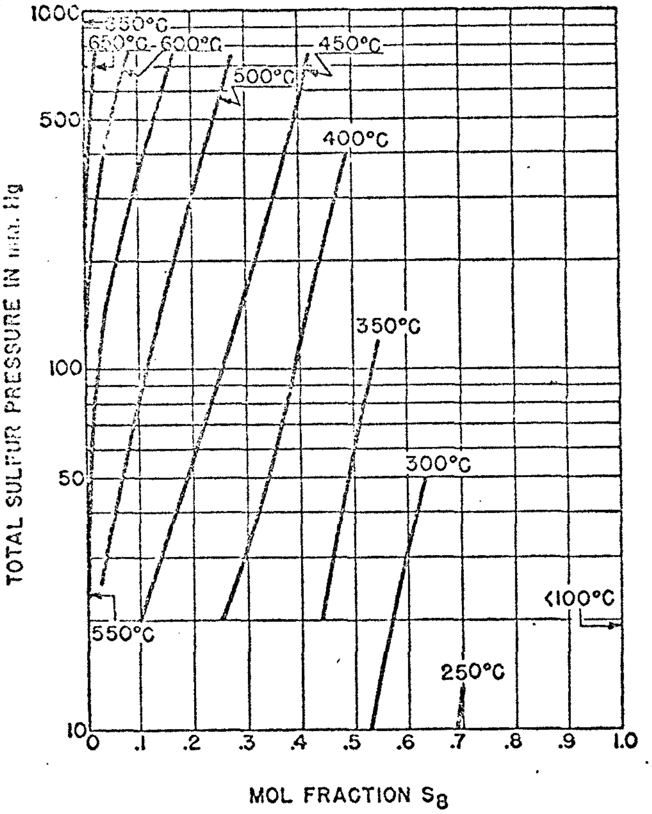
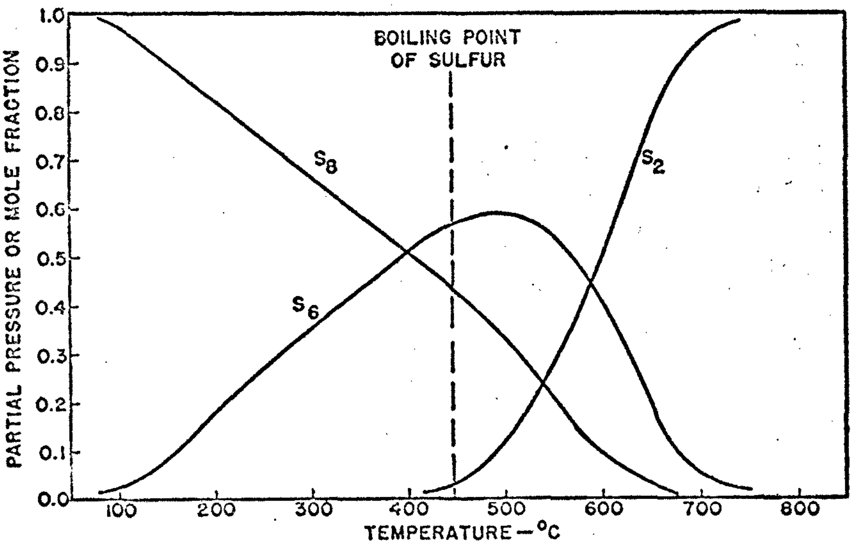


Fig.14. Variation of octatomic sulfur with temperature and pressure when the total pressure is due to sulfur.



$P_{S_8} + P_{S_6} + P_{S_2} + P_S$ = 1 ATMOSPHERE ABOVE BOILING POINT

$P_{S_8} + P_{S_6} + P_{S_2} + P_S$ = VAPOR PRESSURE BELOW BOILING POINT

Fig.15. Equilibrium between the molecular species of sulfur.

ΔC_p=6 for this reaction. Substituting ΔC_p=6 into the standard equations

$$\Delta H_T^\circ = \Delta H_o + \Delta aT + \Delta b/2\ T^2 + \Delta C/3\ T^2 \qquad \text{(E3-10)}$$

$$\Delta F_T^\circ = \Delta H_o - IT\ \Delta b/2\ T^2 - \Delta C/6\ T^3$$

$$- \Delta aT\ell nT \qquad \text{(E3-11)}$$

the following two equations are obtained:

$$\Delta H_T^\circ = \Delta H_o + 6T \qquad \text{(E3-12)}$$

$$\Delta F_T^\circ = \Delta H_o - 13.8T \log T + IT \qquad \text{(E3-13)}$$

where T = temperature, °K

ΔH_T° = standard heat of reaction at temperature T, cal

ΔF_T° = standard free energy change at temperature T, cal

Since $\Delta F_T^\circ = -RT\ell nK$, equation E3-13 was written in the form

$$\sum = -R\ell nK + 13.8T \log T = \Delta H_o/T + I \qquad \text{(E3-14)}$$

Values of Σ were plotted against 1/T and a good approximation to a straight line with a slope that yielded a value of ΔH_o= 95,200 calories was obtained over most of the temperature range. A value of I = -62.28 was calculated by taking an average of values obtained by subtracting $\Delta H_o/T$ from Σ.

The final equations are:

$$\Delta H^\circ_T = 95{,}200 + 6T \quad \text{(E3-15)}$$

$$\Delta F^\circ_T = 95{,}200 - 13.8 \log T - 62.28T \quad \text{(E3-16)}$$

$$\Delta H^\circ_{298.1} = 96{,}990 \text{ cal} \quad \text{(E3-17)}$$

$$\Delta F^\circ_{298.1} = 64{,}670 \text{ cal} \quad \text{(E3-18)}$$

ΔF°_T for the reaction $3S_8 \rightleftarrows 4S_6$. Since the specific heat of S_6 and S_8 are unknown, a value of ΔC_p=2 was assumed for this reaction. Based on this assumption, the equations for ΔH°_T and ΔF°_T take the forms

$$\Delta H^\circ_T = \Delta H_o + 2T \quad \text{(E3-19)}$$

$$\Delta F^\circ_T = \Delta H_o - 4.6T \log T + IT \quad \text{(E3-20)}$$

Using the same procedure as that used for the reaction $S_8 \rightleftarrows 4S_2$, the following equations were obtained:

$$\Delta H^\circ_T = 29{,}250 + 2T \quad \text{(E3-21)}$$

$$\Delta F^\circ_T = 29{,}250 - 4.6T \log T - 27.81T \quad \text{(E3-22)}$$

$$\Delta H^\circ_{298.1} = 29{,}850 \text{ cal} \quad \text{(E3-23)}$$

$$\Delta F^\circ_{298.1} = 17{,}570 \text{ cal} \quad \text{(E3-24)}$$

ΔF°_T for the reaction $S_6 \rightleftarrows 3S_2$. The following expressions for ΔH°_T and ΔF°_T were obtained by combining equations E3-15, E3-16, E3-21, and E3-22:

$$\Delta H_T^\circ = 64{,}090 + 4T \qquad \text{(E3-25)}$$

$$\Delta F_T^\circ = 64{,}090 - 9.2T \log - 44.26T \qquad \text{(E3-26)}$$

$$\Delta H_{298.1}^\circ = 65{,}280 \text{ cal} \qquad \text{(E3-27)}$$

$$\Delta F_{298.1}^\circ = 44{,}110 \text{ cal} \qquad \text{(E3-28)}$$

Equations E3-25 and E3-26 show good agreement with the data of Preuner and Schupp below 873°K.

CHAPTER 4

COMPUTATIONAL AND ASSOCIATED BOUNDS

The exact mechanism for the selective oxidation of hydrogen sulfide to elemental sulfur according to the overall reaction

$$2H_2S + O_2 \rightleftarrows 2H_2O + S_2 \qquad \text{(R4-1)}$$

is unknown. This reaction is conditioned by the equilibria in the vapor phase between S_2, S_6, and S_8 represented by the reactions

$$3S_2 \rightleftarrows S_6 \qquad \text{(R4-2)}$$

$$4S_2 \rightleftarrows S_8 \qquad \text{(R4-3)}$$

and occurs by a complex reaction equilibria which includes the following reactions :

$$2H_2S + 3O_2 \rightleftarrows 2H_2O + 2SO_2 \qquad \text{(R4-4)}$$

$$2H_2S + SO_2 \rightleftarrows 2H_2O + 3/2\ S_2 \qquad \text{(R4-5)}$$

$$S_2 + 2O_2 \rightleftarrows 2SO_2 \qquad \text{(R4-6)}$$

Since the thermodynamic equilibrium constants for the reactions R4-1, R4-4, and R4-6 are so great at the free flame combustion temperature that no elemental oxygen exists in the reaction mixture, the actual equilibria can be solved by considering only reactions R4-2, R4-3, and R4-5.

G. W. Gamson and R. H. Elkins have made a detailed study of the theoretical equilibrium conversion of pure hydrogen sulfide to sulfur vapor by selective oxidation with the stoichiometric quantity of air according to reaction R4-1. Their plot of conversion versus temperature at system pressures of .5, 1.0, and 2.0 atmospheres is shown in Figure 16. The percent conversion is defined in terms of the equilibrium partial pressures by the equation

$$\% \text{ conversion} = \frac{2S_2 + 6S_6 + 8S_8}{2S_2 + 6S_6 + 8S_8 + H_2S + SO_2} \times 100 \quad \text{(E4-1)}$$

It can be seen from this plot that the conversion passes through a minimum in the range of 800-900°K for all three pressures. This minimum point roughly defines two regions of behavior for the reaction; the catalytic region to the left of the minimum, and the thermal region to the right. In the low temperature catalytic region, the presence of a catalyst is required for the reaction to take place and the conversion increases with pressure at a given temperature. In the thermal region, the reaction will take place in free flame combustion without the use of a catalyst and the conversion decreases with pressure at a given temperature. In the thermal region at temperatures above 1300°K, the reaction kinetics are rapid enough to achieve the maximum yield predicted by the thermodynamics of the system. Both the minimum in the conversion curve and the reversal of the pressure-conversion relationship in the two regions are due to a shift in the sulfur specie equilibria with temperature. With increasing temperature, the formation of S_2 by reactions R4-1 and R4-5 increases while the formation of S_6 and S_8 by reactions R4-2 and R4-3 decreases. The pressure-conversion relationship can be explained by analyzing the effect that pressure has on the predominant reactions in each region. Reactions R4-2 and R4-3, which are predominant in the catalytic region, result in a decrease in the number of moles, while reactions R4-1 and R4-5, which predominate in the thermal region, increase and effect no change respectively in the number of moles. Since an increase in pressure tends to drive a reaction in the direction of fewer moles, the conversion increases with pressure in the catalytic region and decreases with pressure in the thermal region.

Although the theoretical yield approaches 100% at around 400°K, the maximum yield in the catalytic region is determined by the theoretical yield at the dew point of the reaction mixture. Below the dew point, sulfur condenses and effectively poisons the catalyst. The total sulfur partial pressure is plotted as a function of temperature and pressure in Figure 17. The intersections of the sulfur vapor pressure curve which is also plotted in Figure 17 with the sulfur partial pressure curves correspond to the dew points at each of the three system pressures. Since the dew point increases

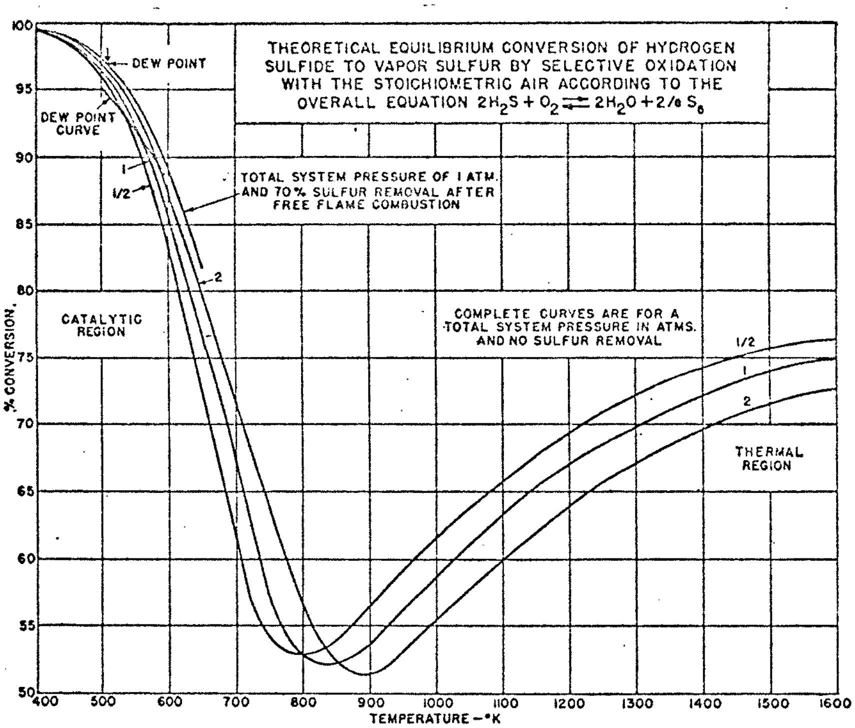


Fig.16. Theoretical equilibrium conversion of hydrogen sulfide to vapor sulfur by selective-oxidation with the stoichiometric air according to the over-all equation $2H_2S + O_2 \rightleftharpoons 2H_2O + 2/eS_e$.

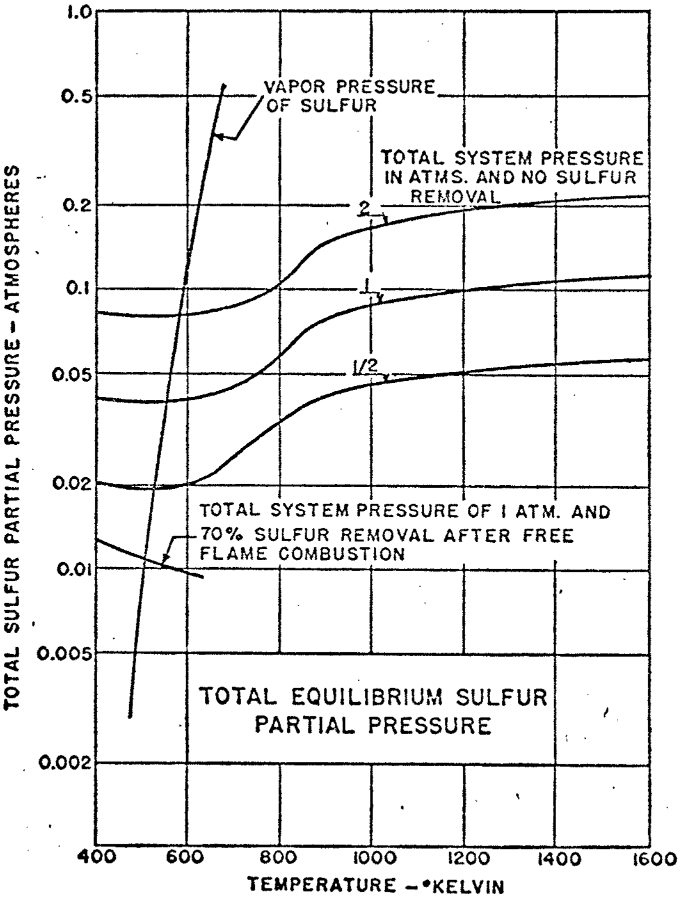


Fig.17. Total equilibrium sulfur partial pressure.

with system pressure, the maximum attainable yield increases inversely with the pressure. However, along an isotherm in the catalytic region, the yield is favored by increasing pressure. The theoretical yields and dew points for the systems shown in Figure 17 are summarized in Table 1 below.

TABLE 1

DEW POINT AND YIELD VERSUS SYSTEM PRESSURE

Total System Pressure atm	Theoretical Dew Point °K	Theoretical Yield %
1/2	527	93.5
1	553	92.0
2	580	89.7

CHAPTER 5

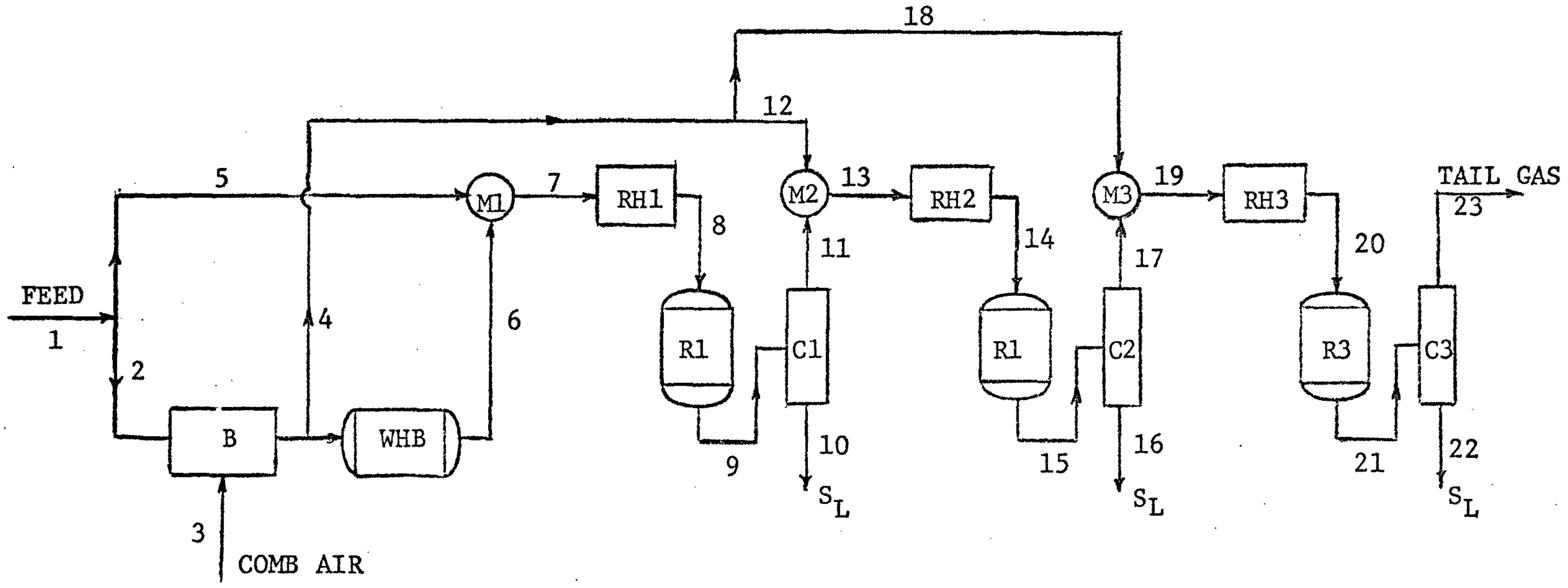
THE COMPUTER PROGRAM

The Main Program

This computer program, which is written in Fortran IV, calculates a complete heat and material balance for a "split feed" Claus sulfur recovery plant with hot gas bypass reheating. All calculations are based on an acid gas feed rate of 100 lb moles per hour and a system pressure of one atmosphere absolute. Plants with one, two, or three catalytic reactors corresponding to eleven, seventeen, and twenty-three streams are provided for. A flow diagram of a three reactor plant with streams numbered as they are in the program is shown in Figure 18. Stream components are represented in the program by a double subscripted variable STRM (i,j), where i is the stream component number and j is the stream number. Each stream has the following components with the associated numbers and units:

COMPONENT NUMBER	COMPONENT	UNITS
1	H_2	lb moles/hr
2	H_2S	lb moles/hr
3	H_2O	lb moles/hr
4	N_2	lb moles/hr
5	O_2	lb moles/hr
6	SO_2	lb moles/hr
7	S_6	lb moles/hr
8	S_8	lb moles/hr
9	S_2	lb moles/hr
10	liquid sulfur	lb atoms/hr
11	total moles	lb moles/hr
12	temperature	°K
13	stream enthalpy	BTU/hr

Fig.18. Computer Process Flow Sheet - Split Feed Claus Process



LEGEND

B	BURNER
WHB	WASTE HEAT BOILER
M	MIXER
RH	REHEATER
R	CATALYTIC REACTOR
C	CONDENSER
S_L	SULFUR LIQUID

Stream data is stored in blank common so that it can be easily accessed from all parts of the program. The program input data includes the acid gas feed composition and temperature, the temperature of the combustion air, the outlet temperature of each condenser, the fraction of burner outlet gas used to heat the feed to each reactor, and the fractional conversion in each reactor. Temperatures are specified in degrees Fahrenheit. Each piece of data is read from a separate data card to provide flexibility when making up the input data. The acid gas feed may contain nitrogen, water vapor, hydrogen, and hydrogen sulfide in any proportion. Feed stream components such as carbonyl sulfide, methane, carbon disulfide, and carbon monoxide are not provided for. The program printout includes the input data, the burner flame temperature, the components of each stream, the cooling loads of the waste heat boiler and condensers, and the heating requirements of the reheaters. The computer program listing and the printout from six sample problems is shown in the APPENDIX.

One-third of the acid gas is fed to a burner where complete conbustion with the stoichiometric quantity of air takes place at the theoretical flame temperature. A subroutine FLAME is called by the main program to calculate the theoretical flame temperature and the material balance around the burner. The fraction of the burner exit gas specified is cooled in a waste heat boiler and then combined with the two thirds of the feed bypassing the burner to form the feed to the first reactor. The remaining burner exit gas is used in the fractions specified as hot gas bypass for heating the feed gas to the second or third reactors. The waste heat boiler subroutine WHB determines the temperature of the gas stream leaving the waste heat boiler and the rate of heat removal in the waste heat boiler. The waste heat boiler exit temperature is initially set to 373°K in the main program before the reactor subroutine REACTR is called to perform the calculations for the first reactor. For a lower limit, it is assumed that this temperature will never be lower than that of steam at atmospheric pressure. If a reheater is required to heat the first reactor feed at this burner exit temperature, the reactor subroutine will set the reheater feed temperature equal to the reactor feed temperature, thus eliminating the first reheater. In this case, the subroutine WHB will calculate the temperature of the burner exit temperature required to meet this condition. In the unusual case where the reheater is not eliminated and a cooler is required, the burner exit temperature remains at its initial value of 373°K. This situation could only occur if the acid gas feed temperature is abnormally high or if the H_2S feed concentration approaches 100%. With the exception of the first reactor, each reactor in the plant is preceded by a mixer and a reheater and followed by a condenser. The outlet gas from the previous condenser and the hot bypass gas are combined in a mixer to form the feed to the next reactor, which is then heated to the desired temperature by the reheater. The mixer has no physical significance as this type of mixing would normally be accomplished in a pipeline in the typical industrial plant. The mixer subroutine MIXER calculates the temperature and composition of the mixer outlet stream taking into account the complex equilibria between S_2, S_6, and S_8. The heater calculations, which are performed by the subroutine REACTR, determine the rate of heat addition in the heater and the reactor feed composition, which changes in passing through the heater due to the equilibria between S_2, S_6, and S_8. It is assumed that no reaction takes place between H_2S and SO_2 in either the mixer or the heater. If the calculated rate of heat addition is negative, a cooler is required to meet the conditions specified in the input data. Although this condition is not automatically corrected by the program, a reduction in the amount of hot gas bypass or the reactor conversion would eliminate the need for cooling. The combination of a mixer, reheater, reactor, and condenser is repeated in the main program by systematically numbering the streams so that there is a mathematical relationship between them.

There is no provision for incinerator tail gas treatment of the gas stream leaving the last condenser.

Each of the subroutines and function programs used in the main program are described below.

Subroutines and Function Programs

In the mathematical expressions used in the descriptions which follow, brackets will be used to identify stream numbers, and the variables names used will be the same as those in the program where possible.

Subroutine FLAME (TADBF). This subroutine calculates the adiabatic flame temperature of the acid gas stream passing through the burner and a material and energy balance around the burner. The quantity of combustion air (steam 3) is calculated from the stoichiometry of the two combustion reactions taking place in the burner shown below.

$$H_2 + 1/2\ O_2 \rightarrow H_2O \qquad (R5\text{-}1)$$

$$H_2S + 3/2\ O_2 \rightarrow SO_2 + H_2O \qquad (R5\text{-}2)$$

The total oxygen is calculated as follows:

$$O_2[3] = 0.5 \times H_2[2] + 1.5 \times H_2O[2] \qquad (E5\text{-}1)$$

The nitrogen in the combustion air is therefore

$$N_2[3] = .79/.21 \times O_2[3] \qquad (E5\text{-}2)$$

The total moles of combustion air is calculated by adding the moles of N_2 and O_2

$$AIR[3] = O_2[3] + N_2[3] \qquad (E5\text{-}3)$$

The components in the burner exit stream are calculated as follows:

$$H_2O[4] = H_2[2] + H_2S[2] + H_2O[2] \tag{E5-4}$$

$$N_2[4] = N_2[3] + N_2[2] \tag{E5-5}$$

$$SO_2[4] = H_2S[2] \tag{E5-6}$$

$$\text{TOTAL MOLES}[4] = H_2O[4] + H_2O[4] + N_2[4] + SO_2[4] \tag{E5-7}$$

To calculate the flame temperature, the variable FUNCT expressing the change in enthalpy in the burner is calculated and checked for convergence with the function program WAYA. The variable FUNCT is defined as

$$\begin{aligned} \text{FUNCT} = {} & \text{SENTH}(2) + \text{SENTH}(3) - \text{SENTH}(4) \\ & - \Delta H_{R5-1} \times H_2[2] - \Delta H_{R5-2} \\ & \times H_2S[2] \end{aligned} \tag{E5-8}$$

where SENTH(N) = enthalpy of stream N, BTU/hr

ΔH_{R5-1} = standard heat of reaction at 25°C for R5-1, BTU/hr

ΔH_{R5-2} = standard heat of reaction at 25°C for R5-2, BTU/hr

The function program SENTH is used to calculate the stream enthalpies in this expression. The upper and lower limits of flame temperature specified with WAYA are 4000°K and 373°K respectively. If these limits do not yield values of FUNCT which bracket zero, the desired value, the message

ADIABATIC FLAME TEMP CALC DID NOT CONVERGE

is printed out and the subroutine is exited without completing the calculation. If FUNCT has not converged, WAYA selects a new value of temperature and FUNCT is recalculated. If FUNCT converges or if 99 trials are exceeded, the calculation is complete and the subroutine returns the adiabatic flame temperature to the main program.

Function WAYA (A, ANS, TOL, START, STOP, LEVEL). The function program WAYA estimates the value of an independent variable START that will make the single valued function A (dependent variable) converge to within ± TOL of the desired value, ANS. The other variables associated with the function are defined as follows:

STOP = upper limit of the dependent variable START

WAYA = a flag used to indicate the status of the convergence. On exit, the value of WAYA is:

- if A has not converged and a new value of START has been estimated

0 if A has converged to within tolerance or 99 trials have been exceeded

\+ if A cannot converge because the values of A calculated at START and STOP respectively do not bracket ANS.

In using WAYA, it is important not to set the tolerance TOL too small or the calculation will not converge within 99 trials and also to select the limits of START so that they yield values of A which bracket ANS. The number of allowable trials is a constant which can be changed to any desirable value.

The algorithm employed is a combination of linear interpolation and the principle of having, each having an equal weight. If the function is not bounded with the first two trials, the subprogram terminates the calculation and returns the respective trial independent variable having the minimum error.

Function SENTH(K). This function program calculates the enthalpy of stream K relative to 25°C by summing the enthalpies of the stream components. The function program EQUA calculates the individual component enthalpies using the constants stored in block data area HFDT. The equation and the source of constants used to calculate component enthalpies is discussed in the APPENDIX. The five constants associated with each component yield an enthalpy value in units of calories per gram mole when the temperature is in °K. The stream enthalpies are therefore multiplied by 1.8 to convert to units of BTU per hour before returning the value to the main program.

Function EQUA (X, C). This function program calculates the value of a polynominal of the form

$$Y = A_0 + A_1X + A_2X^2 + \cdots\cdots A_MX_M + A_{M+1}X^{-1} \qquad \text{(E5-9)}$$

using a nested expansion to calculate the value of Y excluding the last term, which is added on at the end. The X^{-1} term has been included so that the function program can be used for component enthalpy expressions which take this form. Sulfur dioxide is the only one at present. The nested expansion procedure improves the accuracy of the calculation by reducing the round of error. The variable C is the starting address of the array where the polynomial constants are stored in computer memory. The constants are stored in the following order:

$M = C(1)$

$A_0 = C(2)$

$A_1 = C(3)$

$A_2 = C(4)$

....

....

$A_M = C(M+2)$

$A_{M+1} = C(M+3)$

The value of Y is transferred to the main program.

Subroutine MIXER (IN1, IN2, MIX, K). The subroutine calculates the composition and temperature of stream MIX formed by mixing streams IN1 and IN2 in mixer K.

The temperature of the stream MIX is calculated in one iterative loop by setting up an enthalpy balance around the mixer and solving for the temperature which makes the process adiabatic. The reaction equilibria between S_2, S_6, and S_8 is solved at each temperature and included in the enthalpy balance. Before starting the iterative loop, the individual components of stream MIX are calculated by adding streams IN1 and IN2 on a componental basis. At this point, the amounts S_2, S_6, and S_8 have been calculated by straight addition without considering the reaction equilibria because the temperature of stream MIX is unknown. The function program WAYA is used to estimate the temperature of stream MIX and test the following enthalpy expression for convergence:

$$\begin{aligned} H = {} & \mathrm{SENTH[IN1]} + \mathrm{SENTH[IN2]} - \mathrm{SENTH(MIX)} \\ & + \Delta H_{R5-4} \text{ X } \Delta S6 + \Delta H_{R5-5} \text{ X } S8 \end{aligned} \tag{E5-10}$$

If the stream MIX contains any sulfur, the subroutine SPLIT is called to calculate the amounts of S_2, S_6, and S_8 before evaluating equation E5-10. The function program SENTH is used for calculating stream enthalpies. The lower temperature limit is set equal to that of the lower temperature stream entering the mixer. The upper limit is set arbitrarily at 2000°K, a figure which is based on typical operating conditions of a Claus Plant.

If these limits do not yield values of H which bracket the desired value, the message

MIXER K DOES NOT CONVERGE

is printed out and the subroutine is exited without completing the remaining calculations. If H has not converged, WAYA estimates a new value of temperature and the calculation is repeated. If H converges or if 99 trials are exceeded, the subroutine returns to the main program. The components of stream MIX are now stored in blank common.

Subroutine EQUAL (N1, N2). This subroutine sets the first eleven components of stream N2 equal to the corresponding components of stream N1. It is used in many parts of the program where calculations involve two streams differing in only a few components.

Subroutine REACTR (NI, CONV, NO, IR, HEAT, I). This subroutine calculates a heat and material balance around a catalytic reactor and its associated reheater based on the specified conversion and the requirement that the reaction be adiabatic. The variables specified in using the subroutine are as follows:

NI = number of the stream entering the reheater
CONV = conversion of H_2S and SO_2 converted to S_2, S_6, and S_8 based on the entering SO_2

NO = number of the reactor outlet stream

IR = number of the reactor inlet stream

HEAT = reheater heat input, BTU/hr

I = reactor number

In carrying out this calculation, the temperature at which the specified conversion takes place must be determined and then checked to make sure it is above the dew point of the reaction mixture. As explained in CHAPTER 1, only the following three reactions are considered in solving the reaction equilibria:

$$2H_2S + SO_2 \rightleftarrows 2H_2O + 3/2\ S_2 \qquad \text{(R5-3)}$$

$$3S_2 \rightleftarrows S_6 \qquad \text{(R5-4)}$$

$$4S_2 \rightleftarrows S_8 \qquad \text{(R5-5)}$$

The equilibrium expressions for these reactions are:

$$\text{EQK1} = \frac{(\text{WA})^2(\text{S2})^{3/2}}{(\text{H2S})^2(\text{SO2})}\left[\frac{\Pi}{\text{TMOLES}}\right]^{1/2} \qquad \text{(E5-11)}$$

$$\text{EQK2} = \frac{\text{S6}}{(\text{S2})^3}\left[\frac{\text{TMOLES}}{\Pi}\right]^2 \qquad \text{(E5-12)}$$

$$\text{EQK3} = \frac{\text{S8}}{(\text{S2})^4}\left[\frac{\text{TMOLES}}{\Pi}\right]^3 \qquad \text{(E5-13)}$$

where EQKN = equilibrium constant for reaction N at temperature T

TMOLES = total moles in the reactor, lb moles/hr

S2 = moles of S_2 in reactor, lb moles/hr

S6 and S8 are defined similarly.

Because the system pressure has been taken as one atmosphere, the total pressure term Π drops out of these three expressions. The equilibria is solved by performing the calculation in three iterative loops. The reaction temperature, the total moles, and the moles of S_6 are calculated in the outer, middle, and inner loops respectively. The calculation starts in the inner loop with initial values of T and TMOLES by calculating a value of S6. The variable in each loop is tested for convergence by a function program WAYA, which estimates a new value of the variable if it has not converged. Each time a new value of a variable is estimated, the calculation is repeated starting with the inner loop. For example, if a new value of TMOLES is estimated, the calculation is repeated starting with the inner loop using the current value of T and the new value of TMOLES. If a new value of T is estimated, the calculation is repeated starting at the inner loop with TMOLES and S6 equal to their initial values and T equal to the new value.

In the inner loop values of S2 and S8 are calculated from the estimated values of S6, TMOLES, and T using the following two equations:

$$S2 = \frac{(S6)^{1/3}(TMOLES)^{2/3}}{(EQK2)^{1/3}} \qquad (E5\text{-}14)$$

$$S8 = EQK3\ \frac{(S6)^{4/3}}{(EQK2)^{4/3}}\ \frac{1}{(TMOLES)^{1/3}} \qquad (E5\text{-}15)$$

These two equations were obtained by solving equations E5-12 and E5-13 for S2 and S8 respectively in terms of S6. Equilibrium constants EQK2 and EQK3 are calculated by the function program EQK. To see if the estimated value of S6 satisfies the sulfur atom balance, a variable BAL is calculated and tested for convergence by WAYA. The sulfur atom balance can be expressed as

$$2 \times S2[NO] + 6 \times S6[NO] + 8 \times S8[NO] =$$
$$2 \times S2[NI] + 6 \times S6[NI] + 8 \times S8[NI] + SF \qquad (E5\text{-}16)$$

where S2[NO] = S_2 in the reactor outlet stream, 16 moles/hr

Other components are similarly defined

SF = sulfur atoms converted to S_2, S_6, and S_8, lb atoms/hr

The value of SF in this equation is calculated from the specified conversion, CONV, which is defined as

$$\text{CONV} = \frac{\text{SF}}{3 \text{ x } \text{SO2[IR]}} \qquad \text{(E5-17)}$$

The conversion is defined only in terms of SO_2 because the hot gas bypass method of reheating is used, and therefore, the ratio of H_2S/SO_2 in the reactor feed will always be 2.0 or greater. A definition in terms of H S and SO would not represent the true conversion in cases where the H_2S and SO_2 were not present in stoichiometric amounts. The variable BAL is defined in terms of equation E5-16 as follows:

$$\text{BAL} = 1.0 - \frac{(\text{2xS2[NO]} + \text{6xS6[NO]} + \text{8xS8[NO]})}{(\text{2xS2[NI]} + \text{6xS6[NI]} + \text{8xS8[NI]} + \text{SF})} \qquad \text{(E5-18)}$$

If BAL has not converged a new value of S6 is estimated and the inner loop is repeated. The inner loop is repeated until BAL converges of 99 trials are exceeded. If the upper and lower limits of S6 do not yield values of BAL which bracket the desired value, in this case zero, the message

SULFUR BALANCE IN REACTOR DOES NOT CONVERGE

is printed out and subroutine returns to the main program without completing the reactor calculation. If BAL converges, the subroutine proceeds to the middle loop. The initial value of S6 is zero and the upper limit is calculated from the following equation:

$$\text{S6MAX} = \frac{(1\text{xS2[NI]} + 3\text{xS6[NI]} + 4\text{xS8[NI]} + 1.5\text{xSO2[NI]})}{3.0} \qquad \text{(E5-19)}$$

This equation calculates the moles of S_6 in the reactor assuming maximum conversion and that all sulfur is in the form of S_6.

The mole balance is checked in the middle loop by calculating the variable TMCHK defined by

$$\text{TMCHK} = 1.0 - \frac{\text{TMOLES}}{\text{TMCALC}} \qquad \text{(E5-20)}$$

The variable TMCALC in this equation is defined as

$$\text{TMCALC} = N_T\text{[NI]} - \text{SF}/3.0 + \text{S8[NO]} - \text{S8[NI]} + \text{S6[NO]} - \text{S6[NI]} + \text{S2[NO]} - \text{S2[NI]} \qquad \text{(E5-21)}$$

where N_T[NI] = total moles in stream entering the reheater, lb moles/hr

The function program WAYA is used to test the variable TMCHK for convergence and select a new value of TMOLES if TMCHK has not converged. With each new value of TMOLES, the calculation is repeated starting at the inner loop. If TMCHK converges or if WAYA exceeds 99 trials, the calculation proceeds to the outer loop. The initial or lower limit of TMOLES is calculated from the following equation:

$$\text{TMMIN} = N_T\text{[NI]} - .25\text{xS6[NI]} - .75\text{xS2[NI]} - 5/16\text{xH2S[NI]} \qquad \text{(E5-22)}$$

which assumes that all the S_2 and S_6 in the reactor feed stream and all the sulfur that is converted in the reactor takes the form of S_8. The upper limit of TMOLES is calculated with the equation

$$\begin{aligned} \text{TMMAX} = {} & N_T[\text{NI}] + .25\text{xH2S}[\text{NI}] + 2\text{xS6}[\text{NI}] \\ & + 3\text{xS8}[\text{NI}] \end{aligned} \qquad \text{(E5-23)}$$

which assumes that all the S_8 and S_6 in the feed and all the sulfur converted take the form of S_2.

In the outer loop, individual component values are calculated and tested for compliance with the equilibrium expression E5-11 at the current temperature. The component values are calculated from the following equations:

$$\text{H2O}[\text{NO}] = \text{H2O}[\text{NI}] + 2/3 \text{ x SF} \qquad \text{(E5-24)}$$

$$\text{H2S}[\text{NO}] = \text{H2S}[\text{NI}] - 2/3 \text{ SF} \qquad \text{(E5-25)}$$

$$\text{SO2}[\text{NO}] = \text{SO2}[\text{NI}] - \text{SF}/3 \qquad \text{(E5-26)}$$

The variable EQN2, defined by

$$\text{EQN2} = \frac{1.0-(\text{WA}[\text{NO}])^2(\text{S2}[\text{NO}])^{3/2}}{(\text{H2S}[\text{NO}])^2(\text{SO2}[\text{NO}] \text{ TMOLES}^{1/2} \text{ EQK1}} \qquad \text{(E5-27)}$$

is calculated and tested for convergence by the function program WAYA. If the upper and lower limits of temperature do not yield values of EQN2 which bracket zero, the desired value, the message

CALC. FOR TEMP DOES NOT CONVERGE

is printed and the subroutine returns to the main program without completing the remaining calculations. The upper and lower limits of temperature chosen are 850°K and 400°K respectively. These temperatures bracket the catalytic conversion region shown in Figure 16. If EQN2 does not converge, WAYA estimates a new value of temperature and the calculation is repeated from the inner loop. If EQN2 converges, the total sulfur partial pressure is compared with the vapor pressure of sulfur to determine if the reaction temperature is above the des point of the reaction mixture. The partial pressure of sulfur is calculated from the equation

$$P_s = \frac{S2 + S6 + S8}{\text{TMOLES}} \qquad \text{(E5-28)}$$

and the vapor pressure is calculated by the function program VP. If the reaction temperature is below the dew point, the specified conversion is decreased by 0.01 and the calculation is repeated from the beginning. If the reaction temperature is above the dew point, the subroutine proceeds to the heat balance around the reactor and its associated reheater.

In calculating the heat balance, the reactor inlet temperature is first calculated by solving an expression for the enthalpy change in the reactor using the function program WAYA. The expression used is

$$\begin{aligned} \text{HCHG} = \text{SENTH[IR]} - \text{SENTH[NO]} - \Delta H_{R5-3 \text{ at } 25°C} \text{ X} \\ \Delta S02 + \Delta H_{R5-4} \text{ X } \Delta S6 + \Delta H_{R5-5} \text{ X } \Delta S8 \end{aligned} \qquad \text{(E5-29)}$$

where $\Delta SO2$ = the change in flow of SO_2 across the reactor, lb moles/hr

$\Delta S6$, $\Delta S8$ are defined similarly

ΔH_{R5-3} = standard heat of reaction at 25°C for reaction R5-3

ΔH_{R5-4} and ΔH_{R5-5} are similarly defined

SENTH[IR] = the enthalpy of the reactor inlet stream, BTU/hr

SENTH[NO] is similarly defined

The function program SENTH is used to calculate the stream enthalpies in this expression. The calculation of ΔH_{R5-3} is shown in the APPENDIX, while ΔH_{R5-4} and ΔH_{R5-5} were obtained from Kelley's data. Since the second and third reactor inlet streams will contain sulfur, the subroutine SPLIT is used to calculate the equilibrium distribution of S_2, S_6, and S_8 before calculating $\Delta S6$ and $\Delta S8$ in the expression above. In the case of the first reactor, SPLIT is not used. If the upper and lower limits of inlet feed temperature do not yield values of HCHG which bracket the desired value, the subroutine prints out the message

```
CALC FOR REACTOR N INLET TEMPERATURE DOES NOT CONVERGE
```

The upper and lower limits of inlet temperature used are 298°K and 2000°K. These are broad limits chosen to encompass all practical problems. If HCHG has not converged, the calculation is repeated with a new value of inlet temperature. When HCHG converges, the subroutine proceeds to calculate the heat load of the reheater using the following equation:

$$\mathrm{HEAT} = \mathrm{SENTH[IR]} - \mathrm{SENTH[NI]} - \Delta H_{R5-4} \times \Delta S6 - \Delta H_{R5-5} \times \Delta S8 \qquad \text{(E5-30)}$$

where HEAT = reheater heat load, BTU/hr

In the special case of the first reactor, if the reactor inlet temperature is greater than the reheater inlet temperature, the two temperatures are set equal to eliminate the need for a reheater. In the unusual case where this is not true, a cooler is required upstream of the first reactor, the cooling load being calculated by equation E5-30.

Before exiting the subroutine, the initial value of conversion is compared with the current value, and if they are different, the message

```
SPECIFIED CONVERSION IN REACTOR OCCURS BELOW
DEW POINT.  CONVERSION REDUCED TO X X X
```

is printed out.

<u>Function EQK (NO, T)</u>. This function program calculates the equilibrium constant for reaction number NO at temperature T. The three reactions provided for and their respective reaction numbers are listed below:

NO = 1 $2H_2S + SO_2 \rightleftarrows 2H_2O + 3/2\ S_2$ (R5-6)

NO = 2 $3S_2 \rightleftarrows S_6$ (R5-7)

NO = 3 $4S_2 \rightleftarrows S_8$ (R5-8)

The equilibrium constant is calculated with the following equation:

$$EQK = e^{-\frac{FREE}{RT}} \qquad (E5\text{-}31)$$

where FREE = the standard free energy change at temperature T, cal/g mole

T = temperature, °K

R = ideal gas constant = 1.987

= 1.987 g cal/g mole, °K

The value of the standard free energy change FREE used in this equation is calculated using the following general equation:

$$FREE = C_1 + C_2T + C_3T^2 + C_4T^3 + C_5/2T + C_6T\ell nT \qquad (E5\text{-}32)$$

where T = temperature, °K

$C_1, C_2, C_3, C_4, C_5, C_6$ = constants associated with each reaction

The value of the first four terms is calculated first by nested expansion and then the last two terms are added on. The six constants associated with each of the three reactions are stored in a 3x6 array by a data statement at the beginning of the function program. Equation E5-32 and the source of the constants for each of the three reactions are discussed in the APPENDIX.

Subroutine WHB (QOUT). This subroutine calculates the cooling load, QOUT, of the waste heat boiler in BTU per hour. The cooling load is calculated directly from the change in enthalpy of the gas stream passing through the boiler after first calculating the temperature of the outlet stream if this is required. If the first reheater has been eliminated by the reactor subroutine REACTR, this temperature is calculated by satisfying the enthalpy balance around the first mixer. The variable DELH defined as

$$\mathrm{DELH} = \mathrm{SENTH}(5) + \mathrm{SENTH}(6) - \mathrm{SENTH}(7)$$

where SENTH(5) = the enthalpy of the H_2S feed entering mixer 1, BTU/hr
SENTH(6) = the enthalpy of the hot gas bypass entering mixer 1, BTU/hr
SENTH(7) = the enthalpy of the combined stream leaving mixer 1, BTU/hr

is calculated and tested by the function program WAYA for convergence. The upper and lower limits of the temperature of stream 6, which is the unknown in this equation, are set equal to the boiler inlet temperature and 373°K respectively.

Since the boiler is used to generate low pressure steam, this temperature cannot be lower than that of steam at one atmosphere. If these limits do not yield a value of DELH which brackets the desired value, the message

WASTE HEAT BOILER CALC DOES NOT CONVERGE

is printed out and the subroutine is exited without completing the calculation. If DELH has not converged, WAYA selects a new value of temperature and the calculation is repeated. If DELH has converged or 99 trials are exceeded, the cooling load, QOUT, is calculated from the following equation:

$$\begin{aligned}\text{QOUT} = &- \text{SENTH}(4) + \text{SENTH}(12) + \text{SENTH}(18)\\ &+ \text{SENTH}(6)\end{aligned} \tag{E5-33}$$

The streams identified in the equation are shown in Figure 18. If the first reheater has not been eliminated and therefore a cooler is required, QOUT is calculated using equation E5-33 directly, since the temperature of stream 6 is initially set at 373°K in the main program. The value of QOUT is returned by the subroutine to the main program.

<u>Subroutine COND (TCOND, IV, LV, LL, HEAT, I)</u>. The condenser subroutine calculates the condenser cooling load, and the composition and flow rate of the outlet liquid and gas streams. The temperature of the outlet gas stream is specified in the program input data. The variables associated with

the subroutine are defined as follows:

TCOND = condenser outlet temperature, °F
IV = stream number - inlet gas
LV = stream number - outlet gas
LL = stream number - liquid sulfur
HEAT = condenser cooling load, BTU/hr
I = condenser number

The outlet temperature, TCOND, which is read in as part of the input data in °F, is converted to degress Kelvin before any calculations are made.

The first step of the subroutine is to determine if the specified condenser temperature is above the freezing point of sulfur and below the dew point of the inlet stream. The dew point is calculated by the subroutine DEWPT and if it is above the dew point, the error message

```
SPECIFIED TEMP FOR CONDENSER IS ABOVE DEW POINT
```

is printed out and the subroutine returns to the main program without completing the condenser calculations. If the dew point criteria is satisfied, the outlet temperature is compared with the freezing point of sulfur and if it is below, the error message

```
TEMP IS TOO LOW, SULFUR FREEZES AT 392°K
```

is printed out and the outlet temperature is arbitrarily set to 400°K. At this temperature the mole fraction of sulfur in the gas stream is reduced to less than .0006.

To calculate the material balance, the amounts of S_2, S_6, and S_8 in the outlet gas stream are determined in an iterative loop and the flow rate of liquid sulfur is calculated by difference. The total moles of S_2, S_6, and S_8 in the outlet gas stream is calculated from the following equation:

$$\mathrm{TOTSP} = \frac{\mathrm{VP\ X}(N_T[\mathrm{IV}] - \mathrm{S268})}{1-\mathrm{VP}} \qquad \text{(E5-34)}$$

where TOTSP = total moles of S_2, S_6, and S_8 in the outlet gas, lb moles/hr

VP = vapor pressure of sulfur at TCOND, atm

S268 = total moles of S_2, S_6, and S_8 in inlet gas stream, lb moles/hr

N_T[IV] = total moles in inlet stream, lb moles/hr

The combined vapor pressure of S_2, S_6, and S_8 is calculated by the function program VP. The total moles in stream LV is then calculated by difference using the following equation:

$$N_T[\mathrm{LV}] = N_T[\mathrm{IV}] - \mathrm{S268} + \mathrm{TOTSP} \qquad \text{(E5-35)}$$

The moles of S_6 are estimated by the function program WAYA and then used to calculate the moles of S_2 and S_8 from the following two equations:

$$S2 = (S6/EQK2)^{1/3} \text{ X } N_T^{2/3}[LV] \qquad (E5\text{-}36)$$

$$S8 = EQK3 \text{ X } (S6/EQK2)^{4/3}/N_T^{1/3}[LV] \qquad (E5\text{-}37)$$

where EQK2 = equilibrium constant for reaction R5-4 at temp, TCOND

EQK3 = equilibrium constant for reaction R5-5 at temp, TCOND

The equilibrium constants EQK2 and EQK3 are calculated by the function program EQK. The sulfur mole balance is checked by calculating the variable DIFF, which is defined by

$$DIFF = 1.0 - \frac{(S8(LV) + S6[LV] + S2[LV])}{TOTSP} \qquad (E5\text{-}38)$$

and then using the function program WAYA to test for convergence. The upper and lower limits of S_6 specified for use with WAYA are the value of TOTSP and zero respectively. If the upper and lower limits of S_6 do not yield values of DIFF which bracket the desired value, the following error message is printed out:

CONDENSER CALC DOES NOT CONVERGE

If DIFF hasn't converged, WAYA selects a new value of S_6 and DIFF is recalculated. If DIFF has converged or 99 trials are exceeded, the moles of each specie of sulfur condensed are calculated from the following equations:

S2CD = S2(IC) - S2(LV) (E5-39)

S6CD = S6[IV] - S6[LV] (E5-40)

S8CD = S8[IV] - S8[LV] (E5-41)

where S2CD = moles of S_2 condensed, lb moles/hr

S6CD = moles of S_6 condensed, lb moles/hr

S8CD = moles of S_8 condensed, lb moles/hr

Since liquid sulfur exists in several allotropic forms and the thermodynamic data is usually given in terms of atoms, the amount of liquid sulfur is calculated and varried through the program in pound atoms. The amount of liquid sulfur leaving the condenser is calculated from the following equation:

SLIQ = 2 X S2CD + 6 X S6CD + 8 X S8CD (E5-42)

where SLIQ = flow rate of liquid sulfur, lb atoms/hr

The condenser heat load is calculated from the following equation:

HEAT = HVAP(S2CD + S6CD + S8CD)
+ SENTH[IV] + SENTH[LV] (E5-43)

where HEAT = condenser cooling load, BTU/hr

HVAP = latent heat of vaporization of sulfur, BTU/lb mole

SENTH[IV] = enthalpy of inlet gas stream, BTU/hr

SENTH[LV] = enthalpy of inlet gas stream at the condenser exit temperature, BTU/hr

The latent heat of vaporization is calculated from the following equation:

$$HVAP = 1.987(2.3)(4940-4.08x10^{-3}T^2)(1.8) \qquad (E5-44)$$

where T = temperature in °K

HVAP = latent heat of vaporization, BTU/lb mole

This equation is derived from the expression for the vapor pressure of sulfur and the Clausius Clapeyron equation. These equations are shown below.

$$\ell n\ VP = 2.3(-4940.0/T-.00408T + 9.811) \qquad (E5-45)$$

where VP = vapor pressure of sulfur, atm

T = temperature, °K

$$\frac{d\ell nVP}{dT} \qquad \frac{\Delta H_{VAP}}{RT^2} \qquad (E5-46)$$

where R = 1.987 g cal/g mole, °K

ΔH_{VAP} = latent heat of vaporization of sulfur, cal/g moles

T = temperature, °K

The Clausius Clapeyron equation is based on the assumptions that the volume of the liquid phase is negligible compared with the vapor phase and that the vapor obeys the ideal gas law. Equation E5-44 is derived by substituting the value of $d\ell nP/dT$ obtained by differentiating equation E5-45 with respect to temperature into equation E5-46 and solving for ΔH_{VAP}. ΔH_{VAP} is then multiplied by 1.8 to obtain HVAP.

The enthalpy of the liquid sulfur stream in BTU/hr is calculated relative to the gas at 298°K from the following equation:

$$H(LL) = SENTH[IV] - SENTH[LV] + HEAT \qquad (E5\text{-}47)$$

Function VP (T). This function program calculates the combined vapor pressure of sulfur ($S_2 + S_6 + S_8$) using the following equation:

$$VP = 10^{(-4940.0/T-.00408T+9.811)} \qquad (E5\text{-}48)$$

where VP = vapor pressure of sulfur (S_2+S_6+S_8), atm

T = temperature, °K

This equation was obtained from Kelley's data on the properties of sulfur.

Subroutine DEWPT (NO, T). This subroutine calculates the dew point temperature, T, of stream NO containing sulfur vapor. The calculation is made in one iterative loop using the function program WAYA to estimate the temperature. At each temperature, the partial pressure of sulfur is compared with the vapor pressure by calculating the variable DEW, defined as

$$DEW = 1.0 - \frac{(S2[NO] + S6[NO] + S8[NO])}{N_T[NO] \times VP} \qquad (E5\text{-}49)$$

$N_T[NO]$ = total moles in stream NO, lb moles/ℓn

and then using the function program WAYA to check for convergence. The amounts of S_2, S_6, and S_8 and the total moles are calculated by the subroutine SPLIT, and the vapor pressure of sulfur is calculated by the function program VP. The upper and lower limit of temperature are specified as 7178°K and 425°K respectively, corresponding to sulfur vapor pressures of 1.0 atmospheres and .0003 atmospheres. These temperature limits therefore bracket the dew points of streams with sulfur mole fractions between 1.0 and .0003. If these limits do not yield values of DEW which bracket the desired value, the message

DEW POINT CALC ON STREAM NO DOES NOT CONVERGE

is printed out and the subroutine is exited without completing the calculations. If DEW has not converged, WAYA estimates a new value of temperature and the calculation is repeated. If WAYA exceeds 99 trials or the calculation converges, the subroutine returns the value of T to the main program, but the composition of stream NO is not changed.

Subroutine SPLIT (N1, N2, TEMP). This subroutine calculates the composition of stream N1 at temperature TEMP. The composition and total moles in stream N1 change with temperature due to a shift in the equilibria between components S_2, S_6, and S_8. The variables specified when using the subroutine are as follows:

N1 = stream number at the original temperature

N2 = stream number at TEMP

TEMP = temperature of stream N2

It is possible to specify the same number for N1 and N2 if desirable, a feature which has been used several times in the program.

The calculation performed is similar to that of the reactor subroutine REACTR, but is not as complex because the final temperature is known. The calculation therefore only requires two interative calculation procedures. In the inner loop, the moles of S_6 is estimated by the function program WAYA and then this value is used along with the value of total moles estimated in the outer loop to calculate the moles of S_2 and S_8 using equations E5-14 and E5-15. The sulfur balance is checked at the end of the inner loop by calculating the variable BAL, where BAL is defined as

$$\text{BAL} = 1.0 - \frac{(2 \text{ X } \text{S2[N2]} + 6 \text{ X } \text{S6[N2]} + 8 \text{ X } \text{S8[N2]})}{2 \text{ X } \text{S2MAX}} \qquad \text{(E5-50)}$$

and where

$$\text{S2MAX} = \text{S2[N1]} + 3 \text{ X } \text{S6[N1]} + 4 \text{ X } \text{S8[N1]} \qquad \text{(E5-51)}$$

and then using WAYA to test BAL for convergence. The upper and lower limits of S_6 specified for use with WAYA are S2MAX/ 3.0 and zero respectively. If the limits do not yield values of BAL which bracket the desired value, the message

SULFUR BALANCE IN SPLIT CALC ON STREAM N1 DOES NOT CONVERGE

is printed out and the subroutine is exited without completing the calculation. If BAL has not converged, WAYA selects a new value of S_6 and the inner loop calculations are repeated. If BAL has converged, the calculation proceeds to the outer loop where the total moles, TMCALC, is calculated from the following equation:

$$\begin{aligned} \text{TMCALC} = {} & N_T[\text{N1}] - \text{S2}[\text{N1}] - \text{S6}[\text{N1}] - \text{S8}[\text{N1}] \\ & + \text{S2}[\text{N2}] + \text{S6}[\text{N2}] + \text{S8}[\text{N2}] \end{aligned} \tag{E5-52}$$

where $N_T[\text{N1}]$ = total moles in stream N1, lb moles/hr

The total moles calculated, TMCALC, is then compared with the total moles estimated, TMOLES, by calculating the variable TMCHK, where TMCHK is defined as

$$\text{TMCHK} = 1.0 - \frac{\text{TMOLES}}{\text{TMCALC}} \tag{E5-53}$$

and then testing for convergence with WAYA. The lower limit of TMOLES, TMMIN, is calculated from the following equation:

$$\text{TMMIN} = N_T[\text{N1}] - .75 \text{ X } \text{S2}[\text{N1}] - .25 \text{ X } \text{S6}[\text{N1}] \tag{E5-54}$$

This equation is based on the assumption that all the S_2 and S_6 in stream N1 is converted to S_8. The upper limit, TMMAX, is calculated by assuming all the S_6 and S_8 in stream N1 is converted to S_2. The following equation is used to calculate TMMAX:

$$\text{TMMAX} = N_T[\text{N1}] + 3 \times \text{S8}[\text{N1}] + 2 \times \text{S6}[\text{N1}] \qquad \text{(E5-55)}$$

If these limits do not yield values of TMCHK which bracket the desired value, the message

TOTAL MOLE BALANCE IN SPLIT CALC ON STREAM N1 DOES NOT CONVERGE

is printed out and the subroutine is exited without completing the calculations. If TMCHK has not converged, WAYA selects a new value of TMOLES and the calculation is repeated from the inner loop. If convergence occurs or if 99 trials are exceeded, the values of S_2, S_6, and S_8 and TMOLES are assigned to the respective components of stream N2 and the subroutine returns to the main program.

The variable TMOLES was selected for the outer loop because it is the least sensitive variable and its limits are easily calculated. With the least sensitive variable in the outer loop, the calculation converges more rapidly.

Subroutine PRINT (NO). This subroutine prints out the thirteen components of stream NO according to the format shown in the sample in the APPENDIX. The mole fractions are calculated from the stream component data stored in blank common. All stream enthalpies are calculated by the subroutine, except for those of liquid sulfur streams, which are calculated by the condenser subroutine COND.

CHAPTER 6

RESULTS

To verify the accuracy of some of the calculations performed by the computer program, standard free energy values and equilibrium constants for the reactions

$$2H_2S + SO_2 \rightleftarrows 3/2\ S_2 + 2H_2O \qquad (R6\text{-}1)$$

$$3S_2 \rightleftarrows S_6 \qquad (R6\text{-}2)$$

$$4S_2 \rightleftarrows S_8 \qquad (R6\text{-}3)$$

and temperature-conversion data for the overall reaction were calculated and compared with the results of Gamson and Elkins.

Standard free energy and equilibrium constant values are compared in Tables 2 and 3 respectively. The largest percent difference in the free energy values is 21.5%. Of the twenty seven values listed, only three values show a percent difference greater than 2%, and the absolute difference for these three values is less than 30 calories per gram mole. The largest percent difference in the equilibrium constants shown in Table 3 is 10.8% and only five of the twenty three constants differ by more than 2%. Thermodynamic data from several sources (8)(16)(13) were tested to find the best comparison with Gamson and Elkins. The results tabulated were calculated from thermodynamic data from Kelley(8) and Smith

TABLE 2

FREE ENERGY CHANGES IN CALORIES PER GRAM MOLE

TEMP., °K

REACTION		400	600	800	900	1,000	1,100	1,200	1,600	2,000
1	Gamson & Elkins	5,793	2,958	-93	-1,547	-3,000	-4,459	-5,917	-11,598	-17,057
	Computer Program	5,781	2,834	-113	-1,577	-3,032	-4,478	-5,915	-11,567	-17,076
	% Diff.	0.207	4.20	21.5	1.94	1.07	0.427	0.0339	0.268	0.111
2	Gamson & Elkins	-36,815	-22,196	-7,310	203	7,750	15,370	23,016	53,883	85,157
	Computer Program	-36,800	-22,181	-7,291	233	7,801	15,409	23,054	53,944	85,237
	% Diff.	0.0407	0.0677	0.260	14.8	0.658	0.254	0.165	0.113	0.0942
3	Gamson & Elkins	-53,532	-31,225	-8,518	2,940	14,480	26,069	37,727	-84,784	132,450
	Computer Program	-53,508	31,203	-8,490	2,985	14,526	26,128	37,784	84,874	132,570
	% Diff.	0.0448	0.0703	0.329	1.53	0.318	0.226	0.151	0.106	0.0907

TABLE 3

EQUILIBRIUM CONSTANTS = K_p

TEMP., °K

REACTION		400	600	800	900	1,000	1,100	1,200	1,600	2,000
1	Gamson & Elkins	6.84×10^{-4}	8.37×10^{-2}	1.06	2.38	4.53	7.69	1.20×10^{1}	3.84×10^{1}	7.31×10^{1}
	Computer Program	6.93×10^{-4}	9.28×10^{-2}	1.07	2.41	4.60	7.76	1.20×10^{1}	3.80×10^{1}	7.35×10^{1}
	% Diff.	1.32	10.8	0.944	1.26	1.54	0.91	0.0	1.04	0.548
2	Gamson & Elkins	1.30×10^{-20}	1.21×10^{8}	9.93×10^{1}	8.93×10^{-1}	2.03×10^{-2}	8.83×10^{-4}	6.44×10^{-5}	—	—
	Computer Program	1.28×10^{20}	1.20×10^{8}	9.82×10^{1}	8.78×10^{-1}	1.97×10^{-2}	8.67×10^{-4}	6.32×10^{-5}	4.28×10^{-8}	4.84×10^{-10}
	% Diff.	1.54	0.827	1.11	1.68	2.96	1.81	1.86	—	—
3	Gamson & Elkins	1.76×10^{29}	2.36×10^{11}	2.12×10^{2}	1.93×10^{-1}	6.92×10^{-4}	6.45×10^{-6}	1.38×10^{-7}	—	—
	Computer Program	1.73×10^{29}	2.32×10^{11}	2.09×10^{2}	1.88×10^{-1}	6.68×10^{-4}	6.43×10^{-6}	1.31×10^{-7}	2.54×10^{-12}	3.25×10^{-15}
	% Diff.	1.71	1.69	1.42	2.60	3.47	0.310	5.07	—	—

and Van Ness(16) and give the best overall comparison with Gamson and Elkins. All but the water data was obtained from Kelley. The different thermodynamic data were tested to verify that the initial difference in results was due to differences in data and not a mistake in the calculation or a significant difference in calculation method.

The validity of the catalytic reactor subroutine and a general check on the overall program was performed by running ten test problems with specified conversions between .528 and .95 and comparing the results with those of Gamson and Elkins. Since the conversion-temperature data of Gamson and Elkins is for 100% H_2S feed, the ten test problems were for 100% H_2S feed. Except for the specified conversion in the catalytic reactor, the input data for all ten test problems was the same. The following input data was used for the test problems:

NO. OF REACTORS = 1

FEED COMPOSITION	LB MOLES/HR
H_2S	0.0
H_2S	100.0
H_2O	0.0
N_2	0.0

FEED TEMPERATURE = 98°F

COMBUSTION AIR TEMPERATURE = 98°F

CONDENSER 1 EXIT TEMPERATURE = 300°F

CONVERSION IN REACTOR 1 = VARIABLE

BYPASS GAS SPLIT 1 = 1.0

A summary of the results of these test problems and a comparison of the reactor temperature-conversion data with that of Gamson and Elkins is shown in Tables 4 and 5 respectively. All the variables in Table 4 vary with increasing conversion in the direction expected, although some explanation is required for the variable CONDENSER 1 Q, which is the rate of heat removal in CONDENSER 1. From Table 4, it can be seen that the rate of condenser heat removal decreases with increasing conversion, although the opposite might be expected. The condenser inlet temperature decreases with increasing conversion, and since the condenser outlet temperature is fixed, less sensible heat removal is required to cool the gas to the outlet or condensing temperature. With increasing conversion, more sulfur is condensed at a fixed outlet temperature, but apparently the increased cooling requirement for condensing liquid sulfur is more than offset by the decrease in sensible heat removal. The results in Table 4 also show that the reactor inlet temperature did not converge at conversions of .90 and .92. This occurs because the lower limit of reactor inlet temperature is set at 298°K in the reactor subroutine. At conversions of .90 or greater, the inlet temperature would be below 298°K in order to satisfy adiabatic reactor requirement of the subroutine. It should also be pointed out that a cooler is required upstream of the reactor for .868 conversion. This would also have been true for conversions of .90 and .92

TABLE 4

RESULTS OF TEST PROBLEMS

CONVERSION	.528	.55	0.590	.650	.70	.750	.80	.868	.90	(Dew Point) .92
WHB Q, BTU/HR	$-5.101\text{x}10^6$	$-5.39\text{x}10^6$	$-5.76\text{x}10^6$	$-6.189\text{x}10^6$	$-6.478\text{x}10^6$	$-6.736\text{x}10^6$	$-6.987\text{x}10^6$	$-7.22\text{x}10^6$	$-7.22\text{x}10^6$	$-7.22\text{x}10^6$
TEMP. OF SO_2 GAS TO MIXER 1, °K	941.02	867.6	769.9	657.9	579.9	509.1	439.2	373.0	373.0	373.0
REHEATER 1 Q, BTU/HR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	$-1.14\text{x}10^5$	SET=0.0	SET=0.0
REHEATER 1 INLET TEMP. °K	803.86	746.2	669.6	581.9	520.8	465.3	410.7	359.02	359.02	359.02
REACTOR 1 INLET TEMP. °K	803.86	746.2	669.6	581.9	520.8	465.3	410.7	333.29	DID NOT CONVERGE SET=298.0	DID NOT CONVERGE SET=298.0
REACTOR 1 OUTLET TEMP. °K	808.39	787.6	760.1	725.9	699.2	672.3	643.7	599.40	573.9	555.4
CONDENSER 1 Q, BTU/HR	$-2.53\text{x}10^6$	$-2.349\text{x}10^6$	$-2.12\text{x}10^6$	$-1.88\text{x}10^6$	$-1.723\text{x}10^6$	$-1.582\text{x}10^6$	$-1.445\text{x}10^6$	$-1.24\text{x}10^6$	$-1.126\text{x}10^6$	$-1.041\text{x}10^6$
LIQUID SULFUR RATE COND.1, LB ATOMS/HR	52.24	54.4	64.3	64.3	69.4	74.4	79.4	86.22	89.5	91.4

TABLE 5

CONVERSION VERSUS TEMP. FOR 100% H_2S FEED

CONV.	TEMP., °K		% DIFF.
	COMPUTER PROGRAM	GAMSON & ELKINS	
.528	808.4	800	1.05
.55	787.6	770	2.28
.59	760.1	740	2.72
.65	725.9	715	1.53
.70	699.2	685	2.08
.75	672.3	660	1.86
.80	643.7	630	2.17
.868	599.40	600	0.10
.90	573.9	570	0.686
.92 (Dew Point)	555.4	553	0.433

if the reactor inlet temperature had converged. These cases point out the impracticality of using the split feed process for feed streams with extremely high H_2S concentrations, since the required reactor inlet temperature is so low for high conversions that the water in the reactor feed stream would condense out.

The temperature-conversion data comparison in Table 5 shows extremely good agreement between the computer program results and the results of Gamson and Elkins. The maximum percent difference for the ten points is 2.72% at a conversion of .59. Most of the Gamson and Elkins data were read from Figure 16, and is therefore only accurate within about ± 5°K. The dew point (.92 conversion) was calculated in a test problem with a specified conversion of .95. The computer program reduced the specified conversion in increments of .01 until the conversion temperature was equal to or greater than the dew point of the reaction mixture.

Since data for comparison with other program results such as stream enthalpies, burner flame temperature, waste heat boiler cooling load, and reheater heating load were not available in the literature, these quantities were checked for several of the test problems with slide rule calculations and found to be accurate in all cases. In addition to the ten test problems where one reactor was specified, the program has been run successfully several times on problems involving three catalytic reactors.

The general conclusion is that the computer program accurately represents the model intended, and that the results compare extremely well with the data of Gamson and Elkins.

CHAPTER 7

RECOMMENDATIONS FOR FUTURE WORK

There are several minor changes which would improve the existing computer program. They are:

1. The subroutine FLAME should calculate the adiabatic flame temperature of any stream of acceptable composition and not just stream 4.

2. The program user should specify the percentage of sulfur removal in each condenser and not the condenser outlet temperature. By maximizing the sulfur removal in each condenser, the sulfur dew point in the succeeding conversion step is reduced and the maximum conversion therefore increased.

3. The function WAYA should distinguish between the case where it has converged and the case where the allowable number of trials has been exceeded, and in the latter case execution of the program should be terminated by a STOP statement at an appropriate point.

4. The liquid sulfur enthalpy calculation performed in the subroutine COND should be modified so that the enthalpy is calculated relative to rhomic sulfur at

20°C and not relative to sulfur vapor at 25°C and 1 atm.

In addition to the minor changes above, there are several major changes which would greatly improve the existing program. They are listed below.

1. The program should have the flexibility to allow the user to specify as part of the input data the type of Claus flow scheme desired. In addition to the "split feed" flow scheme provided in the existing program, the "once through" and the direct oxidation schemes should be included. This could be accomplished by having the sections in the main program for each flow scheme. A new input variable in the form of an integer with possible values of 1, 2, or 3 should be added to the input data to identify the flow scheme desired.

   The existing reactor subroutine can be modified to be used for either a high temperature non-catalytic converter or a catalytic converter by introducing a variable specified in calling the subroutine which identifies the type of converter required. The reactor subroutine would have to be modified so that a different set of temperature limits is used for each type of conversion. The non-catalytic reactor could also be programmed as a separate subroutine in which the conversion is a constant (.60 to .65 conversion is commonly attained). The subroutine would consist of a simple material balance based on the constant conversion followed by a determination of the reactor outlet temperature using an enthalpy balance. The subroutine SPLIT would be used in the enthalpy balance to account for the change in the sulfur specie equilibria with temperature. A similar enthalpy balance is used at the existing reactor subroutine.

In addition, the subroutines PRINT and FLAME would have to be modified if alternate flow schemes were incorporated in the program. The subroutine PRINT should be modified to print out the proper stream names. This could be done by generating the stream titles in the main program which could then be transferred to the PRINT subroutine in the CALL statement. The stream titles are now stored in the subroutine PRINT. The subroutine FLAME should be modified so that it can be used with either the split feed or straight through flow schemes. In the split feed scheme enough air to burn all the hydrogen sulfide in the burner feed to sulfur dioxide is added, while in the straight through (high temperature non-catalytic oxidation) scheme only enough air to burn one third of the hydrogen sulfide is required.

2. The type of reheat method should be made a variable specified by the user. Since the existing program provides only the hot gas bypass method, several other methods including the direct fired reheater and gas-to-gas exchange should be made available. This modification could be incorporated in the program by writing one subroutine which can perform the calculations for all the reheating methods selected. The type of reheating method could be specified by an integer variable in the input data. The calculations for the hot gas bypass method now performed in the main program and the reheater calculation performed in the reactor should be included in this subroutine.

3. The program should be modified to handle feeds containing the hydrocarbons normally encountered in industry such as CO, CO_2, COS, CH_4, and C_2H_6. The following modifications to the existing program are necessary to add more components to the feed stream:

   a. Modify READ and WRITE statements for the input data.

   b. Renumber stream components in statements throughout the program.

c. Modify material balance calculations in the subroutine flame so that all the hydrocarbons are burned to carbon dioxide and water.

d. Add enthalpy constants for the new feed components to NAMED COMMON area HFDT/COEFF.

e. Modify subroutines EQUAL and SENTH so that the calculations consider the additional components.

4. The temperature of the acid gas stream leaving the waste heat boiler should be set by the required stream pressure in the boiler rather than have the program set this temperature based on the elimination of the first reheater. This would allow the user to specify the stream pressure required at the plant site in question and also increase the flexibility of the Claus plant by including the first reheater. This temperature could be set equal to the temperature of steam at the desired pressure and included in the input data. This would eliminate the provisions for back calculating this temperature in the main program, reactor subroutine, and the waste heat boiler subroutine.

5. The hot bypass gas should be taken off one of the early passes of the waste heat boiler rather than bypassing the gas before it enters the waste heat boiler.

This would require adding the temperature of this gas to the input data and modifying the waste heat boiler subroutine to take this stream into account. This temperature could also be calculated by taking a reasonable percentage of the total temperature drop across the waste heat boiler.

6. Some type of tail gas treatment such as an incinerator should be included in the program. This would require an incinerator subroutine which calculates a material and heat balance around the incinerator. This involves calculating the amount of combustion air and fuel to heat the total gas stream to about 650°C and burn all the hydrogen sulfide to sulfur dioxide. The air temperature, fuel gas temperature, and the incinerator outlet temperature could be specified as part of the input data.

7. The system pressure should be a variable specified by the user. A pressure range between 1 and 3 atmosphere is desirable. To make this modification, a total pressure term should be included in the appropriate equations in the reactor subroutine as mentioned in the discussion of this subroutine in Chapter 5 . A total pressure term should also be included in the calculations in the dew point subroutine, DEW.

8. Modify the program so that the burner air to H_2S gas ratio is a variable specified in the input data. This would provide a means of studying the effect of this ratio on the conversion in each catalytic reactor and the overall plant conversion. This can be done by modifying the subroutine FLAME to use the amount of combustion air specified.

To provide a program with all the above features would require completely rewriting the main program, modifying the existing subroutines and functions, and writing additional subroutines and functions. The above comments on each of the proposed modifications are very general and are not meant to be a complete procedure for expanding the model. The existing program should provide a good foundation for such an undertaking.

Another recommendation for future work is a computer program that calculates a heat, a material balance, sizes the equipment, and estimates the total installed plant cost.

The free energy minimization technique is suggested as a challenging approach for solving the kinetics of the Claus process.

As a check on the assumptions made in this program and the thermodynamic data used, the plant operating conditions predicted by the computer program should be compared with those of an existing plant. This would require that the researcher have access to such information. A cooperative program between industry and engineering schools would be useful in such an endeavor.

APPENDIX

APPENDIX A

CALCULATION OF THERMODYNAMIC PROPERTIES

The methods of calculating specific heat, enthalpy, standard heat of reaction, and the standard free energy change used in the computer program are discussed below. The basic thermodynamic data associated with each component and the sources of data are listed in Table 6.

Individual Component Enthalpy

The enthalpy of individual gas stream components relative to the standard state of 25°C and 1 atm is calculated using the following general equation:

$$H = A_o + A_1T + A_2T^2 + A_3T^3 + A_4T^{-1} \qquad \text{(E-1)}$$

The expression is obtained by integrating the general expression for component heat capacity:

$$C_p = a + bT + CT^2 + dT^{-2} \qquad \text{(E-2)}$$

SO_2 is the only component considered with a T^{-2} term in this expression. Integrating between 298.16°K and T yields

$$H = \int_{298.16°K}^{T} C_p dT = a(T-298.16) + \frac{b}{2}(T^2-\overline{298.16}^2) + \frac{C}{3}(T^3-\overline{298.16}^3)$$
$$- d(T^{-1}-\overline{298.16}^{-1}) \qquad \text{(E-3)}$$

This equation can then be further simplified to yield equation E-1 in which the constants take on the following values:

A_o = the sum of the constant terms
$A_1 = a$
$A_2 = b/2$
$A_3 = C/3$
$A_4 = -d$

The enthalpy equations for the vapor phase components are shown below. These equations yield values of enthalpy in calories per gram mole for temperatures in degrees Kelvin.

$$S_2(g): H = -2350.21 + 7.75T + 0.444 \times 10^{-3}T^2 \qquad (E-4)$$

$$S_6(g): H = -5857.99 + 19.95T + 1.332 \times 10^{-3}T^2 \qquad (E-5)$$

$$S_8(g): H = -7611.88 + 25.0T + 1.776 \times 10^{-3}T^2 \qquad (E-6)$$

$$SO_2(g): H = -4147.74 + 1.14 \times 10^{1}T + 7.07 \times 10^{-4}T^2 + 2.045 \times 10^{5}T^{-1} \qquad (E-7)$$

$$H_2S(g): H = -2279.37 + 7.15T + 1.66 \times 10^{-3}T^2 \qquad (E-8)$$

$$H_2O(g): H = -2268.1 + 7.256T + 1.149 \times 10^{-3}T^2 + 0.0943 \times 10^{-6}T^3 \qquad (E-9)$$

$$H_2(g): H = -2066.67 + 6.947T - 0.1 \times 10^{-3}T^2 + 0.1603 \times 10^{-6}T^3 \qquad (E-10)$$

$$O_2(g): H = -1962.8 + 6.148T + 1.551 \times 10^{-3}T^2 - 0.3087 \times 10^{-6}T^3 \qquad \text{(E-11)}$$

$$N_2(g): H = -2000.7 + 6.524T + 0.625 \times 10^{-3}T^2 - 0.000333 \times 10^{-6}T^3 \qquad \text{(E-12)}$$

The Standard Heat of Reaction at 25°C and 1 Atm

The values of standard heat of reaction used in the computer program were calculated from the following equation:

$$[\Delta H_{REACTION} = \sum \Delta H_{f_{(PRODUCTS)}} - \sum \Delta H_{f_{(REACTANTS)}}]_{25°C} \qquad \text{(E-13)}$$

where ΔH_f = standard heat of formation at 25°C and 1 atm

The calculation for each of the reactions considered in the computer program are shown below.

$$H_2S + \frac{3}{2} O_2 \rightleftarrows SO_2 + H_2O \qquad \text{(R-1)}$$

$\Delta H^\circ_{f\ 25°C}$ for H_2O = -57,798 calories

$\Delta H^\circ_{f\ 25°C}$ for SO_2 = -70,940 calories

$\Delta H^\circ_{f\ 25°C}$ for H_2S = -4,800 calories

$\Delta H^\circ_{f\ 25°C}$ for S_2 = 31,020 calories

$\Delta H^\circ_{25°C}$ = (-70,940 -57,798) - (-4,800) = -123,938 calories

$$2H_2S + SO_2 \rightleftarrows 2H_2O + \frac{3}{2} S_2 \qquad \text{(R-2)}$$

$$\Delta H^\circ_{25^\circ C} = 2(-57{,}798) + \frac{3}{2}(31{,}020) - 2(-4{,}800)$$
$$- (-70{,}940)$$

$$\Delta H^\circ_{25^\circ C} = + 11{,}474 \text{ calories}$$

$$3S_2 \rightleftarrows S_6 \qquad \text{(R-3)}$$

$$\Delta H^\circ_{f\ 25^\circ C} \text{ for } S_6 = 27{,}780 \text{ calories}$$

$$\Delta H^\circ_{25^\circ C} = 27{,}780 - 3(31{,}020) = -65{,}280 \text{ cal/g mole}$$

$$4S_2 \rightleftarrows S_8 \qquad \text{(R-4)}$$

$$\Delta H_{f\ 25^\circ C} \text{ for } S_8 = 27{,}090 \text{ calories}$$

$$\Delta H^\circ_{25^\circ C} = 27{,}090 - 4(31{,}020) = -96{,}990 \text{ cal/g mole}$$

The Standard Free Energy Change

The standard free energy change with temperature for a chemical reaction is calculated by the computer program using the following equation:

$$\Delta F^\circ_T = C_1 + C_2T + C_3T^2 + C_4T^3 \qquad \text{(E-14)}$$
$$+ \frac{C_5}{2T} + C_6 T \ell n T$$

This equation is derived by substituting expressions for ΔH°_T and ΔS°_T which are developed below into the equation

$$\Delta F^\circ_T = \Delta H^\circ_T - T\Delta S^\circ_T \tag{E-15}$$

where ΔH°_T = standard heat of reaction at temperature T and 1 atm

ΔS°_T = standard entropy change at temperature T and 1 atm

Since the heat capacities of all the products and reactants can be expressed as a function of temperature by an equation of the form

$$C_p = a + bT + CT^2 + dT^{-2} \tag{E-16}$$

the following analytical expression for the standard heat of reaction as a function of temperature can be developed:

$$\Delta H^\circ_T = \Delta H^\circ_{298.16^\circ K} + \sum_{\text{PRODUCTS}}(n \int_{298.16^\circ K}^{T} C_p dT) - \sum C_p dT - \sum_{\text{REACTANTS}}(n \int_{298.16^\circ K}^{T} C_p dT) \tag{E-17}$$

$$= \Delta H^\circ_{298.16^\circ K} + \int_{298.16^\circ K}^{T} \Delta C_p dT \tag{E-18}$$

where $\Delta C_p = \Delta a + \Delta bT + \Delta CT^2 + \Delta dT^{-2}$

and $\Delta a = \sum_{\text{PRODUCTS}} na - \sum_{\text{REACTANTS}} na$

Δb, ΔC, and Δd are similarly defined.

Equation E-17 then becomes

$$\Delta H^\circ_T = \Delta H^\circ_{298.16} + \int_{298.16^\circ K}^{T} (\Delta a + \Delta bT + \Delta CT^2 + \Delta dT^{-2})dT \qquad \text{(E-19)}$$

$$= \Delta H^\circ_{298.16} + \Delta a(T-298.16) + \frac{\Delta b}{2}(T^2-\overline{298.16}^2) \qquad \text{(E-20)}$$

$$+ \frac{\Delta C}{3}(T^3-\overline{298.16}^3) - \Delta d(T^{-1}-\overline{298.16}^{-1})$$

Summing all the constant terms and designating the total ΔH_o, the resulting expression is

$$\Delta H^\circ_T = \Delta H_o + \Delta aT + \frac{\Delta b}{2}T^2 + \frac{\Delta C}{3}T^3 - \Delta dT^{-1} \qquad \text{(E-21)}$$

ΔH_o can be calculated from a known value of the standard heat of reaction at a singe temperature. The equation for ΔS°_T is derived by integrating the expression for dS at constant pressure

$$dS = \frac{C_p\,dT}{T} \qquad \text{(E-22)}$$

between absolute zero and T to yield

$$\Delta S^\circ_T = \int_o^T \frac{\Delta C_p\,dT}{T} = \int_o^T \frac{(\Delta a + \Delta bT + \Delta CT^2 + \Delta dT^{-2})dT}{T} \qquad \text{(E-23)}$$

$$= I_S + \Delta a \ln T + \Delta bT + \frac{\Delta C}{2}T^2 - \frac{\Delta dT^{-2}}{2} \qquad \text{(E-24)}$$

The integration constant I_S can be determined from a known value of ΔS°_T. Substituting into equation E-15 for ΔH°_T and ΔS°_T and combining terms gives the following expression for ΔF°_T:

$$\Delta F^\circ_T = \Delta H_o - IT - \frac{\Delta bT^2}{2} - \frac{\Delta CT^3}{6} - \frac{\Delta d}{2T} - T\Delta a\ell nT \qquad \text{(E-25)}$$

$$\text{where } I = \Delta a - I_S$$

Simplifying this expression by substituting a new set of constants yields equation E-14. The expressions for ΔF°_T for reactions R-2, R-3, and R-4 are shown below.

$$2H_2O + SO_2 \rightleftarrows 2H_2O + \frac{3}{2} S_2$$

$$\Delta F^\circ_T = 12119.0 - 12.999T + 1.063 \text{ X } 10^{-3}T^2 \qquad \text{(E-26)}$$

$$- 9.433 \text{ X } 10^{-8}T^3 - \frac{2.045 \text{ X } 10^{+5}}{2T}$$

$$- 4.37 \text{ X } 10^{-1}T\ell nT$$

This expression was calculated as follows:

$$\Delta a = \frac{3}{2}(7.75) + 2(7.256) - 2(7.15) - (11.40) = 0.437$$

$$\Delta b = \frac{3}{2}(0.888) \text{ X } 10^{-3} + 2(2.298) \text{ X } 10^{-3} - 2(3.32) \text{ X } 10^{-3}$$

$$- 1.414 \text{ X } 10^{-3} = - 2.126 \text{ X } 10^{-3}$$

$$\Delta C = \frac{3}{2}(o) + 2(0.283) \text{ X } 10^{-6} - 2(o) - 1(o) = 0.566 \text{ X } 10^{-6}$$

$$\Delta d = -\ (-2.045)\ X\ 10^{-5} = +\ 2.045\ X\ 10^{5}$$

$$\Delta H_{o} = \Delta H^{\circ}_{298.16} - \Delta a\ X\ 298.16 - \frac{\Delta b}{2}(298.16)^{2}$$

$$- \frac{\Delta C}{3}(298.16)^{3} + \frac{\Delta d}{298.16}$$

$$\Delta H_{o} = 11474.0 - 0.437\ X\ 298.16 + 1.063\ X\ 10^{-3}$$

$$X\ (298.16)^{2} - \frac{.566\ X\ 10^{-6}\ X\ (298.16)^{3}}{3}$$

$$+ \frac{204500}{298.16} = 12119.0$$

$$I = \frac{\Delta F^{\circ}_{T} - \Delta H_{o}}{T} + \frac{\Delta bT}{2} + \frac{\Delta CT^{2}}{6} + \frac{\Delta d}{2T^{2}} + \Delta a \ell nT$$

at 298.16°K $I = \frac{7250.0-12119.0}{298.16} - 1.063\ X\ 10^{-3}\ X\ 298.16$

$$+ \frac{0.566\ X\ 10^{-6}\ X\ (298.16)^{2}}{6} + \frac{204500.0}{(2)(298.16)^{2}}$$

$$+ 0.437\ \ell n\ 298.16 = -12.999$$

Substituting into equation E-25 yields equation E-26 above.

$3S_{2} \rightleftarrows S_{6}$

$$\Delta F^{\circ}_{T} = -\ 64090.0 + 44.26T + 4.0T\ell nT \qquad \text{(E-27)}$$

$4S_{2} \rightleftarrows S_{8}$

$$\Delta F^{\circ}_{T} = -\ 95200.0 + 68.28T + 6.0T\ell nT \qquad \text{(E-28)}$$

The last two expressions for ΔF_T° were taken from Kelley (see Chapter 3), but could be calculated in the conventional manner described above using the data in Table 6.

TABLE 6

THERMODYNAMIC PROPERTIES

Constants a, b, c, and d are for specific heat in the form $C_p = a + bT + cT^2 + dT^{-2}$
where T is in °K and C_p in cal/g mole, °K
$\Delta H^\circ_{f\ 298}$ and $\Delta F^\circ_{f\ 298}$ are in units of cal/g mole
Numbers in parenthesis refer to references

COMPONENT	$S_2(g)$	$S_6(g)$	$S_8(g)$	$SO_2(g)$	$H_2S(g)$	$S_\lambda(\ell)$	$H_2O(g)$	$H_2(g)$	$O_2(g)$	$N_2(g)$
CONSTANTS a	7.75 (8)	19.25 (8)	25.0 (8)	11.40 (8)	7.15 (8)	5.4 (8)	7.256 (16)	6.947 (16)	6.148 (16)	6.524 (16)
$b \times 10^3$	0.888	2.664	3.552	1.414	3.32	5.0	2.298	-0.200	3.102	1.250
$c \times 10^6$	0	0	0	0	0	0	0.283	0.481	-0.923	-.001
$d \times 10^{-5}$	0	0	0	-2.045	0	0	0	0	0	0
ΔH°_f 298°K	31,020 (8)	27,780 (8)	27,090 (8)	-70,940 (8)	-4,800 (8)	257 (8)	-57,798 (16)	0	0	0
ΔF°_f 298°K	19,360 (8)	13,970 (8)	12,770 (8)	-71,750 (8)	-7,865 (8)	72 (8)	-54,635 (16)	0	0	0

APPENDIX B

```
      PROGRAM SULPLT
      COMMON//STRM(13,23)
      COMMON/HEDT/COEF(60)
C     CT(I)=TEMP OF CONDENSER I
C     SP(I)=FRACTION OF BURNER OUTLET GAS TO REACTOR I
C     CONV(I)=CONVERSION OF H2S TO S2,S6,OR S8 IN REACTOR I
C     H(I)=HEAT ADDED TO HEATER-COOLER I,BTU/HR
C     HC(I)=HEAT ADDED TO CONDENSER I,BTU/HR
C     THERE ARE 13 COMPONENTS TO A STREAM,1=H2,2=H2S,3=H2O,4=N2,5=O2,
C     6=SO2,7=S6,8=S8,9=S2,10=LIQUID SULFUR,11=TOTAL MOLES,12=TEMP,13=
C     STREAM ENTHALPY
      DIMENSION CT(3),SP(3),CONV(3),H(3),HC(3)
C     SET COMPONENTS OF ALL STEAMS=0
    4 CONTINUE
      WRITE (6,200)
  200 FORMAT ('1')
      DO 5 I=1,23
      DO 5 J=1,13
    5 STRM(J,I)=0                                                          30
C     READ INPUT DATA
C     STREAM 1=FEED STREAM,STREAM 2=BURNER FEED GAS,STREAM 3=BURNER AIR
      READ(5,1,END=2) M,(STRM(J,1),J=1,4),STRM(12,1),STRM(12,3),(CT(I)
     +,SP(I),CONV(I),I=1,M)
    1 FORMAT(I1/(F10.3))
C     WRITE INPUT DATA
      WRITE(6,7)M,(STRM(J,1),J=1,4),STRM(12,1),STRM(12,3),(I,CT(I),
     +CONV(I),SP(I),I=1,M)
    7 FORMAT(T1,' 'T7,'INPUT DATA'/T1,' 'T2,'NO. OF REACTORS=',I1/
     +T1,' 'T7,'LB MOLES/HR'/T1,' 'T2,'H2'
     +T9,F6.2/T1,' 'T2,'H2S'T9,F6.2/T1,' 'T2,'H2O'T9,F6.2/T1,' 'T2
     +,'N2'T9,F6.2/T1,'0'T7,'TEMP,DEGREES F'/T1,' 'T2,'FEED'T9,F6.2/
     +T1,' 'T2,'AIR'T9,F6.2//T1,' 'T2,'REACTOR'T12,'COND. TEMP.,F'
     +T28,'CONVERSION'T41,'BYPASS GAS SPLIT'/(T1,' 'T5,I1,T16,F6.2,T29,
     +F6.3,T46,F6.2))
C     CONVERT FEED GAS TEMP FROM FAHRENHEIT TO KELVIN
      STRM(12,1)=(STRM(12,1)+460.0)/1.8
C     SET TOTAL MOLES IN STREAM 1=100.
      STRM(11,1)=100.0
C     SET STREAM 1=1/3*STREAM 1,STREAM 5=2/3*STREAM 1
      DO 50 I=1,4
      STRM(I,2)=STRM(I,1)/3.0
   50 STRM(I,5)=STRM(I,2)*2.0
      STRM(11,5)=200.0/3.0
      STRM(11,2)=100.0/3.0
      STRM(12,5)=STRM(12,1)
      STRM(12,2)=STRM(12,1)
C     CALCULATE ADIABATIC FLAME TEMP OF STREAM 4
      CALL FLAME(FLTP)
      WRITE(6,40)FLTP
   40 FORMAT(/' FLAME TEMP,DEGREES K=',F7.2)
```

```
C     SET TEMP OF HOT BYPASS GAS TO EACH REACTOR
      STRM(12,6)=373.0
      STRM(12,12)=FLTP
      STRM(12,18)=FLTP
      DO 68 I=1,M
      K=6+(I-1)*6
      DO 69 J=1,11
C     CALCULATE FRACTION OF BURNER OUTLET GAS TO HEATER-COOLER I
   69 STRM(J,K)=STRM(J,4)*SP(I)
C     MIX STREAMS K&K-1
      CALL MIXER(K-1,K,K+1,I)
C     CALCULATE HEAT AND MAT'L BALANCE AROUND REACTOR I USING SPECIFIED
C     CONVERSION
      CALL REACTR(K+1,CONV(I),K+3,K+2,H(I),I)
C     IS THIS THE FIRST REACTOR ?
      IF(I-1)66,62,66
C     YES,CALCULATE HEAT REMOVED IN WASTE HEAT BOILER
   62 CALL WHB(QOUT)
      WRITE(6,65) QOUT
   65 FORMAT(' WASTE HEAT BOILER Q,BTU/HR=',E20.5)
C     CALCULATE HEAT AND MAT'L BALANCE AROUND CONDENSER I
   66 CALL COND(CT(I),K+3,K+5,K+4,HC(I),I)
   68 WRITE(6,67)I,H(I),I,HC(I)
   67 FORMAT(' HEATER-COOLER ',I1,' Q,BTU/HR=',E20.5/' CONDENSER ',I1,
     +' Q,BTU/HR=',E20.5)
      L=23+(M-3)*6
C     PRINT OUT ALL STREAMS WITH 3 STREAMS ON A PAGE
      K=1
      DO 70 I=1,L
      IF(I-K)70,21,21
   21 K=K+3
   23 WRITE(6,22)
   22 FORMAT('1')
   70 CALL PRINT(I)
      GO TO 4
    2 STOP
      END
```

```
      SUBROUTINE FLAME(TADBF)
C     SUBROUTINE CALCULATES THE ADIABATIC FLAME TEMP OF STREAM 4
      COMMON//STRM(13,23)
      COMMON/HFDT/COEF(60)
C     THERE ARE 13 COMPONENTS TO A STREAM.1=H2,2=H2S,3=H2O,4=N2,5=O2,
C     6=SO2,7=S6,8=S8,9=S2,10=LIQUID SULFUR,11=TOTAL MOLES,12=TEMP,13=
C     STREAM ENTHALPY
C     SET LOWER LIMIT OF FLAME TEMP=373.0
      STRM(12,4)=373.0
      TBIG=4000.0
C     CONVERT AIR TEMP FROM FAHRENHEIT TO KELVIN
      STRM(12,3)=(STRM(12,3)+460.0)/1.8
C     CALCULATE TOTAL MOLES OF OXYGEN REQUIRED
      STRM(5,3)=.5*STRM(1,2)+1.5*STRM(2,2)
C     CALCULATE TOTAL MOLES OF N2 REQUIRED
      STRM(4,3)=.79/.21*STRM(5,3)
C     CALCULATE TOTAL MOLES OF AIR
      STRM(11,3)=STRM(5,3)+STRM(4,3)
C     CALC. MOLES OF H2O IN STREAM 4
      STRM(3,4)=STRM(3,2)+STRM(2,2)+STRM(1,2)
C     CALC. MOLES OF N2 IN STREAM 4
      STRM(4,4)=STRM(4,2)+STRM(4,3)
C     CALC. MOLES OF SO2 IN STREAM 4
      STRM(6,4)=STRM(2,2)
      STRM(11,4)=STRM(3,4)+STRM(4,4)+STRM(6,4)
C     FUNCT=TOTAL CHANGE IN ENTHALPY
    7 FUNCT=SENTH(2)+SENTH(3)-SENTH(4)+57798.0*1.8*STRM(1,2)+123938.0*
     +1.8*STRM(2,2)
C     TEST FOR CONVERGENCE USING FUNCTION WAYA
      IF(WAYA(FUNCT,0.0,1.0,STRM(12,4),TBIG,1))7,8,9
    9 WRITE(6,100)
  100 FORMAT(////10X,'ADIABATIC FLAME TEMP CALC DID NOT CONVERGE'////)
      TADBF=2114.47
      RETURN
    8 TADBF=STRM(12,4)
      RETURN
      END
```

```
      SUBROUTINE REACTR(NI,CONV,NO,IR,HEAT,I)
C     SUBROUTINE DETERMINES IF SPECIFIED CONVERSION OCCURS ABOVE DEW
C     POINT.IF IT DOESN'T THE SUBR. DETERMINES THE MAX CONVERSION
C     WITHIN .01 WHICH SATISFIES THE DEW POINT CRITERIA.A HEAT AND MAT'L
C     BALANCE AROUND THE REACTOR ARE THEN CALCULATED
C     THERE ARE 13 COMPONENTS TO A STREAM.1=H2,2=H2S,3=H2O,4=N2,5=O2,
C     6=SO2,7=S6,8=S8,9=S2,10=LIQUID SULFUR,11=TOTAL MOLES,12=TEMP,13=
C     STREAM ENTHALPY
C     CONV=CONVERSION OF H2S AND SO2 TO SULFUR BASED ON ENTERING SO2
C     NO=REACTOR OUTLET STREAM
C     IR=STREAM ENTERING REACTOR
C     NI=STREAM ENTERING HEATER-COOLER
C     I=REACTOR NO.
C     HEAT=HEAT ADDED IN HEATER-COOLER,BTU/HR
C     S2LIM=MAX VALUE OF MOLES OF S2 IN REACTOR AT EQUILIBRIUM
C     TMMAX=MAX TOTAL MOLES
C     TMMIN=MIN TOTAL MOLES
C     SF=ATOMS OF SULFUR CONVERTED TO S2,S6,OR S8
C     T=TEMP IN REACTOR
C     TMOLES =TOTAL MOLES
      COMMON//STRM(13,23)
      COMMON/HPDT/COEF(60)
      S2LIM=(STRM(9,NI)+STRM(8,NI)*4.0+STRM(7,NI)*3.0+STRM(6,NI)*1.5)
      S6MAX=S2LIM/3.0
C     CALC. MAXIMUM TOTAL MOLES
      TMMAX=STRM(11,NI)+.25*STRM(2,NI)+STRM(7,NI)*2.0+STRM(8,NI)*3.0
C     CALC. MINIMUM TOTAL MOLES
      TMMIN=STRM(11,NI)-.25*STRM(7,NI)-.75*STRM(9,NI)-5./16.*STRM(2,NI)
      CONV1=CONV
C     CALC. TOTAL ATOMS OF SULFUR CONVERTED
    1 SF=3.0*STRM(6,NI)*CONV
C     SET TEMP. EQUAL TO LOWER LIMIT
      T=400.0
   13 TMOLES=TMMIN
C     SET S6 EQUAL TO LOWER LIMIT
    4 S6=0.0
   45 S2=(S6/EQK(2,T))**(1./3.)*TMOLES**(2./3.)
      S8=EQK(3,T)*(S6/EQK(2,T))**(4./3.)/TMOLES**(1./3.)
C     CALCULATE SULFUR BALANCE
      BAL=1.0-(2.0*S2+6.0*S6+8.0*S8)/(SF+2.0*STRM(9,NI)+6.0*STRM(7,NI)
     ++8.0*STRM(8,NI))
C     CHECK SULFUR BALANCE WITH FUNCTION WAYA
      IF(WAYA(BAL,0.0,.001,S6,S6MAX,1))45,46,47
C     TMCALC=CALCULATED TOTAL MOLES
   46  TMCALC=STRM(11,NI)-SF/3.0+S8-STRM(8,NI)+S6-STRM(7,NI)+S2-
     +STRM(9,NI)
      TMCHK=1.0-TMOLES/TMCALC
C     CHECK MOLE BALANCE USING FUNCTION WAYA
      IF(WAYA(TMCHK,0.0,.001,TMOLES,TMMAX,2))4,49,52
   49 WA=STRM(3,NI)+2./3.*SF
```

```
      H2S=STRM(2,NI)-2./3.*SF
      SO2=STRM(6,NI)-1./3.*SF
      EQN2=1.0-WA**2*S2**1.5/(H2S**2*SO2*SQRT(TMOLES)*EQK(1,T))
C     USE FUNCTION WAYA TO SEE IF CALCULATED VALUES SATISFY EQUILIBRIUM
C     CONSTANT FOR THE MAIN REACTION
      IF(WAYA(EQN2,0.0,.005,T,850.0,3))13,7,15
    7 STRM(2,NO)=H2S
      STRM(3,NO)=WA
      STRM(4,NO)=STRM(4,NI)
      STRM(6,NO)=SO2
      STRM(7,NO)=S6
      STRM(8,NO)=S8
      STRM(9,NO)=S2
      STRM(11,NO)=TMOLES
      STRM(12,NO)=T
C     VP(T)=VAPOR PRESSURE IN ATMOS. FOR S2,S6,AND S8 COMBINED
C     IS VAPOR PRESSURE > PARTIAL PRESSURE ?
      IF(VP(T)-(S2+S6+S8)/TMOLES)8,10,10
C     YES,REACTION TEMP IS ABOVE DEW POINT.
   10 STRM(12,IR)=298.0
C     IS THIS THE FIRST REACTOR (I.E. NO S2,S6,OR S8)
      IF(STRM(7,NI)+STRM(8,NI)+STRM(9,NI))40,40,20
C      YES
   40 L=2
C     SET COMPONENTS OF STREAMS IR AND NI EQUAL
      CALL EQUAL(NI,IR)
      GO TO 51
C     NO
   20 L=1
C     DETERMINE TEMP OF STREAM IR SO THAT REACTOR IS ADIABATIC
C     CALC S2,S6,AND S8 IN STREAM IR AT SELECTED TEMP
   50 CALL SPLIT(NI,IR,STRM(12,IR))
C     CALCULATED HEAT ADDED TO REACTOR
   51 HCHG=SENTH(IR)-SENTH(NO)-11524.0*1.8*(STRM(6,IR)-STRM(6,NO))+
     +65280.0*1.8*(STRM(7,NO)-STRM(7,IR))+96990.0*1.8*(STRM(8,NO)-STRM(8
     +,IR))
C     TEST VALUE OF HEAT ADDED FOR CONVERGENCE
      IF(WAYA(HCHG,0.0,1.0,STRM(12,IR),2000.0,3))24,21,22
C     NOT CONVERCED,RECALC. HCHG WITH NEW VALUE OF TEMP
   24 GO TO(50,51),L
   21 GO TO (70,71),L
C     IS REACTOR INLET TEMP. GREATER THAN 1ST HEATER INLET TEMP.
   71 IF(STRM(12,IR)-STRM(12,NI))70,70,72
C     YES,SET TEMP OF NI =IR SO THAT HEATER IS NOT REQUIRED.CAN TAKE OUT
C     LESS HEAT IN WASTE HEAT BOILER
   72 STRM(12,NI)=STRM(12,IR)
C     CALC HEATER-COOLER LOAD
   70 HEAT=SENTH(IR)-SENTH(NI)-65280.0*1.8*(STRM(7,IR)-STRM(7,NI))-
     +96990.0*1.8*(STRM(8,IR)-STRM(8,NI))
   30 IF(CONV1-CONV)25,25,26
```

```
   25 RETURN
   26 WRITE(6,12)I,CONV
   12 FORMAT(' SPECIFIED CONVERSION IN REACTOR ',I1,' OCCURS BELOW DEW'/
     +' POINT. CONVERSION REDUCED TO',F7.3)
      RETURN
   22 WRITE(6,23)I
   23 FORMAT(' CALC FOR REACTOR',I1,' INLET STREAM DOES NOT CONVERGE')
      GO TO 30
C     NO,REDUCE CONV. BY .01
    8 CONV=CONV-.01
      GO TO 1
   15 WRITE(6,16)I
   16 FORMAT(' REACTOR ',I1,' CALC. FOR TEMP DOES NOT CONVERGE')
      RETURN
   52 WRITE(6,53)I
   53 FORMAT(' CALC. FOR TOTAL MOLES IN REACTOR ',I1,' DOES NOT'/
     +' CONVERGE')
      RETURN
   47 WRITE(6,48)I
   48 FORMAT(' SULFUR BALANCE IN REACTOR ',I1,' DOES NOT CONVERGE')
      RETURN
      END
```

```
      SUBROUTINE SPLIT(N1,N2,TEMP)
      COMMON//STRM(13,23)
      CALL EQUAL(N1,N2)
      S2MAX=STRM(9,N1)+4.0*STRM(8,N1)+3.0*STRM(7,N1)
      TMMIN=STRM(11,N1)-.75*STRM(9,N1)-.25*STRM(7,N1)
      TMMAX=STRM(11,N1)+3.0*STRM(8,N1)+2.0*STRM(7,N1)
      S6MAX=S2MAX/3.0
      TMOLES=TMMIN
    1 S6=0.0
    4 S2=(S6/EQK(2,TEMP))**(1./3.)*TMOLES**(2./3.)
      S8=EQK(3,TEMP)*(S6/EQK(2,TEMP))**(4./3.)/TMOLES**(1./3.)
      BAL=1.0-(2.0*S2+6.0*S6+8.0*S8)/(S2MAX*2.0)
      IF(WAYA(BAL,0.0,.001,S6,S6MAX,1))4,2,3
    2 TMCALC=STRM(11,N1)-STRM(9,N1)-STRM(8,N1)-STRM(7,N1)+S8+S6+S2
      TMCHK=1.0-TMOLES/TMCALC
      IF(WAYA(TMCHK,0.0,.005,TMOLES,TMMAX,2))1,5,6
    5 STRM(7,N2)=S6
      STRM(8,N2)=S8
      STRM(9,N2)=S2
      STRM(11,N2)=TMOLES
      STRM(12,N2)=TEMP
      RETURN
    3 WRITE(6,20)N1
   20 FORMAT(' SULFUR BALANCE IN SPLIT CALC. ON STREAM',I2,' DOES NOT '/
     +' CONVERGE')
      RETURN
    6 WRITE(6,7) N1
    7 FORMAT(' TOTAL MOLE BALANCE IN SPLIT CALC. ON STREAM ',I2,' DOES '
     +/' NOT CONVERGE')
      RETURN
      END
```

```
      SUBROUTINE MIXER(IN1,IN2,MIX,K)
      COMMON//STRM(13,23)
      DO 2 I=1,11
    2 STRM(I,MIX)=STRM(I,IN1)+STRM(I,IN2)
      STRM(12,MIX)=AMIN1(STRM(12,IN1),STRM(12,IN2))
      TMAX=2000.0
    9 IF(STRM(7,MIX)+STRM(8,MIX)+STRM(9,MIX))7,7,4
    4 CALL SPLIT(MIX,MIX,STRM(12,MIX))
    7 H=SENTH(IN1)+SENTH(IN2)-SENTH(MIX)+1.8*65280.0*(STRM(7,MIX)-
     +STRM(7,IN1)-STRM(7,IN2))+96990.0*1.8*(STRM(8,MIX)-STRM(8,IN1)-
     +STRM(8,IN2))
      IF(WAYA(H,0.0,1.0,STRM(12,MIX),TMAX,3))9,5,6
    5 RETURN
    6 WRITE(6,8)K
    8 FORMAT(' MIXER ',I1,' TEMP DOES NOT CONVERGE')
      RETURN
      END
```

```
      FUNCTION     EQUA  ( X, C )
C
C     THIS FUNCTION EVALUATES A SET OF POLYNOMINAL COEFFICIENTS BY
C     NESTED EXPANSION ---- AS GENERATED BY FUNCTION FITIT.
C
C           Y = A0 + A1*X + A2*X**2 + ..... + AM*X**M
C
C                 M = C(1)
C
C                 A0  = C(2)
C                 A1  = C(3)
C                 A2  = C(4)
C                 .. . ....
C                 .. . ....
C                 AM  = C(M+2)
C
      REAL        C(1)
C
      M = C(1)
      Y = C(M+2)
      DO  1  J=1,M
      MM=M+2-J
      Y=Y*X+C(MM)
    1 CONTINUE
      Y=Y+C(M+3)/X
      EQUA = Y
      RETURN
      END
```

```
      FUNCTION WAYA(A,ANS,TOL,START,STOP,LEVEL)
C
C        ROUTINE TO CONVERGE ON SINGLE VALUED FUNCTION
C
C   A     =CURRENT VALUE OF DEPENDENT VARIABLE
C   ANS   =DESIRED VALUE OF DEPENDENT VARIABLE
C   TOL   =TOLERANCE
C   START=CURRENT VALUE OF INDEPENDENT VARIABLE. A BETTER VALUE RETURNED.
C   STOP =LIMIT OF INDEPENDENT VARIABLE. ANSWER BETWEEN START AND STOP.
C   LEVEL= 1,2, OR 3 AS AN INDEX FOR MULTILEVEL USE.
C
C   WAYA WILL VARY START BETWEEN ITS INITIAL VALUE AND STOP UNTIL
C         ABS( ANS- A) .LE. TOL OR 30 TRIALS TAKEN.
C
C   ON EXIT WAYA IS:
C    - FOR NOT CONVERGED. REPEAT CALCULATION WITH NEW VALUE IN START.
C    0 FOR CONVERGED IN LIMITS OR 30 TRIALS TAKEN.
C    + FOR CANNOT CONVERGE. START WILL BE ITS INITIAL VALUE OR STOP,
C          WHICHEVER GIVES LESSER ERROR, OR ITS INITIAL VALUE IF LEVEL
C          IS NEGATIVE.
C
      DIMENSION X1(4),X2(4),Y1(4),Y2(4),KOUNT(4)
      DATA  KOUNT/ 4*0 /
C
C        SET X,Y & LEVEL
      X=START
      Y=ANS-A
      L=IABS(LEVEL)
      WAYA=1.0
C
C         SEE IF CONVERGED
C
      IF(ABS(Y).LE. TOL) GO TO 70
C
C         NOT CONVERGED. SEE WHICH CALL.
C
      IF(KOUNT(L)) 80,30,10
C
C         SECOND OR HIGHER CALL. SEE IF Y AND Y1(L) BRACKET ANSWER.
C
   10 IF(Y*Y1(L) .LT. 0.0) GO TO 20
C
C         NO Y-Y1 BRACKET. SEE IF SECOND OR HIGHER CALL.
C
      IF(KOUNT(L) .GT. 1) GO TO 30
C
C         NO BRACKET AT ALL. RE-DO AT START IF THAT LIMIT IS CLOSER OR IF
C         LEVEL IS MINUS
C
      IF(ABS(Y) .LE. ABS(Y1(L)) .AND. LEVEL .GT. 0) GO TO 80
```

```
      X=X1(L)
      KOUNT(L)= -1
      GO TO 60
C
C        Y-Y1 BRACKET. STORE X & Y IN X2(L) AND Y2(L)
C
 20   X2(L)=X
      Y2(L)=Y
      GO TO 40
C
C        FIRST CALL OR CONVERGING Y-Y2 BRACKET CALL.  STORE X & Y IN X1
C        & Y1.
C
 30   X1(L)=X
      Y1(L)=Y
      X=STOP
      IF(KOUNT(L).EQ. 0) GO TO 50
C
C        INTERPOLATE NEW X AND CONTINUE OR QUIT DEPENDING ON KOUNT(L).
C
 40   X=(X1(L)*(3.*Y2(L)-Y1(L))+X2(L)*(Y2(L)-3.*Y1(L)))/(4.*(Y2(L)-Y1(L)
     1))
      IF(KOUNT(L) .GE. 99) GO TO 70
 50   KOUNT(L)=KOUNT(L)+1
 60   WAYA=-1.0
      GO TO 90
C
C        CONVERGED OR TOO MANY TRIALS
C
 70   WAYA=0.0
 80   KOUNT(L)=0
C
C        SET NEW VALUE OF INDEPENDENT VARIABLE.
C
 90   START=X
      RETURN
C
C
      END
```

```
      BLOCK DATA
      COMMON/HFDT/COEF(60)
      DATA COEF/3.0,-2066.7,6.947,-1.0F-4,1.603E-7,0.0,
     +2.0,-2279.37,7.15,1.66E-3,0.0,0.0,
     +3.0,-2268.1,7.256,1.149E-3,9.43E-8,0.0,
     +3.0,-2000.7,6.524,6.25E-4,-3.33E-10,0.0,
     +3.0,-1962.8,6.148,1.551E-3,-3.076E-7,0.0,
     +2.0,-4147.74,1.14E+1,7.07E-4,2.045E+5,0.0,
     +2.0,-5357.99,19.25,1.332E-3,0.0,0.0,
     +2.0,-7611.88,25.0,1.776E-3,0.0,0.0,
     +2.0,-2350.21,7.75,4.44E-4,0.0,0.0,
     +2.0,-1832.31,5.4,2.5E-3,0.0,0.0/
      END
```

```
      FUNCTION   EQK(NO,T)
      REAL FENG(6,3)/12119.00,-12.999,1.063E-3,-9.433E-9,-4.37E-1,
     +-2.045E+5,
     +-64090.0,+44.26,2*0.0,4.0,0.0,
     +-95200.0,68.28,2*0.0,6.0,0.0/
      FREE=FENG(4,NO)
      DO 10 J=1,3
      J4=4-J
   10 FREE=FREE*T+FENG(J4,NO)
      FREE=FREE+FENG(5,NO)*ALOG(T)*T+FENG(6,NO)/(2.0*T)
      EQK=EXP(-FREE/(1.987*T))
      RETURN
      END
```

```
      FUNCTION VP(T)
      VP=10.0**(-4940.0/T-.00408*T+9.811)
      RETURN
      END
```

```
      SUBROUTINE DEWPT(NO,I)
      COMMON//STRM(13,23)
      T=425.0
      I=23
    1 CALL SPLIT(NO,I,T)
      DEW=1.0-(STRM(7,I)+STRM(8,I)+STRM(9,I))/(STRM(11,I)*VP(T))
      IF(WAYA(DEW,0.0,.005,T,0717.8,3))1,2,3
    2 RETURN
    3 WRITE(6,4)NO
    4 FORMAT(' DEW POINT CALC ON STREAM ',I2,' DOES NOT CONVERGE')
      RETURN
      END
```

```
      SUBROUTINE COND(TCOND,IV,LV,LL,HEAT,I)
      COMMON//STRM(13,23)
C     IV=NO. OF INLET STREAM
C     LV=NO OF OUTLET GAS STREAM
C     LL=NO. OF OUTLET LIQUID STREAM
C     CONVERT COND. TEMP. FROM FAHRENHEIT TO CENTIGRADE
      TCOND=(TCOND+460.0)/1.8
      IF(TCOND-392.0) 5,5,2
    2 CALL DEWPT(IV,T)
      IF(T-TCOND)10,10,1
    1 S268=STRM(7,IV)+STRM(8,IV)+STRM(9,IV)
C     CALC. TOTAL MOLES OF SULFUR IN VAPOR PHASE AT THE DEW POINT
      TOTSP=VP(TCOND)*(STRM(11,IV)-S268)/(1.0-VP(TCOND))
      TMOLES=STRM(11,IV)-S268+TOTSP
      S2MAX=TOTSP
      S8MAX=TOTSP
      S6MAX=TOTSP
      S6=0.0
    3 S2=(S6/EQK(2,TCOND))**(1./3.)*TMOLES**(2./3.)
      S8=EQK(3,TCOND)*(S6/EQK(2,TCOND))**(4./3.)/TMOLES**(1./3.)
C     CHECK MOLE BALANCE
      DIFF=1.0-(S8+S6+S2)/TOTSP
      IF(WAYA(DIFF,0.0,.001,S6,S6MAX,1))3,4,7
    4 CALL EQUAL(IV,LV)
      STRM(12,LV)=TCOND
      S2CD=STRM(9,IV)-S2
      S6CD=STRM(7,IV)-S6
      S8CD=STRM(8,IV)-S8
      SLIQ=6.0*S6CD+8.0*S8CD+2.0*S2CD
      HVAP=2.303*(4940.0-.00408*TCOND**2)*1.987*1.8
      HEAT=-HVAP*(S2CD+S6CD+S8CD)-SENTH(IV)+SENTH(LV)
      STRM(7,LV)=S6
      STRM(8,LV)=S8
      STRM(9,LV)=S2
      STRM(11,LV)=TMOLES
      STRM(12,LL)=TCOND
      STRM(10,LL)=SLIQ
      STRM(11,LL)=SLIQ
      STRM(13,LL)=SENTH(IV)-SENTH(LV)+HEAT
      RETURN
    5 WRITE(6,6) I
    6 FORMAT(' CONDENSER ',I1,' TEMP IS TOO LOW,SULFUR FREEZES AT 392K,'
     +/' TEMP SET=400K')
      TCOND=400.0
      GO TO 2
   10 WRITE(6,16)I
   16 FORMAT(' SPECIFIED TEMP FOR CONDENSER ',I1,' IS ABOVE DEW POINT')
      RETURN
    7 WRITE(6,8)I
    8 FORMAT(' CONDENSER ',I1,' CALC. DOES NOT CONVERGE')
```

```
   51          RETURN
   52          END
```

```
      SUBROUTINE EQUAL(N1,N2)
      COMMON//STRM(13,23)
      DO 1 I=1,11
    1 STRM(I,N2)=STRM(I,N1)
      RETURN
      END
```

```
      SUBROUTINE PRINT(NO)
      COMMON//STRM(13,23)
      DIMENSION FRAC(11),C(11)
      DATA C/'H2  ','H2S ','H2O ','N2  ','O2  ','SO2 ','S6  ','S8  ',
     +'S2  ','SLIQ','MOLS'/
      REAL*8 TITLE(3,23)/'     FEE','D STREAM','(1)     ',
     +'   BURNE','R H2S GA','S(2)    ',
     +'      BUR','NER AIR(','3)      ',
     +'      BUR','NER OUTL','ET(4)   ',
     +'INLET H2','S GAS MI','XER 1(5)',
     +'SO2 GAS ','TO MIXER','1(6)    ',
     +'   INLET',' HEATER ','1(7)    ',
     +'   INLET',' REACTOR',' 1(8)   ',
     +'  OUTLET',' REACTOR',' 1(9)   ',
     +'LIQUID S','ULFUR CO','ND 1(10)',
     +'  OUTLET',' GAS CON','D 1(11) ',
     +'SO2 GAS ','TO MIXER','2(12)   ',
     +'   INLET',' HEATER ','2(13)   ',
     +'   INLET',' REACTOR',' 2(14)  ',
     +'  OUTLET',' REACTOR',' 2(15)  ',
     +'LIQUID S','ULFUR CO','ND 2(16)',
     +'  OUTLET',' GAS CON','D 2(17) ',
     +'SO2 GAS ','TO MIXER','3(18)   ',
     +'   INLET',' HEATER ','3(19)   ',
     +'   INLET',' REACTOR',' 3(20)  ',
     +'  OUTLET',' REACTOR',' 3(21)  ',
     +'LIQUID S','ULFUR CO','ND 3(22)',
     +'  OUTLET',' GAS CON','D 3(23) '/
      DO 1 J=1,11
    1 FRAC(J)=STRM(J,NO)/STRM(11,NO)
      IF(STRM(10,NO))3,3,4
    3 STRM(13,NO)=SENTH(NO)
    4 WRITE(6,2)(TITLE(I,NO),I=1,3),(C(I),FRAC(I),STRM(I,NO),I=1,11),
     +STRM(12,NO),STRM(13,NO)
    2 FORMAT(//T1,' 'T13,3A8/T1,' 'T10,'MOLE FRAC.'T33,'LB MOLES/HR'
     +11(/T1,' 'T2,A4,T6,E20.5,T26,E20.5),/' TEMP,DEGREES K=',E20.5/
     +' ENTHALPY,BTU/HR=',E20.5)
      RETURN
      END
```

```
      FUNCTION SENTH(K)
      COMMON//STRM(13,23)
      COMMON/HFD1/COEF(60)
      SENTH=0.0
      DO 1 I=1,10
      M=1+6*(I-1)
    1 SENTH=SENTH+EQUA(STRM(12,K),COEF(M))*STRM(I,K)*1.8
      RETURN
      END
```

```
      SUBROUTINE WHB(QOUT)
      COMMON//STRM(13,23)
C     1ST HEATER COOLER ELIMINATED ?
      IF(STRM(12,8)-STRM(12,7))6,5,6
C     CALC. TEMP. OF GAS LEAVING WHB REQD TO YIELD DESIRED TEMP AT
C     REACTOR INLET
    5 TMAX=STRM(12,4)
      STRM(12,6)=373.0
    1 DELH=SENTH(5)+SENTH(6)-SENTH(7)
      IF(WAYA(DELH,0.0,1.0,STRM(12,6),TMAX,1))1,6,3
C     NO,CALC.HEAT REMOVED IN WHB
    6 QOUT=-SENTH(4)+SENTH(12)+SENTH(18)+SENTH(6)
    2 RETURN
    3 WRITE(6,4)
    4 FORMAT(' WASTE HEAT BOILER CALC DOES NOT CONVERGE')
      RETURN
      END
```

```
      INPUT DATA
 NO. OF REACTORS=1
      LB MOLES/HR
 H2        0.00
 H2S     100.00
 H2O       0.00
 N2        0.00

      TEMP,DEGREES F
 FEED     98.00
 AIR      98.00

 REACTOR   COND. TEMP.,F   CONVERSION   BYPASS GAS SPLIT
    1          300.00         0.550              1.00

 FLAME TEMP,DEGREES K=2114.47
 WASTE HEAT BOILER Q,BTU/HR=            -0.53919E 07
 HEATER-COOLER 1 Q,BTU/HR=              0.00000E 00
 CONDENSER 1 Q,BTU/HR=           -0.23492E 07
```

```
                     FEED STREAM(1)
        MOLE FRAC.                  LB MOLES/HR
 H2           0.00000E 00              0.00000E 00
 H2S          0.10000E 01              0.10000E 03
 H2O          0.00000E 00              0.00000E 00
 N2           0.00000E 00              0.00000E 00
 O2           0.00000E 00              0.00000E 00
 SO2          0.00000E 00              0.00000E 00
 S6           0.00000E 00              0.00000E 00
 S8           0.00000E 00              0.00000E 00
 S2           0.00000E 00              0.00000E 00
 SLIQ         0.00000E 00              0.00000E 00
 MOLS         0.10000E 01              0.10000E 03
 TEMP,DEGREES K=               0.31000E 03
 ENTHALPY,BTU/HR=               0.17398E 05


                   BURNER H2S GAS(2)
        MOLE FRAC.                  LB MOLES/HR
 H2           0.00000E 00              0.00000E 00
 H2S          0.10000E 01              0.33333E 02
 H2O          0.00000E 00              0.00000E 00
 N2           0.00000E 00              0.00000E 00
 O2           0.00000E 00              0.00000E 00
 SO2          0.00000E 00              0.00000E 00
 S6           0.00000E 00              0.00000E 00
 S8           0.00000E 00              0.00000E 00
 S2           0.00000E 00              0.00000E 00
 SLIQ         0.00000E 00              0.00000E 00
 MOLS         0.10000E 01              0.33333E 02
 TEMP,DEGREES K=               0.31000E 03
 ENTHALPY,BTU/HR=               0.57992E 04


                     BURNER AIR(3)
        MOLE FRAC.                  LB MOLES/HR
 H2           0.00000E 00              0.00000E 00
 H2S          0.00000E 00              0.00000E 00
 H2O          0.00000E 00              0.00000E 00
 N2           0.79000E 00              0.18810E 03
 O2           0.21000E 00              0.50000E 02
 SO2          0.00000E 00              0.00000E 00
 S6           0.00000E 00              0.00000E 00
 S8           0.00000E 00              0.00000E 00
 S2           0.00000E 00              0.00000E 00
 SLIQ         0.00000E 00              0.00000E 00
 MOLS         0.10000E 01              0.23810E 03
 TEMP,DEGREES K=               0.31000E 03
 ENTHALPY,BTU/HR=               0.35159E 05
```

```
                    BURNER OUTLET(4)
          MOLE FRAC.                   LB MOLES/HR
 H2              0.00000E 00             0.00000E 00
 H2S             0.00000E 00             0.00000E 00
 H2O             0.13084E 00             0.33333E 02
 N2              0.73832E 00             0.18810E 03
 O2              0.00000E 00             0.00000E 00
 SO2             0.13084E 00             0.33333E 02
 S6              0.00000E 00             0.00000E 00
 S8              0.00000E 00             0.00000E 00
 S2              0.00000E 00             0.00000E 00
 SLIQ            0.00000E 00             0.00000E 00
 MOLS            0.10000E 01             0.25476E 03
 TEMP,DEGREES K=               0.21145E 04
 ENTHALPY,BTU/HR=               0.74772E 07


                INLET H2S GAS MIXER 1(5)
          MOLE FRAC.                   LB MOLES/HR
 H2              0.00000E 00             0.00000E 00
 H2S             0.10000E 01             0.66667E 02
 H2O             0.00000E 00             0.00000E 00
 N2              0.00000E 00             0.00000E 00
 O2              0.00000E 00             0.00000E 00
 SO2             0.00000E 00             0.00000E 00
 S6              0.00000E 00             0.00000E 00
 S8              0.00000E 00             0.00000E 00
 S2              0.00000E 00             0.00000E 00
 SLIQ            0.00000E 00             0.00000E 00
 MOLS            0.10000E 01             0.66667E 02
 TEMP,DEGREES K=               0.31000E 03
 ENTHALPY,BTU/HR=               0.11598E 05


                SO2 GAS TO MIXER1(6)
          MOLE FRAC.                   LB MOLES/HR
 H2              0.00000E 00             0.00000E 00
 H2S             0.00000E 00             0.00000E 00
 H2O             0.13084E 00             0.33333E 02
 N2              0.73832E 00             0.18810E 03
 O2              0.00000E 00             0.00000E 00
 SO2             0.13084E 00             0.33333E 02
 S6              0.00000E 00             0.00000E 00
 S8              0.00000E 00             0.00000E 00
 S2              0.00000E 00             0.00000E 00
 SLIQ            0.00000E 00             0.00000E 00
 MOLS            0.10000E 01             0.25476E 03
 TEMP,DEGREES K=               0.86764E 03
 ENTHALPY,BTU/HR=               0.20862E 07
```

```
                  INLET HEATER 1(7)
          MOLE FRAC.                   LB MOLES/HR
 H2                0.00000E 00            0.00000E 00
 H2S               0.20741E 00            0.66667E 02
 H2O               0.10370E 00            0.33333E 02
 N2                0.58519E 00            0.18810E 03
 O2                0.00000E 00            0.00000E 00
 SO2               0.10370E 00            0.33333E 02
 S6                0.00000E 00            0.00000E 00
 S8                0.00000E 00            0.00000E 00
 S2                0.00000E 00            0.00000E 00
 SLIQ              0.00000E 00            0.00000E 00
 MOLS              0.10000E 01            0.32143E 03
 TEMP,DEGREES K=              0.74629E 03
 ENTHALPY,BTU/HR=              0.20978E 07


                  INLET REACTOR 1(8)
          MOLE FRAC.                   LB MOLES/HR
 H2                0.00000E 00            0.00000E 00
 H2S               0.20741E 00            0.66667E 02
 H2O               0.10370E 00            0.33333E 02
 N2                0.58519E 00            0.18810E 03
 O2                0.00000E 00            0.00000E 00
 SO2               0.10370E 00            0.33333E 02
 S6                0.00000E 00            0.00000E 00
 S8                0.00000E 00            0.00000E 00
 S2                0.00000E 00            0.00000E 00
 SLIQ              0.00000E 00            0.00000E 00
 MOLS              0.10000E 01            0.32143E 03
 TEMP,DEGREES K=              0.74629E 03
 ENTHALPY,BTU/HR=              0.20978E 07


                  OUTLET REACTOR 1(9)
          MOLE FRAC.                   LB MOLES/HR
 H2                0.00000E 00            0.00000E 00
 H2S               0.93502E-01            0.30000E 02
 H2O               0.21817E 00            0.70000E 02
 N2                0.58624E 00            0.18810E 03
 O2                0.00000E 00            0.00000E 00
 SO2               0.46751E-01            0.15000E 02
 S6                0.12935E-01            0.41501E 01
 S8                0.15482E-02            0.49673E 00
 S2                0.40788E-01            0.13087E 02
 SLIQ              0.00000E 00            0.00000E 00
 MOLS              0.10000E 01            0.32085E 03
 TEMP,DEGREES K=              0.78765E 03
 ENTHALPY,BTU/HR=              0.22919E 07
```

```
              LIQUID SULFUR COND 1(10)
         MOLE FRAC.                    LB MOLES/HR
H2            0.00000E 00              0.00000E 00
H2S           0.00000E 00              0.00000E 00
H2O           0.00000E 00              0.00000E 00
N2            0.00000E 00              0.00000E 00
O2            0.00000E 00              0.00000E 00
SO2           0.00000E 00              0.00000E 00
S6            0.00000E 00              0.00000E 00
S8            0.00000E 00              0.00000E 00
S2            0.00000E 00              0.00000E 00
SLIQ          0.10000E 01              0.54480E 02
MOLS          0.10000E 01              0.54480E 02
TEMP,DEGREES K=             0.42222E 03
ENTHALPY,BTU/HR=           -0.56796E 06


              OUTLET GAS COND 1(11)
         MOLE FRAC.                    LB MOLES/HR
H2            0.00000E 00              0.00000E 00
H2S           0.98948E-01              0.30000E 02
H2O           0.23088E 00              0.70000E 02
N2            0.62039E 00              0.18810E 03
O2            0.00000E 00              0.00000E 00
SO2           0.49474E-01              0.15000E 02
S6            0.42189E-04              0.12791E-01
S8            0.20233E-03              0.61345E-01
S2            0.29457E-07              0.89310E-05
SLIQ          0.00000E 00              0.00000E 00
MOLS          0.10000E 01              0.30319E 03
TEMP,DEGREES K=             0.42222E 03
ENTHALPY,BTU/HR=            0.51068E 06
```

```
      INPUT DATA
NO. OF REACTORS=1
      LB MOLES/HR
H2        0.00
H2S     100.00
H2O       0.00
N2        0.00

      TEMP,DEGREES F
FEED     98.00
AIR      98.00

REACTOR   COND. TEMP.,F   CONVERSION   BYPASS GAS SPLIT
   1            300.00         0.650                 1.00

FLAME TEMP,DEGREES K=2114.47
WASTE HEAT BOILER Q,BTU/HR=          -0.61896E 07
HEATER-COOLER 1 Q,BTU/HR=           0.00000E 00
CONDENSER 1 Q,BTU/HR=          -0.18810E 07
```

```
                    FEED STREAM(1)
          MOLE FRAC.                  LB MOLES/HR
H2                  0.00000E 00          0.00000E 00
H2S                 0.10000E 01          0.10000E 03
H2O                 0.00000E 00          0.00000E 00
N2                  0.00000E 00          0.00000E 00
O2                  0.00000E 00          0.00000E 00
SO2                 0.00000E 00          0.00000E 00
S6                  0.00000E 00          0.00000E 00
S8                  0.00000E 00          0.00000E 00
S2                  0.00000E 00          0.00000E 00
SLIQ                0.00000E 00          0.00000E 00
MOLS                0.10000E 01          0.10000E 03
TEMP,DEGREES K=               0.31000E 03
ENTHALPY,BTU/HR=               0.17398E 05


                   BURNER H2S GAS(2)
          MOLE FRAC.                  LB MOLES/HR
H2                  0.00000E 00          0.00000E 00
H2S                 0.10000E 01          0.33333E 02
H2O                 0.00000E 00          0.00000E 00
N2                  0.00000E 00          0.00000E 00
O2                  0.00000E 00          0.00000E 00
SO2                 0.00000E 00          0.00000E 00
S6                  0.00000E 00          0.00000E 00
S8                  0.00000E 00          0.00000E 00
S2                  0.00000E 00          0.00000E 00
SLIQ                0.00000E 00          0.00000E 00
MOLS                0.10000E 01          0.33333E 02
TEMP,DEGREES K=               0.31000E 03
ENTHALPY,BTU/HR=               0.57992E 04


                    BURNER AIR(3)
          MOLE FRAC.                  LB MOLES/HR
H2                  0.00000E 00          0.00000E 00
H2S                 0.00000E 00          0.00000E 00
H2O                 0.00000E 00          0.00000E 00
N2                  0.79000E 00          0.18810E 03
O2                  0.21000E 00          0.50000E 02
SO2                 0.00000E 00          0.00000E 00
S6                  0.00000E 00          0.00000E 00
S8                  0.00000E 00          0.00000E 00
S2                  0.00000E 00          0.00000E 00
SLIQ                0.00000E 00          0.00000E 00
MOLS                0.10000E 01          0.23810E 03
TEMP,DEGREES K=               0.31000E 03
ENTHALPY,BTU/HR=               0.35159E 05
```

```
                  BURNER OUTLET(4)
         MOLE FRAC.                    LB MOLES/HR
 H2          0.00000E 00                0.00000E 00
 H2S         0.00000E 00                0.00000E 00
 H2O         0.13084E 00                0.33333E 02
 N2          0.73832E 00                0.18810E 03
 O2          0.00000E 00                0.00000E 00
 SO2         0.13084E 00                0.33333E 02
 S6          0.00000E 00                0.00000E 00
 S8          0.00000E 00                0.00000E 00
 S2          0.00000E 00                0.00000E 00
 SLIQ        0.00000E 00                0.00000E 00
 MOLS        0.10000E 01                0.25476E 03
 TEMP,DEGREES K=              0.21145E 04
 ENTHALPY,BTU/HR=              0.74772E 07

              INLET H2S GAS MIXER 1(5)
         MOLE FRAC.                    LB MOLES/HR
 H2          0.00000E 00                0.00000E 00
 H2S         0.10000E 01                0.66667E 02
 H2O         0.00000E 00                0.00000E 00
 N2          0.00000E 00                0.00000E 00
 O2          0.00000E 00                0.00000E 00
 SO2         0.00000E 00                0.00000E 00
 S6          0.00000E 00                0.00000E 00
 S8          0.00000E 00                0.00000E 00
 S2          0.00000E 00                0.00000E 00
 SLIQ        0.00000E 00                0.00000E 00
 MOLS        0.10000E 01                0.66667E 02
 TEMP,DEGREES K=              0.31000E 03
 ENTHALPY,BTU/HR=              0.11598E 05

              SO2 GAS TO MIXER1(6)
         MOLE FRAC.                    LB MOLES/HR
 H2          0.00000E 00                0.00000E 00
 H2S         0.00000E 00                0.00000E 00
 H2O         0.13084E 00                0.33333E 02
 N2          0.73832E 00                0.18810E 03
 O2          0.00000E 00                0.00000E 00
 SO2         0.13084E 00                0.33333E 02
 S6          0.00000E 00                0.00000E 00
 S8          0.00000E 00                0.00000E 00
 S2          0.00000E 00                0.00000E 00
 SLIQ        0.00000E 00                0.00000E 00
 MOLS        0.10000E 01                0.25476E 03
 TEMP,DEGREES K=              0.65798E 03
 ENTHALPY,BTU/HR=              0.12876E 07
```

```
                    INLET HEATER 1(7)
          MOLE FRAC.                    LB MOLES/HR
H2                 0.00000E 00             0.00000E 00
H2S                0.20741E 00             0.66667E 02
H2O                0.10370E 00             0.33333E 02
N2                 0.58519E 00             0.18810E 03
O2                 0.00000E 00             0.00000E 00
SO2                0.10370E 00             0.33333E 02
S6                 0.00000E 00             0.00000E 00
S8                 0.00000E 00             0.00000E 00
S2                 0.00000E 00             0.00000E 00
SLIQ               0.00000E 00             0.00000E 00
MOLS               0.10000E 01             0.32143E 03
TEMP,DEGREES K=              0.58193E 03
ENTHALPY,BTU/HR=              0.12992E 07


                    INLET REACTOR 1(8)
          MOLE FRAC.                    LB MOLES/HR
H2                 0.00000E 00             0.00000E 00
H2S                0.20741E 00             0.66667E 02
H2O                0.10370E 00             0.33333E 02
N2                 0.58519E 00             0.18810E 03
O2                 0.00000E 00             0.00000E 00
SO2                0.10370E 00             0.33333E 02
S6                 0.00000E 00             0.00000E 00
S8                 0.00000E 00             0.00000E 00
S2                 0.00000E 00             0.00000E 00
SLIQ               0.00000E 00             0.00000E 00
MOLS               0.10000E 01             0.32143E 03
TEMP,DEGREES K=              0.58193E 03
ENTHALPY,BTU/HR=              0.12992E 07


                   OUTLET REACTOR 1(9)
          MOLE FRAC.                    LB MOLES/HR
H2                 0.00000E 00             0.00000E 00
H2S                0.74489E-01             0.23333E 02
H2O                0.24475E 00             0.76667E 02
N2                 0.60048E 00             0.18810E 03
O2                 0.00000E 00             0.00000E 00
SO2                0.37245E-01             0.11667E 02
S6                 0.22285E-01             0.69807E 01
S8                 0.55792E-02             0.17476E 01
S2                 0.14512E-01             0.45457E 01
SLIQ               0.00000E 00             0.00000E 00
MOLS               0.10000E 01             0.31324E 03
TEMP,DEGREES K=              0.72596E 03
ENTHALPY,BTU/HR=              0.19751E 07
```

```
                LIQUID SULFUR COND 1(10)
         MOLE FRAC.                  LB MOLES/HR
 H2             0.00000E 00               0.00000E 00
 H2S            0.00000E 00               0.00000E 00
 H2O            0.00000E 00               0.00000E 00
 N2             0.00000E 00               0.00000E 00
 O2             0.00000E 00               0.00000E 00
 SO2            0.00000E 00               0.00000E 00
 S6             0.00000E 00               0.00000E 00
 S8             0.00000E 00               0.00000E 00
 S2             0.00000E 00               0.00000E 00
 SLIQ           0.10000E 01               0.64395E 02
 MOLS           0.10000E 01               0.64395E 02
 TEMP,DEGREES K=             0.42222E 03
 ENTHALPY,BTU/HR=           -0.40851E 06

                 OUTLET GAS COND 1(11)
         MOLE FRAC.                  LB MOLES/HR
 H2             0.00000E 00               0.00000E 00
 H2S            0.77767E-01               0.23333E 02
 H2O            0.25552E 00               0.76667E 02
 N2             0.62690E 00               0.18810E 03
 O2             0.00000E 00               0.00000E 00
 SO2            0.38883E-01               0.11667E 02
 S6             0.42189E-04               0.12658E-01
 S8             0.20233E-03               0.60709E-01
 S2             0.29457E-07               0.88383E-05
 SLIQ           0.00000E 00               0.00000E 00
 MOLS           0.10000E 01               0.30004E 03
 TEMP,DEGREES K=              0.42222E 03
 ENTHALPY,BTU/HR=              0.50269E 06
```

```
       INPUT DATA
 NO. OF REACTORS=1
       LB MOLES/HR
 H2         0.00
 H2S      100.00
 H2O        0.00
 N2         0.00

       TEMP,DEGREES F
 FEED     98.00
 AIR      98.00

 REACTOR    COND. TEMP.,F    CONVERSION    BYPASS GAS SPLIT
    1            300.00          0.700               1.00

 FLAME TEMP,DEGREES K=2114.47
 WASTE HEAT BOILER Q,BTU/HR=          -0.64785E 07
 HEATER-COOLER 1 Q,BTU/HR=             0.00000E 00
 CONDENSER 1 Q,BTU/HR=           -0.17234E 07
```

```
                    FEED STREAM(1)
           MOLE FRAC.                LB MOLES/HR
 H2              0.00000E 00            0.00000E 00
 H2S             0.10000E 01            0.10000E 03
 H2O             0.00000E 00            0.00000E 00
 N2              0.00000E 00            0.00000E 00
 O2              0.00000E 00            0.00000E 00
 SO2             0.00000E 00            0.00000E 00
 S6              0.00000E 00            0.00000E 00
 S8              0.00000E 00            0.00000E 00
 S2              0.00000E 00            0.00000E 00
 SLIQ            0.00000E 00            0.00000E 00
 MOLS            0.10000E 01            0.10000E 03
 TEMP,DEGREES K=             0.31000E 03
 ENTHALPY,BTU/HR=             0.17398E 05


                  BURNER H2S GAS(2)
           MOLE FRAC.                LB MOLES/HR
 H2              0.00000E 00            0.00000E 00
 H2S             0.10000E 01            0.33333E 02
 H2O             0.00000E 00            0.00000E 00
 N2              0.00000E 00            0.00000E 00
 O2              0.00000E 00            0.00000E 00
 SO2             0.00000E 00            0.00000E 00
 S6              0.00000E 00            0.00000E 00
 S8              0.00000E 00            0.00000E 00
 S2              0.00000E 00            0.00000E 00
 SLIQ            0.00000E 00            0.00000E 00
 MOLS            0.10000E 01            0.33333E 02
 TEMP,DEGREES K=             0.31000E 03
 ENTHALPY,BTU/HR=             0.57992E 04


                    BURNER AIR(3)
           MOLE FRAC.                LB MOLES/HR
 H2              0.00000E 00            0.00000E 00
 H2S             0.00000E 00            0.00000E 00
 H2O             0.00000E 00            0.00000E 00
 N2              0.79000E 00            0.18810E 03
 O2              0.21000E 00            0.50000E 02
 SO2             0.00000E 00            0.00000E 00
 S6              0.00000E 00            0.00000E 00
 S8              0.00000E 00            0.00000E 00
 S2              0.00000E 00            0.00000E 00
 SLIQ            0.00000E 00            0.00000E 00
 MOLS            0.10000E 01            0.23810E 03
 TEMP,DEGREES K=             0.31000E 03
 ENTHALPY,BTU/HR=             0.35159E 05
```

```
                 BURNER OUTLET(4)
          MOLE FRAC.                 LB MOLES/HR
H2              0.00000E 00           0.00000E 00
H2S             0.00000E 00           0.00000E 00
H2O             0.13084E 00           0.33333E 02
N2              0.73832E 00           0.18810E 03
O2              0.00000E 00           0.00000E 00
SO2             0.13084E 00           0.33333E 02
S6              0.00000E 00           0.00000E 00
S8              0.00000E 00           0.00000E 00
S2              0.00000E 00           0.00000E 00
SLIQ            0.00000E 00           0.00000E 00
MOLS            0.10000E 01           0.25476E 03
TEMP,DEGREES K=              0.21145E 04
ENTHALPY,BTU/HR=              0.74772E 07


             INLET H2S GAS MIXER 1(5)
          MOLE FRAC.                 LB MOLES/HR
H2              0.00000E 00           0.00000E 00
H2S             0.10000E 01           0.66667E 02
H2O             0.00000E 00           0.00000E 00
N2              0.00000E 00           0.00000E 00
O2              0.00000E 00           0.00000E 00
SO2             0.00000E 00           0.00000E 00
S6              0.00000E 00           0.00000E 00
S8              0.00000E 00           0.00000E 00
S2              0.00000E 00           0.00000E 00
SLIQ            0.00000E 00           0.00000E 00
MOLS            0.10000E 01           0.66667E 02
TEMP,DEGREES K=              0.31000E 03
ENTHALPY,BTU/HR=              0.11598E 05


             SO2 GAS TO MIXER1(6)
          MOLE FRAC.                 LB MOLES/HR
H2              0.00000E 00           0.00000E 00
H2S             0.00000E 00           0.00000E 00
H2O             0.13084E 00           0.33333E 02
N2              0.73832E 00           0.18810E 03
O2              0.00000E 00           0.00000E 00
SO2             0.13084E 00           0.33333E 02
S6              0.00000E 00           0.00000E 00
S8              0.00000E 00           0.00000E 00
S2              0.00000E 00           0.00000E 00
SLIQ            0.00000E 00           0.00000E 00
MOLS            0.10000E 01           0.25476E 03
TEMP,DEGREES K=              0.57997E 03
ENTHALPY,BTU/HR=              0.99878E 06
```

```
                   INLET HEATER 1(7)
         MOLE FRAC.                    LB MOLES/HR
 H2           0.00000E 00               0.00000E 00
 H2S          0.20741E 00               0.66667E 02
 H2O          0.10370E 00               0.33333E 02
 N2           0.58519E 00               0.18810E 03
 O2           0.00000E 00               0.00000E 00
 SO2          0.10370E 00               0.33333E 02
 S6           0.00000E 00               0.00000E 00
 S8           0.00000E 00               0.00000E 00
 S2           0.00000E 00               0.00000E 00
 SLIQ         0.00000E 00               0.00000E 00
 MOLS         0.10000E 01               0.32143E 03
 TEMP,DEGREES K=             0.52082E 03
 ENTHALPY,BTU/HR=             0.10104E 07
```

```
                   INLET REACTOR 1(8)
         MOLE FRAC.                    LB MOLES/HR
 H2           0.00000E 00               0.00000E 00
 H2S          0.20741E 00               0.66667E 02
 H2O          0.10370E 00               0.33333E 02
 N2           0.58519E 00               0.18810E 03
 O2           0.00000E 00               0.00000E 00
 SO2          0.10370E 00               0.33333E 02
 S6           0.00000E 00               0.00000E 00
 S8           0.00000E 00               0.00000E 00
 S2           0.00000E 00               0.00000E 00
 SLIQ         0.00000E 00               0.00000E 00
 MOLS         0.10000E 01               0.32143E 03
 TEMP,DEGREES K=             0.52082E 03
 ENTHALPY,BTU/HR=             0.10104E 07
```

```
                   OUTLET REACTOR 1(9)
         MOLE FRAC.                    LB MOLES/HR
 H2           0.00000E 00               0.00000E 00
 H2S          0.64420E-01               0.20000E 02
 H2O          0.25768E 00               0.80000E 02
 N2           0.60586E 00               0.18810E 03
 O2           0.00000E 00               0.00000E 00
 SO2          0.32210E-01               0.10000E 02
 S6           0.24046E-01               0.74653E 01
 S8           0.80931E-02               0.25126E 01
 S2           0.82451E-02               0.25598E 01
 SLIQ         0.00000E 00               0.00000E 00
 MOLS         0.10000E 01               0.31046E 03
 TEMP,DEGREES K=             0.69926E 03
 ENTHALPY,BTU/HR=             0.18422E 07
```

```
              LIQUID SULFUR COND 1(10)
         MOLE FRAC.                  LB MOLES/HR
H2             0.00000E 00             0.00000E 00
H2S            0.00000E 00             0.00000E 00
H2O            0.00000E 00             0.00000E 00
N2             0.00000E 00             0.00000E 00
O2             0.00000E 00             0.00000E 00
SO2            0.00000E 00             0.00000E 00
S6             0.00000E 00             0.00000E 00
S8             0.00000E 00             0.00000E 00
S2             0.00000E 00             0.00000E 00
SLIQ           0.10000E 01             0.69455E 02
MOLS           0.10000E 01             0.69455E 02
TEMP,DEGREES K=              0.42222E 03
ENTHALPY,BTU/HR=            -0.37988E 06


              OUTLET GAS COND 1(11)
         MOLE FRAC.                  LB MOLES/HR
H2             0.00000E 00             0.00000E 00
H2S            0.67115E-01             0.20000E 02
H2O            0.26846E 00             0.80000E 02
N2             0.63120E 00             0.18810E 03
O2             0.00000E 00             0.00000E 00
SO2            0.33556E-01             0.10000E 02
S6             0.42189E-04             0.12572E-01
S8             0.20233E-03             0.60295E-01
S2             0.29457E-07             0.87780E-05
SLIQ           0.00000E 00             0.00000E 00
MOLS           0.10000E 01             0.29800E 03
TEMP,DEGREES K=              0.42222E 03
ENTHALPY,BTU/HR=              0.49869E 06
```

```
       INPUT DATA
 NO. OF REACTORS=1
       LB MOLES/HR
 H2        0.00
 H2S     100.00
 H2O       0.00
 N2        0.00

       TEMP,DEGREES F
 FEED     98.00
 AIR      98.00

 REACTOR   COND. TEMP.,F   CONVERSION   BYPASS GAS SPLIT
    1          300.00        0.800              1.00

 FLAME TEMP,DEGREES K=2114.47
 WASTE HEAT BOILER Q,BTU/HR=         -0.69870E 07
 HEATER-COOLER 1 Q,BTU/HR=          0.00000E 00
 CONDENSER 1 Q,BTU/HR=          -0.14450E 07
```

```
                   FEED STREAM(1)
        MOLE FRAC.                    LB MOLES/HR
 H2            0.00000E 00             0.00000E 00
 H2S           0.10000E 01             0.10000E 03
 H2O           0.00000E 00             0.00000E 00
 N2            0.00000E 00             0.00000E 00
 O2            0.00000E 00             0.00000E 00
 SO2           0.00000E 00             0.00000E 00
 S6            0.00000E 00             0.00000E 00
 S8            0.00000E 00             0.00000E 00
 S2            0.00000E 00             0.00000E 00
 SLIQ          0.00000E 00             0.00000E 00
 MOLS          0.10000E 01             0.10000E 03
 TEMP,DEGREES K=              0.31000E 03
 ENTHALPY,BTU/HR=              0.17398E 05

                  BURNER H2S GAS(2)
        MOLE FRAC.                    LB MOLES/HR
 H2            0.00000E 00             0.00000E 00
 H2S           0.10000E 01             0.33333E 02
 H2O           0.00000E 00             0.00000E 00
 N2            0.00000E 00             0.00000E 00
 O2            0.00000E 00             0.00000E 00
 SO2           0.00000E 00             0.00000E 00
 S6            0.00000E 00             0.00000E 00
 S8            0.00000E 00             0.00000E 00
 S2            0.00000E 00             0.00000E 00
 SLIQ          0.00000E 00             0.00000E 00
 MOLS          0.10000E 01             0.33333E 02
 TEMP,DEGREES K=              0.31000E 03
 ENTHALPY,BTU/HR=              0.57992E 04

                   BURNER AIR(3)
        MOLE FRAC.                    LB MOLES/HR
 H2            0.00000E 00             0.00000E 00
 H2S           0.00000E 00             0.00000E 00
 H2O           0.00000E 00             0.00000E 00
 N2            0.79000E 00             0.18810E 03
 O2            0.21000E 00             0.50000E 02
 SO2           0.00000E 00             0.00000E 00
 S6            0.00000E 00             0.00000E 00
 S8            0.00000E 00             0.00000E 00
 S2            0.00000E 00             0.00000E 00
 SLIQ          0.00000E 00             0.00000E 00
 MOLS          0.10000E 01             0.23810E 03
 TEMP,DEGREES K=              0.31000E 03
 ENTHALPY,BTU/HR=              0.35159E 05
```

```
                    BURNER OUTLET(4)
          MOLE FRAC.                      LB MOLES/HR
 H2             0.00000E 00                0.00000E 00
 H2S            0.00000E 00                0.00000E 00
 H2O            0.13084E 00                0.33333E 02
 N2             0.73832E 00                0.18810E 03
 O2             0.00000E 00                0.00000E 00
 SO2            0.13084E 00                0.33333E 02
 S6             0.00000E 00                0.00000E 00
 S8             0.00000E 00                0.00000E 00
 S2             0.00000E 00                0.00000E 00
 SLIQ           0.00000E 00                0.00000E 00
 MOLS           0.10000E 01                0.25476E 03
 TEMP,DEGREES K=                 0.21145E 04
 ENTHALPY,BTU/HR=                 0.74772E 07


                INLET H2S GAS MIXER 1(5)
          MOLE FRAC.                      LB MOLES/HR
 H2             0.00000E 00                0.00000E 00
 H2S            0.10000E 01                0.66667E 02
 H2O            0.00000E 00                0.00000E 00
 N2             0.00000E 00                0.00000E 00
 O2             0.00000E 00                0.00000E 00
 SO2            0.00000E 00                0.00000E 00
 S6             0.00000E 00                0.00000E 00
 S8             0.00000E 00                0.00000E 00
 S2             0.00000E 00                0.00000E 00
 SLIQ           0.00000E 00                0.00000E 00
 MOLS           0.10000E 01                0.66667E 02
 TEMP,DEGREES K=                 0.31000E 03
 ENTHALPY,BTU/HR=                 0.11598E 05


                SO2 GAS TO MIXER1(6)
          MOLE FRAC.                      LB MOLES/HR
 H2             0.00000E 00                0.00000E 00
 H2S            0.00000E 00                0.00000E 00
 H2O            0.13084E 00                0.33333E 02
 N2             0.73832E 00                0.18810E 03
 O2             0.00000E 00                0.00000E 00
 SO2            0.13084E 00                0.33333E 02
 S6             0.00000E 00                0.00000E 00
 S8             0.00000E 00                0.00000E 00
 S2             0.00000E 00                0.00000E 00
 SLIQ           0.00000E 00                0.00000E 00
 MOLS           0.10000E 01                0.25476E 03
 TEMP,DEGREES K=                 0.43922E 03
 ENTHALPY,BTU/HR=                 0.49019E 06
```

```
                    INLET HEATER 1(7)
          MOLE FRAC.                    LB MOLES/HR
 H2             0.00000E 00              0.00000E 00
 H2S            0.20741E 00              0.66667E 02
 H2O            0.10370E 00              0.33333E 02
 N2             0.58519E 00              0.18810E 03
 O2             0.00000E 00              0.00000E 00
 SO2            0.10370E 00              0.33333E 02
 S6             0.00000E 00              0.00000E 00
 S8             0.00000E 00              0.00000E 00
 S2             0.00000E 00              0.00000E 00
 SLIQ           0.00000E 00              0.00000E 00
 MOLS           0.10000E 01              0.32143E 03
 TEMP,DEGREES K=             0.41071E 03
 ENTHALPY,BTU/HR=             0.50179E 06


                    INLET REACTOR 1(8)
          MOLE FRAC.                    LB MOLES/HR
 H2             0.00000E 00              0.00000E 00
 H2S            0.20741E 00              0.66667E 02
 H2O            0.10370E 00              0.33333E 02
 N2             0.58519E 00              0.18810E 03
 O2             0.00000E 00              0.00000E 00
 SO2            0.10370E 00              0.33333E 02
 S6             0.00000E 00              0.00000E 00
 S8             0.00000E 00              0.00000E 00
 S2             0.00000E 00              0.00000E 00
 SLIQ           0.00000E 00              0.00000E 00
 MOLS           0.10000E 01              0.32143E 03
 TEMP,DEGREES K=             0.41071E 03
 ENTHALPY,BTU/HR=             0.50179E 06


                   OUTLET REACTOR 1(9)
          MOLE FRAC.                    LB MOLES/HR
 H2             0.00000E 00              0.00000E 00
 H2S            0.43437E-01              0.13333E 02
 H2O            0.28234E 00              0.86667E 02
 N2             0.61277E 00              0.18810E 03
 O2             0.00000E 00              0.00000E 00
 SO2            0.21718E-01              0.66667E 01
 S6             0.23297E-01              0.71513E 01
 S8             0.14610E-01              0.44847E 01
 S2             0.20488E-02              0.62889E 00
 SLIQ           0.00000E 00              0.00000E 00
 MOLS           0.10000E 01              0.30696E 03
 TEMP,DEGREES K=             0.64373E 03
 ENTHALPY,BTU/HR=             0.15719E 07
```

```
                 LIQUID SULFUR COND 1(10)
             MOLE FRAC.                    LB MOLES/HR
 H2                0.00000E 00               0.00000E 00
 H2S               0.00000E 00               0.00000E 00
 H2O               0.00000E 00               0.00000E 00
 N2                0.00000E 00               0.00000E 00
 O2                0.00000E 00               0.00000E 00
 SO2               0.00000E 00               0.00000E 00
 S6                0.00000E 00               0.00000E 00
 S8                0.00000E 00               0.00000E 00
 S2                0.00000E 00               0.00000E 00
 SLIQ              0.10000E 01               0.79492E 02
 MOLS              0.10000E 01               0.79492E 02
 TEMP,DEGREES K=                 0.42222E 03
 ENTHALPY,BTU/HR=               -0.36376E 06


                   OUTLET GAS COND 1(11)
             MOLE FRAC.                    LB MOLES/HR
 H2                0.00000E 00               0.00000E 00
 H2S               0.45234E-01               0.13333E 02
 H2O               0.29402E 00               0.86667E 02
 N2                0.63812E 00               0.18810E 03
 O2                0.00000E 00               0.00000E 00
 SO2               0.22617E-01               0.66667E 01
 S6                0.42189E-04               0.12436E-01
 S8                0.20233E-03               0.59641E-01
 S2                0.29457E-07               0.86828E-05
 SLIQ              0.00000E 00               0.00000E 00
 MOLS              0.10000E 01               0.29477E 03
 TEMP,DEGREES K=                 0.42222E 03
 ENTHALPY,BTU/HR=                 0.49069E 06
```

```
      INPUT DATA
NO. OF REACTORS=1
      LB MOLES/HR
H2         0.00
H2S      100.00
H2O        0.00
N2         0.00

      TEMP,DEGREES F
FEED      98.00
AIR       98.00

REACTOR   COND. TEMP.,F   CONVERSION   BYPASS GAS SPLIT
   1          300.00         0.900               1.00

FLAME TEMP,DEGREES K=2114.47
CALC FOR REACTOR1 INLET STREAM DOES NOT CONVERGE
WASTE HEAT BOILER Q,BTU/HR=           -0.72200E 07
HEATER-COOLER 1 Q,BTU/HR=           0.00000E 00
CONDENSER 1 Q,BTU/HR=           -0.11265E 07
```

```
                    FEED STREAM(1)
          MOLE FRAC.                LB MOLES/HR
 H2               0.00000E 00          0.00000E 00
 H2S              0.10000E 01          0.10000E 03
 H2O              0.00000E 00          0.00000E 00
 N2               0.00000E 00          0.00000E 00
 O2               0.00000E 00          0.00000E 00
 SO2              0.00000E 00          0.00000E 00
 S6               0.00000E 00          0.00000E 00
 S8               0.00000E 00          0.00000E 00
 S2               0.00000E 00          0.00000E 00
 SLIQ             0.00000E 00          0.00000E 00
 MOLS             0.10000E 01          0.10000E 03
 TEMP,DEGREES K=             0.31000E 03
 ENTHALPY,BTU/HR=             0.17398E 05


                  BURNER H2S GAS(2)
          MOLE FRAC.                LB MOLES/HR
 H2               0.00000E 00          0.00000E 00
 H2S              0.10000E 01          0.33333E 02
 H2O              0.00000E 00          0.00000E 00
 N2               0.00000E 00          0.00000E 00
 O2               0.00000E 00          0.00000E 00
 SO2              0.00000E 00          0.00000E 00
 S6               0.00000E 00          0.00000E 00
 S8               0.00000E 00          0.00000E 00
 S2               0.00000E 00          0.00000E 00
 SLIQ             0.00000E 00          0.00000E 00
 MOLS             0.10000E 01          0.33333E 02
 TEMP,DEGREES K=             0.31000E 03
 ENTHALPY,BTU/HR=             0.57992E 04


                    BURNER AIR(3)
          MOLE FRAC.                LB MOLES/HR
 H2               0.00000E 00          0.00000E 00
 H2S              0.00000E 00          0.00000E 00
 H2O              0.00000E 00          0.00000E 00
 N2               0.79000E 00          0.18810E 03
 O2               0.21000E 00          0.50000E 02
 SO2              0.00000E 00          0.00000E 00
 S6               0.00000E 00          0.00000E 00
 S8               0.00000E 00          0.00000E 00
 S2               0.00000E 00          0.00000E 00
 SLIQ             0.00000E 00          0.00000E 00
 MOLS             0.10000E 01          0.23810E 03
 TEMP,DEGREES K=             0.31000E 03
 ENTHALPY,BTU/HR=             0.35159E 05
```

```
                    BURNER OUTLET(4)
           MOLE FRAC.                    LB MOLES/HR
H2            0.00000E 00               0.00000E 00
H2S           0.00000E 00               0.00000E 00
H2O           0.13084E 00               0.33333E 02
N2            0.73832E 00               0.18810E 03
O2            0.00000E 00               0.00000E 00
SO2           0.13084E 00               0.33333E 02
S6            0.00000E 00               0.00000E 00
S8            0.00000E 00               0.00000E 00
S2            0.00000E 00               0.00000E 00
SLIQ          0.00000E 00               0.00000E 00
MOLS          0.10000E 01               0.25476E 03
TEMP,DEGREES K=               0.21145E 04
ENTHALPY,BTU/HR=               0.74772E 07


                INLET H2S GAS MIXER 1(5)
           MOLE FRAC.                    LB MOLES/HR
H2            0.00000E 00               0.00000E 00
H2S           0.10000E 01               0.66667E 02
H2O           0.00000E 00               0.00000E 00
N2            0.00000E 00               0.00000E 00
O2            0.00000E 00               0.00000E 00
SO2           0.00000E 00               0.00000E 00
S6            0.00000E 00               0.00000E 00
S8            0.00000E 00               0.00000E 00
S2            0.00000E 00               0.00000E 00
SLIQ          0.00000E 00               0.00000E 00
MOLS          0.10000E 01               0.66667E 02
TEMP,DEGREES K=               0.31000E 03
ENTHALPY,BTU/HR=               0.11598E 05


                SO2 GAS TO MIXER1(6)
           MOLE FRAC.                    LB MOLES/HR
H2            0.00000E 00               0.00000E 00
H2S           0.00000E 00               0.00000E 00
H2O           0.13084E 00               0.33333E 02
N2            0.73832E 00               0.18810E 03
O2            0.00000E 00               0.00000E 00
SO2           0.13084E 00               0.33333E 02
S6            0.00000E 00               0.00000E 00
S8            0.00000E 00               0.00000E 00
S2            0.00000E 00               0.00000E 00
SLIQ          0.00000E 00               0.00000E 00
MOLS          0.10000E 01               0.25476E 03
TEMP,DEGREES K=               0.37300E 03
ENTHALPY,BTU/HR=               0.25721E 06
```

```
                   INLET HEATER 1(7)
          MOLE FRAC.                    LB MOLES/HR
 H2            0.00000E 00               0.00000E 00
 H2S           0.20741E 00               0.66667E 02
 H2O           0.10370E 00               0.33333E 02
 N2            0.58519E 00               0.18810E 03
 O2            0.00000E 00               0.00000E 00
 SO2           0.10370E 00               0.33333E 02
 S6            0.00000E 00               0.00000E 00
 S8            0.00000E 00               0.00000E 00
 S2            0.00000E 00               0.00000E 00
 SLIQ          0.00000E 00               0.00000E 00
 MOLS          0.10000E 01               0.32143E 03
 TEMP,DEGREES K=                0.35902E 03
 ENTHALPY,BTU/HR=                0.26880E 06


                   INLET REACTOR 1(8)
          MOLE FRAC.                    LB MOLES/HR
 H2            0.00000E 00               0.00000E 00
 H2S           0.20741E 00               0.66667E 02
 H2O           0.10370E 00               0.33333E 02
 N2            0.58519E 00               0.18810E 03
 O2            0.00000E 00               0.00000E 00
 SO2           0.10370E 00               0.33333E 02
 S6            0.00000E 00               0.00000E 00
 S8            0.00000E 00               0.00000E 00
 S2            0.00000E 00               0.00000E 00
 SLIQ          0.00000E 00               0.00000E 00
 MOLS          0.10000E 01               0.32143E 03
 TEMP,DEGREES K=                0.29800E 03
 ENTHALPY,BTU/HR=               -0.67534E 03


                  OUTLET REACTOR 1(9)
          MOLE FRAC.                    LB MOLES/HR
 H2            0.00000E 00               0.00000E 00
 H2S           0.21921E-01               0.66667E 01
 H2O           0.30690E 00               0.93333E 02
 N2            0.61850E 00               0.18810E 03
 O2            0.00000E 00               0.00000E 00
 SO2           0.10961E-01               0.33333E 01
 S6            0.16649E-01               0.50632E 01
 S8            0.24486E-01               0.74467E 01
 S2            0.22286E-03               0.67777E-01
 SLIQ          0.00000E 00               0.00000E 00
 MOLS          0.10000E 01               0.30412E 03
 TEMP,DEGREES K=                0.57398E 03
 ENTHALPY,BTU/HR=                0.12415E 07
```

```
                 LIQUID SULFUR COND 1(10)
            MOLE FRAC.                    LB MOLES/HR
 H2               0.00000E 00               0.00000E 00
 H2S              0.00000E 00               0.00000E 00
 H2O              0.00000E 00               0.00000E 00
 N2               0.00000E 00               0.00000E 00
 O2               0.00000E 00               0.00000E 00
 SO2              0.00000E 00               0.00000E 00
 S6               0.00000E 00               0.00000E 00
 S8               0.00000E 00               0.00000E 00
 S2               0.00000E 00               0.00000E 00
 SLIQ             0.10000E 01               0.89543E 02
 MOLS             0.10000E 01               0.89543E 02
 TEMP,DEGREES K=               0.42222E 03
 ENTHALPY,BTU/HR=             -0.36769E 06

                  OUTLET GAS COND 1(11)
            MOLE FRAC.                    LB MOLES/HR
 H2               0.00000E 00               0.00000E 00
 H2S              0.22862E-01               0.66667E 01
 H2O              0.32006E 00               0.93333E 02
 N2               0.64502E 00               0.18810E 03
 O2               0.00000E 00               0.00000E 00
 SO2              0.11431E-01               0.33333E 01
 S6               0.42189E-04               0.12303E-01
 S8               0.20233E-03               0.59003E-01
 S2               0.29457E-07               0.85899E-05
 SLIQ             0.00000E 00               0.00000E 00
 MOLS             0.10000E 01               0.29161E 03
 TEMP,DEGREES K=               0.42222E 03
 ENTHALPY,BTU/HR=               0.48269E 06
```

```
       INPUT DATA
  NO. OF REACTORS=1
       LB MOLES/HR
  H2          0.00
  H2S       100.00
  H2O         0.00
  N2          0.00

       TEMP,DEGREES F
  FEED     98.00
  AIR      98.00

  REACTOR    COND. TEMP.,F    CONVERSION    BYPASS GAS SPLIT
     1           300.00         0.950               1.00

  FLAME TEMP,DEGREES K=2114.47
  CALC FOR REACTOR1 INLET STREAM DOES NOT CONVERGE
  SPECIFIED CONVERSION IN REACTOR 1 OCCURS BELOW DEW
  POINT. CONVERSION REDUCED TO  0.920
  WASTE HEAT BOILER Q,BTU/HR=           -0.72200E 07
  HEATER-COOLER 1 Q,BTU/HR=           0.00000E 00
  CONDENSER 1 Q,BTU/HR=          -0.10416E 07
```

```
                         FEED STREAM(1)
          MOLE FRAC.                    LB MOLES/HR
H2              0.00000E 00               0.00000E 00
H2S             0.10000E 01               0.10000E 03
H2O             0.00000E 00               0.00000E 00
N2              0.00000E 00               0.00000E 00
O2              0.00000E 00               0.00000E 00
SO2             0.00000E 00               0.00000E 00
S6              0.00000E 00               0.00000E 00
S8              0.00000E 00               0.00000E 00
S2              0.00000E 00               0.00000E 00
SLIQ            0.00000E 00               0.00000E 00
MOLS            0.10000E 01               0.10000E 03
TEMP,DEGREES K=              0.31000E 03
ENTHALPY,BTU/HR=              0.17398E 05
```

```
                       BURNER H2S GAS(2)
          MOLE FRAC.                    LB MOLES/HR
H2              0.00000E 00               0.00000E 00
H2S             0.10000E 01               0.33333E 02
H2O             0.00000E 00               0.00000E 00
N2              0.00000E 00               0.00000E 00
O2              0.00000E 00               0.00000E 00
SO2             0.00000E 00               0.00000E 00
S6              0.00000E 00               0.00000E 00
S8              0.00000E 00               0.00000E 00
S2              0.00000E 00               0.00000E 00
SLIQ            0.00000E 00               0.00000E 00
MOLS            0.10000E 01               0.33333E 02
TEMP,DEGREES K=              0.31000E 03
ENTHALPY,BTU/HR=              0.57992E 04
```

```
                         BURNER AIR(3)
          MOLE FRAC.                    LB MOLES/HR
H2              0.00000E 00               0.00000E 00
H2S             0.00000E 00               0.00000E 00
H2O             0.00000E 00               0.00000E 00
N2              0.79000E 00               0.18810E 03
O2              0.21000E 00               0.50000E 02
SO2             0.00000E 00               0.00000E 00
S6              0.00000E 00               0.00000E 00
S8              0.00000E 00               0.00000E 00
S2              0.00000E 00               0.00000E 00
SLIQ            0.00000E 00               0.00000E 00
MOLS            0.10000E 01               0.23810E 03
TEMP,DEGREES K=              0.31000E 03
ENTHALPY,BTU/HR=              0.35159E 05
```

```
                    BURNER OUTLET(4)
         MOLE FRAC.                    LB MOLES/HR
 H2             0.00000E 00             0.00000E 00
 H2S            0.00000E 00             0.00000E 00
 H2O            0.13084E 00             0.33333E 02
 N2             0.73832E 00             0.18810E 03
 O2             0.00000E 00             0.00000E 00
 SO2            0.13084E 00             0.33333E 02
 S6             0.00000E 00             0.00000E 00
 S8             0.00000E 00             0.00000E 00
 S2             0.00000E 00             0.00000E 00
 SLIQ           0.00000E 00             0.00000E 00
 MOLS           0.10000E 01             0.25476E 03
 TEMP,DEGREES K=              0.21145E 04
 ENTHALPY,BTU/HR=              0.74772E 07


                 INLET H2S GAS MIXER 1(5)
         MOLE FRAC.                    LB MOLES/HR
 H2             0.00000E 00             0.00000E 00
 H2S            0.10000E 01             0.66667E 02
 H2O            0.00000E 00             0.00000E 00
 N2             0.00000E 00             0.00000E 00
 O2             0.00000E 00             0.00000E 00
 SO2            0.00000E 00             0.00000E 00
 S6             0.00000E 00             0.00000E 00
 S8             0.00000E 00             0.00000E 00
 S2             0.00000E 00             0.00000E 00
 SLIQ           0.00000E 00             0.00000E 00
 MOLS           0.10000E 01             0.66667E 02
 TEMP,DEGREES K=              0.31000E 03
 ENTHALPY,BTU/HR=              0.11598E 05


                 SO2 GAS TO MIXER1(6)
         MOLE FRAC.                    LB MOLES/HR
 H2             0.00000E 00             0.00000E 00
 H2S            0.00000E 00             0.00000E 00
 H2O            0.13084E 00             0.33333E 02
 N2             0.73832E 00             0.18810E 03
 O2             0.00000E 00             0.00000E 00
 SO2            0.13084E 00             0.33333E 02
 S6             0.00000E 00             0.00000E 00
 S8             0.00000E 00             0.00000E 00
 S2             0.00000E 00             0.00000E 00
 SLIQ           0.00000E 00             0.00000E 00
 MOLS           0.10000E 01             0.25476E 03
 TEMP,DEGREES K=              0.37300E 03
 ENTHALPY,BTU/HR=              0.25721E 06
```

```
                    INLET HEATER 1(7)
             MOLE FRAC.                  LB MOLES/HR
H2                 0.00000E 00             0.00000E 00
H2S                0.20741E 00             0.66667E 02
H2O                0.10370E 00             0.33333E 02
N2                 0.58519E 00             0.18810E 03
O2                 0.00000E 00             0.00000E 00
SO2                0.10370E 00             0.33333E 02
S6                 0.00000E 00             0.00000E 00
S8                 0.00000E 00             0.00000E 00
S2                 0.00000E 00             0.00000E 00
SLIQ               0.00000E 00             0.00000E 00
MOLS               0.10000E 01             0.32143E 03
TEMP,DEGREES K=               0.35902E 03
ENTHALPY,BTU/HR=               0.25860E 06
```

```
                    INLET REACTOR 1(8)
             MOLE FRAC.                  LB MOLES/HR
H2                 0.00000E 00             0.00000E 00
H2S                0.20741E 00             0.66667E 02
H2O                0.10370E 00             0.33333E 02
N2                 0.58519E 00             0.18810E 03
O2                 0.00000E 00             0.00000E 00
SO2                0.10370E 00             0.33333E 02
S6                 0.00000E 00             0.00000E 00
S8                 0.00000E 00             0.00000E 00
S2                 0.00000E 00             0.00000E 00
SLIQ               0.00000E 00             0.00000E 00
MOLS               0.10000E 01             0.32143E 03
TEMP,DEGREES K=               0.29800E 03
ENTHALPY,BTU/HR=              -0.67534E 03
```

```
                   OUTLET REACTOR 1(9)
             MOLE FRAC.                  LB MOLES/HR
H2                 0.00000E 00             0.00000E 00
H2S                0.17567E-01             0.53333E 01
H2O                0.31181E 00             0.94667E 02
N2                 0.61954E 00             0.18810E 03
O2                 0.00000E 00             0.00000E 00
SO2                0.87834E-02             0.26667E 01
S6                 0.14375E-01             0.43644E 01
S8                 0.27052E-01             0.82130E 01
S2                 0.11130E-03             0.33792E-01
SLIQ               0.00000E 00             0.00000E 00
MOLS               0.10000E 01             0.30361E 03
TEMP,DEGREES K=               0.55549E 03
ENTHALPY,BTU/HR=               0.11551E 07
```

```
              LIQUID SULFUR COND 1(10)
          MOLE FRAC.                    LB MOLES/HR
 H2              0.00000E 00               0.00000E 00
 H2S             0.00000E 00               0.00000E 00
 H2O             0.00000E 00               0.00000E 00
 N2              0.00000E 00               0.00000E 00
 O2              0.00000E 00               0.00000E 00
 SO2             0.00000E 00               0.00000E 00
 S6              0.00000E 00               0.00000E 00
 S8              0.00000E 00               0.00000E 00
 S2              0.00000E 00               0.00000E 00
 SLIQ            0.10000E 01               0.91413E 02
 MOLS            0.10000E 01               0.91413E 02
 TEMP,DEGREES K=              0.42222E 03
 ENTHALPY,BTU/HR=            -0.36757E 06


                OUTLET GAS COND 1(11)
          MOLE FRAC.                    LB MOLES/HR
 H2              0.00000E 00               0.00000E 00
 H2S             0.18324E-01               0.53333E 01
 H2O             0.32524E 00               0.94667E 02
 N2              0.64623E 00               0.18810E 03
 O2              0.00000E 00               0.00000E 00
 SO2             0.91618E-02               0.26667E 01
 S6              0.42189E-04               0.12280E-01
 S8              0.20233E-03               0.56892E-01
 S2              0.29457E-07               0.85739E-05
 SLIQ            0.00000E 00               0.00000E 00
 MOLS            0.10000E 01               0.29107E 03
 TEMP,DEGREES K=              0.42222E 03
 ENTHALPY,BTU/HR=             0.48110E 06
```

REFERENCES

1. Boas, A. H. and R. C. Andrade, "Simulate Sulfur Recovery Plants," Hydrocarbon Processing, Vol. 50, March, 1971, pp. 81-84.

2. Braune, H., S. Peter and V. Neveling, "Die Dissoziation des Schwefeldampfes," Naturforschg, Vol. 62, 1951, pp. 32-37.

3. Gamson, B. W. and R. H. Elkins, "Sulfur from Hydrogen Sulfide," Chemical Engineering Progress, Vol. 49, No. 4, April, 1953, pp. 203-215.

4. Grekel, H., L. V. Kunkel and R. McGalliard, "Package Plants for Sulfur Recovery," Chemical Engineering Progress, Vol. 61, No. 9, September, 1965, pp. 70-73.

5. Hays, H. L. and F. T. Barber, "Sulfur Recovery from H_2S," The Oil and Gas Journal, April 26, 1954, pp. 218-222.

6. Hougen, Olaf A., Kenneth M. Watson and Roland A. Ragatz, Chemical Process Principles Part I. Second Edition. New York: John Wiley & Sons, Inc., London: Chapman & Hall, Ltd., 1959, pp. 78-79, 345-355.

7. Hougen, Olaf A., Kenneth M. Watson and Roland A. Ragatz, Chemical Process Principles Part II, Second Edition. New York, London, Sydney: John Wiley & Sons, Inc., 1966, pp. 982-988, 1015-1026.

8. Kelley, K. K., "Contributions to the Data on Theoretical Metallurgy," U.S. Bureau of Mines Bulletin 406, 1937, pp. 1-23, 99-100.

9. Moses, H., G. H. Strom and J. E. Carson, "Effects of Meteorological and Engineering Factors on Stack Plume Rise," Nuclear Safety, Vol. 6, No. 1, Fall, 1964, pp. 1-19.

10. Oliver, R. C., S. E. Stephanou and R. W. Baier, "Calculating Free Energy Minimization," Chemical Engineering, February 19, 1962, pp. 121-128.

11. Opekar, P. C. and G. B. Goar, "The Computer Optimizes Sulfur Plant Design and Operation," Hydrocarbon Processing, Vol. 45, No. 6, June, 1966, pp. 181-185.

REFERENCES

12. Parker, J. L., "Sulfur From H_2S," The Oil and Gas Journal, Vol. 50, March 31, 1952, pp. 84-85, 95-97.

13. Perry's Chemical Engineers' Handbook, Robert H. Perry, Cecil H. Chilton, and Sidney D. Kirkpatrick (eds.), Fourth Edition. New York, Toronto, London: McGraw-Hill Book Company, Inc., 1963, pp. (3-134)-(3-141).

14. Preuner, G. and W. Schupp, "Dissociationsisothermen des Schwefels zwischen 300 and 850°," Z. Physik-Chem., Vol. 68, July 20, 1909, pp. 129-156.

15. Sawyer, F. G., R. N. Hader, I. K. Herndon and E. Morningstar, "Sulfur from Sour Gases," Industrial and Engineering Chemistry, Vol. 42, No. 10, October, 1950, pp. 1938-1950.

16. Smith, J. M. and H. C. Van Ness, Introduction to Chemical Engineering Thermodynamics, Second Edition. New York, Toronto, London: McGraw-Hill Book Company, Inc., 1959, pp. 138-139, 404-433.

17. Stull, D. R., "Thermodynamics of Carbon Disulfide Production," Industrial and Engineering Chemistry, Vol. 41, No. 9, September, 1949, pp. 1968-1973.

18. Valdes, A. R., "New Look at Sulfur Plants," Hydrocarbon Processing and Petroleum Refiner, Vol. 43, No. 3, March, 1964, pp. 104-108.

19. Webb, M., "Production of Sulfur from Hydrogen Sulfide," The Oil and Gas Journal, January 11, 1951, pp. 71-72.

20. West, James R., "Thermodynamic Properties of Sulfur," Industrial and Engineering Chemistry, Vol. 42, No. 4, April, 1950, pp. 713-718.

21. West, W. A. and A. W. C. Menzies, "The Vapor Pressures of Sulfur Between 100° and 550° with Related Thermal Data," Journal of Physical Chemistry, Vol. 33, December, 1929, pp. 1880-1892.

22. White, W. B., S. M. Johnson and G. B. Dantzig, "Chemical Equilibrium in Complex Mixtures," The Journal of Chemical Physics, Vol. 28, No. 5, May, 1958, pp. 751-755.

REFERENCES

23. Zelenik, F. J. and S. Gordon, "Calculation of Complex Chemical Equilibria," *Industrial and Engineering Chemistry*, Vol. 60, No. 6, June, 1968, pp. 28-57.

24. Zurcher, P., "Sulfur from Industrial Gases," *Petroleum Processing*, Vol. 7, March, 1952, pp. 333-338.