SIMULATION OF ALKANOLAMINE SWEETENING PROCESSES

BY

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SWEETENING PROCESSES

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PREFACE

This research is directed toward the development of a reliable, dependable and accurate calculation procedure for alkanolamine sweetening. A convergence algorithm has been developed. A simulation program, based on the algorithm along with reliable data and equilibrium calculation models has been written and tested. Major equipment of amine processes and commonly used amines are included to provide the process and design engineer a powerful tool for evaluation of alkanolamine processes.

I with to express my sincere gratitude and deep appreciation to my major adviser, Dr. Robert N. Maddox. His concern, help and intelligent guidance are the most cheerful and memorable part throughout my graduate work.

My sincere thanks are due to the committee members, Dr. Gary L. Foutch, Dr. Arland H. Johannes, Dr. Faye C. McQuiston, and the late Dr. John H. Erbar for their advisement in the course of this work.

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INTRODUCTION

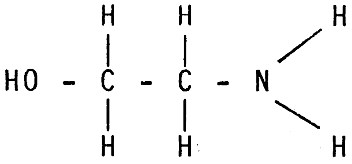
Industrial Requirements

Industrial processes for the removal of hydrogen sulfide and carbon dioxide from sour gas streams have been in use for a long time. Hydrogen sulfide and carbon dioxide are frequently present in natural gas, refinery gas, and synthesis gas. Their removal is of concern environmentally and economically. Because of the toxicity of H_2S, the lack of heating value of CO_2, and the corrosiveness of H_2S and/or CO_2 in the presence of water, sales gas is required to be sweetened to contain no more than one quarter grain of H_2S per one hundred standard cubic feet of gas. This is equivalent to four parts per million on a gas volume basis. The heating value is required to be no less than 920 to 980 BTU per standard cubic feet of gas, depending on the contract (13). The most widely used processes to sweeten gas streams are those using alkanolamines as a reactive solvent.

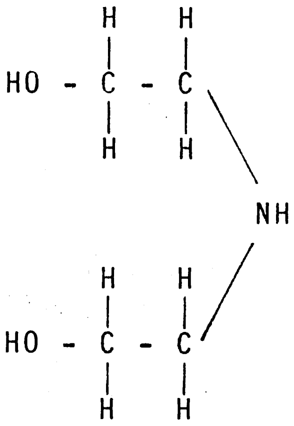
Amines of Commercial Interest

Credit for the first process using aqueous alkanolamine goes to R. R. Bottoms, who was granted a patent in 1930 for natural gas sweetening application. Triethanolamine (TEA) was the first commercially applied, but it has been displaced because of its low reactivity as a tertiary amine and its low capacity because of high equivalent weight. The amines covered in this research are monoethanolamine (MEA), diethanolamine (DEA), diglycolamine (DGA), diisopropanolamine (DIPA), and methyldiethanolamine (MDEA). The chemical formulas of these alkanolamines are shown in Figure 1. The physical and thermodynamic properties of the alkanolamines are presented in Appendix A. The commercial application of these amines is discussed briefly.

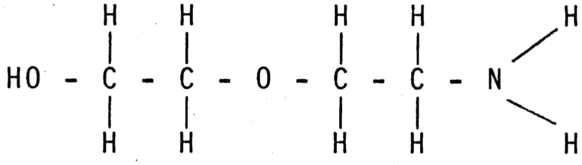
Monoethanolamine, as a primary amine, reacts most rapidly with acid gas to remove both hydrogen sulfide and carbon dioxide. The rate of CO_2 reaction in MEA is slower than that of H_2S (40). However, the process is not considered selective, because the carbon dioxide is readily absorbed and will be removed completely when sweetening natural gas to sweet gas specification. The irreversible reaction products with COS and CS_2 result in chemical losses and solid build-up in MEA solution. The higher vapor pressure of MEA than other amines causes greater solution losses through vaporization. The low molecular weight of monoethanolamine results in high solution carrying capacity for acid gases on a weight basis. MEA is chemically stable and relatively easy to regenerate by steam stripping. The MEA solutions are appreciably more corrosive than other



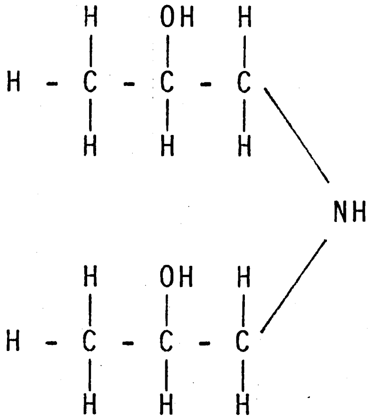
Monoethanolamine



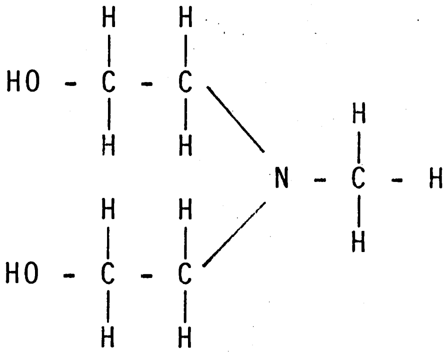
Diethanolamine



Diglycolamine



Diisopropanolamine



Methyldiethanolamine

Figure 1. Chemical Structural Formulas for Alkanolamines Covered in This Research

amine solutions, especially when MEA concentrations exceed 20 weight percent and the solution loaded with acid gases (36). This feature limits the application of MEA solution in case of higher partial pressures of the acid gases permitting higher loadings. Monoethanolamine is still the preferred amine for gases treated at low pressure, relatively low composition of H_2S and CO_2, and no COS and CS_2 contaminants along with maximum removal of H_2S and CO_2 required.

The reactions of DEA with COS and CS_2 result in different products than those from the irreversible chemical reactions between MEA and these components. Unlike MEA units, a large part of the COS and CS_2 is hydrolyzed or absorbed and will be released in the flash gas and acid gas (60). High removal of COS and CS_2 can be attained with DEA without high solution losses through chemical degradation (18). Diethanolamine solutions are not particularly corrosive (60) and are a better choice for the treatment of refinery and manufactured gases which normally contain appreciable amounts of COS and CS_2. The low vapor pressure of DEA and its reversible reactions with COS and CS_2 cause negligible chemical loss. Aqueous solutions of diethanolamine normally have much lower concentrations of residual acid gases than those of MEA solutions after steam stripping. The S.N.P.A.-DEA process developed by Societe Nationale des Petroles d'Aquitaine of France is applicable for sweetening of high pressure gases with high concentrations of acid gases and appreciable amounts of COS and CS_2 present (18, 59). The aqueous DEA solution used is 20 to 30 weight percent with high carrying capacity of acid gases up to 1.0 to 1.3 mole of DEA per mole of acid gases (60). An S.N.P.A.-DEA treating has smaller size major equipment owing to the reduced solution circulation rate because of the high acid gas carrying capacity of the solution.

Diglycolamine is the trade name of 2-(2-aminoethoxy)-ethanol. The process is proprietary and has been named the Fluor Econamine process. DGA is a primary amine reacting non-selectively with acid gases in much the same way as MEA. It has a relatively low vapor pressure which permits its use in relatively high concentrations, typically 40 to 60 weight percent (12, 36). This feature results in lower circulation rate and lower steam consumption when compared to monoethanolamine solution. DGA reacts reversibly with carbonyl sulfide, carbon disulfide and carbon dioxide to form urea type degradation products (27,28). These degradation products are thermally regenerated at elevated temperatures and regenerator pressures. DGA generally is non-corrosive to carbon steel and has little tendency to foam. Aqueous solutions are comparable to ethylene glycol in freezing point, viscosity, and dew point depression of natural gas (12). It is thermally stable at temperatures in excess of 400°F and is suitable for use in the Arctic as well as hot desert areas short of cooling water (11, 12).

In Saudi Arabia, DGA is successfully treating large amounts of low pressure, about 150 psia, associated gas to 0.25 grain pipeline specification (27, 28).

Diisopropanolamine is the reactive solvent used in the ADIP process (33) and the Sulfinol process (36). It is used together with a physical organic solvent in the Sulfinol process. In the ADIP process, the use of 30 to 40 weight percent aqueous solutions of diisopropanolamine has been reported (22). Aqueous DIPA solutions are reported to have a low heat requirement for regeneration and to be non-corrosive (33). Of the secondary amines, DIPA reacts with COS to form thiocarbonates which can be regenerated under normal process conditions (33). Furthermore, DIPA will yield somewhat better selectivity toward H_2S than the other primary or secondary amines due to steric hindrance or partial blockage by the amine molecule itself of its reactive sites reducing carbamate reaction (54).

Methyldiethanolamine is most commonly used in 30 to 50 weight percent concentration range without appreciable evaporation losses because of its low vapor pressure. MDEA also is highly resistant to thermal and chemical degradation and is non-corrosive (36). As a tertiary amine, MDEA has become the subject of recent interest for its selective reaction with hydrogen sulfide in the presence of carbon dioxide (1, 4, 5, 38, 61). It is a more economic process particularly in the purification of non-hydrocarbon gases such as coke-oven gas, the products from coal gasification processes, and Claus plant tail gas. Aqueous MDEA or MDEA based solutions are reported capable of treating sour gas to sweet gas specification for H_2S while permitting a major fraction of the CO_2 to pass through unabsorbed (16, 26, 51, 52). MDEA is also used as a non-selective solvent with the addition of small amount of monomethylmonoethanolamine or piperazine as absorption activators. The activators increase the rate of hydration of CO_2 and thus increase the rate of absorption (46, 47, 48).

Plan of Work

Calculations of the basic vapor-liquid equilibrium of the alkanolamine-H_2S-CO_2-water system made computer simulation of amine sweetening installations feasible. Reliable models based on experimental data have been developed to predict vapor-liquid equilibrium of the alkanolamine-H_2S-CO_2-water system for different concentrations and temperatures (31, 49). These models will be introduced in Chapter II. Reaction mechanisms of primary and secondary amines, such as MEA, DEA, DGA, and DIPA, have been covered in these equilibrium models. One of the objectives of this research is to establish the equilibrium model for the tertiary amine, MDEA.

Selection of amine sweetening processes and design procedures have historically been based on approximate calculations. A simulation program with reliable, dependable and accurate calculation procedures is certainly a useful tool to evaluate the design and operation systematically and economically. There are several ethanolamine calculation procedures available. One was developed earlier by Vaz (57, 58) at Oklahoma State University. Others are available on commercial computer programs. None of these is capable of reliable and dependable calculations to a converged solution. The problems encountered will be discussed in Chapter III. A converged rigorous stage-by-stage calculation simulation program was developed in this research to overcome these problems and provide flexible design abilities by allowing rigorous calculations on major equipment in an amine sweetening process. The calculations on major process units include contactor, regenerator, flash tank, and amine-to-amine heat exchanger. Calculation options such as assigned stage efficiencies, intercoolers, sidefeeds, condenser, and sidedraws, are also included in the proposed simulation program.

Since equilibrium models are used in the program, equilibrium stage calculations or calculations based on assigned Murphree vapor stage efficiencies are performed in the program.

Common practice is to assign an overall stage efficiency under certain operating conditions by the experience of the designer. Then, the number of actual stages needed in the column is calculated by the ratio of the number of the calculated equilibrium stages required to the assigned overall stage efficiency. However, the Murphree vapor stage efficiencies required to simulate the actual stage column are unknown. Knowledge of the Murphree stage efficiencies is required to scale-up from equilibrium stage calculation to actual stage calculation. A relationship between the Murphree vapor stage efficiency and the overall stage efficiency is established in Chapter III. The accuracy of this model is shown in Chapter IV.

CHAPTER II

BASIC EQUILIBRIUM CALCULATIONS

Model Review

Relatively large amounts of experimental data on the equilibrium of H_2S and/or CO_2 over aqueous MEA or DEA solutions are available. However, most of these data are for the equilibrium of a single acid gas-amine-water system and very few data fall in the regions of low acid gas loadings and low acid gas partial pressures where most commercial units operate. Less data are available on DIPA, DGA, and MDEA. For the rational design of an amine process, knowledge of the equilibrium solubility of the H_2S and CO_2 in the aqueous amine solution is necessary.

Several authors have proposed thermodynamic models based on reaction equilibrium to correlate the published equilibrium solubility data and to extrapolate and interpolate for different concentrations and temperatures. Atwood, et al. (2) proposed a method using the "mean ionic activity coefficient" for the calculation of equilibrium in the H_2S-amine-water system. The activity coefficients of all ionic species are assumed to be equal. This assumption is good at low ionic strength or if only single type anions and cations are present. However, this is generally not the case for amine sweetening process. The Atwood, et al. model was modified by Klyamer, et al. for the CO_2-amine-water system (34, 35) and later generalized to make it applicable to the H_2S-CO_2-amine-water system. They established equations based on proposed reaction mechanisms and thermodynamic equilibrium constants to relate the equilibrium partial pressures of acid gases, the solution loadings, and the temperature. However, the equilibrium constants of the reactions, the Henry's law constants, and the mean ion activity coefficients must be known to apply those equations, and they depend on the ionic strength.

Danckwerts and McNeil (20) used pseudo-equilibrium constants which do not contain activity coefficients to predict the equilibrium partial pressure of carbon dioxide over the CO_2-amine-water solution. The central feature of this model is the use of pseudo-equilibrium constants and their dependence on ionic strength. However, the predicted vapor pressure using their values for the amine equilibrium constants deviates substantially from the experimental data. The lack of agreement, which may be due to the nonidealities caused by the many ionic species in the solution, suggests that the ionic strength alone is insufficient to determine the concentration dependence of the pseudo-equilibrium constants. Danckwerts (19) recommends ionic characterization factors to correct the Henry's law constants for highly ionized solutions. However, this method is complicated and requires information not readily available.

Kent and Eisenberg (30, 31) have proposed an expansion of the work by Danckwerts and McNeil. They first tried to correlate the solubility data using published equilibrium constants without any dependence on ionic strength. Significant deviations between predicted data and experimental data were observed. Instead of using ionic characterization factors for the dependence of the pseudo-equilibrium constants on ionic strength, they accepted the published values of all but two amine related reaction pseudo-equilibrium constants. Then they treated these two pseudo-equilibrium constants as variables and obtained them by fitting experimental data for the H_2S-amine-water system and the CO_2-amine-water system. These two variables were found to exhibit an Arrhenius type dependence with temperature. The model was extended to predict H_2S-CO_2-amine-water data at different temperatures. Satisfactory comparison of the predicted data and the experimental data were reported by the original authors, and by Moshfeghian, et al. (49) and Maddox, et al. (44).

Batt, et al. (6) fitted the Kent and Eisenberg model to MEA and DEA with improved pseudo-equilibrium and also extended the application of Kent and Eisenberg model to DGA and DIPA. The Kent and Eisenberg model with both the original and the improved variables is included in the proposed program as a tool to calculate the vapor-liquid equilibrium of the H_2S-CO_2-amine-water system. One of the objectives of this research is to extend the Kent and Eisenberg type model to the tertiary amine, MDEA. A brief discussion on the expression and implementation of the Kent and Eisenberg model and the model development for MDEA will be presented in the following two sections.

Kent and Eisenberg Model

The equilibrium vapor pressures of the acid gas species are related to the free acid gas concentrations in the liquid phase by the Henry's law relationship.

$$P_{H2S} = H_{H2S}\,[H_2S] \qquad (2.1)$$

$$P_{CO2} = H_{CO2}\,[CO_2] \qquad (2.2)$$

Kent and Eisenberg suggested that the free or unreacted acid gas concentrations in the liquid phase can be determined by the following set of reactions which describe the system.

$$RR'NH_2^+ \overset{K_1}{\rightleftharpoons} H^+ + RR'NH \qquad (2.3)$$

$$RR'NCOO^- + H_2O \overset{K_2}{\rightleftharpoons} RR'NH + HCO_3^- \qquad (2.4)$$

$$H_2O + CO_2 \overset{K_3}{\rightleftharpoons} H^+ + HCO_3^- \qquad (2.5)$$

$$H_2O \overset{K_4}{\rightleftharpoons} H^+ + OH^- \qquad (2.6)$$

$$HCO_3^- \overset{K_5}{\rightleftharpoons} H^+ + CO_3^= \qquad (2.7)$$

$$H_2S \overset{K_6}{\rightleftharpoons} H^+ + HS^- \qquad (2.8)$$

$$HS^- \overset{K_7}{\rightleftharpoons} H^+ + S^= \qquad (2.9)$$

RR'NH represents the primary or secondary amine. For example, R represents C_2H_4OH, R' represents H for MEA, and both R and R' represent C_2H_4OH for DEA.

Batt, et al. (6) conducted several experiments using Nuclear Magnetic Resonance (NMR) spectra and C^{13} NMR spectroscopy to determine the dominant processes for reactions in the MEA-CO_2 and MEA-H_2S systems. Their studies suggest that water is not a necessary reactant, but merely serves as a diluent for the ethanolamines and provides for better mixing of the solution on the stages of the contactor and regenerator. When hydrogen sulfide and carbon dioxide react with ethanolamine solutions, the following overall reactions are confirmed by their study.

$$RR'NH + H_2S \overset{K_1}{\rightleftharpoons} RR'NH_2^+ + HS^- \qquad (2.10)$$

$$2RR'NH + CO_2 \overset{K_2}{\rightleftharpoons} RR'NH_2^+ + RR'NCOO^- \qquad (2.11)$$

Reaction (2.11) includes two steps of reaction. The rate determining step in reaction (2.11) is

$$RR'NH + CO_2 \rightleftharpoons RR'NCOOH \qquad (2.12)$$

and reaction (2.10) is a simple protonation of the amine.

Reactions (2.3) and (2.4) used in the Kent and Eisenberg model are different from reactions (2.10) and (2.11), so different solutions and different expressions for K_1 and K_2 are expected. However, the combined stoichiometry of reactions (2.3) and (2.4) is the same as that of reactions (2.10) and (2.11). Solution of the two different sets of equations is essentially the same. Therefore, only the expression of pseudo-equilibrium constants and solution development for the Kent and Eisenberg model are discussed here. The pseudo-equilibrium constants for reactions of (2.3) to (2.9) are expressed in equations (2.13) to (2.19).

$$K_1 = [H^+]\,[RR'NH] \,/\, [RR'NH_2{}^+] \qquad (2.13)$$

$$K_2 = [HCO_3{}^-]\,[RR'NH] \,/\, [RR'NCOO^-] \qquad (2.14)$$

$$K_3 = [H^+]\,[HCO_3{}^-] \,/\, [CO_2] \qquad (2.15)$$

$$K_4 = [H^+]\,[OH^-] \qquad (2.16)$$

$$K_5 = [H^+]\,[CO_3{}^=] \,/\, [HCO_3{}^-] \qquad (2.17)$$

$$K_6 = [H^+]\,[HS^-] \,/\, [H_2S] \qquad (2.18)$$

$$K_7 = [H^+]\,[S^=] \,/\, [HS^-] \qquad (2.19)$$

The charge balance for the reacting species of the system can be expressed as follows.

$$[RR'NH_2^+] + [H^+] = [RR'NCOO^-] + [HCO_3^-] + 2\,[CO_3^=] + [HS^-] + 2\,[S^=] + [OH^-] \qquad (2.20)$$

Component mass balances for the reacting species of alkanolamine, hydrogen sulfide, and carbon dioxide in the system are shown in equations (2.21) to (2.23).

$$[RR'NH] + [RR'NCOO^-] + [RR'NH_2^+] = M \qquad (2.21)$$

$$[H_2S] + [HS^-] + [S^=] = L_{H2S}M \qquad (2.22)$$

$$[CO_2] + [RR'NCOO^-] + [HCO_3^-] + [CO_3^=] = L_{CO2}M \qquad (2.23)$$

M is the molality of amine. L_{H2S} and L_{CO2} are the solution loadings of hydrogen sulfide and carbon dioxide in the liquid phase.

The values of the pseudo-equilibrium constants for K_3 to K_7 and the Henry's law constants of hydrogen sulfide and carbon dioxide were published by different authors and collected by Kent and Eisenberg (30). The pseudo-equilibrium constant K_1 was obtained by fitting the published data for the H_2S-amine-water system using equations (2.1), (2.3), (2.6), (2.8), and (2.9). A similar approach was used to obtain K_2 by using the value found for K_1, and the equation group of (2.2) to (2.7) to fit the experimental data for the CO_2-amine-water system. A value of K_1 or K_2 was obtained at each temperature level for which data are available. The values obtained for K_1 and K_2 were correlated by an Arrhenius type dependence with temperature.

Through suitable algebraic manipulation, the thirteen equations of (2.1), (2.2), and (2.13) to (2.23) can be reduced to three non-linear equations. The three equations are:

$$P_{H2S} = (H_{H2S}\ A[H^+]^2/K_6K_7) * [1/(1+[H^+]/K_7)] \qquad (2.24)$$

$$P_{CO2} = (H_{CO2}\ B[H^+]^2/K_3K_5) * [1/(1+[H^+]/K_5+M[H^+]/K_2K_5C)] \qquad (2.25)$$

$$[H^+] = \left\{ A * [1+1/(1+[H^+]/K_7)] + B * [1+1/(1+[H^+]/K_5+M[H^+]/K_2K_5C)] + K_4/[H^+] \right\} * [1/(1+M/CK_1)] \qquad (2.26)$$

where

$$A = L_{H2S}M - P_{H2S}/H_{H2S}$$

$$B = L_{CO2}M - P_{CO2}/H_{CO2}$$

$$C = 1 + [H^+]/K_1 + P_{CO2}K_3/(K_2\ [H^+]\ H_{CO2})$$

Since the pseudo-equilibrium constants from K_1 to K_7 are known, there will be only three unknowns left in the three non-linear equations by assigning either the solution loadings or the partial pressures of the acid gases for a H_2S-CO_2-amine-water system at a specified amine concentration and temperature. Therefore, the non-linear equations (2.24) to (2.26) can be solved by suitable numerical techniques. All the ion concentrations in the H_2S-CO_2-amine-water system will then be able to calculated.

Model Development for MDEA

In order to develop the Kent and Eisenberg type equilibrium model for the tertiary amine, MDEA, the reaction nature of the H_2S-CO_2-MDEA-water system will be discussed and compared to the primary and secondary amines oriented Kent and Eisenberg model.

Methyldiethanolamine can be represented as $R_2R'N$, where R_2 is $(C_2H_4OH)_2$ and R' is CH_3. Since there is no hydrogen attached to the nitrogen in MDEA, the formation of carbamate as in reaction (2.11) will not happen for a tertiary amine (4, 10). However, the same instantaneous proton transfer reaction (2.3) still occurs when hydrogen sulfide reacts with MDEA directly. Since carbon dioxide can not react with MDEA directly, it must react slowly with water to form bicarbonate as in equation (2.5). Equation (2.5) is slow and rate controlling of the CO_2 reactions. The selective reaction of aqueous MDEA solution with H_2S is achieved by the fast proton transfer reaction for H_2S absorption and the slow bicarbonate reaction for CO_2. The selectivity of MDEA will be further discussed in Chapter V.

To develop the equilibrium model for the H_2S-CO_2-MDEA-water system, the reactions of CO_2 hydrolysis and dissociation are the same as equations (2.5) to (2.9), and the reaction of proton transfer is the same as equation (2.3). Reaction (2.11) of carbamate formation is eliminated. The equilibrium partial pressures and the free solution concentrations of acid gases are related by equations (2.1) and (2.2). The expression for the pseudo-equilibrium constants K_1, and K_3 to K_7 are the same as equations (2.13) and (2.15) to (2.19).

In the same way as for primary and secondary amines, the pseudo-equilibrium constant K_1 will be fitted to available experimental data. The value of K_1 should be the same for the H_2S-MDEA-water system and the CO_2-MDEA-water system. K_1 is obtained by using experimental H_2S-MDEA-water and CO_2-MDEA-water solubility data and the equation group of (2.1), (2.2), (2.3), (2.5), (2.6), (2.7), (2.8), and (2.9). The pseudo-equilibrium constant K_1 will be correlated with the Arrhenius dependence with temperature.

The charge balance and component mass balances for the reacting species for the H_2S-CO_2-MDEA-water system can be derived as the following expressions.

$$[R_2R'NH^+] + [H^+] = [HCO_3^-] + 2\,[CO_3^=] + [HS^-] + 2\,[S^=] + [OH^-] \tag{2.27}$$

$$[R_2R'N] + [R_2R'NH^+] = M \tag{2.28}$$

$$[H_2S] + [HS^-] + [S^=] = L_{H2S}M \tag{2.29}$$

$$[CO_2] + [HCO_3^-] + [CO_3^=] = L_{CO2}M \quad (2.30)$$

By algebraic rearrangement, the following expressions for the three non-linear equations are derived.

$$P_{H2S} = (H_{H2S}\ A[H^+]^2/K_6K_7) * [1/(1+[H^+]/K_7)] \quad (2.31)$$

$$P_{CO2} = (H_{CO2}\ B[H^+]^2/K_3K_5) * [1/(1+[H^+]/K_5)] \quad (2.32)$$

$$\begin{aligned}[H^+] = \{ & A * [1+1/(1+[H^+]/K_7)] + \\ & B * [1+1/(1+[H^+]/K_5)] + \\ & K_4/[H^+] \} * [1/(1+M/CK_1)] \end{aligned} \quad (2.33)$$

where

$$A = L_{H2S}M - P_{H2S}/H_{H2S}$$

$$B = L_{CO2}M - P_{CO2}/H_{CO2}$$

$$C = 1 + [H^+]/K_1$$

The three non-linear equations are solved by the same numerical method as for the primary and secondary amines, and the concentrations of all ions in the H_2S-CO_2-MDEA-water system are then calculated algebraically. The comparison of the predicted values and the experimental data will be presented in Chapter IV.

CHAPTER III

AMINE PROCESS UNIT CALCULATIONS

Sweetening Processes and Equipment

Industrial applications of alkanolamines for sweetening natural gases have been used for several decades. When first introduced, MEA was used almost exclusively. DEA became popular later. In recent years, several new amines such as DGA, DIPA, and MDEA have come into use. The characteristics of these amines have been briefly discussed in Chapter I.

Selection of the desired amine and the design of sweetening process are still largely based on gross approximations and operating experience (40). The need for rigorous calculations when designing alkanolamine sweetening process is apparent. Optimum performance and economic overall cost can only be achieved by proper process simulation. The equilibrium model of the acid gases and aqueous amine solution system provides an adequate and feasible basis for the development of rigorous design calculations.

The flow schemes and major equipment in an amine sweetening plant are similar, regardless of the amine used. A basic flow scheme for an amine sweetening process is shown in Figure 2. Different process flow schemes and discussion of amine selection and the operation of the equipment have been presented by many authors (36, 50, 53, 55, 62). The equipment such as the contactor, regenerator, flash tank, and amine-amine heat exchanger are always major process units of concern. Process options on the choice of location of intercoolers, sidefeeds to the contactor, condenser, and liquid sidedraws from the regenerator together with the associated pumps, air or water cooler and piping provide for variety in the process scheme.

The simulation program developed in this research allows rigorous stage-by-stage calculations of the contactor and the regenerator along with calculation options on sidestreams, intercoolers, Murphree vapor efficiencies, etc. Rigorous calculations on the flash tank and amine-amine heat exchanger are also included. Therefore, it provides a flexible flow sheet with rigorous calculation procedures to design and evaluate different amine sweetening processes. The computation algorithms of the major process units will be discussed in the following sections.

Contactor Calculations

Rigorous calculations of any multistage separation process are always a combination of the material conservation, energy conservation and phase equilibrium relationships to determine the temperatures and component flowrates of each phase on each stage of the separation

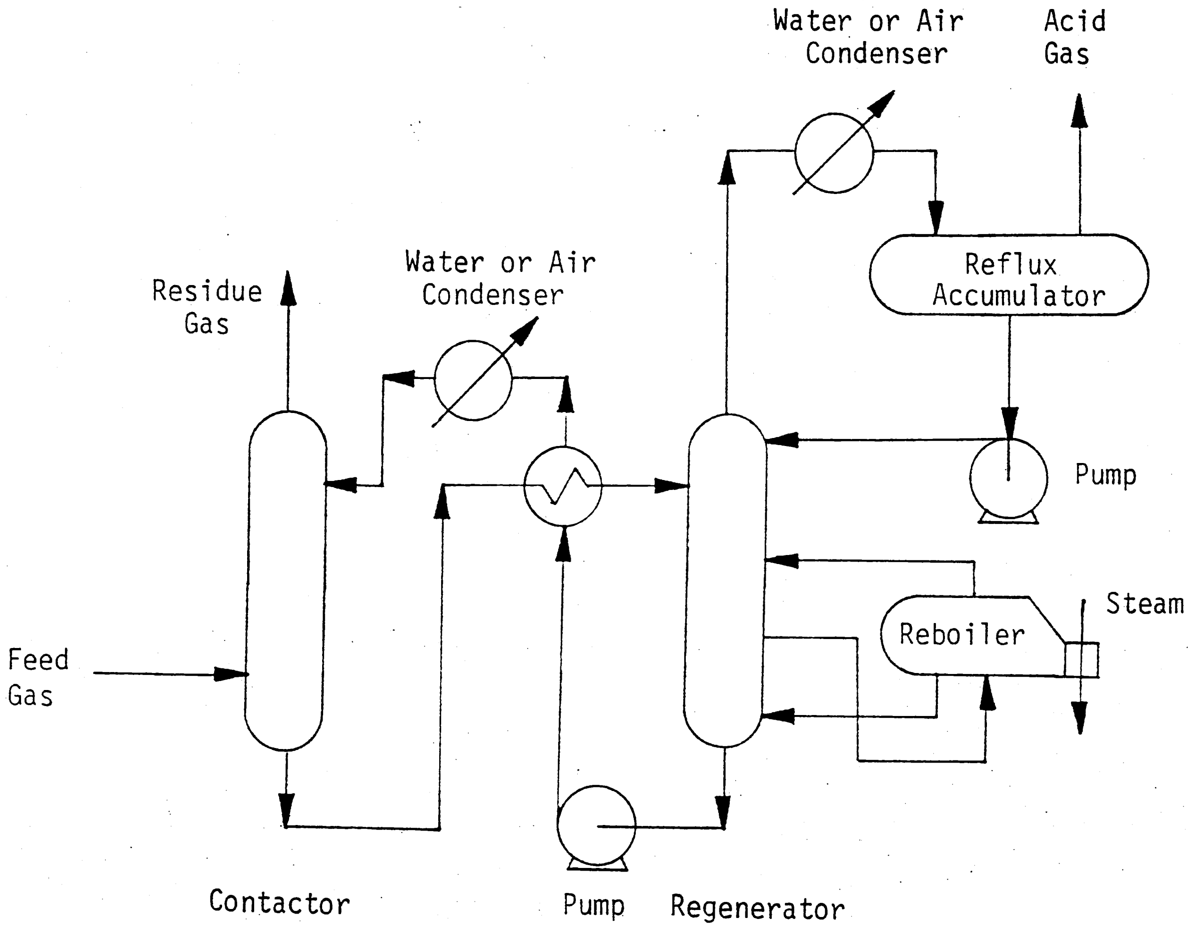


Figure 2. Basic Flow Scheme for An Amine Sweetening Process.

process. The procedures used here are no exception. Simultaneous relationships for each stage in the stage-by-stage calculations are presented and solved to simulate the column at steady-state operation.

Convergence algorithms used to solve non-linear simultaneous equations can be matrix or successive iteration methods. Matrix methods are numerical and need to overcome truncation errors, stability, and convergence problems especially in the case of non-linear equations. A successive iteration method is a good alternative to the matrix methods. It ensures fast and stable convergence and simplifies the calculations (32). Both algorithms are discussed extensively in numerical methods text books (15). The application of the basic successive iteration method to stage-by-stage contactor or regenerator calculations with a given correlation, such as the vapor-liquid equilibrium model used in this research, need proper calculation procedures and special program implementation to overcome the physical and numerical limitations encountered in the successive iteration process.

The equations governing the contactor calculations are based on the contactor model presented in Figure 3. The temperature, flow rate and composition of each component in the lean solvent, L_0, and sour gas, V_{n+1}, are specified. The contactor pressure is also specified. Calculation of the whole column is started from the bottom stage of the column with assumed initial conditions for each stage. The

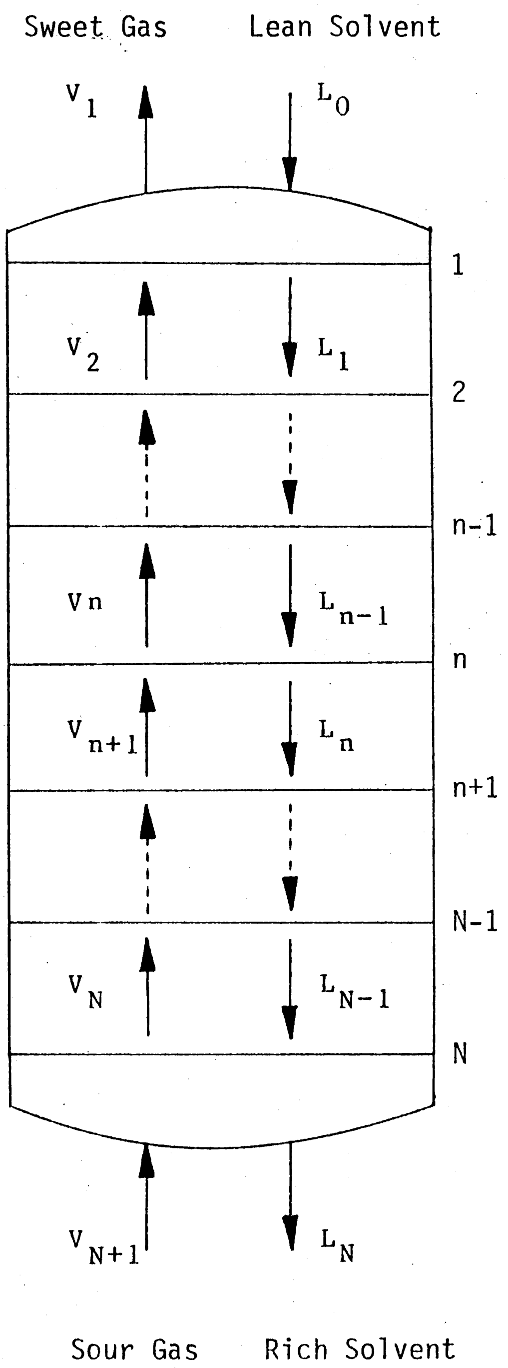


Figure 3. Model for a Multistage Contactor.

initial conditions for each stage are assigned as the conditions of lean solvent. The nomenclature for streams leaving and entering the nth stage of the contactor are shown in Figure 4. Since the temperature and flow rate of each component are known for entering gas, V_{n+1}, and entering liquid, L_{n-1}, the temperature and flow rate of each component can be solved for by manipulation of the equations of material balance, heat balance and phase equilibrium relationship on this stage. The degree of equilibrium approach for hydrogen sulfide and carbon dioxide are adjusted by the implementation of Murphree vapor stage efficiencies. The computational approach on a single contactor stage are summarized as follows:

1. Assume a stage temperature for the amine solution and gas leaving the stage.
2. Assume the compositions of gas components in the gas leaving the stage.
3. Calculate the loadings of components in the liquid amine solution by stage material balance,

$$l_{i,n} = l_{i,n-1} + (v_{i,n+1} - v_{i,n}) / C_r , \qquad (3.1)$$

   where C_r is the amine circulation rate, mole amine/mole sour gas.
4. Calculate the loadings of components in liquid amine solution by the basic equilibrium model and adjust with specified Murphree vapor efficiencies

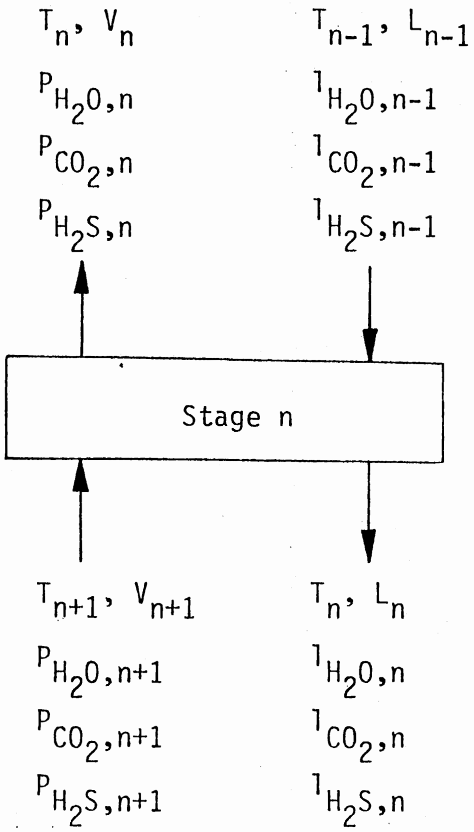


Figure 4. Nomenclature for Streams Leaving and Entering a Single Contactor Stage.

for the stage.

5. Compare the results of step 3 and step 4. Repeat step 2 to step 4 until convergence.

6. Calculate a stage temperature by energy balance. The energy balance includes the heat of reaction of acid gases and amine solution, $\Delta H_{R,n}$, the heat pick-up of the sweet gas, $\Delta H_{G,n}$, the heat of water vaporization or condensation, $\Delta H_{W,n}$, and the temperature changes in the amine solution affected by the energy balance. The temperature of the amine solution leaving stage n can then be calculated as,

$$T_n = T_{n-1} + (\Delta H_{R,n} - \Delta H_{G,n} - \Delta H_{W,n}) / C_{P,n} \qquad (3.2)$$

where $C_{P,n}$ is the heat capacity of the amine solution leaving stage n.

7. Compare the stage temperature calculated by step 6 and the stage temperature assumed in step 1. Repeat step 1 to step 7 until temperature converges.

The computation of each stage will go through the whole column according to the above procedure. The calculated stage temperature and component flow rates in gas and liquid will then be compared to the values of the initial conditions or the last iteration. The newly calculated values will be used as initial values for the next column iteration. The successive iteration procedure on the whole column will be carried out until the whole column converges. When a converged solution of the column is obtained, the iteration variables such as stage temperature and flow rates of components in gas and liquid become fixed and represent the steady-state operation of the column.

The heat of reaction of acid gases in amine solutions is estimated by the method of Crynes and Maddox (17, 45). The heat of reaction is calculated by using acid gas partial pressures which can be provided by the equilibrium model calculation. Appropriate numerical techniques are used to improve the speed of convergence and to avoid the blow-ups caused by model limitations or improper intermediate values generated during each convergence step of the whole successive iteration scheme.

Regenerator Calculations

Like the contactor calculations, the regenerator calculations in this research are based on a successive iteration scheme. The regenerator model is represented in Figure 5. The nomenclature of streams leaving and entering the nth stage of the regenerator is shown in Figure 6. In regenerator operations, heat is supplied to the column by a heat medium such as saturated steam to evaporate water into steam vapor in the reboiler. The generated steam vapor with stripped acid gases, V_{N+1}, will be passed through the column

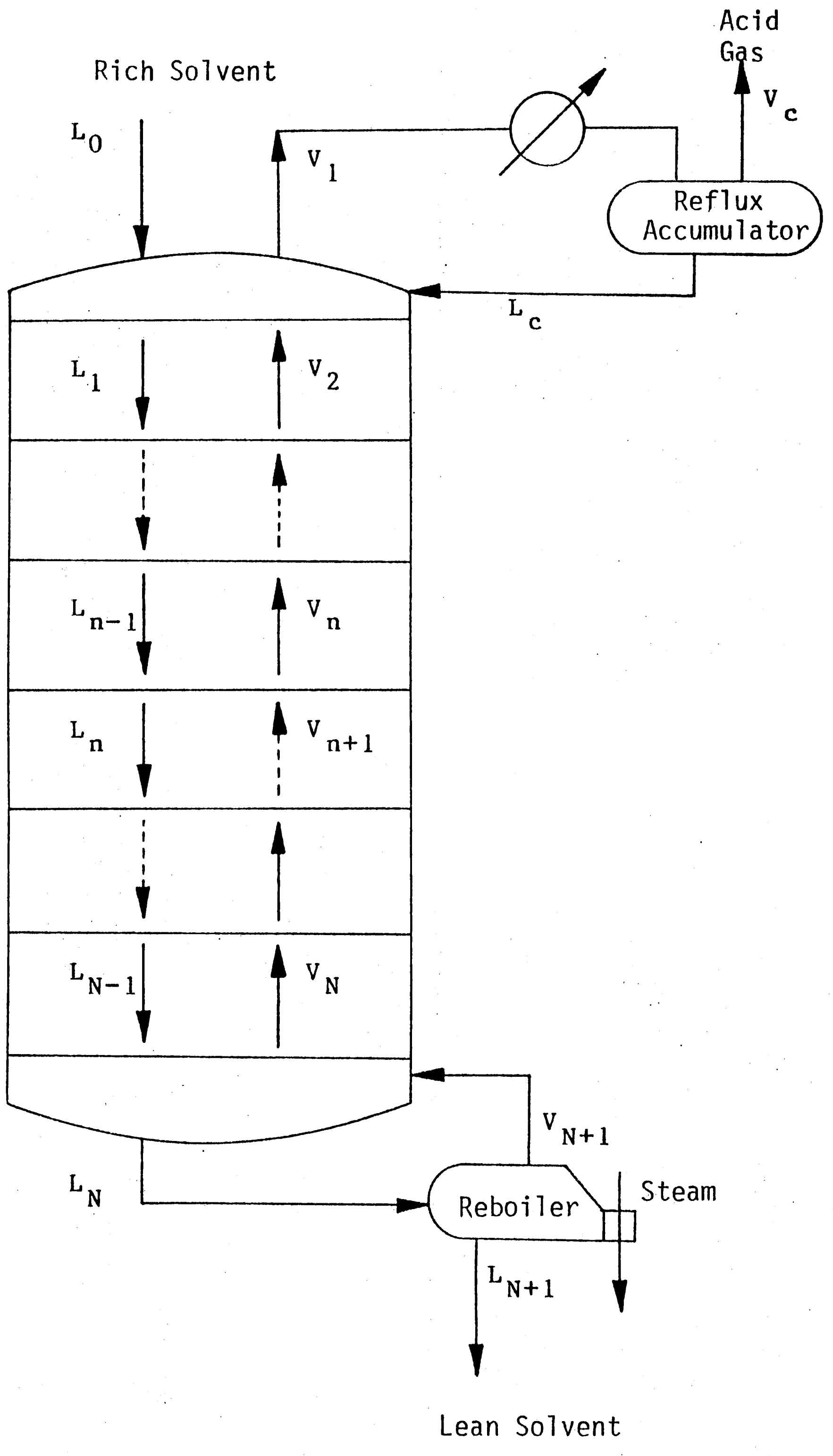


Figure 5. Model for a Multistage Regenerator.

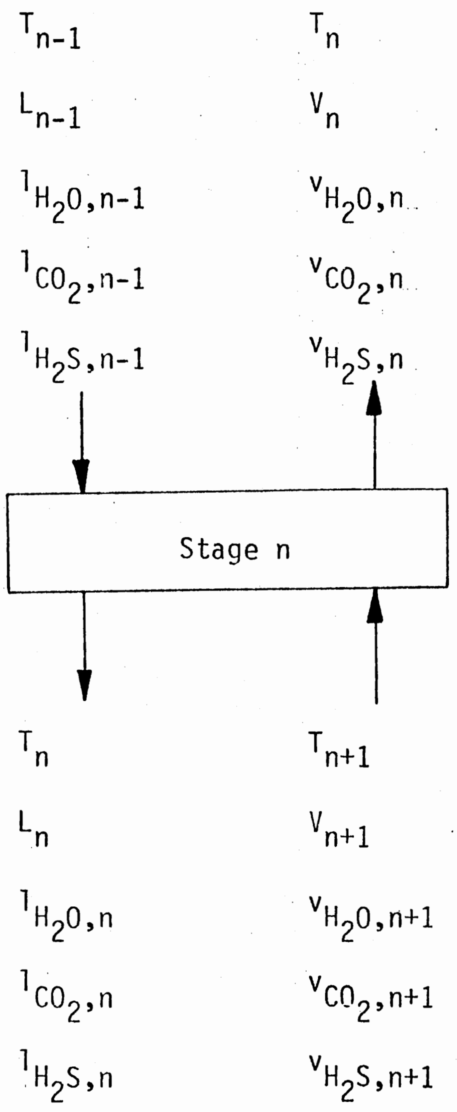


Figure 6. Nomenclature for Streams Leaving and Entering a Single Regenerator Stage.

and condensed in a air or water cooled overhead condenser and then returned to the regenerator as reflux, L_c.

The objective of the proposed regenerator calculations is to get converged results of the regenerator column at steady-state operation. The regenerator calculations are based on the specified rich amine solution, L_0, entering the column, the reboiler duty, and the condenser temperature to calculate the converged performance profiles of temperatures and constituents across the regenerator. Calculations of theoretical stages or actual stages with assigned Murphree stage efficiencies are performed for each stage with the help of the basic equilibrium model. The heat of regeneration required to dissolve acid gases in the amine solutions is also estimated by the method of Crynes and Maddox (17). Vapor pressures and Raoult's law of ideal solutions are used for estimating stage temperature by a bubblepoint calculation. The ideal solution is acceptable since water exists as the principal component even in concentrated solutions of amines so that the liquid phase nonideality effects on the partial pressure of water are negligible (3).

The heat effects in regenerator calculations include the sensible heat, the heat of dissolution, and the heat of vaporization/condensation. In the reboiler, the reboiler duty is consumed by the sensible heat required to raise the temperature of the entering amine solution to the temperature of the reboiler, the heat of regeneration required to break the chemical bonds between the acid gas molecules and the amine, and the heat of vaporization of water to produce stripping steam. In single stage calculations, the heat release from the condensation of steam is compensated by the sensible heat required to raise the temperature of the entering amine solution to the temperature of the stage and the heat of regeneration required for the stage. The overhead condenser duty is calculated by the sensible heat released from the temperature of the entering acid gas-steam vapor to the temperature of the condenser and the heat released from the steam condensed.

In the regenerator calculations, the reboiler and the overhead condenser are each treated as a single stage applied with their own physical characteristics. The regenerator column calculation scheme is similar to the contactor column calculation scheme. Proper initialization of the vapor phase can be obtained from the specified conditions of the feed amine solution and the reboiler duty. The column calculations are started from top to bottom for each stage. The outline of the single regenerator stage calculation with specified conditions of entering amine solutions and entering acid gases and steam vapor is as follows.

1. Assume the amount of steam leaving the stage.
2. Assume the loadings of acid gas components in the

amine solution leaving the stage.

3. At specified stage pressure, calculate the stage temperature by bubblepoint calculation using the reaction equilibrium model, the specified Murphree stage efficiencies, and Raoult's law.
4. Calculate the amounts of components leaving the stage in the vapor by using the assumed amount of steam leaving the stage and the partial pressure of each component at the stage temperature.
5. Calculate the loadings of acid gas components in the amine solution leaving the stage by material balance.
6. Compare the loadings assumed in step 2 and the loadings calculated in step 5. Repeat step 2 to step 5 until convergence.
7. Calculate the amount of steam leaving the stage by energy balance as discussed earlier.
8. Compare the assumed amount of steam in step 1 and the calculated result of step 7. Repeat step 1 to step 7 until convergence.

The stage temperature and each component flow rate in leaving amine solution and acid gas vapor are determined for each stage at the specified entering gas and liquid conditions. Similar to the contactor calculations, a successive iteration scheme is then applied to the regenerator column calculations to get a converged result as the performance at the steady-state operation.

Flash Tank and Heat Exchanger

At high pressure contactor operations, appreciable amounts of nonacidic gases such as hydrocarbons are carried by the solution from the contactor to the regenerator. A flash tank is often used to recover hydrocarbons that may have dissolved or condensed in the amine solution leaving the contactor. Hydrocarbon contamination in the amine solution often promotes foaming. Equipment fouling may be more severe and occur faster in the absence of a flash separator. Sulfur plant operation may be hindered if hydrocarbons are volatilized in the regenerator (13).

The pressure of the amine solution from the contactor is dropped as it enters the flash tank allowing the lightest hydrocarbons such as methane and ethane to flash. The heavier hydrocarbons remain as a liquid, but separate from the aqueous amine to form a separate upper layer due to lower density, and can be skimmed off from the top (13). The hydrocarbon considered in the flash tank calculation is therefore only included methane and ethane. The scheme of a flash tank is shown in Figure 7. The flash tank calculation is similar to a single stage calculation in the regenerator without steam. Outlines of a single stage regenerator calculation were carried out with the proper modification in mass and energy balance for the flash tank with the inclusion of methane and ethane.

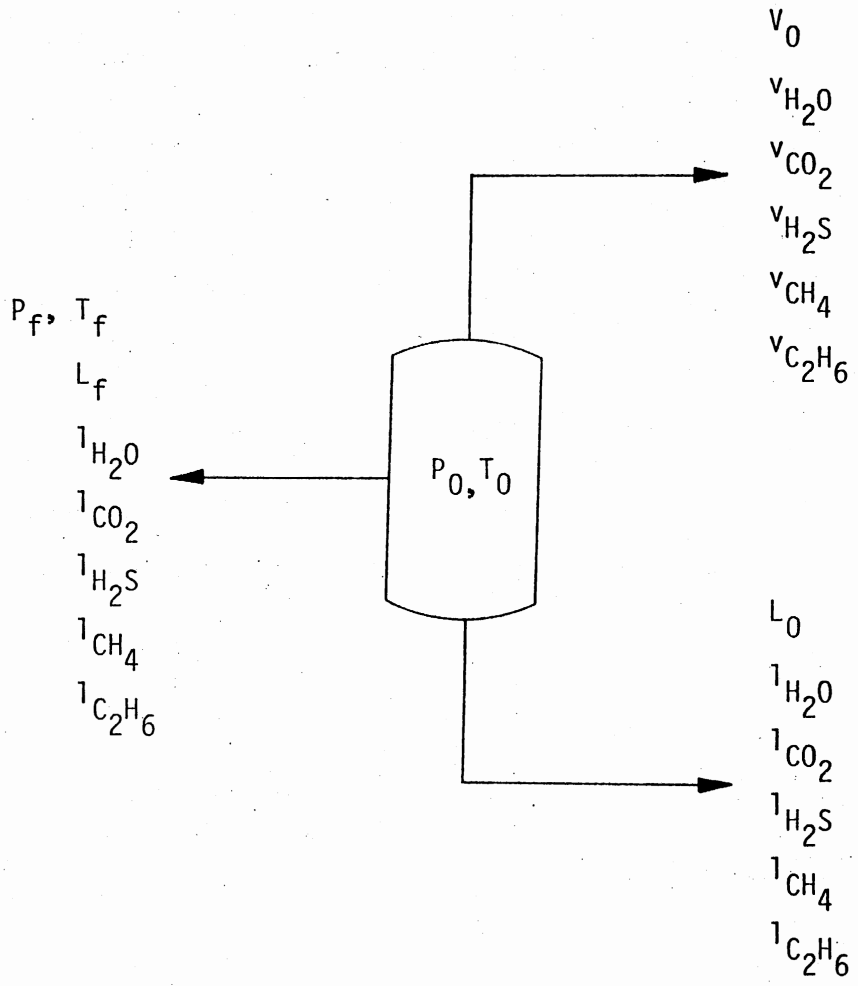


Figure 7. Nomenclature for a Flash Tank.

Since the rich amine solution from the contactor needs to be preheated before entering the regenerator and the lean amine solution from the reboiler must be cooled before entering the contactor, an amine-amine heat exchanger is often used to reduce the heat load on the reboiler. Heat exchanger duty is calculated in the program with standard procedures and heat capacity data.

Relationship Between Overall Stage Efficiency and Murphree Vapor Stage Efficiency

It is a common practice to assign an overall stage efficiency for a particular type of plate by some prediction method or the experience of the designer. The number of actual stages required in the column is calculated from the ratio of the required number of equilibrium stages to the assigned overall stage efficiency. The required number of equilibrium stages is decided by equilibrium stage calculation for specified sour gas removal.

The Murphree vapor stage efficiency for the actual stage column is unknown but would be useful to scale-up from equilibrium stage contactor to actual stage contactor. A model to predict the Murphree stage efficiency from the assigned overall stage efficiency and the required number of equilibrium stages is established here.

At an assigned overall stage efficiency, the performance of the contactor with required number of equilibrium stages is the same as the performance of the contactor with equivalent number of actual stages. This criterion can be met with correct Murphree stage efficiencies applied to actual stage contactor calculations.

If the Murphree vapor stage efficiency of component i is assumed to be the same for each stage, the Murphree stage efficiency of component i on the top stage is the same as that on the bottom stage,

$$E_{MV,i,1} = E_{MV,i,N} \tag{3.3}$$

where $E_{MV,i,1}$ and $E_{MV,i,N}$ are the Murphree vapor stage efficiencies of component i on the top and bottom stages, respectively.

From the definition of the Murphree vapor stage efficiency and the constant total pressure assumption in the contactor, equation (3.3) can be expressed as

$$\begin{aligned}(P_{i,1} - P_{i,2}) \;/\; (P^*_{i,1} - P_{i,2}) &= \\ (P_{i,N} - P_{i,N+1}) \;/\; (P^*_{i,N} - P_{i,N+1})\end{aligned} \tag{3.4}$$

where $P^*_{i,1}$ and $P^*_{i,N}$ are the equilibrium partial pressures of component i leaving the top and bottom stages respectively.

Since the specified conditions for the bottom stage sour gas feed and the top stage lean amine solution for the actual stage contactor are the same as those of the equilibrium stage contactor, $P_{i,N+1}$ is known. Because the performance of the actual stage contactor and the equilibrium stage contactor should be the same, the partial pressure of component i, $P_{i,1}$, leaving the top of the actual stage contactor can be obtained by running the program on the equivalent equilibrium stage contactor.

Assuming the temperature and loadings of the amine solution leaving the equilibrium stage contactor are the same as those of the actual stage contactor, the equilibrium partial pressure of component i, $P_{i,N}$, leaving the bottom stage can be calculated from the temperature and loadings of the amine solution leaving the contactor by using the reaction equilibrium model. The equilibrium partial pressure of the top stage $P^*_{i,1}$ is small and can be reasonably estimated from the temperature and loadings of the top stage lean amine solution by using the reaction equilibrium model.

The pressure change of component i across the whole equilibrium stage column is the same as that across the whole actual stage column:

$$\triangle P_{i,E} = \triangle P_{i,A} \qquad (3.5)$$

where $\triangle P_{i,E}$ and $\triangle P_{i,A}$ are the total pressure change of component i across the equilibrium and actual stage column respectively. With the introduction of the number of stages, N_E and N_A, for the equilibrium and actual stage column, equation (3.5) can be expressed as:

$$(\overline{\Delta P}_{i,E})\, N_E = (\overline{\Delta P}_{i,A})\, N_A \qquad (3.6)$$

where $\overline{\Delta P}_{i,E}$ and $\overline{\Delta P}_{i,A}$ are the general expressions for the pressure change of component i across a single equilibrium stage and a single actual stage respectively. The overall stage efficiency is defined as:

$$E_0 = N_E / N_A \qquad (3.7)$$

By introducing overall stage efficiency E_0 into (3.6),

$$\overline{\Delta P}_{i,A} = (\overline{\Delta P}_{i,E})\, E_0 \qquad (3.8)$$

$\overline{\Delta P}_{i,A}$ is assumed to be the logarithmic mean of the pressure change of the top stage and the pressure change of the bottom stage in the actual stage column,

$$\overline{\Delta P}_{i,A} = (\Delta P_{T,A} - \Delta P_{B,A}) / \ln(\Delta P_{T,A}/\Delta P_{B,A}) \qquad (3.9)$$

where

$$\Delta P_{T,A} = (P_{i,2} - P_{i,1})_A \qquad (3.10)$$

and

$$\Delta P_{B,A} = (P_{i,N+1} - P_{i,N})_A \qquad (3.11)$$

$\overline{\Delta P}_{i,E}$ is assumed to be expressed as the geometric mean of the average pressure change of the equilibrium stage column and the logarithmic mean of the pressure change of the top stage and the pressure change of the bottom stage in the equilibrium stage column.

$$\overline{\triangle P}_{i,E} = \left\{ [(P_{i,N+1} - P_{i,1})/N_E] * [(\triangle P_{T,E} - \triangle P_{B,E})/\ln(\triangle P_{T,E} / \triangle P_{B,E})] \right\}^{1/2} \quad (3.12)$$

where

$$\triangle P_{T,E} = (P_{i,2} - P_{i,1})_E \quad (3.13)$$

and

$$\triangle P_{B,E} = (P_{i,N+1} - P_{i,N})_E \, . \quad (3.14)$$

There are only two unknowns, $P_{i,2}$ and $P_{i,N}$, in the two non-linear equations (3.4) and (3.8). After $P_{i,2}$ and $P_{i,N}$ are obtained by solving equations (3.4) and (3.8) numerically, the Murphree vapor stage efficiency of component i can be calculated by equation (3.4). The accuracy of the proposed model will be presented in Chapter IV.

CHAPTER IV

RESULTS

Equilibrium MDEA Model

A reaction equilibrium model for prediction of vapor-liquid equilibrium in the MDEA-H_2S-CO_2-H_2O system has been developed in Chapter II. Solubility data for the H_2S-MDEA-H_2O system and the CO_2-MDEA-H_2O system have been reported by Jou, et al. (29) and Bhairi (8).

The solubility data from Bhairi's research were used to obtain K_1. The solubility data used are 20 weight percent MDEA solution at 100°F, 150°F, and 240°F for both H_2S-MDEA-H_2O and CO_2-MDEA-H_2O systems. The comparison of the experimental data and the fitted model are presented in Figure 8 for the H_2S-MDEA-H_2O system and in Figure 9 for the CO_2-MDEA-H_2O system. The absolute average percent deviations are 10.4 percent for the CO_2-MDEA-H_2O system and 17.7 percent for the H_2S-MDEA-H_2O system. Both Figures 8 and 9 show reasonable agreement between the proposed model and the experimental data.

The proposed model with the generated K_1 value was then used to predict the partial pressures of acid gases for the CO_2-MDEA-H_2O system over 2.0N MDEA solution at 25°C and the

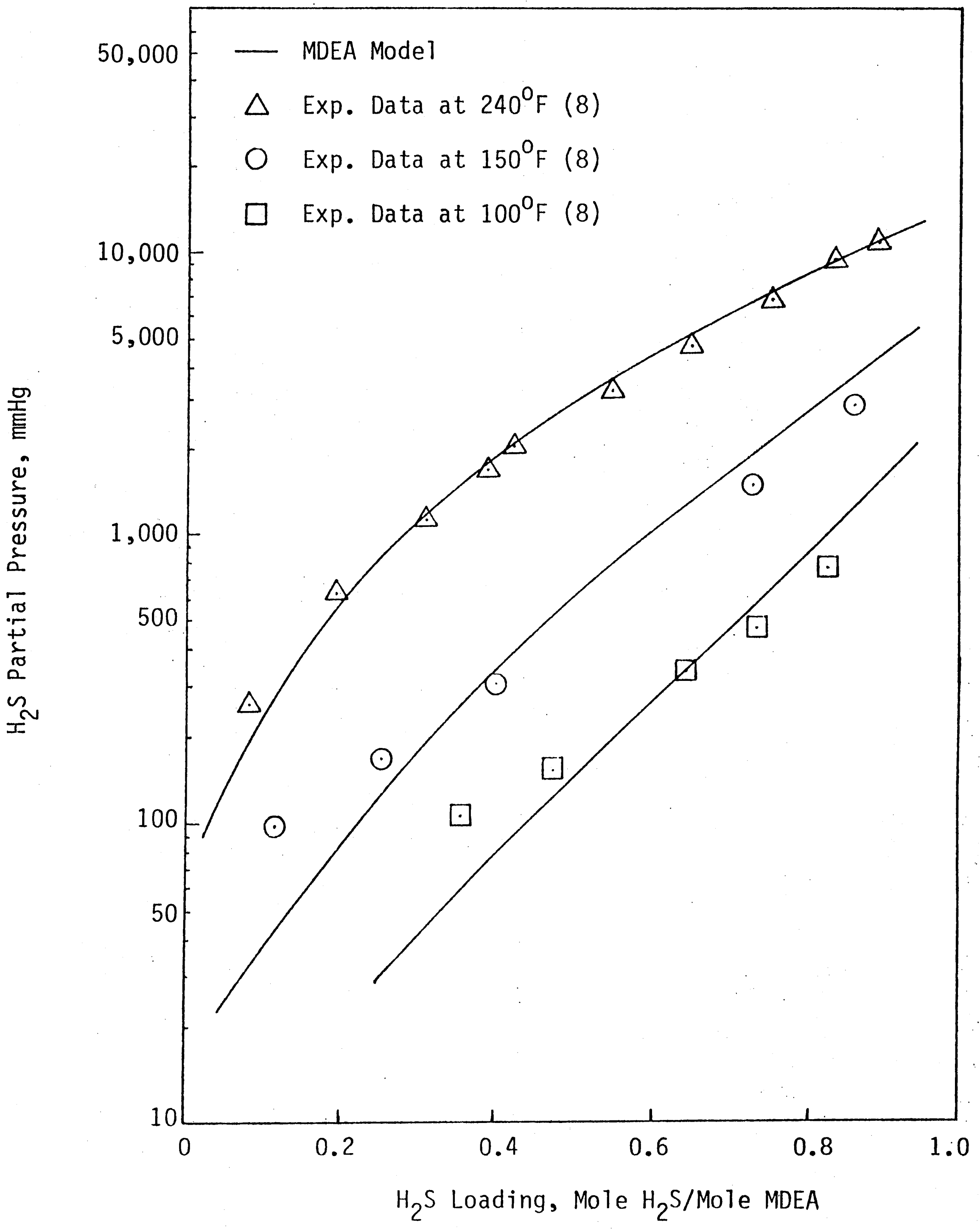


Figure 8. Comparison of Experimental Data and Fitted Curve for H_2S Partial Pressure Over 20% by Weight MDEA Aqueous Solutions at 100, 150 and 240°F.

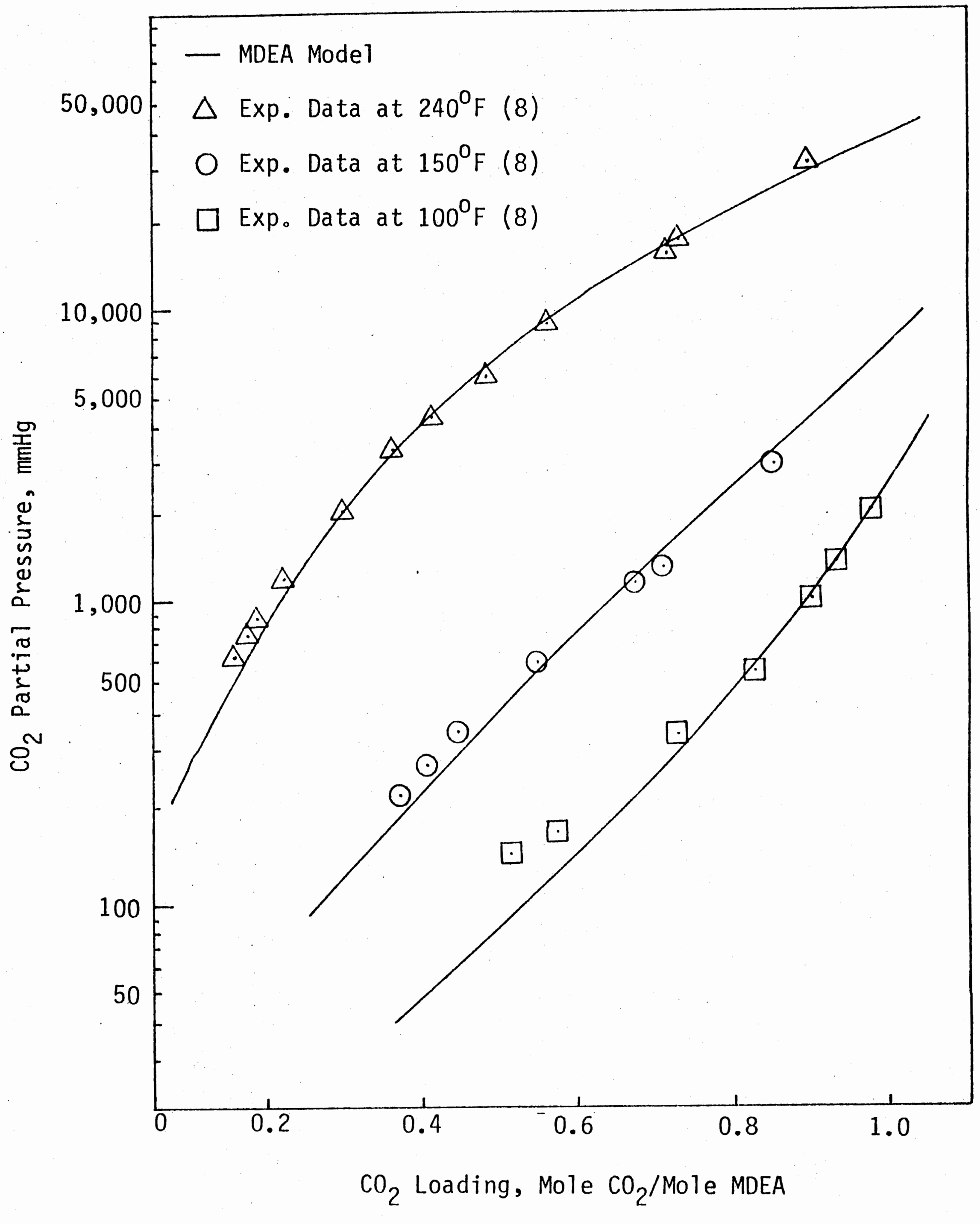


Figure 9. Comparison of Experimental Data and Fitted Curve for CO_2 Partial Pressure Over 20% by Weight MDEA Aqueous Solutions at 100, 150, and 240°F.

H_2S-MDEA-H_2O system over 1.0N MDEA solution at 25°C. Experimental data on the conditions of the above-mentioned system were reported by Jou, et al. (29) and Bhairi (8). The predicted model along with the experimental data are shown in Figures 10 and 11 for the two ternary systems respectively.

From the experimental data shown in Figures 10 and 11, essential discrepancies exist between the experimental data of Jou, et al. and the data of Bhairi. The deviations shown in Figure 10 and 11 appear to be caused by the differences in reported experimental values rather than the weakness in the proposed reaction equilibrium models. This trend is in agreement with that experienced by other researchers (44, 49, 57) in their studies on other amine solution systems. In general, the proposed model can reproduce the experimental data of the CO_2-MDEA-H_2O system and the H_2S-MDEA-H_2O system reasonably well and provides a way for the prediction of the MDEA-H_2S-CO_2-H_2O mixtures.

Amine Process Simulation Model

The amine process simulation model developed in Chapter III is based on rigorous calculation procedures for amine sweetening units. Equilibrium calculations described in Chapter II and reliable physical and thermodynamic data are applied to the calculations of mass and energy balances.

There are several ethanolamine calculations have been reported. One was developed earlier by Vaz (57) at Oklahoma

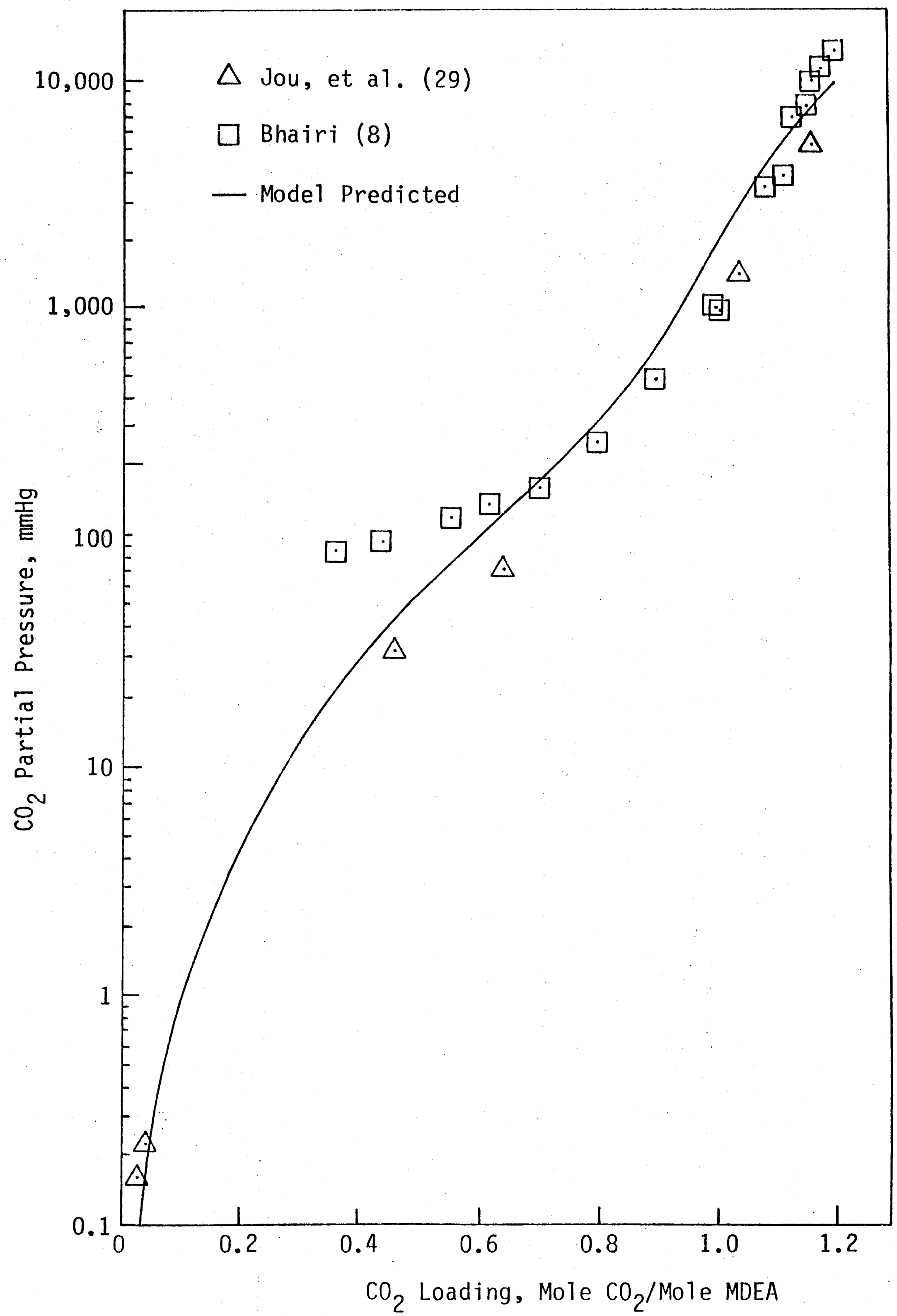


Figure 10. Comparison of Experimental and Predicted Data for CO_2 Partial Pressure Over 2.0N MDEA Solution at 25°C.

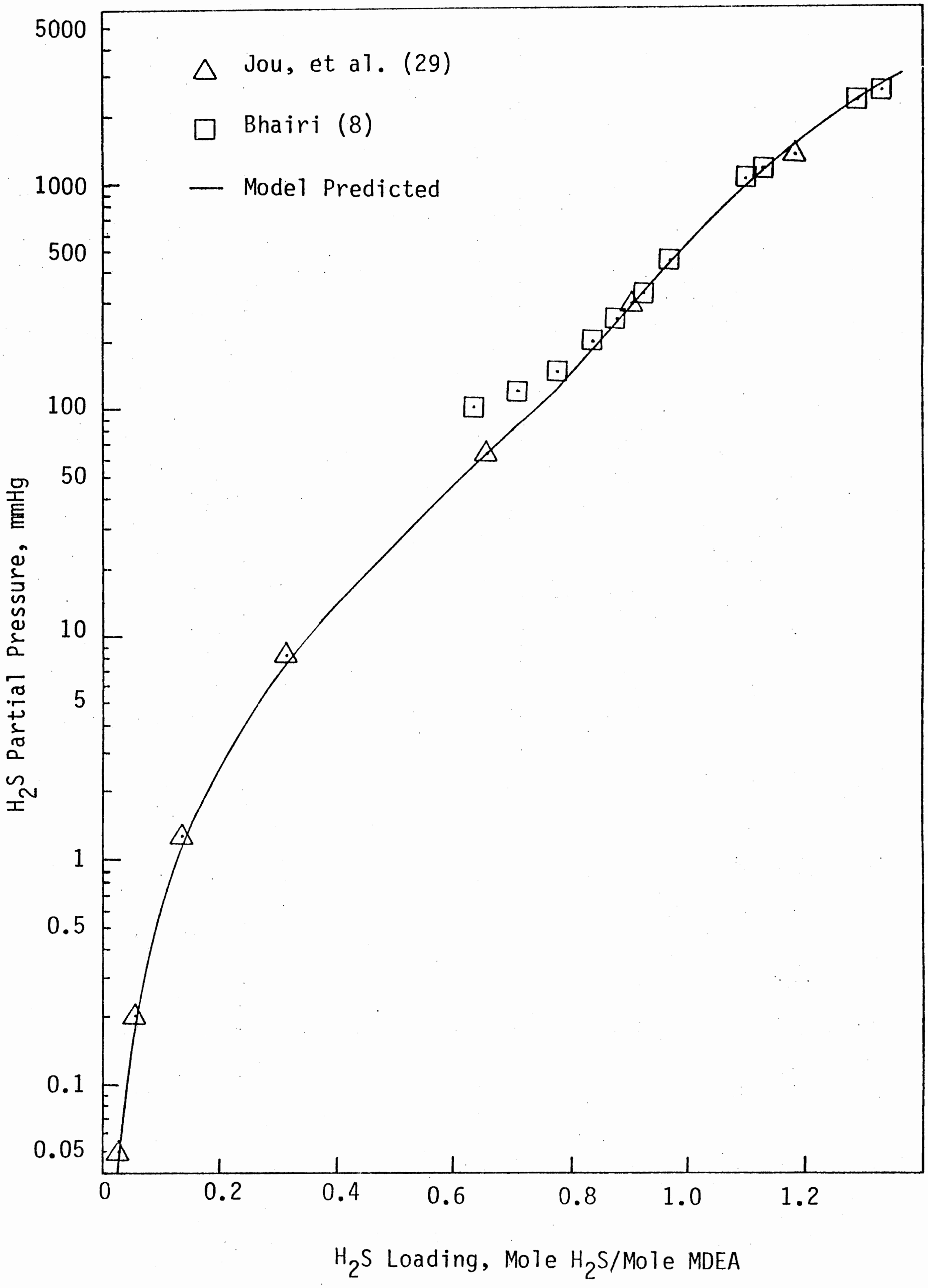


Figure 11. Comparison of Experimental and Predicted Data for H_2S Partial Pressure Over 1.0N MDEA Solution at 25°C.

State University. Others are available on commercial computer programs. All of those programs are very slow to converge and do not reach solutions for all ranges of conditions. None is capable of obtaining a fast, reliable and dependable converged solution at all the possible design conditions.

The proposed program has been tested extensively over wide ranges of operating conditions. Fast and converged results have been obtained in every case. Generally, it takes less than 5 seconds of CPU time on a VAX 11/780 system to run a 20 stage column. The program is also implemented on an IBM compatible personal computer and takes about 20 minutes to run a 20 stage column. Less time is required for fewer stages. The convergence tolerances used in the contactor calculations, regenerator calculations, and equilibrium calculations are summarized in Table I. Converged results are also obtained for flash and amine-amine heat exchanger calculations. Sample runs of those calculations are illustrated in Appendix B.

It is desirable to compare the program result with operating data in commercial sweetening units. However, only inconsistent and incomplete information are available. Extensive checks have been made against available operating data along with design data. The results are summarized below.

TABLE I

SUMMARY OF CONVERGENCE TOLERANCES USED IN THE PROGRAM

	Absolute Tolerance (%)		Relative Tolerance (%)
Contactor Calculation:			
Whole column:			
Liquid loadings	-		1.00
Acid gases	-		1.00
Temperature, °F	0.30	AND	0.10
Single stage:			
Liquid loadings	1.E-6	OR	1.00
Acid gases	-		0.10
Temperature, °F	0.01		-
Regenerator Calculation:			
Whole column:			
Liquid Loadings	-		1.00
Steam and acid gases	-		1.00
Temperature, °F	0.30	AND	0.10
Single stage:			
Liquid loadings	-		1.00
Steam, mole	0.01		-
Pressure, mmHg	1.00		-
Equilibrium Calculation:			
Partial pressure,			
CO_2, mmHg	1.E-4	AND	1.E-5
H_2S, mmHg	1.E-4	AND	1.E-5
Hydrogen ion concentration	1.E-13		-

Monoethanolamine (MEA)

An example of a rough design of a MEA contactor and regenerator has been presented by Maddox and Burns (40, 42, 43). Table II shows comparison of the program results with those from other calculations for the contactor. The example was based on 4 ppm H_2S sweet gas specification. The program shows that the sweet gas will contain less than this amount. Two equilibrium stages will be required in the contactor. The MEA regenerator comparison is shown in Table III. Approximately four equilibrium stages are required in the regenerator. The original example determined the lean MEA concentrations from the work of Fitzgerald and Richardson (24) which is based on plant test data. Agreement of the lean solution loadings obtained from the program and the example are excellent. Steam to the reboiler is saturated at 250^{o}F.

Operating data for a commercial natural gas treating plant was presented by Kohl and Riesenfeld (36). A 17 weight percent aqueous MEA solution was used to treat natural gas with low acid gas content. The operating data and the results of the program simulation are shown in Table IV. The solution loadings of lean and rich amine solution are obtained from the recycle simulation of the contactor and the regenerator. The rich solution loadings from the contactor are used as feed for the regenerator and the lean solution from the regenerator is used as feed for the

TABLE II

COMPARISON OF THE PROGRAM CALCULATIONS WITH DESIGN DATA FOR A MEA CONTACTOR

Contactor Specification:

Sour gas feed at 90°F, 900 PSIG, 2.5% CO_2, 0.5% H_2S

Lean MEA solution at 122°F, 2.5N with loadings of 0.1275 moel CO_2/mole MEA, 0.0025 mole H_2S/mole MEA

Top tray amine circulation rate at 0.0817 mole MEA/Mole sour gas

Sweet Gas PP, mmHg		Sweet Gas ppm		Rich Amine mole/mole		Rich Amine Temperature	Equilibrium Plates	Source
CO_2	H_2S	CO_2	H_2S	CO_2	H_2S	°F		
-	0.189	-	4	0.396	0.067	135-140		Ref. (40)
22.774	17.327	469	356	0.427	0.059	132.87	1	Program
0.072	0.121	1	2	0.433	0.064	135.50	2	Program
0.050	0.031	1	1	0.433	0.064	136.60	3	Program

TABLE III

COMPARISON OF THE PROGRAM CALCULATIONS WITH DESIGN DATA FOR A MEA REGENERATOR

Regenerator Variables	Ref. (43)	Program
Rich Solution Analysis:		
Concentration, 15 wt. % (2.5N) MEA		
Temperature, °F	190.	190.*
CO_2, mole/mole amine	0.4607	0.4607*
H_2S, mole/mole amine	0.0611	0.0611*
Lean Solution Analysis:		
CO_2, mole/mole amine	0.15	0.1482
H_2S, mole/mole amine	Negligible	0.0032
Number of Stages	12 - 20	4*
Top Tray Pressure, PSIA	20.0	20.0*
Bottom Tray Pressure, PSIA	24.0	24.0*
Top Tray Temperature, °F	200.0	215.5
Condenser Temperature, °F	150.0	150.0*
Reboiler Temperature, °F	240.0	239.9
Reflux, mole H_2O/mole acid gas	3.0	2.52
Steam to Reboiler, lb steam/Gal	1.17	1.17
Top Vapor to Condenser:		
CO_2, mole/mole amine feed	0.3107	0.3125
H_2S, mole/mole amine feed	0.0611	0.0579
Water Condensed mole/mole amine feed	1.1152	1.0175
Bottom Vapor from Reboiler:		
CO_2, mole/mole amine feed	-	0.0476
H_2S, mole/mole amine feed	-	0.0028
Steam, mole/mole amine feed	3.0350	2.8550

* Specified values

TABLE IV

COMPARISON OF THE PROGRAM SIMULATION WITH A LARGE COMMERCIAL MEA TREATING PLANT FOR NATURAL GAS SERVICE

Plant Variables	Ref. (36)	Program
Solution:		
Concentration, MEA, wt. %	17	17*
Flow Rate, Gal/MSCF Gas	2.0 - 3.0	2.5*
Contactor:		
Pressure, PSIG	200	200*
No. of Stages	20	3*
Feed Gas, MMSCFD	50	50*
CO_2, %	0.300 - 0.400	0.350*
H_2S, %	0.255 - 0.287	0.271*
Outlet Gas,		
CO_2, ppm	-	1.3
H_2S, ppm	0.3	4.6
Feed Temperature, °F		
Sour Gas	-	90*
Solution	-	100*
Regenerator:		
Pressure, PSIG	12	11 - 13*
No. of Stages	20	5*
Feed Temperature, °F	200	200*
Top Temperature, °F	240	236.3
Bottom Temperature, °F	250	248.6
Steam Consumption, lb/MSCF Gas	3.2	3.2*
Lean Solution Analysis:		
CO_2, mole/mole amine	-	0.1062
H_2S, mole/mole amine	-	0.0073
Rich Solution Analysis:		
H_2S, mole/mole amine	-	0.1289
CO_2, mole/mole amine	-	0.2633

* Specified values

contactor. The temperature of solution feeds to the contactor and the regenerator are assumed values rather than calculated. The comparison is satisfactory and indicates that the proposed model is capable of simulating and describing the process.

Diethanolamine (DEA)

Performance data for aqueous diethanolamine plant contactors used to remove CO_2 and H_2S from synthesis gas are also presented by Kohl and Riesenfeld (36). The program results along with operating data are presented in Table V. Two to three equilibrium stages are required for both plants. No regenerator data for these plants are available. Berthier (7) presents operating data for a DEA plant in high pressure natural gas service. The comparison with the program simulation of recycling solution between contactor and regenerator is shown in Table VI. The calculated results are in excellent agreement with plant data.

Diglycolamine (DGA)

Description of large DGA plants in Saudi Arabia has been reported by Huval, et al (27, 28). Large amounts of low pressure natural and associated gases were treated to 0.25 grain gas pipeline specification. The operating data reported are in ranges or graphical results of process conditions. With the introduction of the sidecooler on the contactor, the bulk of the heat of reaction can be removed

TABLE V

COMPARISON OF THE PROGRAM CALCULATIONS WITH OPERATING DATA OF DEA CONTACTORS FOR SYNTHESIS GAS

Contactor	Plant 1		Plant 2	
	Ref. (36)	Program	Ref. (36)	Program
Gas Feed, SCF/hr	87000	87000*	71900	71900*
CO_2, %	15.0	15.0*	19.4	19.4*
H_2S, ppm	2073	2073*	1196	1196*
Outlet Gas,				
CO_2, %	2.5	0.3	4.2	0.0031
H_2S, ppm	191	154	33	15
Solution Rate, gpm	36	36*	41	41*
DEA Solution, wt. %	35	35*	41	41*
Temperature, ^{o}F				
Feed Gas	-	100*	-	100*
Lean Solution	-	100*	-	100*
Pressure, PSIG	350	350*	340	340*
No. of Stages	-	3*	-	2*
Lean Solution Analysis:				
CO_2 mole/mole amine	.1181	.1181*	.0385	.0385*
H_2S mole/mole amine	.0024	.0024*	.0047	.0047*
Rich Solution Analysis:				
CO_2 mole/mole amine	.5634	.6564	.4008	.4752
H_2S mole/mole amine	.0080	.0094	.0068	.0073

*Specified values

TABLE VI

COMPARISON OF THE PROGRAM SIMULATION WITH A HIGH PRESSURE NATURAL GAS PLANT USING AQUEOUS DEA SOLUTION

Plant Variables	Ref. (7)	Program
Solution:		
Concentration, DEA, wt. %	20	20*
Flow Rate, gpm	1540	1540*
Contactor:		
Pressure, PSIG	1000	1000*
No. of Stages	30	2*
Feed Gas, MMSCFD	35.5	35.5*
CO_2, %	10.0	10.0*
H_2S, %	15.0	15.0*
Sweet Gas,		
CO_2, ppm	19.7	0.4
H_2S, ppm	4.5	4.1
Regenerator:		
Pressure, PSIG	25	23 - 27*
No. of Stages	20	4*
Reboiler Temperature, ^oF	272	272.1
Steam to Reboiler, lb/hr	92000	92000*
Lean Solution Analysis:		
CO_2, mole/mole amine	-	0.0021
H_2S, mole/mole amine	-	0.0275
Rich Solution Analysis:		
CO_2, mole/mole amine	-	0.2610
H_2S, mole/mole amine	-	0.4158

* Specified values

and the cooled rich amine solution returned to the contactor increasing the removal of acid gases. With the sidecooler to control the temperature inside the contactor, gas specification was reportedly achieved. When the rich amine solution is allowed or forced to go above 185°F, the sweet gas drifts off specification. The sidecooler is usually located about 3 to 5 trays up from the bottom. Table VII shows the comparison of the program results with the operating data. Without a sidecooler, the rich amine temperature reaches 187.8°F after four equilibrium stages. The gas specification can not be achieved even with more stages. With a sidecooler to control the temperature of the amine solution entering stage number four at 140°F, the gas specification is achieved by five equilibrium stages. The heat effect will be further discussed in Chapter V.

Diisopropanolamine (DIPA)

Partial operating data from the ADIP process for three plants using diisopropanolamine (DIPA) was presented by Klein (33). The comparisons of the program results with the operating data are shown in Table VIII. The first plant applies to a contactor treating synthesis gas from an oil gasification unit. The second contactor treats cracked gases from a catalytic cracking unit. The third column shows operating data for the removal of H_2S from the residual gas obtained in the hydrodesulfurization of gas oil. Though the data are incomplete, there is sufficient

TABLE VII

COMPARISON OF THE PROGRAM CALCULATIONS WITH OPERATING DATA ON A LARGE DGA GAS SWEETENING PLANT FOR CONTACTOR

Contactor	Ref. (28)	Run 1	Run 2
Gas Feed, MMSCFD	500 - 600	550*	550*
Temperature, °F	100 - 125	110*	110*
CO_2, %	8 - 14	10*	10*
H_2S, %	3 - 8	4*	4*
Outlet Gas,			
CO_2, ppm	< 100	5893	1
H_2S, ppm	4	9848	< 1
Pressure, PSIG	170	170*	170*
No. of Stages	20	4*	5*
Sidecooler,	Yes	No*	Yes*
Location (from top)	-	-	4*
Temperature, °F	-	-	140*
DGA Solution, wt. %	45 - 65	62*	62*
Solution Rate, gpm	6000 - 7000	7000*	7000*
Lean Solution Analysis,			
Temperature, °F	130 - 150	130*	130*
CO_2, mole/mole amine	-	.001*	.001*
H_2S, mole/mole amine	-	.001*	.001*
Rich Solution Analysis,			
Temperature, °F	< 185	187.8	176.7
CO_2, mole/mole amine	-	.2603	.2765
H_2S, mole/mole amine	-	.0841	.1112

* Specified values

TABLE VIII

COMPARISON OF THE PROGRAM CALCULATIONS WITH CONTACTOR OPERATING DATA IN ADIP PLANTS

Contactor	Plant 1		Plant 2		Plant3	
	Ref. (33)	Program	Ref. (33)	Program	Ref. (33)	Program
Gas Throughput, cu ft/hr	71000	71000*	83000	83000*	120000	120000*
CO_2, % vol	5.5	5.5*	2.5	2.5*	-	-
H_2S, % vol	0.5	0.5*	10.4	10.4*	15.6	15.6*
Pressure, PSIA	367.4	367.4*	293.9	293.9*	73.5	73.5*
Temperature, ^oF	104.0	104.0*	95.0	95.0*	104.0	104.0*
No. of Stages	25	2*	20	3*	15	4*
Purified Gas CO_2, ppm	100	0	-	-	-	-
H_2S, ppm	2	2	< 10	1	100	70
Rich Amine Temperature, ^oF	-	151.4	-	150.63	-	150.29
Circulation Rate, mole amine/mole feed gas	-	0.15*	-	0.19*	-	0.255*
DIPA Solution, wt. %	-	40.0*	-	40.0*	-	40.0*

* Specified values

information to conclude that the program results are in the same range so far as sweet gas composition is concerned.

Methyldiethanolamine (MDEA)

Since the removal of CO_2 is much less than the removal of H_2S sweetening with MDEA solution, the equilibrium stage calculation is desired to incorporate stage efficiencies for the selective MDEA process. Stage efficiency with selective reaction will be discussed in Chapter V. The program has incorporated the option of Murphree vapor stage efficiencies in the model for contactor and regenerator. Operating data for commercial scale operation with MDEA in a refinery treating plant has been reported by Kohl and Miller (37). Table IX shows the comparison of operating data and the program calculation with empirically assigned Murphree vapor stage efficiencies. More examples with specified Murphree vapor efficiencies will be presented in Chapter V.

Prediction of Murphree Vapor Stage Efficiency from Overall Stage Efficiency

A model is proposed in Chapter III to predict the Murphree vapor stage efficiencies for CO_2 and H_2S in an actual stage contactor with knowledge of the equivalent number of equilibrium stages and the overall stage efficiency.

By running the proposed program on the specified actual

TABLE IX

COMPARISON OF THE PROGRAM RESULTS WITH OPERATING DATA FOR MDEA TREATING PLANT

	Ref. (37)	Program
Solution,		
MDEA, wt. %	20	20[a]
Feed Gas,		
Temperature, °F	-	90[a]
CO_2, %	1 - 2	1.2[a]
H_2S, %	5 - 6	5.3[a]
Outlet Gas,		
CO_2, % passed	75	75.2
H_2S, ppm	5824	5834
No. of Stages	8	8[a]
Pressure, psig	150	150[a]
Stage Efficiencies,		
CO_2, %	-	2.9[a]
H_2S, %	-	24.5[a]
Lean Solution Analysis:		
Temperature, °F	90 - 100	90[a]
CO_2, mole/mole amine	.0005[b]	.0005[a]
H_2S, mole/mole amine	.0025[b]	.0025[a]
Rich Solution Analysis:		
Temperature, °F	-	104.4
CO_2, mole/mole amine	-	.0258
H_2S, mole/mole amine	-	.4039
Top Tray Circulation Rate, mole amine/mole feed	.1175[b]	.1175[a]

a. Specified value
b. Estimated from Ref. (37)

stage contactor with trial-and-error Murphree stage efficiencies, the actual used Murphree stage efficiencies are obtained by matching the performance of the equivalent equilibrium stage contactor at the same operating conditions of sour gas and lean amine solution. The so-call actual used Murphree stage efficiencies are then compared to the model predicted Murphree stage efficiencies for different alkanolamines at different overall stage efficiency.

Comparisons of the predicted and the actual used Murphree vapor stage efficiencies at different overall stage efficiencies for different alkanolamines for various sweetening conditions are presented in Figure 12 and Figure 13 for H_2S and CO_2 respectively. The overall stage efficiency covered in these two charts ranges from 5 percent to 70 percent. The amine concentration ranges from 20 weight percent for MEA and DEA up to 60 weight percent for DGA. The absolute average deviations between the predicted and actual used Murphree efficiencies are 1.75 percent for H_2S and 4.67 percent for CO_2. The proposed model is capable of predicting correctly Murphree stage efficiencies for the actual stage column at a specified overall stage efficiency for a required number of equilibrium stages.

The overall stage efficiencies are also plotted against the Murphree stage efficiencies for CO_2 and H_2S as shown in Figure 14 and Figure 15 for the same conditions used in Figure 12 and Figure 13. Figure 14 and Figure 15 serve as a quick guide to the relationship between overall stage

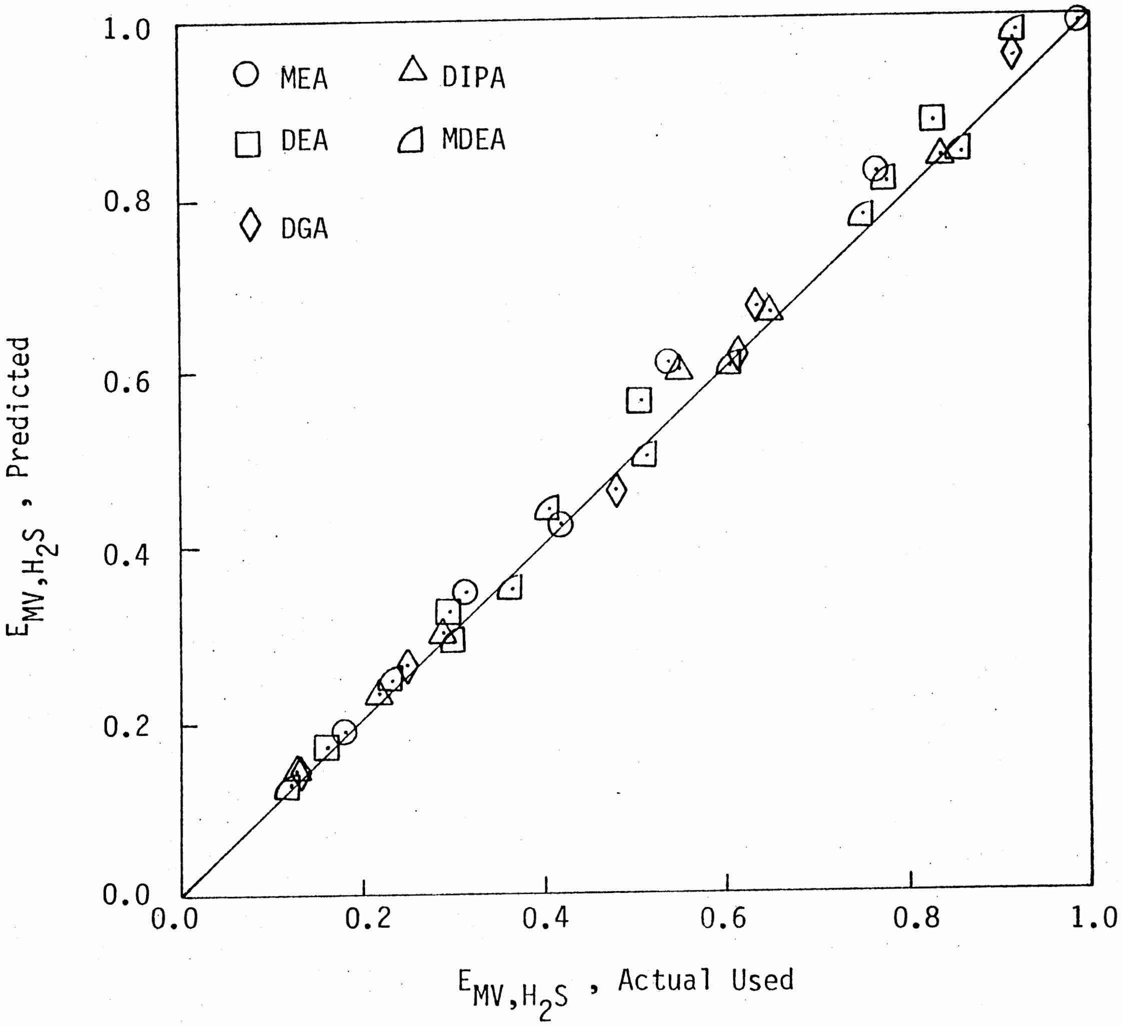


Figure 12. Comparison of Actual Used and Predicted Murphree Vapor Stage Efficiencies at Different Overall Efficiencies and Different Amine Sweetening Conditions for H_2S.

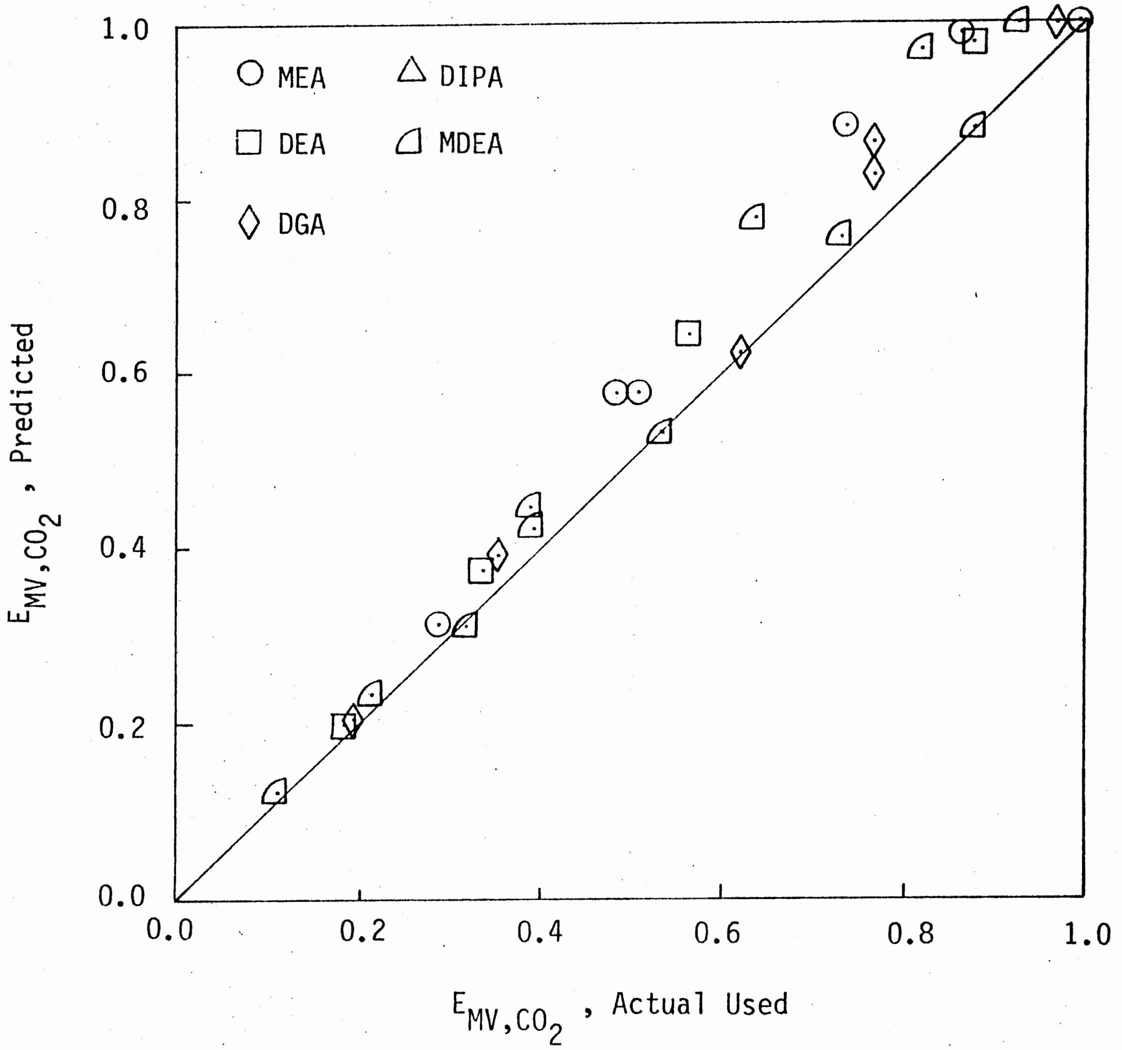


Figure 13. Comparison of Actual Used and Predicted Murphree Vapor Stage Efficiencies at Different Overall Efficiencies and Different Amine Sweetening Conditions for CO_2.

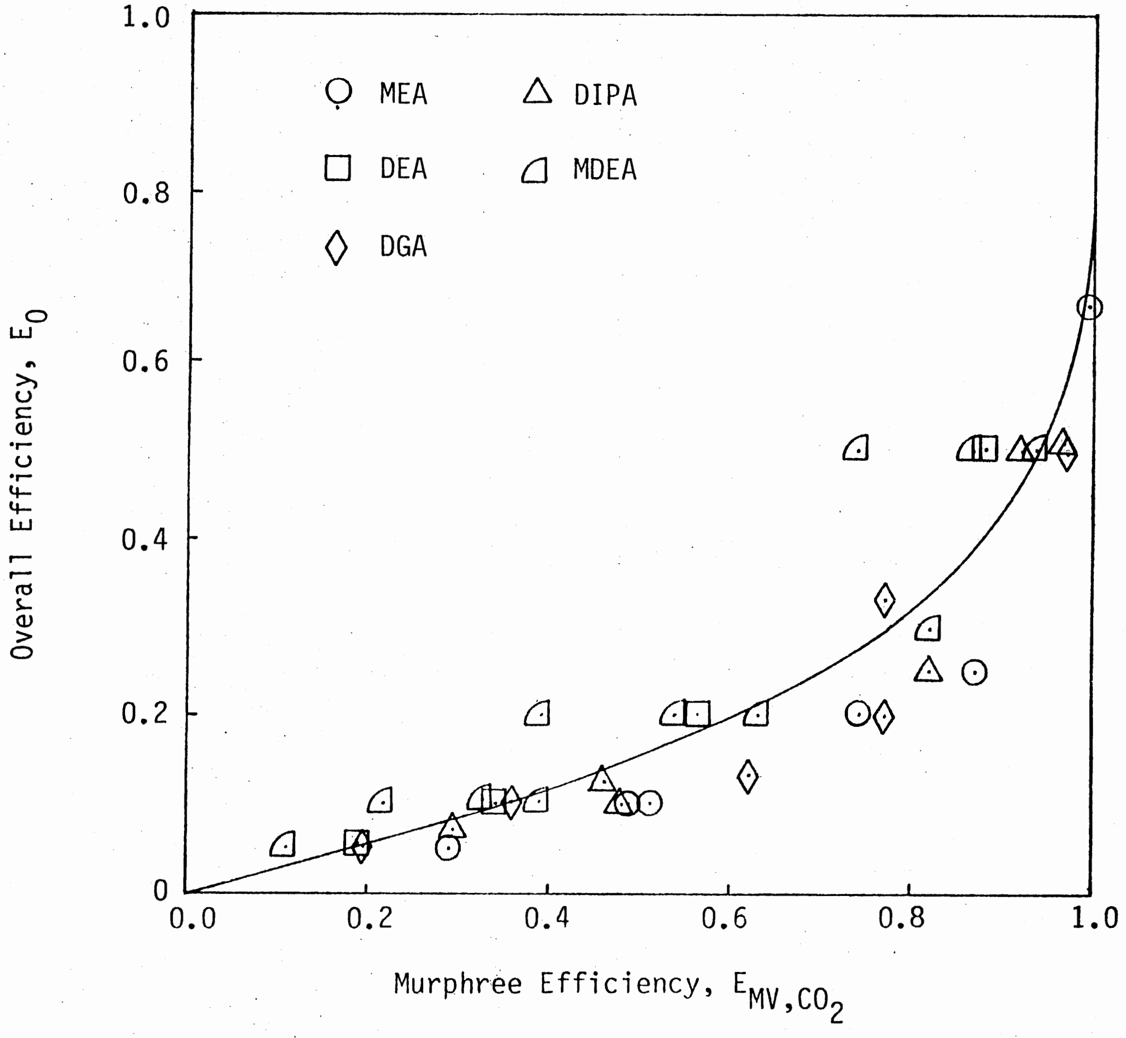


Figure 14. Overall Stage Efficiencies Versus Murphree Stage Efficiencies at Different Amine Sweetening Conditions for CO_2.

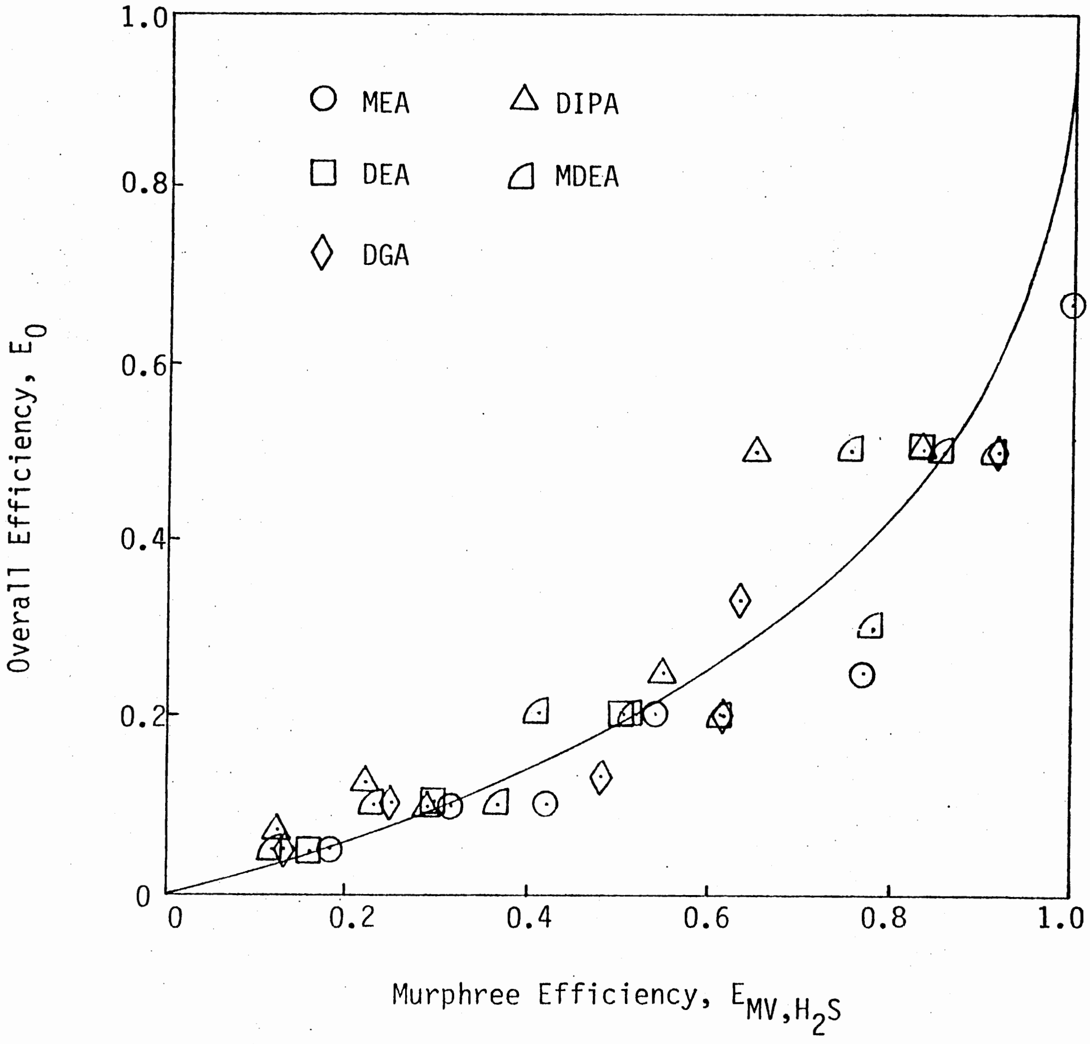


Figure 15. Overall Stage Efficiencies Versus Murphree Stage Efficiencies at Different Amine Sweetening Conditions for H_2S.

efficiency and Murphree stage efficiencies for carbon dioxide and hydrogen sulfide in sweetening process design.

CHAPTER V

DISCUSSION

Heat Effect and Amine Circulation Rate

The rigorous contactor calculations presented in this research are based on an adiabatic process. The competing heat effects include the heat released from the reaction, the heat pick-up in the gas phase, and the heat changes in the liquid phase. The heat of evaporation of the solution is usually negligible. The temperatures of the gas and liquid streams leaving the same stage are assumed to be the same. This assumption is not necessarily true but it is acceptable, because the efficiency of thermal equilibrium generally is greater than the efficiency of mass equilibrium. The temperature profile of the column is determined by the energy balance of the combined heat effects. In addition to reliable values of the heat capacities in the gas and liquid phases and the heats of reaction, the amounts of these heat effects and the patterns of the temperature profiles are strongly influenced by the ratio of the liquid to gas flow rates.

When the amine circulation rate is very small in the extreme case, the quantity of gas is very large relative to the amount of liquid. Essentially all of the heat of reaction will be taken out of the column by the gas stream. The gas leaves at a higher temperature and the gas temperature generally decreases downward in the contactor.

The required amine circulation rate is normally large to purify gas streams containing relatively large concentrations of acid gases. The temperature profile of the column is a combination of the effects of the heat of reaction taken up by the gas and liquid streams. Since a large quantity of amine solution is supplied, the exit gas is cooled by the lean amine solution at the top of the column. In such case, essentially all of the heat of reaction is taken up by the amine solution which leaves the column at an elevated temperature. When the temperature of the feed gas is cool, the heat is picked up by the gas from the rich amine solution at the bottom of the column and later will be lost to the cooler amine solution near the upper part of the column. Therefore, the temperature profile of the column starts from the top to increase and reach a maximum value, a hot spot, to show a temperature bulge, at an intermediate point then decreases to the bottom of the column.

If the amine solution is heated too much by the heat of reaction released, the equilibrium line and operating line will touch causing the contactor to become inoperable without concentration change in gas and liquid phase. It is obvious that an inoperable condition must be avoided by providing sufficient amine circulation rate to absorb the acid gases and, in addition, to absorb the heat of solution. In an isothermal column, the minimum amine circulation rate can be calculated with the available temperature of exit amine solution and the equilibrium pinch at the bottom of the column for removing a specified amount of acid gases by straightforward procedures. Since the contactor operation is assumed adiabatic, the operating and equilibrium lines may touch at an intermediate point and the temperature of the exit rich amine solution is not known initially. The calculations for the minimum amine circulation rate are not as simple as for an isothermal column. The minimum amine circulation rate for a specified amount of acid gas removal can be found by a trial-and-error procedure running the proposed program at different amine circulation rates for a given set of conditions. Consideration of the intermediate pinch point and the hot spot in the column complicates the calculation procedure and justifies the contactor calculation scheme used in this research.

A first guess of the approximate minimum amine circulation rate is desirable and procedure for doing this has been included in the program. The exit temperature of the rich amine solution is calculated by assuming that the acid gas content of the rich amine solution will approach to specified percentages, 75 to 80 percent normally, of the equilibrium values with respect to the feed gas composition. The approximate amine circulation rate required is then calculated at this exit temperature from the reaction equilibrium model, mass and energy balance.

Residual Gas Composition and Stripping Steam Rate

Residual gas composition of H_2S and CO_2 in the lean amine solution is a critical parameter for sour gas purification. The residual loadings determine the limiting equilibrium condition at the top of the contactor, and so the H_2S content of the sweet gas. The residual acid gas left depends on the heat supplied to the regenerator and the sour gas composition. The heat requirement depends upon the ratio of H_2S to CO_2 in the feed gas, the amine solution used, the height of the regenerator, and the temperature of the reboiler. It is customary to express the heat requirements for solution stripping in terms of pounds of steam per gallon of circulated rich amine solution. In commercial practice, the stripping steam rate often ranges from less than 1.0 to as much as 1.5 pounds, or more, of steam per gallon of rich amine solution.

A correlation for MEA of the effect on residual gas composition of the ratio of H_2S to CO_2 in the sour gas feed and the stripping steam rate to the regenerator has been presented by Fitzgerald and Richardson (23, 24). Their graph was based on a study of thirteen Canadian MEA sweetening units. The concentrations of amine solution studied ranged from 11.1 to 20.0 percent by weight for widely varying H_2S to CO_2 ratios in the sour gas. Figure 16

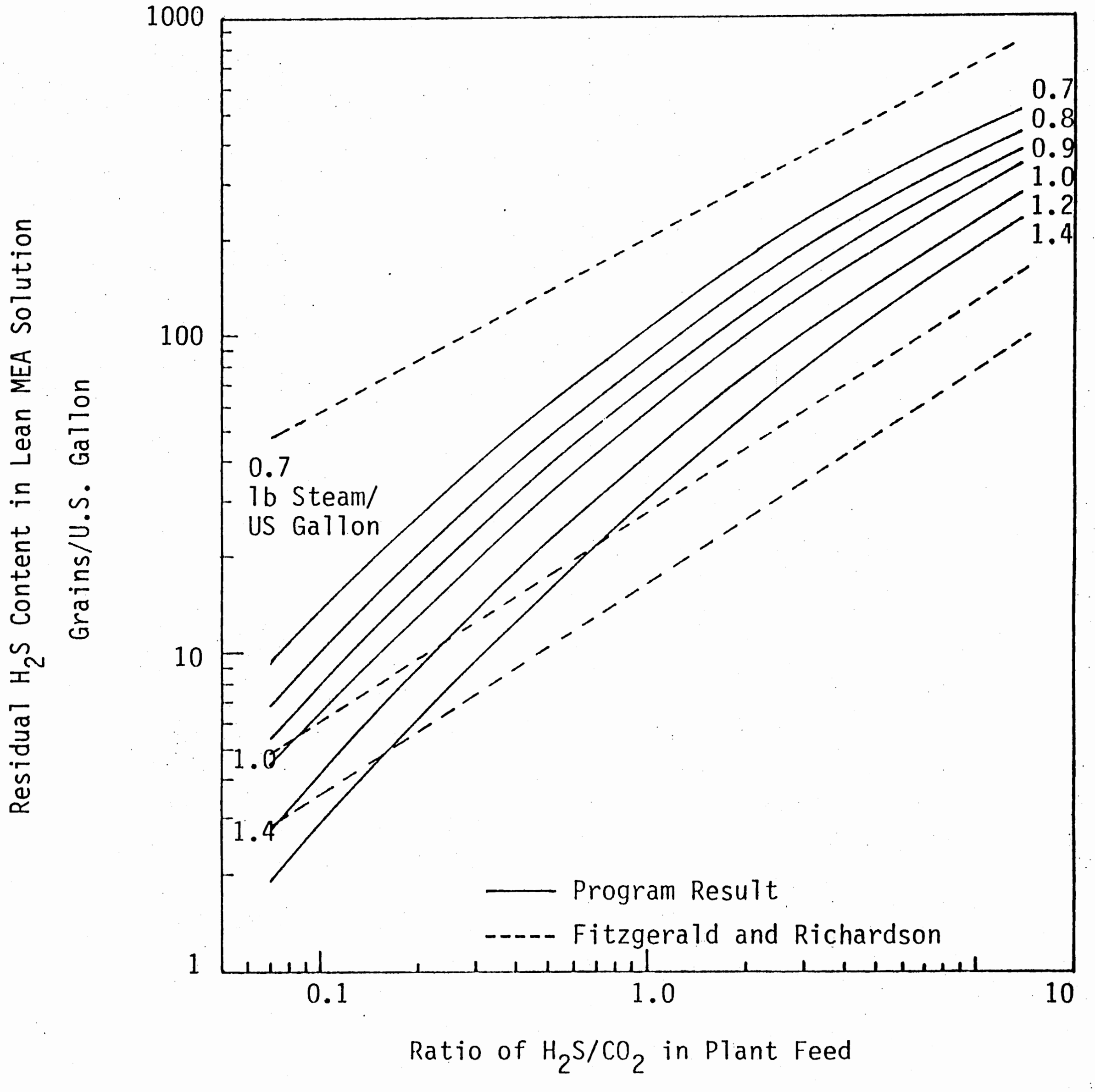


Figure 16. Effect of Acid Gas Ratio ans Stripping Rate on Residual H_2S Content Over 15 Wt. % Lean MEA Solution.

shows comparisons for the Fitzgerald and Richardson correlation and the results calculated by the proposed program. The program results are made with 15 percent by weight MEA solution over various ratios of H_2S to CO_2 in feed gas composition over normal operating conditions. Considering the large number of variables, many without proper definition, the results calculated by the program agree reasonably well and show the same trends as the Fitzgerald and Richardson correlation. Similar charts for H_2S residuals were prepared using the proposed program and are presented in Figure 17 to Figure 20 for DEA, DGA, DIPA and MDEA treating units at different amine concentrations normally used in industrial practice. It is interesting to note that the amount of steam required to obtain a given H_2S residual decreases with decreasing ratio of H_2S to CO_2. This fact indicates that CO_2 acts as stripping vapor for H_2S. The effect of CO_2 on H_2S residual is obvious on MEA treating and on the low ratio of H_2S to CO_2 for other amines. The low H_2S residual for DIPA may contribute to its lower value of heat of dissolution than other amines as reported by Klein (33).

Although carbon dioxide has a tendency to assist in stripping hydrogen sulfide in the regenerator by effecting an increase in hydrogen sulfide vapor pressure above predicted values for systems lacking carbon dioxide, a reverse and frequently detrimental effect occurs on the top stage of the contactor. The partial pressure of H_2S is

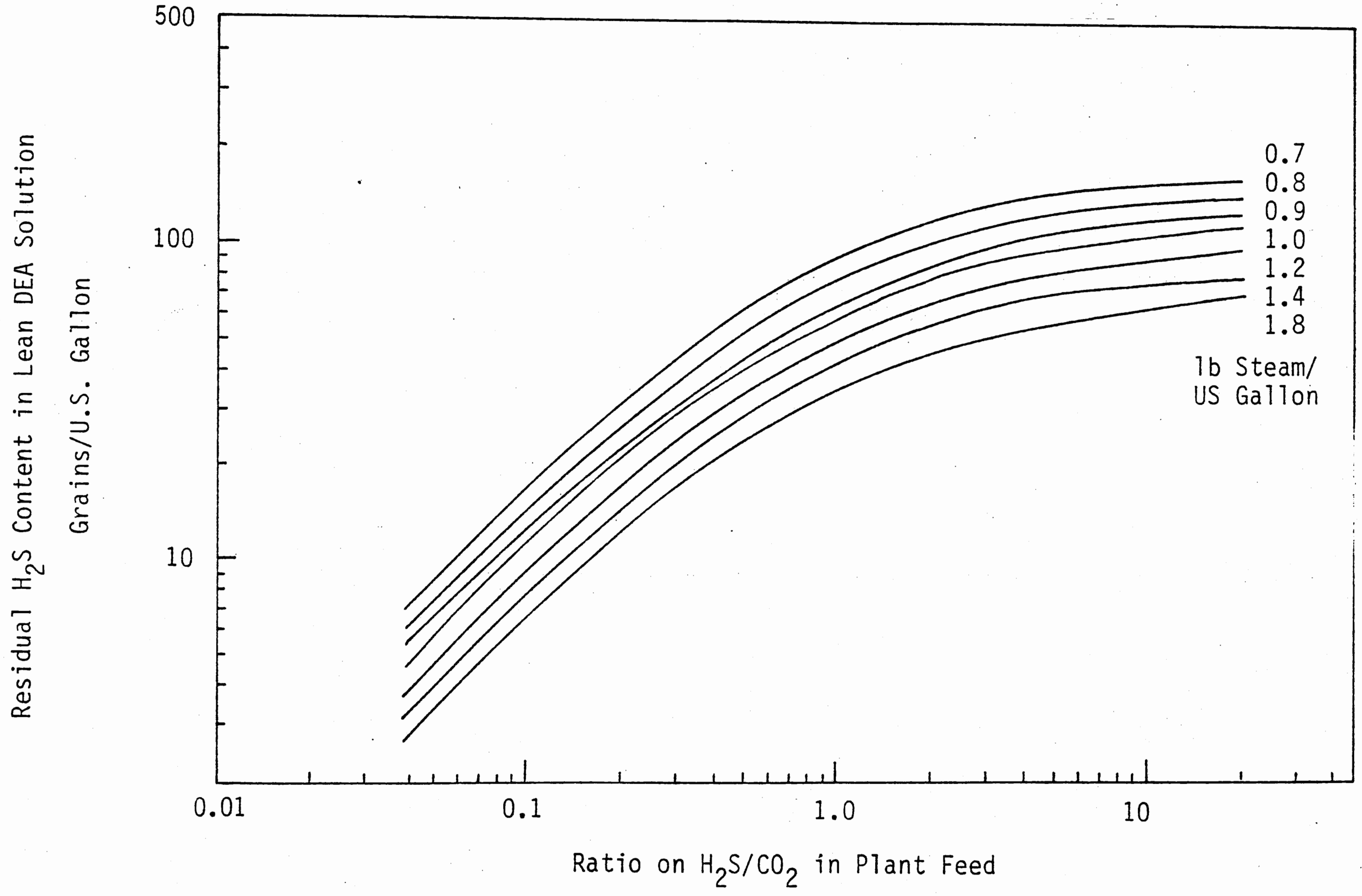


Figure 17. Effect of Acid Gas Ratio and Stripping Rate on Residual H_2S Content Over 20 Wt. % Lean DEA Solution.

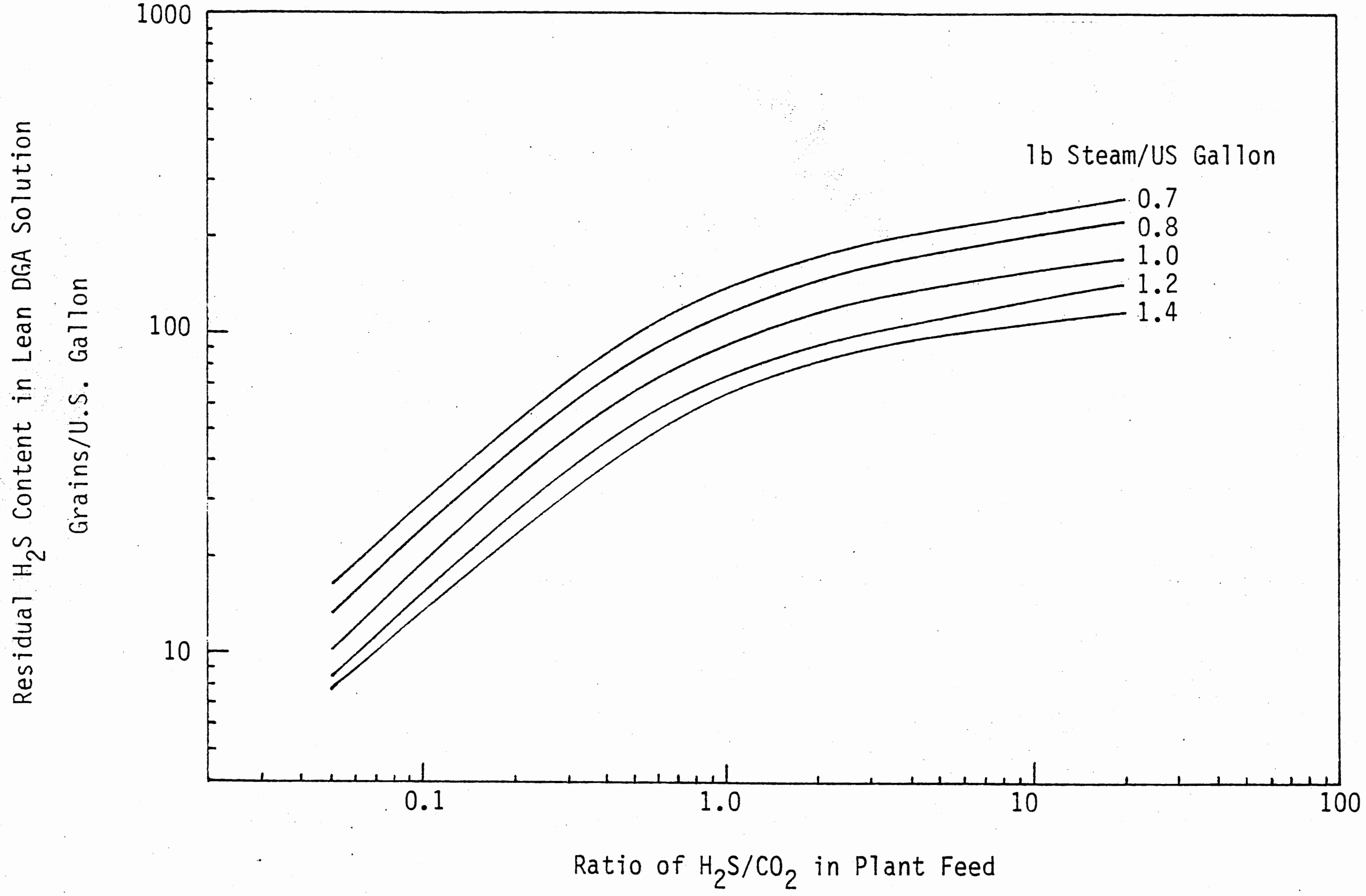


Figure 18. Effect of Acid Gas Ratio and Stripping Rate on Residual H_2S Content Over 50 Wt. % Lean DGA Solution.

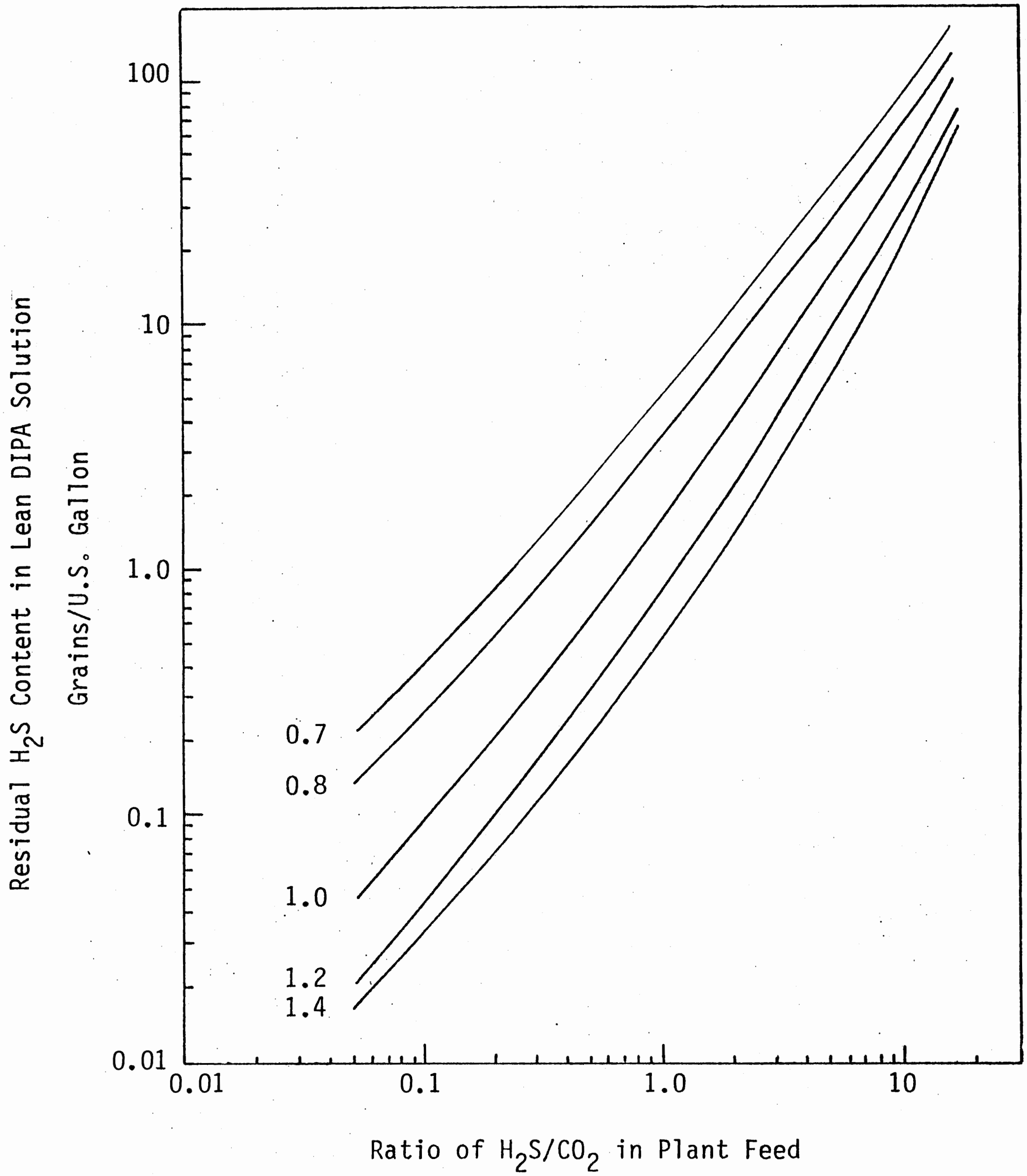


Figure 19. Effect of Acid Gas Ratio and Stripping Rate on Redisual H_2S Content Over 35 Wt. % Lean DIPA Solution.

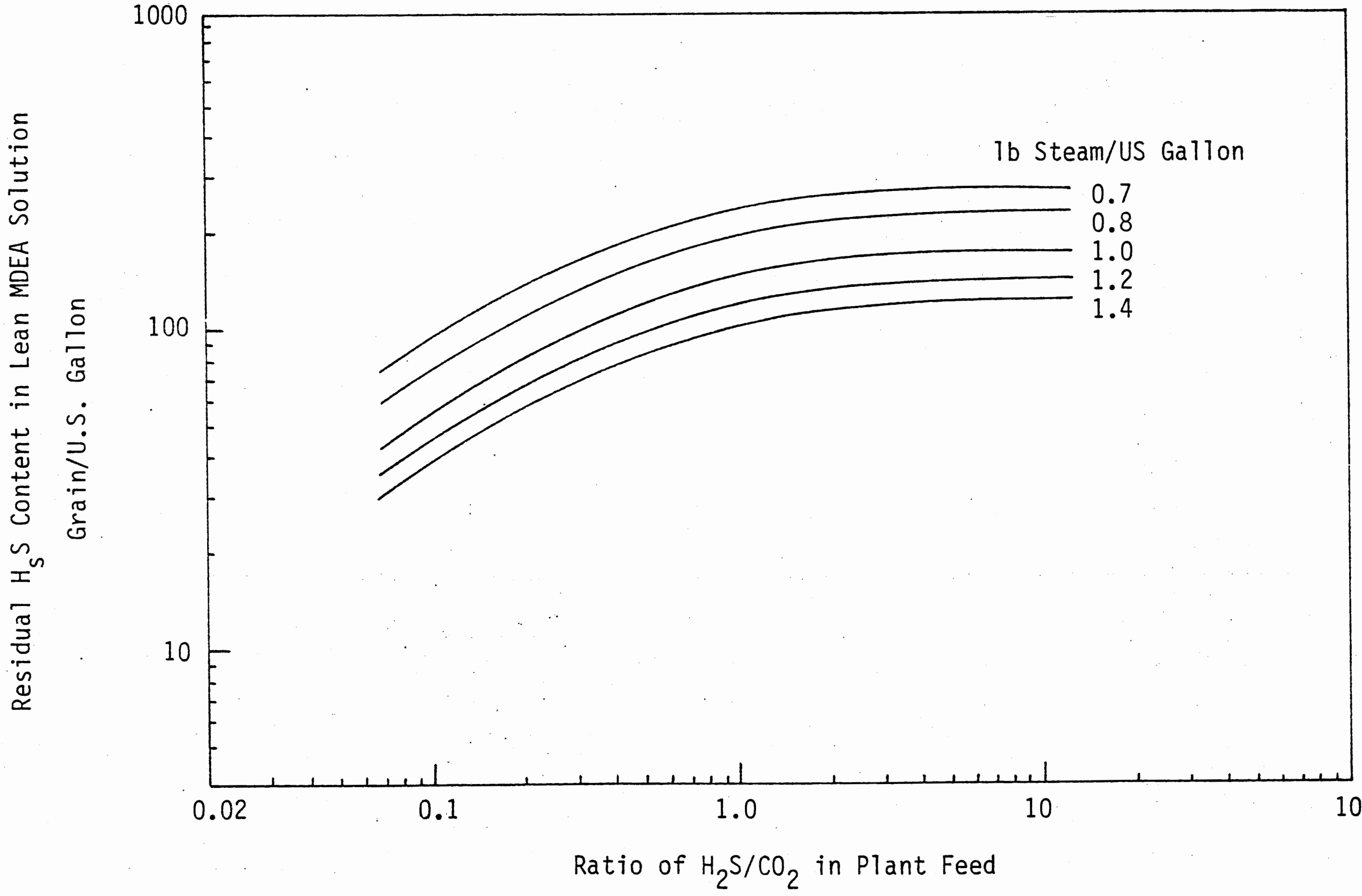


Figure 20. Effect of Acid Gas Ratio and Stripping Rate on Residual H_2S Content Over 45 Wt. % Lean MDEA Solution.

increased due to the CO_2 retained in the regenerated amine solution. Fitzgerald and Richardson also studied the effect of the H_2S to CO_2 ratio in the sour gas and the stripping steam rate on the retention of CO_2 in the regenerated amine solution. Comparison of the Fitzgerald and Richardson correlation and the results obtained by the proposed program for CO_2 residuals are shown in Figure 21 for MEA treating units. Figures 22 to Figure 25 show the effect of the ratio of H_2S to CO_2 in sour gas and the stripping steam rate on the CO_2 residual for DEA, DGA, DIPA and MDEA treating units at different amine concentrations. The CO_2 residual in the regenerated amine is only marginally influenced by the H_2S to CO_2 ratio in the sour gas when the ratio is small. Since the reaction rate of CO_2 and MDEA is very slow, Figure 25 is only used as a guide for sweetening processes using MDEA as a non-selective solvent for removing acid gases. Figure 16 to Figure 24 provide vital information to be used in process design for alkanolamine treating units.

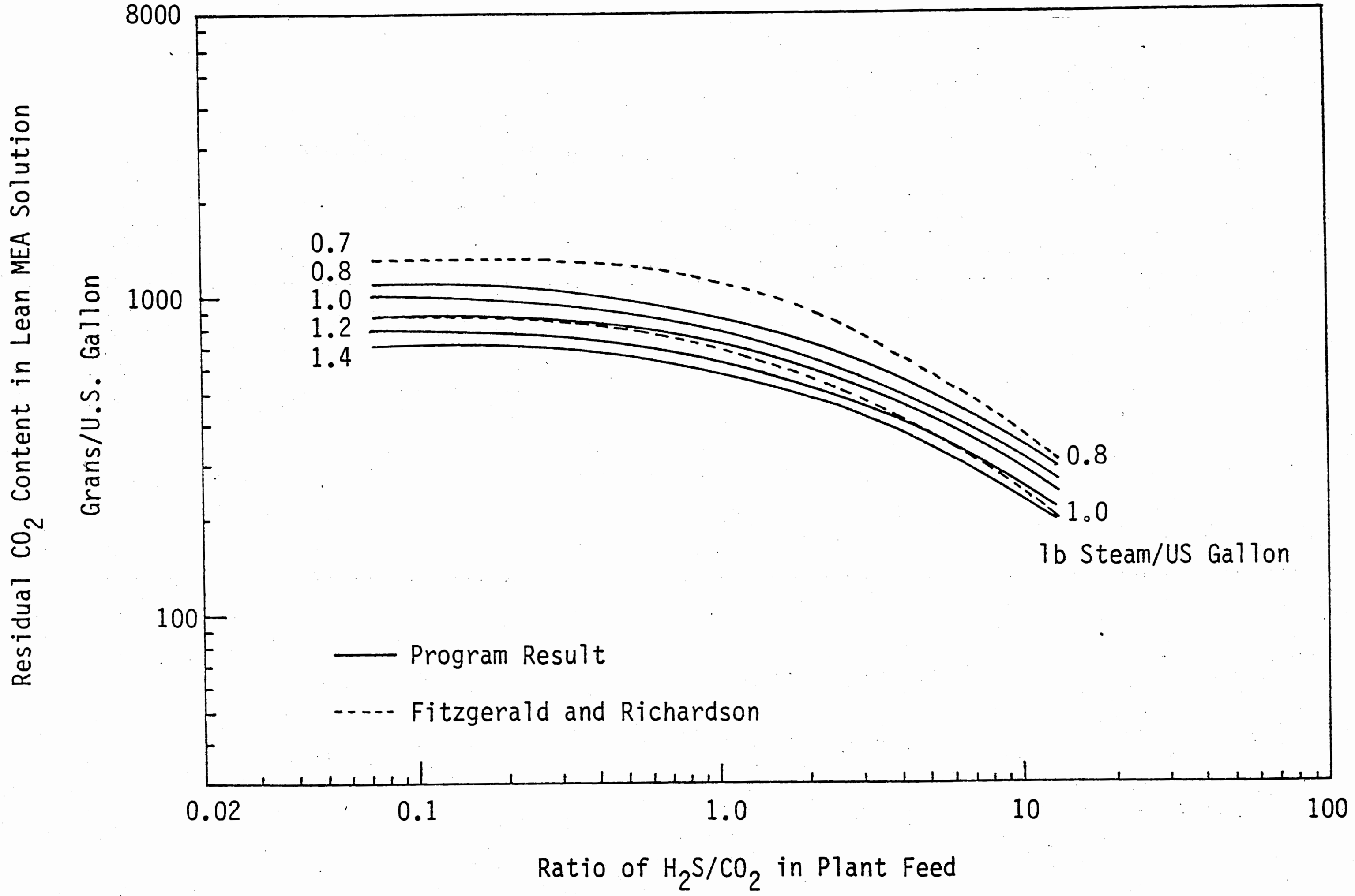


Figure 21. Effect of Acid Gas Ratio and Stripping Rate on Residual CO_2 Content Over 15 Wt. % Lean MEA Solution.

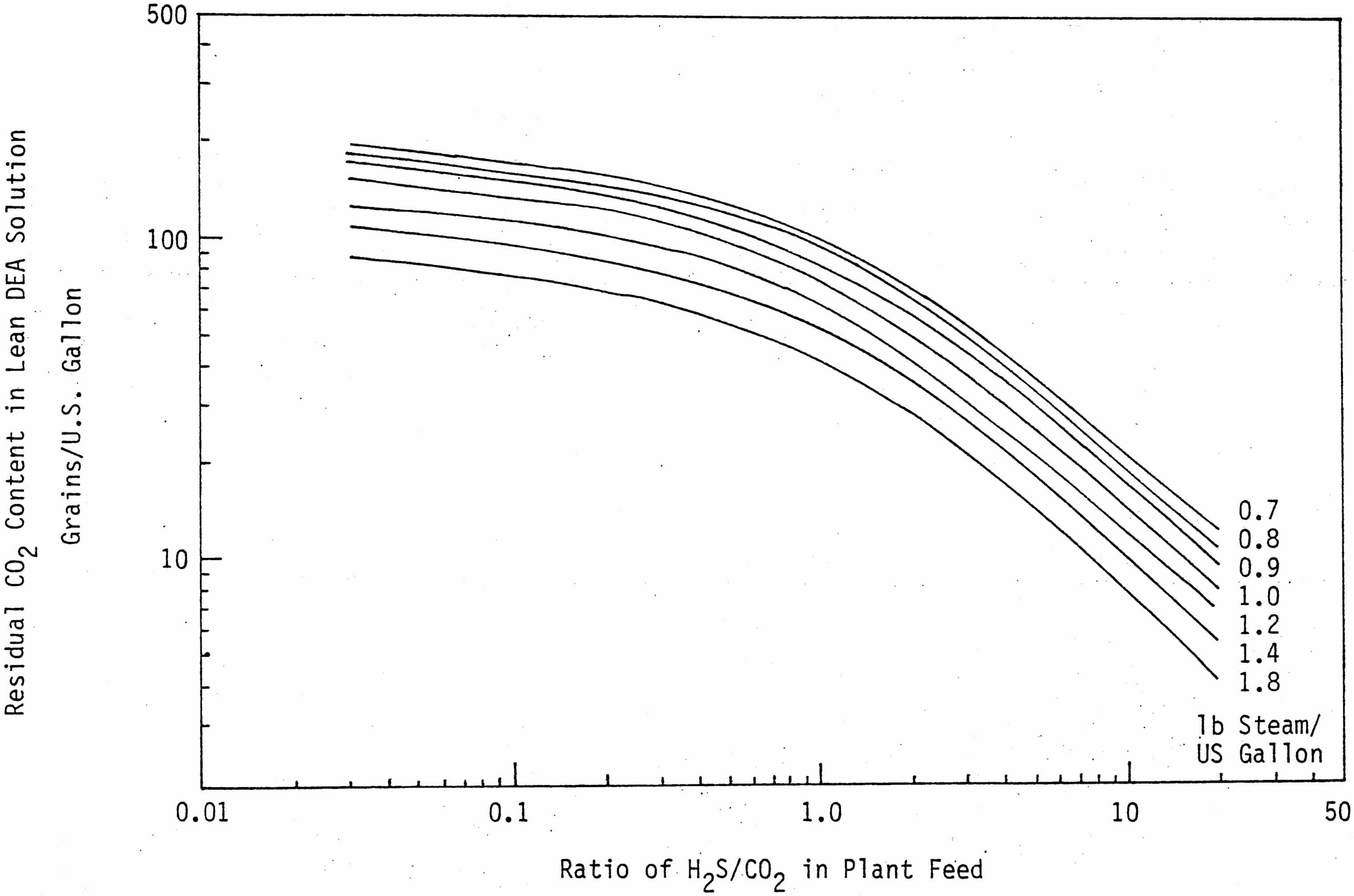


Figure 22. Effect of Acid Gas Ratio and Stripping Rate on Residual CO_2 Content Over 20 Wt. % Lean DEA Solution.

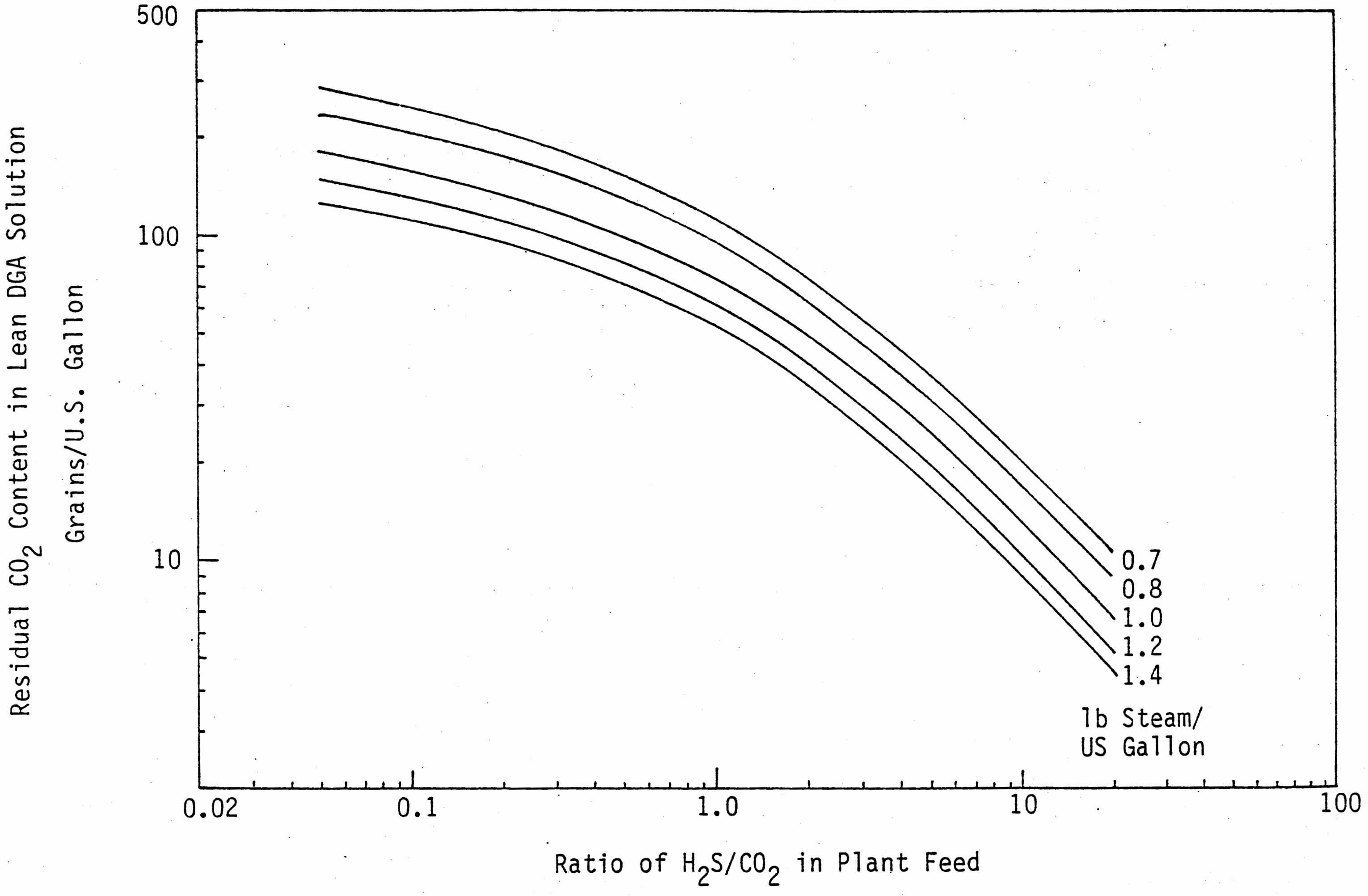


Figure 23. Effect of Acid Gas Ratio and Stripping Rate on Redisual CO_2 Content Over 50 Wt. % Lean DGA Solution.

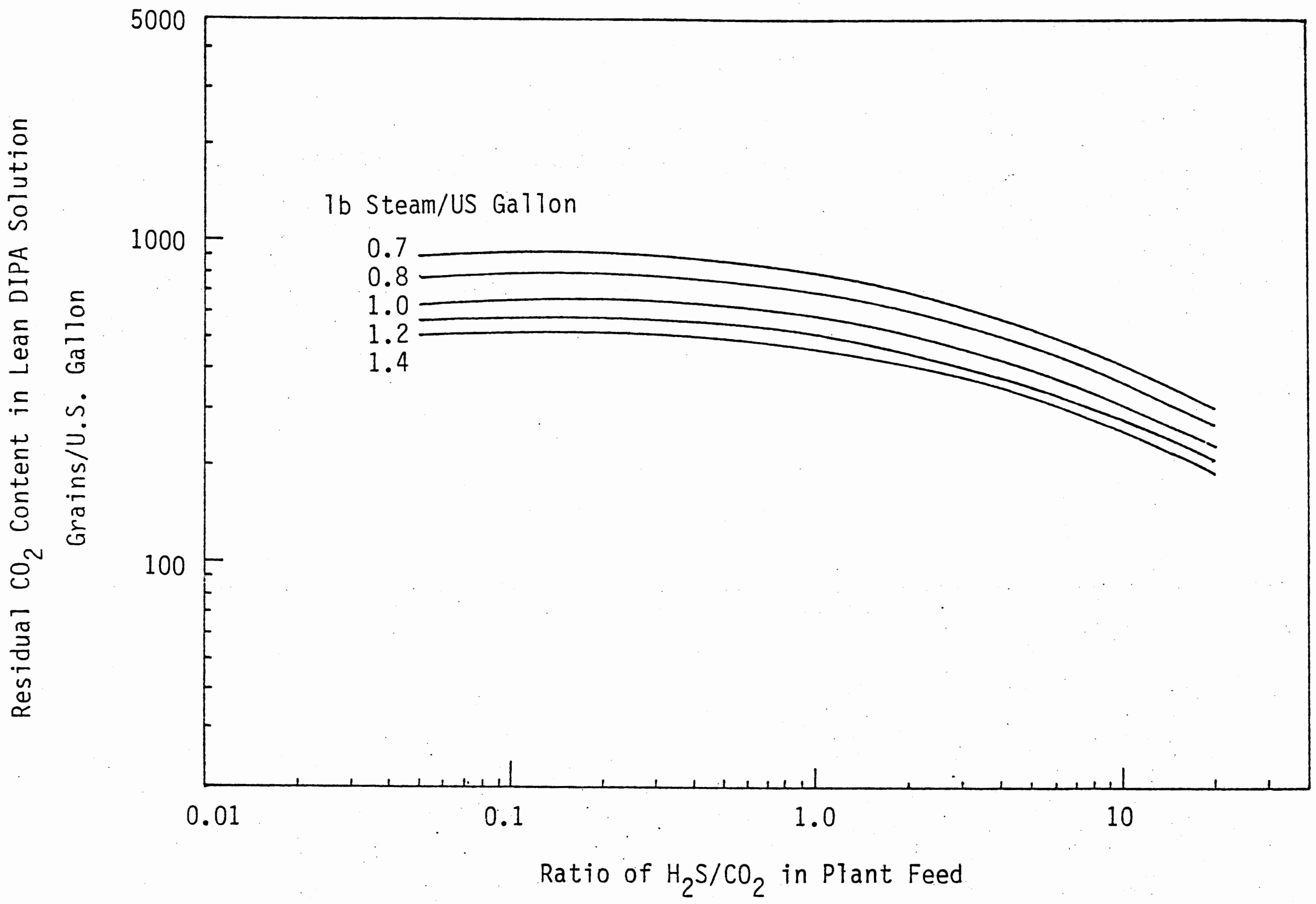


Figure 24. Effect of Acid Gas Ratio and Stripping Rate on Residual CO_2 Content Over 35 Wt. % Lean DIPA Solution.

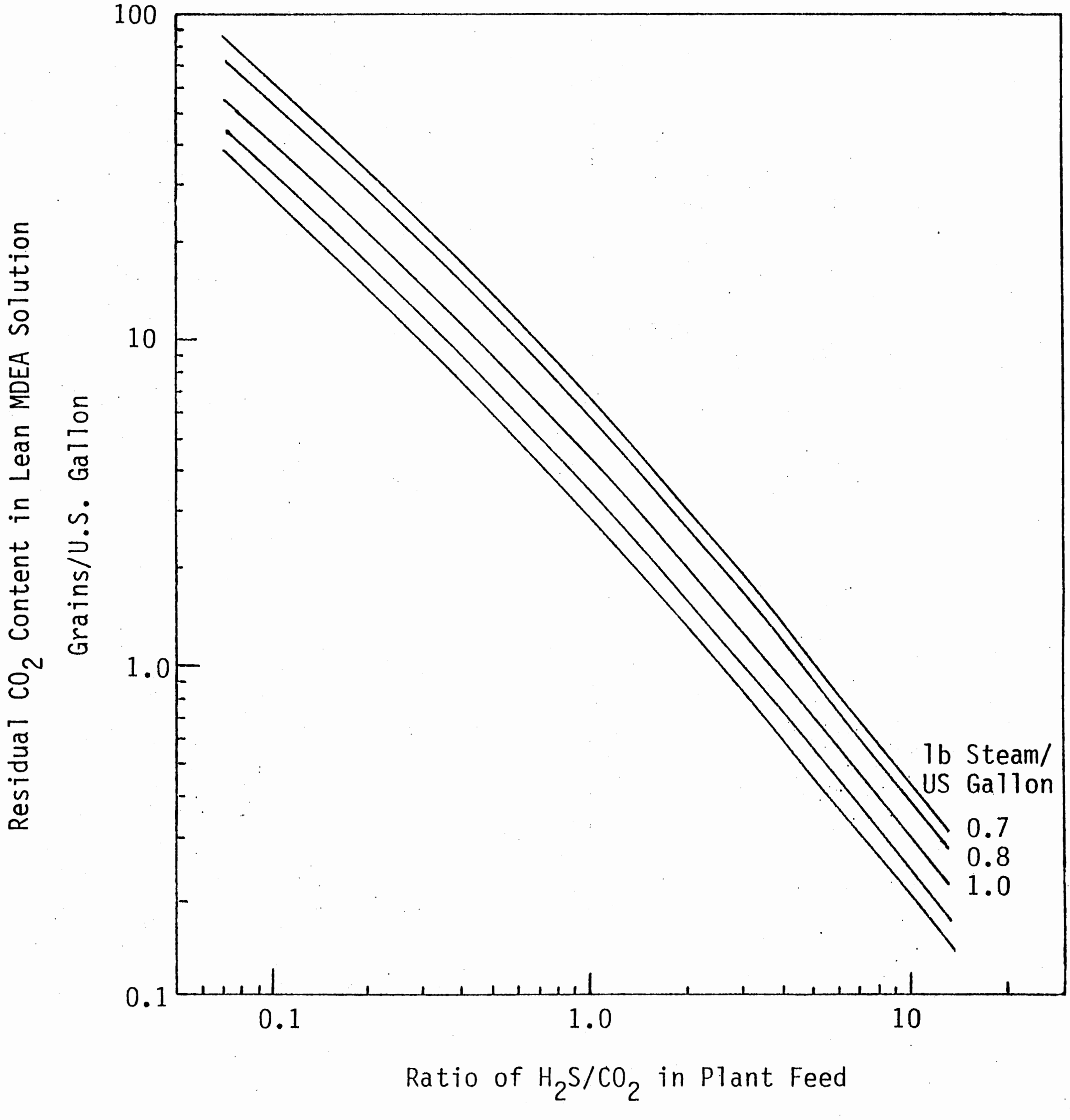


Figure 25. Effect of Acid Gas Ratio and Stripping Rate on Residual CO_2 Content Over 45 Wt. % Lean MDEA Solution.

Mass Transfer Coefficient and Murphree Vapor Stage Efficiency

The model proposed in Chapter IV to predict the Murphree vapor efficiency from the overall stage efficiency and the required number of equilibrium stages is useful to scale-up the design from the equilibrium stage column to the actual stage column. The proposed model is especially useful for non-selective amine sweetening processes in which both H_2S and CO_2 react with aqueous amine solutions very fast and the sweetening operations can be accurately described by equilibrium stage calculations.

In case of selective sweetening process such as using MDEA as a selective solvent, the reaction rate of H_2S with aqueous MDEA solution is appreciably faster than that of CO_2 with aqueous MDEA solution (5, 9). In order to account for the selectivity when modeling MDEA sweetening processes, it is necessary to incorporate the Murphree stage efficiency into equilibrium stage models for selective sweetening units (9, 56). The difficulty is to find the correct Murphree stage efficiencies to use.

The Murphree stage efficiency, E_{MV}, is a function of the mass transfer rate and mass transfer coefficients. A fundamental approach to estimating Murphree stage efficiency from mass transfer coefficients is given from the concept of local efficiency, E', and the number of transfer units. The relation between E_{MV} and E' has been established mathematically for different situations by Lewis (39). For the simplest case in which vapor and liquid are assumed completely mixed on the tray, the local and Murphree efficiencies are equal.

$$E_{MV} = E' \tag{5.1}$$

The local efficiency is related to the number of overall gas phase transfer units (25), N_{OG}, by

$$E' = 1 - \exp(-N_{OG}) \tag{5.2}$$

where N_{OG} can be expressed in terms of gas flow rate, G, depth of pool of liquid on plate, Z, total pressure, P, interfacial area, a, and overall gas phase mass transfer coefficient, K_{OG}, by

$$N_{OG} = K_{OG}\ aZP/G \tag{5.3}$$

The overall gas phase mass transfer coefficient and the individual gas and liquid mass transfer coefficients, k_G and k_L, are related (56) by

$$1 / K_{OG} = 1 / k_G + H / Ek_L \tag{5.4}$$

where H is the Henry constant and E is the enhancement factor due to the liquid phase chemical reaction.

By rearranging equations (5.1), (5.2), (5.3), and (5.4), the Murphree stage efficiency can be expressed as

$$E_{MV} = 1 - \exp \left\{ - [1/(1/k_G + H/EK_L)] (aZP/G) \right\} \quad (5.5)$$

Particular attention must be paid to the enhancement factor E which accounts for the effect of the chemical reactions that take place in the liquid phase. In certain cases, explicit values of E can be given. Danckwerts and Sharma (21) expressed the enhancement factor for absorption of CO_2 in primary and secondary amine solutions, in the case of pseudo-first order reaction, by

$$E = (1 + k_2 D M / k_L^2)^{1/2} \quad (5.6)$$

where D is the diffusivity of CO_2 dissolved in the liquid phase, M is the amine concentration, and k_2 is the second order chemical reaction kinetic constant for the reaction between amine and dissolved CO_2.

In the general case of simultaneous reaction of H_2S and CO_2, there are no explicit expressions for the enhancement factor E which are valid for all amine types of interest over the entire range of concentrations encountered. In addition, reliable data on kinetic rate constants, diffusivities, interfacial area, and individual mass transfer coefficients in liquid and gas phases are required. Essentially, equation (5.5) is a kinetic approach. Its application is subject to the above-mentioned uncertainties and available small amount of unreliable data.

The program proposed in this research is capable of simulating non-selective amine sweetening processes with equilibrium stage modeling. The equilibrium stage column can then be scaled-up to an actual stage column with the Murphree vapor stage efficiency predicted by the model proposed in Chapter III at specified overall stage efficiency. As for the simulation of selective processes using MDEA solution, the proposed program is also capable of describing the process in case reliable values of Murphree stage efficiencies are provided. The Murphree stage efficiency can be obtained either by prediction such as using equation (5.5) or specified from experience.

Since equation (5.5) is complicated and difficult to apply, empirical knowledge on the range of Murphree stage efficiencies is useful for design purposes. Table X shows the comparison of program results with design data using a commercial selective solvent to treat sour gas containing only CO_2 without H_2S (41). The commercial selective solvent is a MDEA based solution. The Murphree stage efficiencies of CO_2 are 7.4 and 8.7 percent with respect to amine circulation rates of 0.0716 and 0.0146 mole amine per mole feed gas for a 20 stage contactor as shown in Table X. The CO_2 capacities are 0.402 and 0.171 mole CO_2 per mole amine for plant 1 and plant 2 respectively. The average CO_2 Murphree stage efficiency used for the design of sweetening process of sour gas containing CO_2 without H_2S is about eight percent.

Table XI shows the comparison of program results with

TABLE X

COMPARISON OF THE PROGRAM RESULTS WITH DESIGN DATA OF MDEA SOLUTION TREATING SOUR GAS CONTAINING ONLY CO_2 WITHOUT H_2S

	Plant 1		Plant 2	
	Ref.(41)	Program	Ref.(41)	Program
Solution, wt %				
Selective Solvent	50	-	50	-
MDEA	-	50[a]	-	50[a]
Feed Gas,				
Flow rate, MMSCFD	3.0	3.0[a]	94.45	94.45[a]
Temperature, °F	100	100[a]	60	60[a]
CO_2, %	4.88	4.88[a]	0.30	0.30[a]
C_1^+, %	95.12	95.12[a]	99.70	99.70[a]
Outlet Gas,				
CO_2, %	2.0	2.002	0.050	0.0498
No. of Stages	-	20[a]	-	20[a]
Pressure, psig	1000	1000[a]	875	875[a]
Stage Efficiencies,				
CO_2, %	-	7.4[a]	-	8.7[a]
Circulation Rate, GPM	11.0	11.0[a]	71.0	71.0[a]
Lean Solution Analysis:				
Temperature, °F	-	100[a]	-	100[a]
CO2, mole/mole amine	0.01	0.01[a]	0.01	0.01[a]
Rich Solution Analysis:				
Temperature, °F	-	139.8	-	60.4
CO2, mole/mole amine	0.41	.4118	0.20	0.180
Top Tray Circulation Rate, mole amine/mole feed	.072[b]	.0716	.0132[b]	.0146

a. Specified values
b. Estimated from original references (41)

TABLE XI

COMPARISON OF THE PROGRAM RESULTS WITH DESIGN DATA OF MDEA TREATING PLANTS

	Plant 1		Plant 2		Plant 3		Plant 4	
	Ref.[b]	Program	Ref.[b]	Program	Ref.[b]	Program	Ref.[b]	Program
Solution, wt %								
Selective Solvent	50	-	50	-	50	-	50	-
MDEA	-	50[a]	-	50[a]	-	50[a]	-	50[a]
Feed Gas,								
Flow rate, MMSCFD	10	10[a]	25	25[a]	6.5	6.5[a]	8.3	8.3[a]
Temperature, °F	100	100[a]	110	110[a]	100	100[a]	100	100[a]
CO_2, %	12.	12.[a]	5.5	5.5[a]	1.83	1.83[a]	1.83	1.83[a]
H_2S, ppm	16.	16.[a]	16.	16.[a]	135.5	135.5[a]	135.5	135.5[a]
C_1+, %	88.	88.[a]	94.5	94.5[a]	-	-	-	-
Outlet Gas,								
CO_2, %	3.	3.027	3.	2.974	1.098	1.101	.9882	.9885
H_2S, ppm	< 4.	3.5	< 4.	4.0	< 4.	3.4	< 4.	3.3
No. of Stages	-	20[a]	-	20[a]	-	20[a]	-	20[a]
Pressure, psig	1100	1100[a]	900	900[a]	700	700[a]	700	700[a]
Stage Efficiencies,								
CO_2, %	-	6.4[a]	-	4.7[a]	-	2.6[a]	-	3.2[a]
H_2S, %	-	12.0[a]	-	43.0[a]	-	24.0[a]	-	35.0[a]

TABLE XI (Continued)

	Plant 1		Plant 2		Plant 3		Plant 4	
	Ref.[b]	Program	Ref.[b]	Program	Ref.[b]	Program	Ref.[b]	Program
Circulation rate, GPM	106	106[a]	86	86[a]	7.5	7.5[a]	8.3	8.3[a]
Lean Solution Analysis,								
Temperature, °F	-	100[a]	-	100[a]	120	120[a]	110	110[a]
CO_2, mole/mole amine	.01	.01[a]	.01	.01[a]	.01	.01[a]	.01	.01[a]
H_2S, mole/mole amine	-	.001[a]	-	.001[a]	-	.001[a]	-	.001[a]
Rich Solution Analysis,								
CO_2, mole/mole amine	.45	.44345	.39	.38596	.39	.3334	-	.347
H_2S, mole/mole amine	-	.00106	-	.00118	-	.0069	-	.055
Top Tray Circulation rate, mole amine/mole feed	.2045[c]	.2070	.0658[c]	.0672	.0193[c]	.0225	-	.0249

a. Specified values
b. From reference (41)
c. Estimated from reference (41)

design data of a selective solvent for simultaneous CO_2 and H_2S removal. The Murphree vapor stage efficiency of CO_2 ranges from 6.4 to 2.6 percent with respect to amine circulation rates from 0.207 to 0.022 mole amine per mole feed gas for a 20 stage contactor. The largest Murphree vapor stage efficiency of H_2S required to treat the sour gas to gas specification is 43.0 percent as shown in Table XI. However, the solution loadings of H_2S are uncertain for these plants, no attempt is made to plot empirical H_2S Murphree stage efficiency. The results of CO_2 Murphree stage efficiencies in Table VIII and Table XI are plotted in Figure 26 versus amine circulation rates and amine concentrations. Figure 26 can be used to estimate the CO_2 Murphree stage efficiency of simultaneous absorption processes for design purposes.

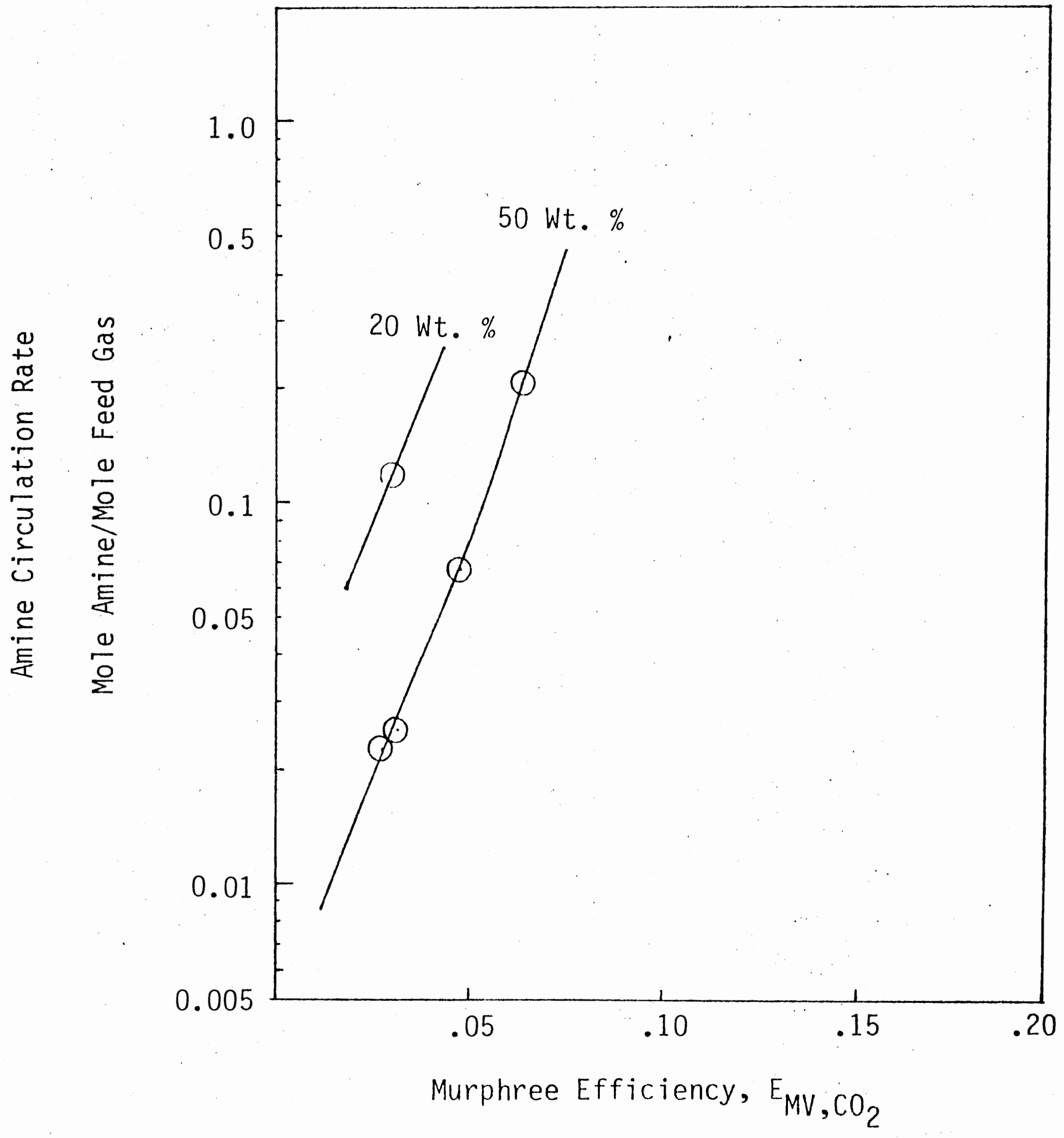


Figure 26. Murphree Stage Efficiencies Versus Amine Circulation Rates at 20 and 50 Wt. Percent MDEA Solution for Simultaneous Absorption.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

The following conclusions are drawn from the results of this study.

1. Rigorous calculation procedures for the stage-by-stage calculation of contactor and regenerator in amine processes have been established. Fast and converged results for steady-state operation have been obtained at a wide variety of operating conditions.
2. The reaction equilibrium model is capable of predicting the partial pressures of CO_2 and H_2S over alkanolamines. The application of the equilibrium model is well executed in the proposed program. A reaction equilibrium model for MDEA has been developed. Results of the MDEA equilibrium model agree well with experimental data.
3. An amine process simulation program has been completed with proposed calculation procedures for major amine sweetening units. Calculations for contactor, regenerator, flash tank, and amine-amine

heat exchanger have been tested satisfactorily against experimental or plant data. Process options such as sidefeed to contactor, intercooler, sidedraws of regenerator, condenser duty, reboiler duty, cycling of contactor and regenerator, and stage efficiencies are also included in the program. Flexible flow sheet design ability is provided by the proposed program for amine sweetening processes.

4. A model for the prediction of Murphree vapor stage efficiencies at specified overall stage efficiency has been developed. Satisfactory results have been obtained for the prediction of stage efficiencies. Knowledge of stage efficiencies is required to scale-up design from the equilibrium stage column to the actual stage column at specified overall stage efficiency.

Recommendations

The following recommendations are made based on the results of amine process simulation model in this study.

1. The reaction equilibrium model is the key to correctly describing the relationship of vapor-liquid equilibrium of the acid gases, water, and amine system. Since the prediction of partial pressures of acid gases is sensitive to the two fitted constants, K_1 and K_2, in the equilibrium

model, more reliable solubility data, especially on quaternary systems, are desired to improve the prediction of reaction equilibrium relationship.

2. In case of a selective sweetening process, it is desirable to incorporate the Murphree vapor stage efficiency into the equilibrium model as suggested in Chapter V. Further study on the knowledge of the Murphree vapor stage efficiencies is desired for the selective processes.

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APPENDICES

APPENDIX A

PHYSICAL PROPERTIES OF AMINE SOLUTIONS

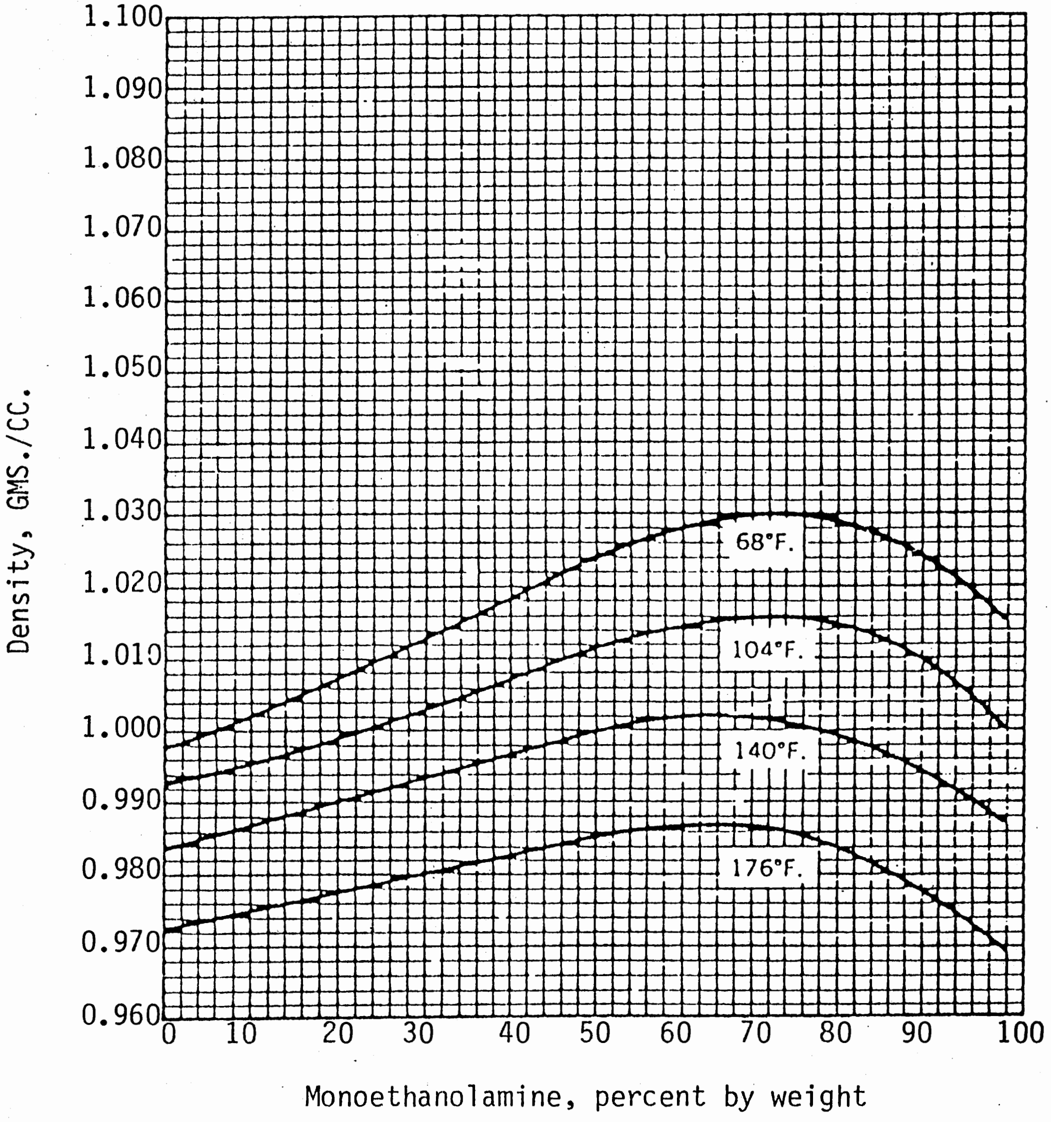

Figure 27. Density of MEA Solutions (40).

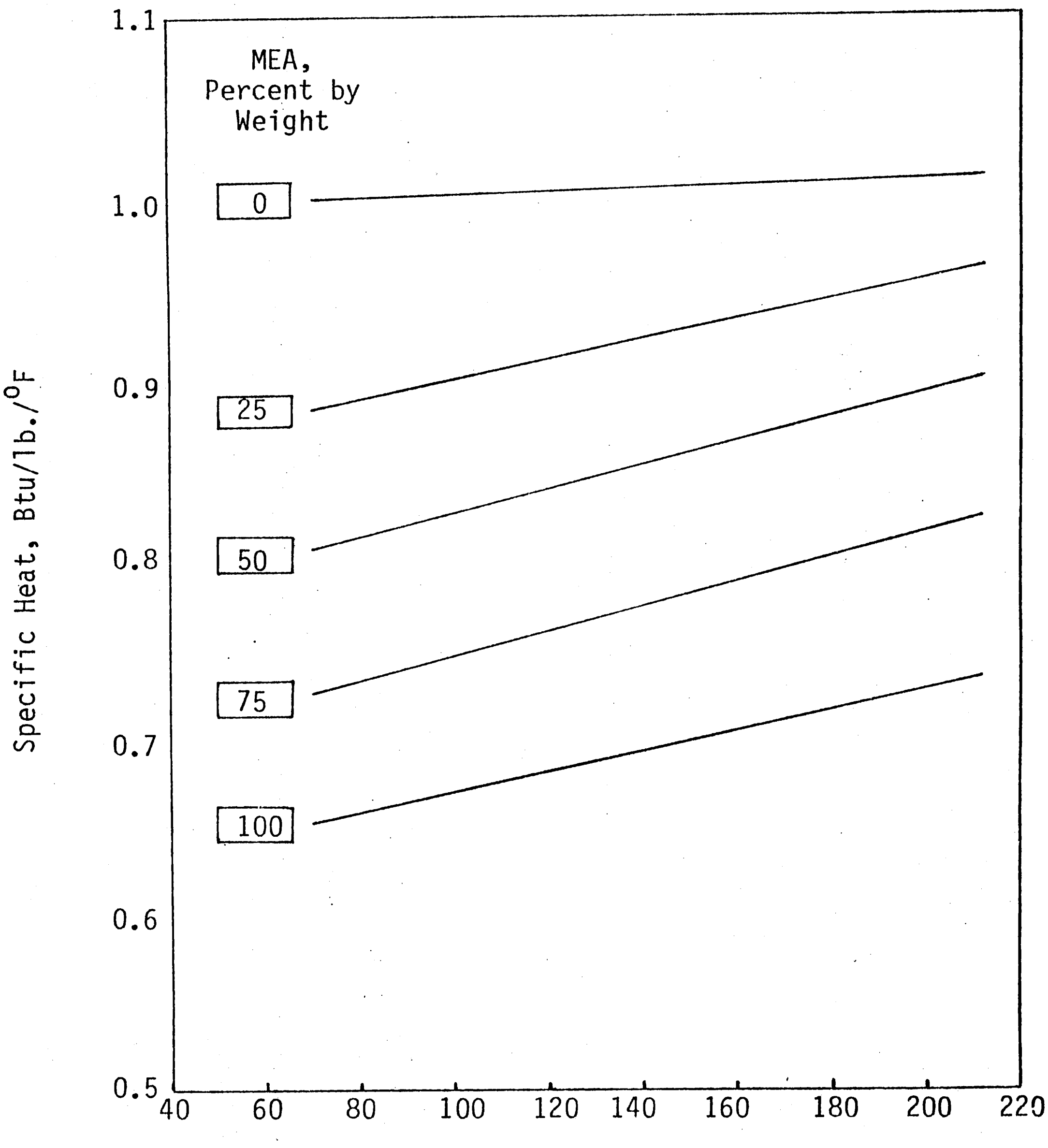

Figure 28. Specific Heat of MEA Solutions (40).

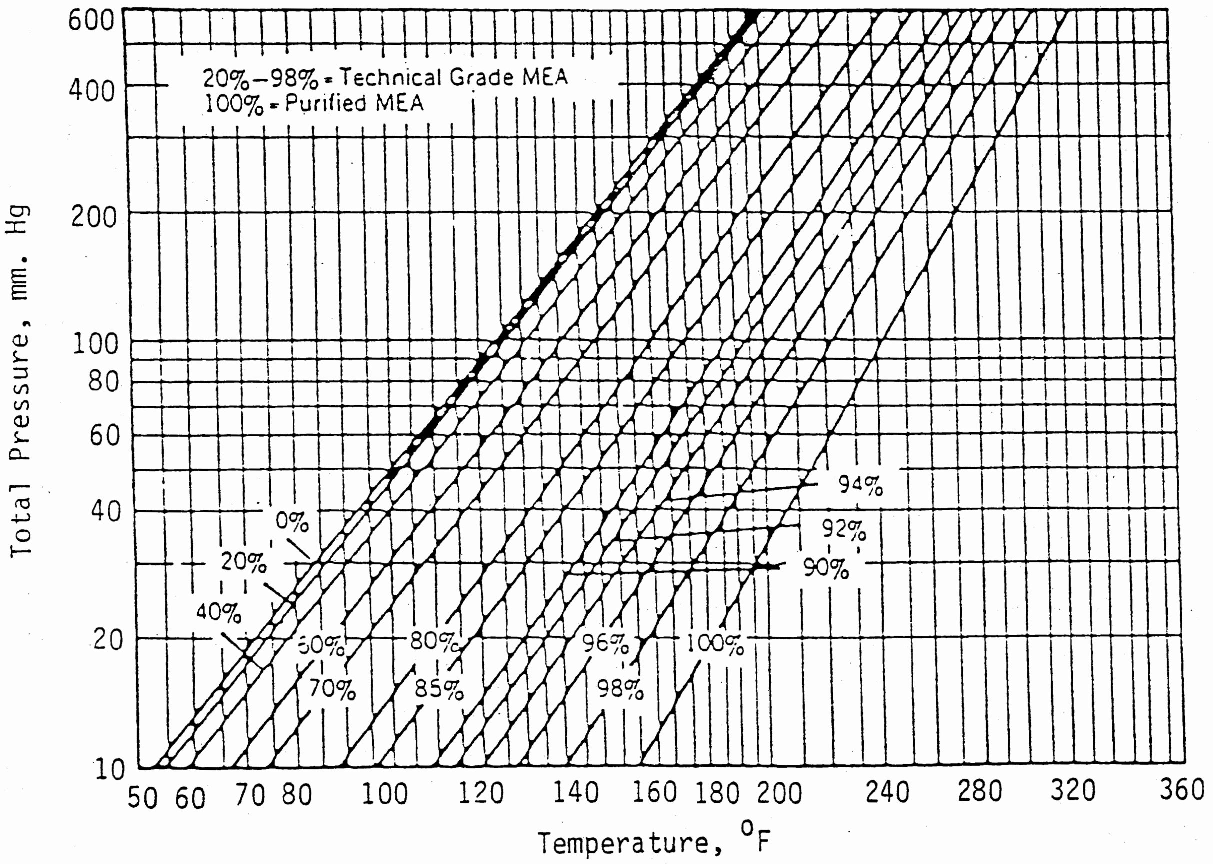

Figure 29. Vapor Pressure of MEA Solutions (40).

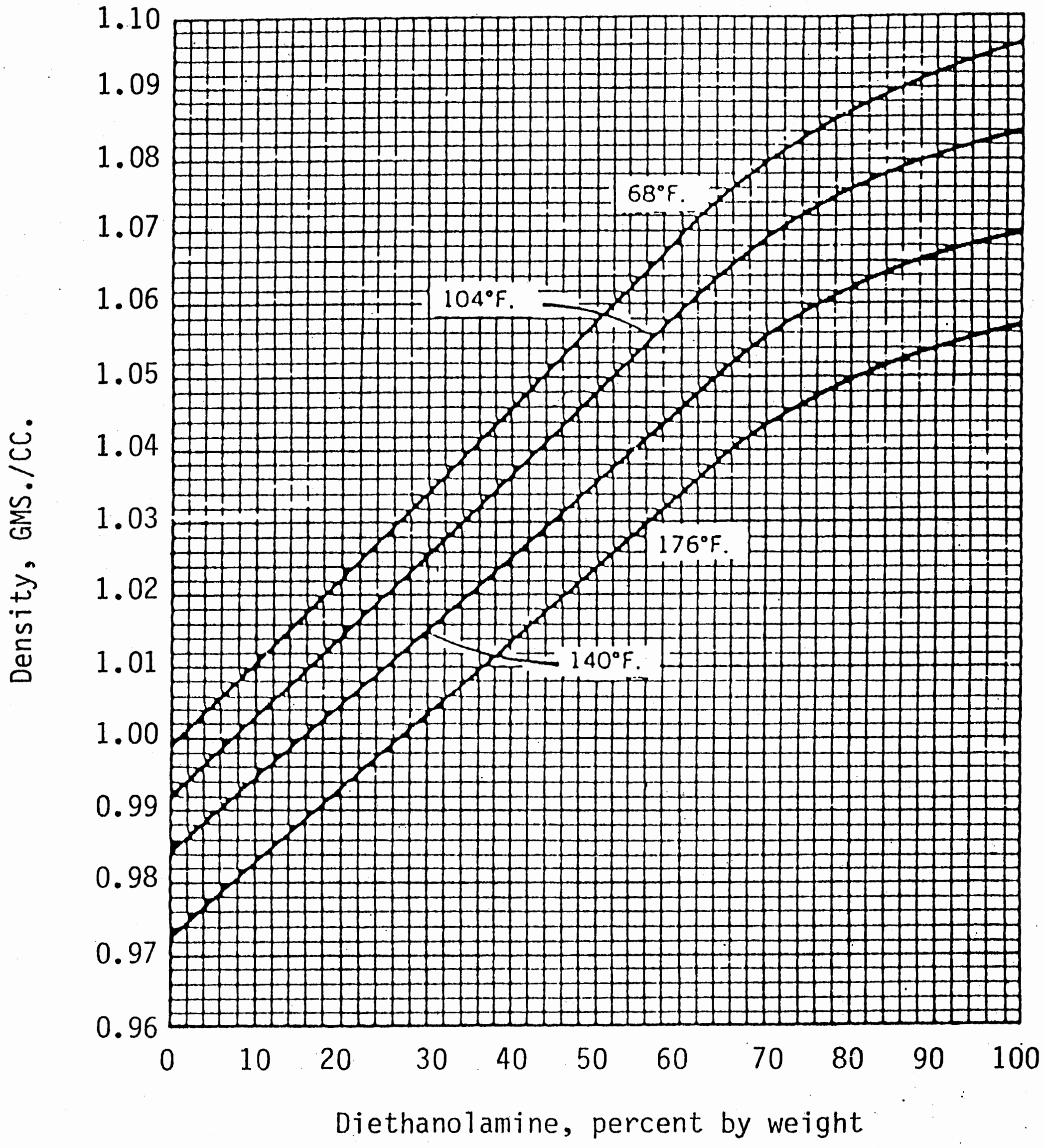

Figure 30. Density of DEA Solutions (40).

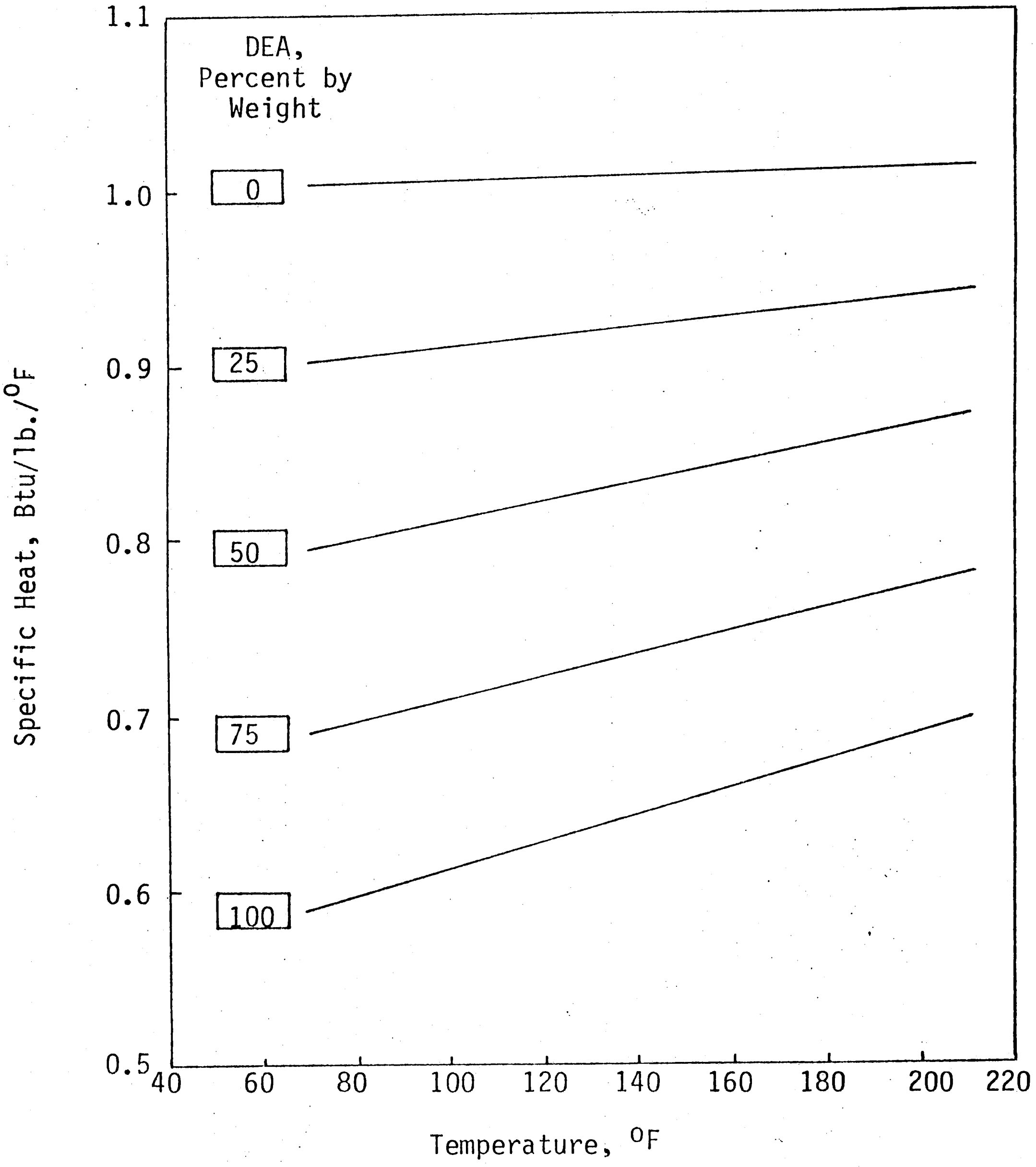

Figure 31. Specific Heat of DEA Solutions (40).

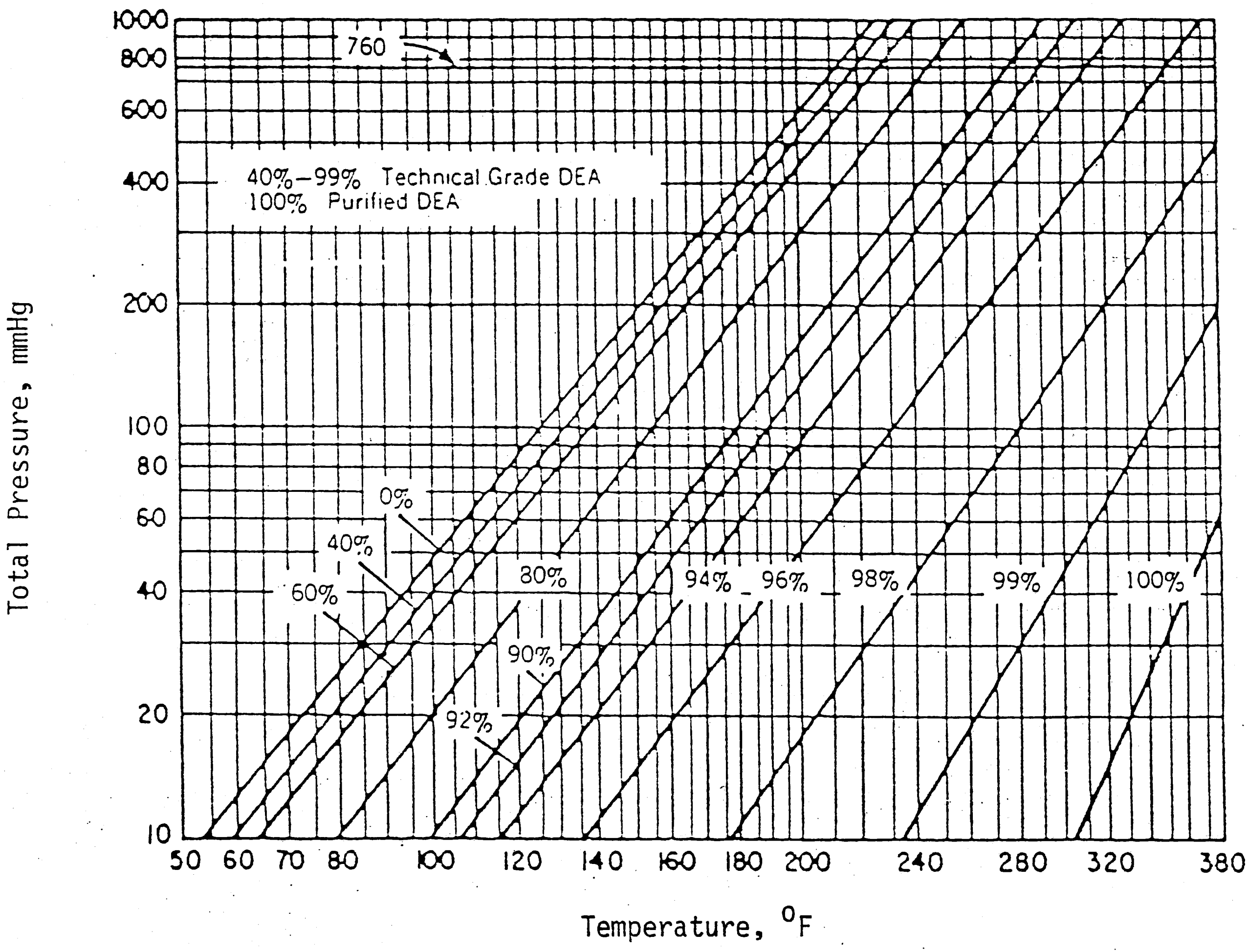

Figure 32. Vapor Pressure of DEA Solutions (40).

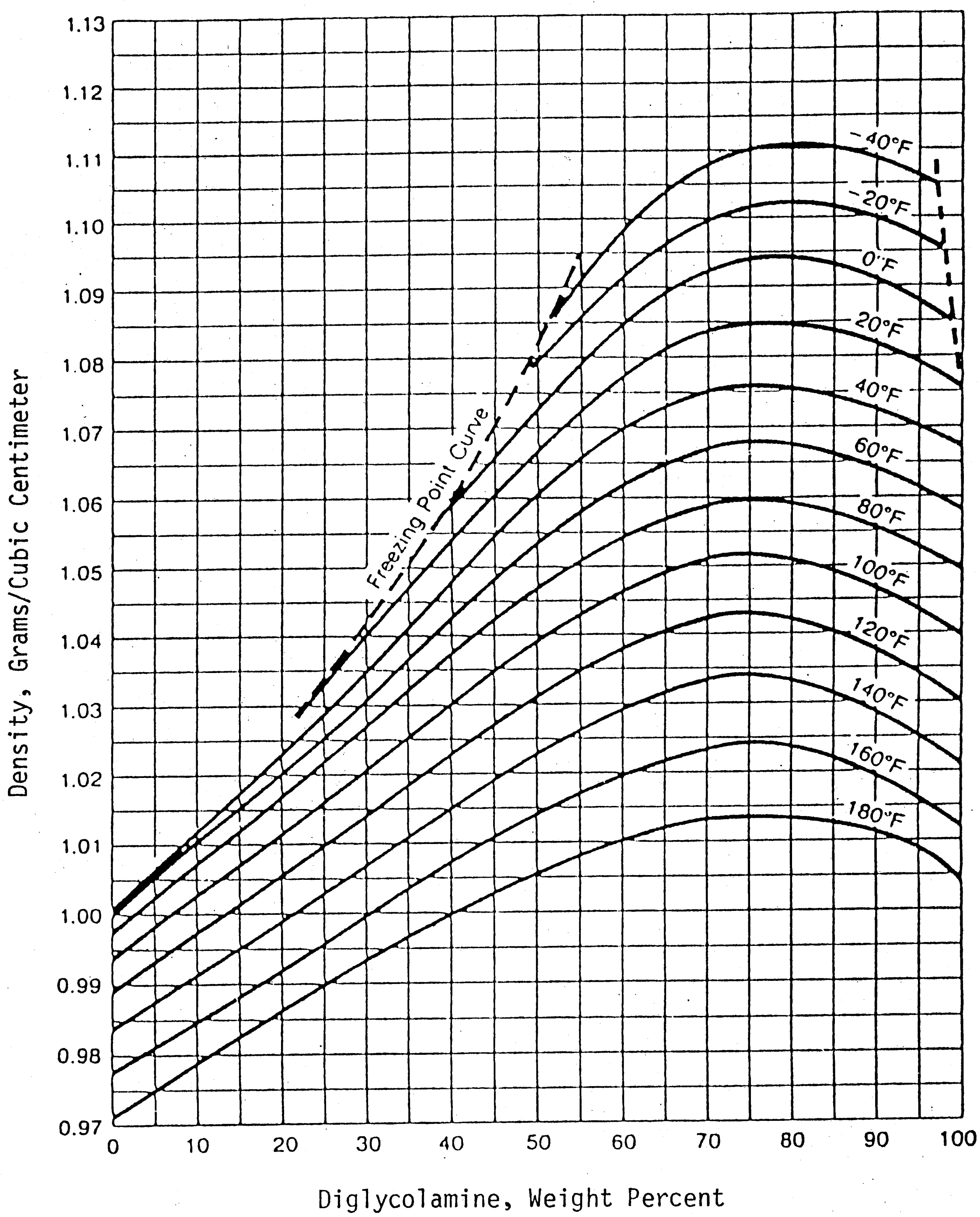

Figure 33. Density of DGA Solutions (40).

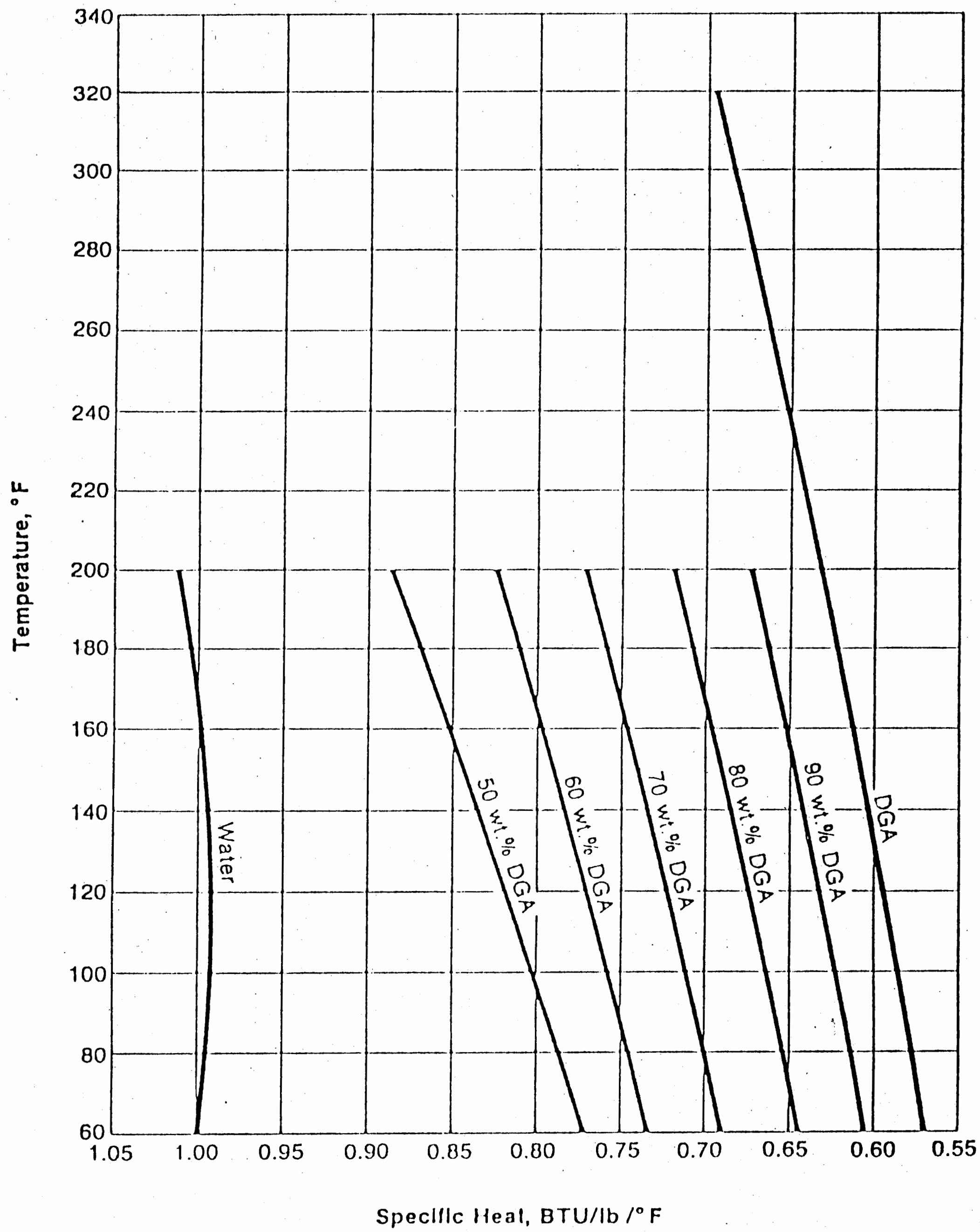

Figure 34. Specific Heat of DGA Solutions (40).

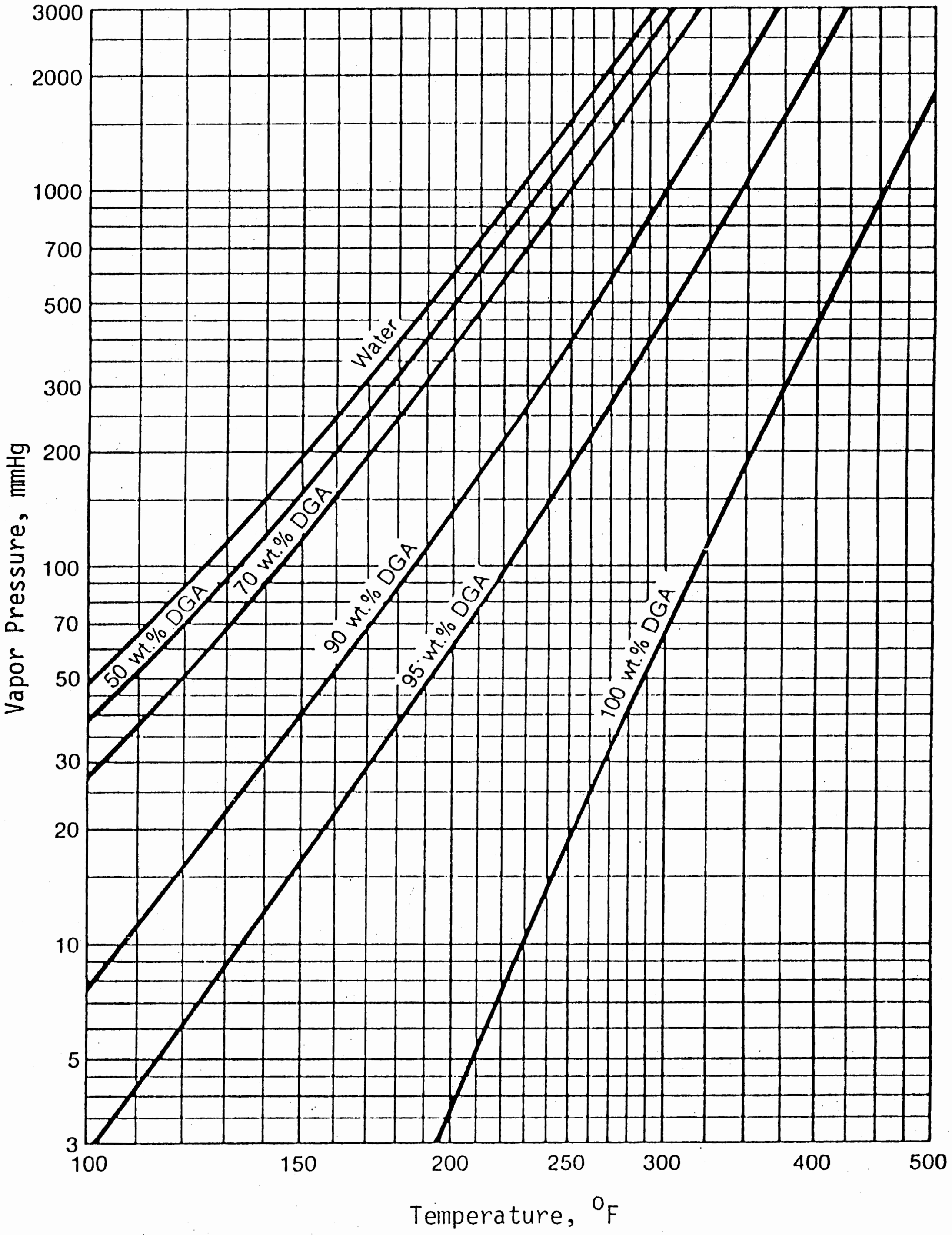

Figure 35. Vapor Pressure of DGA Solutions (40).

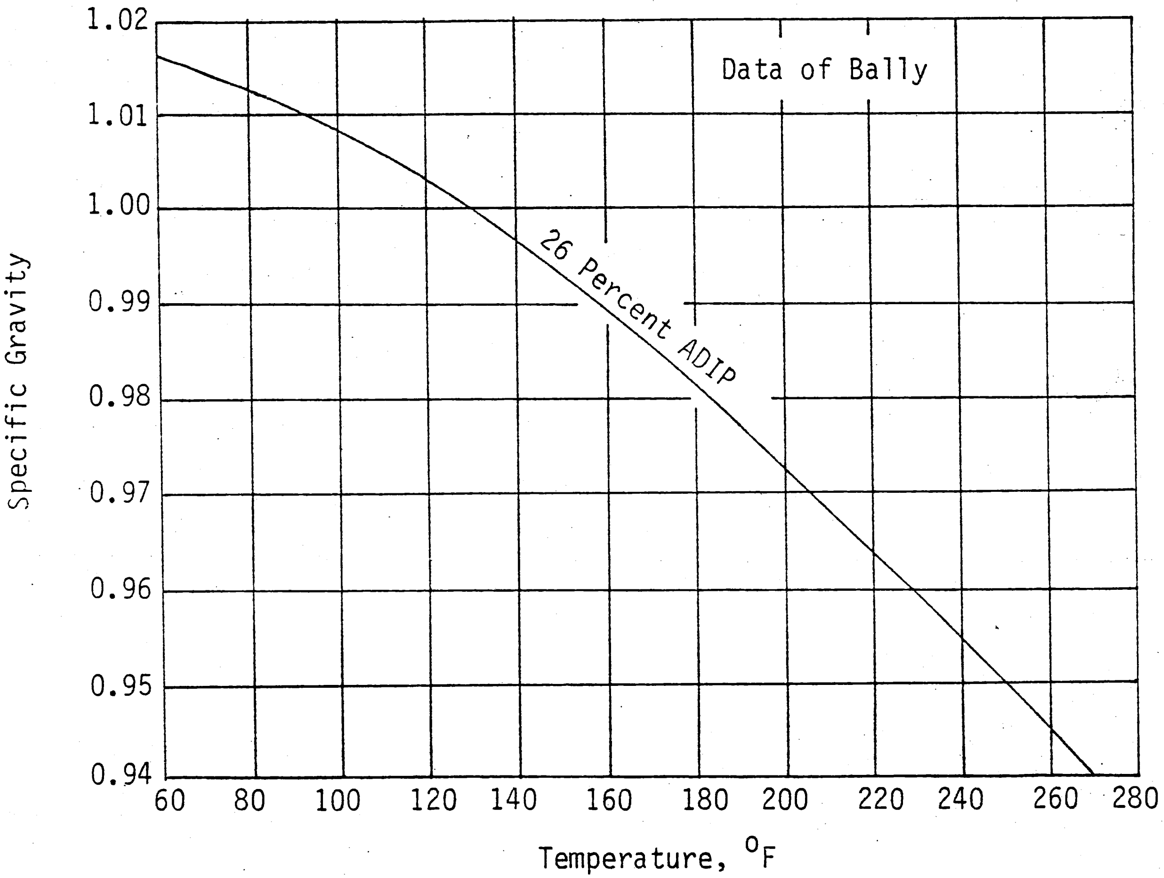

Figure 36. Specific Gravity of DIPA Based ADIP Solution (36).

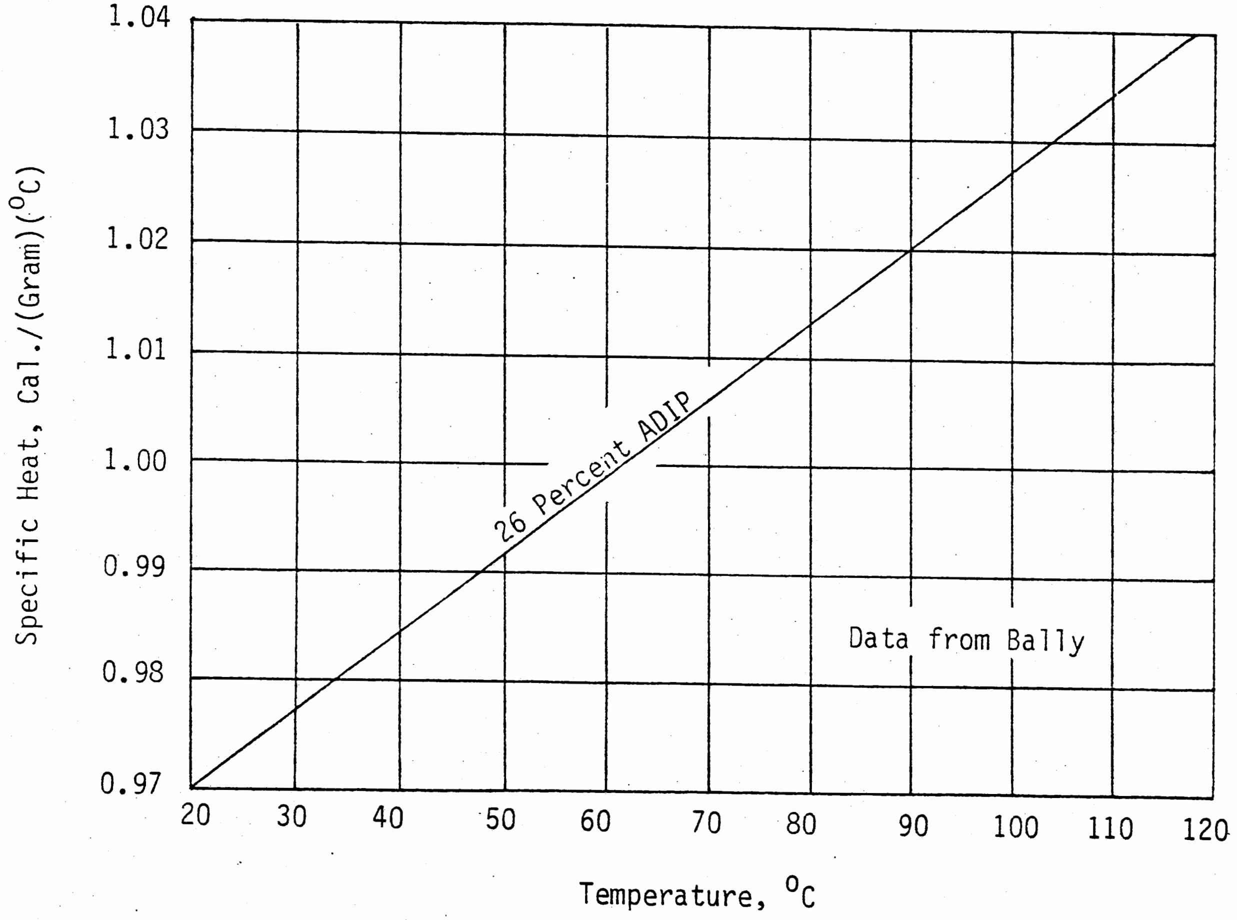

Figure 37. Specific Heat of DIPA Based ADIP Solution (36).

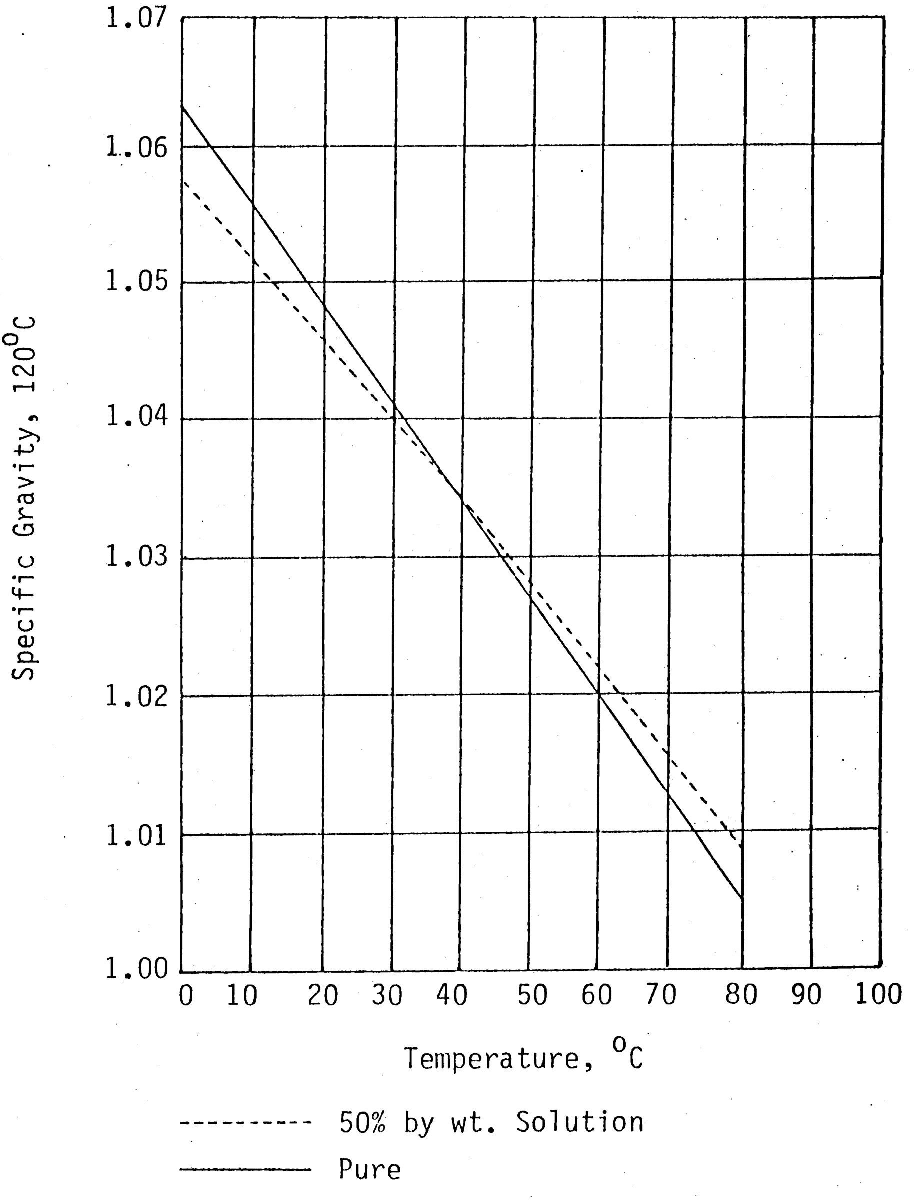

Figure 38. Specific Gravity of Pure and Aqueous MDEA Based UCARSOL HS Solvent 101 (36).

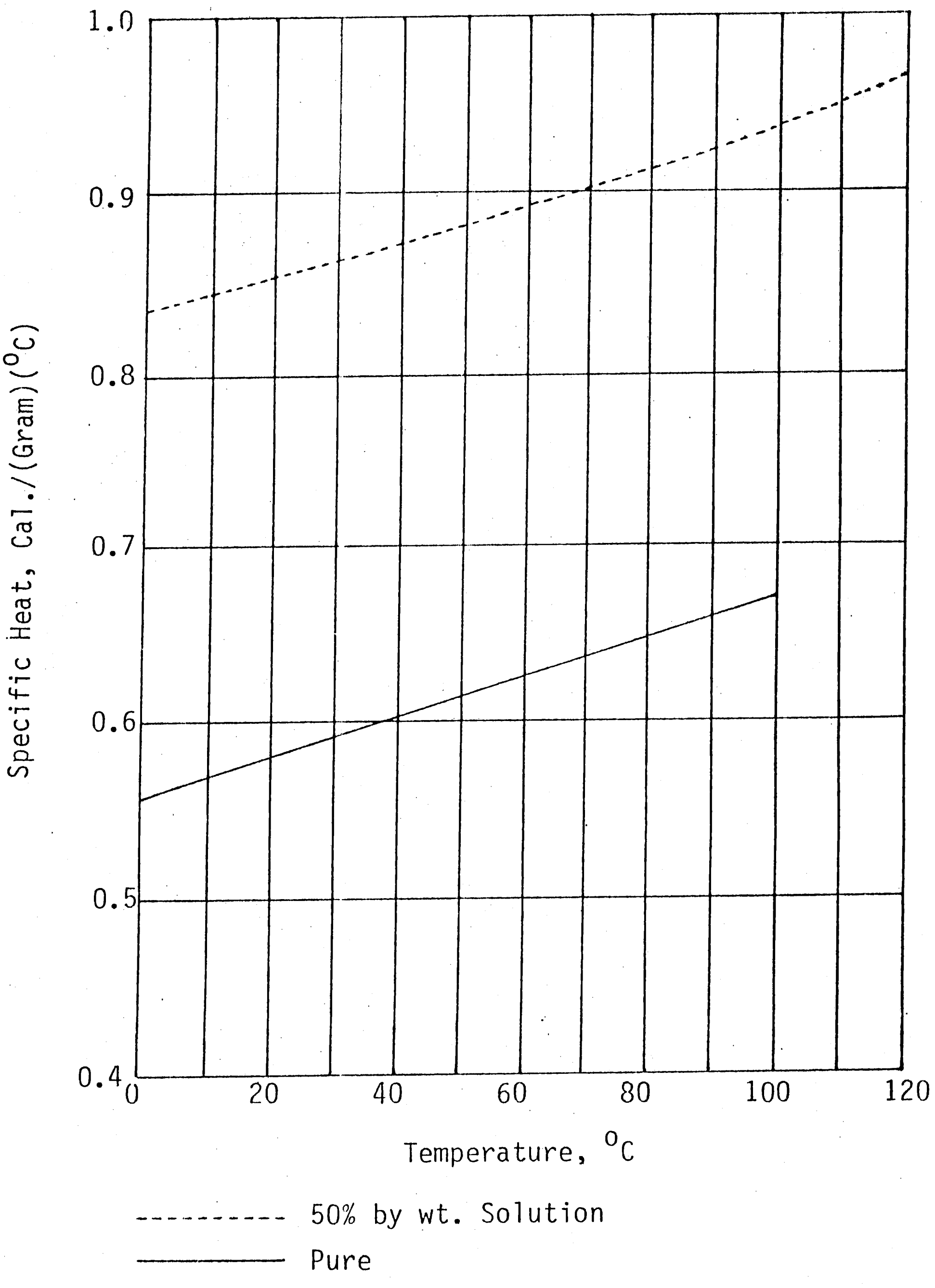

Figure 39. Specific Heat of Pure and Aqueous MDEA Based UCARSOL Solvent 101 (36).

APPENDIX B

COMPUTER PRINTOUT OF SAMPLE RUNS

```
                    AMINE PROCESS SIMULATION


                          James H. Loh
                               and
                        Robert N. Maddox



                        September 1, 1987

Would you like to see the HELP MENU? (Y/N)


Problem Title: SAMPLE RUN OF CONTACTOR CALCULATION
Calculation Option:
    0-Contactor,
    1-Regenerator,
    2-Contactor & Regenerator? . . . . . . . . . . . . . . . . .   0
Amine Type:0-MEA,1-DEA,2-DGA,3-DIPA,4-MDEA? . . . . . . . . . .   0
Amine Concentration Unit:0-Weight percent,1-Normality? . . . .   1
Concentration of Amine Solution? . . . . . . . . . . . . .     2.50
Reaction Equilibrium Model:
    0-Kent & Eisenberg,          (For MEA,DEA)
    1-Improved Kent & Eisenberg,(For MEA,DEA,DGA,DIPA)
    2-Smoothed Data,             (For MEA,DEA,DGA,DIPA)
    3-MDEA? . . . . . . . . . . . . . . . . . . . . . . . . . .   0
Output:0-Key Stages,1-All Stages? . . . . . . . . . . . . . . .   0
Temperature Unit:0-F,1-R,2-C,3-K? . . . . . . . . . . . . . . .   0
Pressure Unit:0-Psia,1-Atm,2-KPa,3-Bar,4-MPa,5-Kg/Cm2,6-MMHg?.   0
Energy Unit:0-BTU/Lb Mole Amine/F,1-KCal/Kg Mole Amine/C? . .   0
Gas Flow Rate Unit:0-Lb Mole/Min,1-Kg Mole/Min,
    2-MMSCF/D,3-MMSCM/D? . . . . . . . . . . . . . . . . . . .   0
Liquid Flow Rate Unit:0-Lb Mole Amine/Min,
    1-Kg Mole Amine/Min,2-Lb Amine Solution/Min,
    3-Kg Amine Solution/Min,4-GPM Amine Solution? . . . . . .   0
Steam Flow Rate Unit:0-Lb Mole/Min,1-Kg Mole/Min,2-Lb/Min,
    3-Kg/Min,4-GPM,5-Lb Steam/Gallon Amine Solution? . . . . .   0
Please enter data or press "ESC" key to accept all data.
```

```
Contactor Data:
    Pressure? Psia     . . . . . . . . . . . . . . .   500.0000
    Number of Stages?  . . . . . . . . . . . . . . .         20
    CO2 Murphree Vapor Efficiency, percent?  . . . .      30.00
    H2S Murphree Vapor Efficiency, percent?  . . . .      30.00
Sour Gas Data:
    Temperature? F . . . . . . . . . . . . . . . . .     100.00
    Flow Rate? Lb Mole/Min . . . . . . . . . . . . .     1.0000
    CO2 concentration, percent?  . . . . . . . . . .    3.00000
    H2S concentration, percent?  . . . . . . . . . .    1.00000
    CH4 concentration, percent?  . . . . . . . . . .   90.00000
    C2H6 concentration, percent? . . . . . . . . . .    5.00000
First Guess on Amine Circulation Rate:0-No,1-Yes?  .          0
    If yes, % Approach CO2 Equilibrium Loading?  . .       0.00
    If yes, % Approach H2S Equilibrium Loading?  . .       0.00
Lean Amine Solution Data:
    Temperature? F . . . . . . . . . . . . . . . . .     120.00
    Flow Rate? Lb Mole Amine/Min       . . . . . . .     0.1200
    Loading Unit:0-Mole/Mole Amine,1-Grain/Gallon? .          0
    CO2 loading? . . . . . . . . . . . . . . . . . .   0.010000
    H2S loading? . . . . . . . . . . . . . . . . . .   0.005000
Number of Sidecoolers? . . . . . . . . . . . . . . .          0
Number of Sidefeeds? . . . . . . . . . . . . . . . .          0
Estimate equivalent stage efficiencies:0-No,1-Yes? .          0
Please enter data or press "ESC" key to accept all data.
```

```
Sidecooler Data:
    Specify:0-Temperature Drop of Cooled Solution in Sidecooler,
            1-Temperature of Cooled Solution from Sidecooler?  . . . . .    0

    Sidecooler       Liquid Taken from       Temperature Drop
       No.              Stage No.            or Temperature
                    (Counted from Top)              F
        1                   0                     0.00
        2                   0                     0.00
        3                   0                     0.00

Sidefeed Data:

    Sidefeed    Liquid Added on     Sidefeed     Sidefeed          Loading
       No.         Stage No.       Temperature   Flow Rate     Mole/Mole Amine
               (Counted from Top)       F                      CO2        H2S
        1              0               0.00        0.0000    0.000000  0.000000
        2              0               0.00        0.0000    0.000000  0.000000
        3              0               0.00        0.0000    0.000000  0.000000
    (Sidefeed Flow Rate Unit:Lb Mole Amine/Min     )


Please enter data or press "ESC" key to accept all data.
```

```
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             SUMMARY OF CONTACTOR SPECIFICATIONS
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  TITLE -  SAMPLE RUN OF CONTACTOR CALCULATION


  EQUILIBRIUM REACTION MODEL - Kent and Eisenberg Model

  AMINE - MEA
  CONCENTRATION OF AMINE SOLUTION =  2.50 N (OR 15.13 WT PCT)

  TEMPERATURE OF FEED GAS =   100.00 DEG F
  GAS FEED FLOW RATE =          1.0000 Lb Mole/Min

  COMPOSITION OF FEED GAS -
                       CO2 =   3.0000 PCT
                       H2S =   1.0000 PCT
                       CH4 =  90.0000 PCT
                      C2H6 =   5.0000 PCT
                    OTHERS =   1.0000 PCT

  TEMPERATURE OF AMINE SOLUTION FEED =   120.00 DEG F
  LIQUID FEED FLOW RATE =         .120000 Lb Mole Amine/Min

  LOADINGS OF AMINE SOLUTION FEED -
       CO2 =   .010000 MOLE/MOLE AMINE(OR    64.26 GRAINS/GALLON SOLUTION)
       H2S =   .005000 MOLE/MOLE AMINE(OR    24.83 GRAINS/GALLON SOLUTION)
       H2O = 19.038230 MOLE/MOLE AMINE

  CONTACTOR PRESSURE =   500.00 Psia     (OR  25857.3800 MMHG)
  NUMBER OF STAGES SPECIFIED =  20
  VAPOR MURPHREE STAGE EFFICIENCY - CO2 =  30.00 PCT
                                    H2S =  30.00 PCT

  BASIS FOR CONTACTOR CALCULATION - 1.0 Lb MOLE FEED GAS/MIN
  TOP TRAY AMINE CIRCULATION RATE =   .120000 MOLE AMINE/MOLE FEED GAS

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RUNNING... PLEASE WAIT...

      ..... CONTACTOR CALCULATIONS CONVERGED AFTER  24 ITERATIONS .....
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                      STAGE --   1

  TITLE -  SAMPLE RUN OF CONTACTOR CALCULATION


  TEMPERATURE OF STAGE =   120.02 DEG F

  PARTIAL PRESSURE OF GAS ENTERING STAGE -
           CO2 =         .8852 MMHG (OR  .00003297 MOLE/MOLE FEED GAS)
           H2S =         .3125 MMHG (OR  .00001164 MOLE/MOLE FEED GAS)
           H2O =       83.1342 MMHG (OR  .00309660 MOLE/MOLE FEED GAS)

  PARTIAL PRESSURE OF GAS LEAVING STAGE -
           CO2 =         .6197 MMHG (OR  .00002308 MOLE/MOLE FEED GAS)
           H2S =         .2206 MMHG (OR  .00000822 MOLE/MOLE FEED GAS)
           H2O =       83.0947 MMHG (OR  .00309508 MOLE/MOLE FEED GAS)

  TOTAL ACID GASES REMOVED FROM FEED GAS -
           CO2 =   99.9231 PERCENT OF CO2 IN FEED GAS
           H2S =   99.9178 PERCENT OF H2S IN FEED GAS

  LOADINGS OF AMINE SOLUTION ENTERING STAGE -
              CO2 =   .010000 MOLE/MOLE AMINE
              H2S =   .005000 MOLE/MOLE AMINE

  LOADINGS OF AMINE SOLUTION LEAVING STAGE -
              CO2 =   .010082 MOLE/MOLE AMINE
              H2S =   .005029 MOLE/MOLE AMINE

  AMINE STAGE CIRCULATION RATE =  .120000 Lb MOLE AMINE/Lb MOLE FEED GAS

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                         STAGE --  20

  TITLE -  SAMPLE RUN OF CONTACTOR CALCULATION

  TEMPERATURE OF STAGE =    143.80 DEG F

  PARTIAL PRESSURE OF GAS ENTERING STAGE -
           CO2 =      774.2526 MMHG (OR  .03000000 MOLE/MOLE FEED GAS)
           H2S =      258.0842 MMHG (OR  .01000000 MOLE/MOLE FEED GAS)
           H2O =       48.9570 MMHG (OR  .00189694 MOLE/MOLE FEED GAS)

  PARTIAL PRESSURE OF GAS LEAVING STAGE -
           CO2 =      542.8143 MMHG (OR  .02086315 MOLE/MOLE FEED GAS)
           H2S =      183.6334 MMHG (OR  .00705798 MOLE/MOLE FEED GAS)
           H2O =      153.7929 MMHG (OR  .00591105 MOLE/MOLE FEED GAS)

  LOADINGS OF AMINE SOLUTION ENTERING STAGE -
              CO2 =   .183667 MOLE/MOLE AMINE
              H2S =   .063748 MOLE/MOLE AMINE

  LOADINGS OF AMINE SOLUTION LEAVING STAGE -
              CO2 =   .259808 MOLE/MOLE AMINE
              H2S =   .088265 MOLE/MOLE AMINE

  AMINE STAGE CIRCULATION RATE =  .120000 Lb MOLE AMINE/Lb MOLE FEED GAS

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    HYDROCARBON SOLUBILITY :

           GAS FEED COMPOSITION :
                 CH4 = 90.0000 PCT
                C2H6 =  5.0000 PCT

           HYDROCARBON IN RICH AMINE :
                 CH4 =  .008633 MOLE/MOLE AMINE
                C2H6 =  .000484 MOLE/MOLE AMINE

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Problem Title: SAMPLE RUN OF REGENERATOR CALCULATION
Calculation Option:
    0-Contactor,
    1-Regenerator,
    2-Contactor & Regenerator? . . . . . . . . . . . . . . . . .  1
Amine Type:0-MEA,1-DEA,2-DGA,3-DIPA,4-MDEA? . . . . . . . . .  1
Amine Concentration Unit:0-Weight percent,1-Normality? . . . .  0
Concentration of Amine Solution? . . . . . . . . . . . . .  20.00
Reaction Equilibrium Model:
    0-Kent & Eisenberg,          (For MEA,DEA)
    1-Improved Kent & Eisenberg,(For MEA,DEA,DGA,DIPA)
    2-Smoothed Data,             (For MEA,DEA,DGA,DIPA)
    3-MDEA? . . . . . . . . . . . . . . . . . . . . . . . . . .  0
Output:0-Key Stages,1-All Stages?  . . . . . . . . . . . . . .  0
Temperature Unit:0-F,1-R,2-C,3-K?  . . . . . . . . . . . . . .  0
Pressure Unit:0-Psia,1-Atm,2-KPa,3-Bar,4-MPa,5-Kg/Cm2,6-MMHg?.  0
Energy Unit:0-BTU/Lb Mole Amine/F,1-KCal/Kg Mole Amine/C?  . .  0
Gas Flow Rate Unit:0-Lb Mole/Min,1-Kg Mole/Min,
    2-MMSCF/D,3-MMSCM/D? . . . . . . . . . . . . . . . . . . .  0
Liquid Flow Rate Unit:0-Lb Mole Amine/Min,
    1-Kg Mole Amine/Min,2-Lb Amine Solution/Min,
    3-Kg Amine Solution/Min,4-GPM Amine Solution?  . . . . . .  0
Steam Flow Rate Unit:0-Lb Mole/Min,1-Kg Mole/Min,2-Lb/Min,
    3-Kg/Min,4-GPM,5-Lb Steam/Gallon Amine Solution? . . . . .  5
Please enter data or press "ESC" key to accept all data.


Regenerator Data:
    Top Pressure? Psia     . . . . . . . . . . . . . .      20.0000
    Bottom Pressure? Psia      . . . . . . . . . . . .      24.0000
    Number of Stages?  . . . . . . . . . . . . . . . .            4
    CO2 Murphree Vapor Efficiency, percent?  . . . . .        50.00
    H2S Murphree Vapor Efficiency, percent?  . . . . .        50.00
    Condenser Temperature? F . . . . . . . . . . . . .       120.00
    Saturated Steam Rate to Reboiler? Lb/Gal Soln  . .       1.0000
        At Steam Temperature?(Default 250F) F  . . . .       250.00
        Or Pressure?(Default 29.82 Psia) Psia      . .         0.00
Rich Amine Solution Data:
    Temperature? F . . . . . . . . . . . . . . . . . .       200.00
    Flow Rate? Lb Mole Amine/Min       . . . . . . . .       1.0000
    CO2 Loading, mole/mole amine?  . . . . . . . . . .     0.400000
    H2S Loading, mole/mole amine?  . . . . . . . . . .     0.300000

Number of Sidestreams Withdrawn? (Max. 3). . . . . . .            0
    Sidestream      Withdrawn From      Fraction of
    Withdrawn         Stage No.          Sidestream
       No.         (Counted from Top)      Removed
        1                 0                0.0000
        2                 0                0.0000
        3                 0                0.0000

Please enter data or press "ESC" key to accept all data.
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              SUMMARY OF REGENERATOR SPECIFICATIONS
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  TITLE -  SAMPLE RUN OF REGENERATOR CALCULATION


  EQUILIBRIUM REACTION MODEL - Kent and Eisenberg Model

  AMINE - DEA
  CONCENTRATION OF AMINE SOLUTION =  1.95 N (OR 20.00 WT PCT)

  REGENERATOR TOP PRESSURE =     20.00 Psia
           BOTTOM PRESSURE =     24.00 Psia

  TEMPERATURE OF AMINE SOLUTION FEED =   200.00 DEG F
  AMINE SOLUTION FEED RATE =       1.000000 Lb Mole Amine/Min

  LOADINGS OF AMINE SOLUTION FEED -
                CO2 =   .400000 MOLE/MOLE AMINE
                H2S =   .300000 MOLE/MOLE AMINE
                H2O = 23.364440 MOLE/MOLE AMINE

  SATURATED STEAM TO REBOILER AT  250.00 DEG F(OR     29.82 PSIA)
  STEAM RATE TO REBOILER =     1.0000 LB STEAM/GALLON AMINE SOLUTION
                     (OR =     3.4091 Lb MOLE STEAM/MIN)

  CONDENSER TEMPERATURE =   120.00 DEG F

  NUMBER OF STAGES SPECIFIED =   4
  VAPOR MURPHREE STAGE EFFICIENCY - CO2 =  50.00 PCT
                                    H2S =  50.00 PCT

  REGENERATOR CALCULATION BASIS - 1.0 Lb MOLE AMINE FEED/MIN

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RUNNING... PLEASE WAIT...

      ..... REGENERATOR CALCULATIONS CONVERGED AFTER   8 ITERATIONS .....
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                        STAGE --    1

  TITLE -  SAMPLE RUN OF REGENERATOR CALCULATION


  TEMPERATURE OF STAGE =   206.66 DEG F

  PRESSURE OF STAGE =      20.00 Psia

  CONCENTRATION OF LIQUID IN =  1.95 N (OR 20.00 WT PCT)
  LOADINGS OF LIQUID ENTERING STAGE -
              CO2 =    .400000 MOLE/MOLE AMINE
              H2S =    .300000 MOLE/MOLE AMINE
              H2O = 23.364440 MOLE/MOLE AMINE

  CONCENTRATION OF LIQUID OUT =  1.84 N (OR 18.87 WT PCT)
  LOADINGS OF LIQUID LEAVING STAGE -
          CO2 =   .222001 MOLE/MOLE AMINE(OR   1114.21 GRAINS/GAL SOLUTION)
          H2S =   .168286 MOLE/MOLE AMINE(OR    652.66 GRAINS/GAL SOLUTION)
          H2O = 25.106360 MOLE/MOLE AMINE

  TOTAL LIQUID LEAVING =       1.000000 Lb Mole Amine/Min
                 (OR =      26.496640 Lb MOLE LIQUID/MIN)

  VAPOR ENTERING STAGE PER MOLE RICH AMINE FEED -
                      CO2 =    .190303 MOLE/MOLE AMINE FEED
                      H2S =    .142599 MOLE/MOLE AMINE FEED
                    STEAM =   1.801212 MOLE/MOLE AMINE FEED

  VAPOR LEAVING STAGE PER MOLE RICH AMINE FEED -
                      CO2 =    .368302 MOLE/MOLE AMINE FEED
                      H2S =    .274313 MOLE/MOLE AMINE FEED
                    STEAM =   1.070513 MOLE/MOLE AMINE FEED

  TOTAL VAPOR LEAVING =        1.713128 Lb MOLE VAPOR/MIN

  ... CONDENSER DUTY =      1223861.00  BTU/HR
               (OR =        20397.69  BTU/Lb MOLE AMINE FEED/MIN)
               (OR =          313.24  BTU/GPM AMINE FEED)
        CONDENSER TEMPERATURE =   120.00 DEG F
        WATER CONDENSED = 1.011212 MOLE/MOLE AMINE FEED
        AMINE LOSS =  .00000000 MOLE/MOLE AMINE FEED
        AMINE CONDENSED =   .00002255 MOLE/MOLE AMINE FEED
                 (OR =   .013026 WEIGHT PERCENT OF REFLUX SOLUTION)
        REFLUX RATIO =   1.57 Lb MOLE CONDENSED WATER/Lb MOLE ACID GASES
               (OR =    .71 Lb CONDENSED WATER/Lb ACID GASES)

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                     STAGE --    4

  TITLE -  SAMPLE RUN OF REGENERATOR CALCULATION


  TEMPERATURE OF STAGE =   236.01 DEG F

  PRESSURE OF STAGE =     23.00 Psia

  CONCENTRATION OF LIQUID IN =  1.77 N (OR 18.19 WT PCT)
  LOADINGS OF LIQUID ENTERING STAGE -
              CO2 =   .084987 MOLE/MOLE AMINE
              H2S =   .068141 MOLE/MOLE AMINE
              H2O = 26.276520 MOLE/MOLE AMINE

  CONCENTRATION OF LIQUID OUT =  1.76 N (OR 18.07 WT PCT)
  LOADINGS OF LIQUID LEAVING STAGE -
          CO2 =   .057927 MOLE/MOLE AMINE(OR    290.73 GRAINS/GAL SOLUTION)
          H2S =   .047640 MOLE/MOLE AMINE(OR    184.76 GRAINS/GAL SOLUTION)
          H2O = 26.492520 MOLE/MOLE AMINE

  TOTAL LIQUID LEAVING =       1.000000 Lb Mole Amine/Min
                  (OR =       27.598090 Lb MOLE LIQUID/MIN)

  VAPOR ENTERING STAGE PER MOLE RICH AMINE FEED -
                    CO2 =   .026229 MOLE/MOLE AMINE FEED
                    H2S =   .021953 MOLE/MOLE AMINE FEED
                  STEAM =  3.187376 MOLE/MOLE AMINE FEED

  VAPOR LEAVING STAGE PER MOLE RICH AMINE FEED -
                    CO2 =   .053290 MOLE/MOLE AMINE FEED
                    H2S =   .042454 MOLE/MOLE AMINE FEED
                  STEAM =  2.971378 MOLE/MOLE AMINE FEED

  TOTAL VAPOR LEAVING =       3.067122 Lb MOLE VAPOR/MIN
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                        REBOILER

  TITLE -  SAMPLE RUN OF REGENERATOR CALCULATION


  TEMPERATURE OF STAGE =   239.45 DEG F

  PRESSURE OF STAGE =     24.00 Psia

  CONCENTRATION OF LIQUID IN =  1.76 N (OR 18.07 WT PCT)
  LOADINGS OF LIQUID ENTERING STAGE -
              CO2 =   .057927 MOLE/MOLE AMINE
              H2S =   .047640 MOLE/MOLE AMINE
              H2O = 26.492520 MOLE/MOLE AMINE

  CONCENTRATION OF LIQUID OUT =  1.96 N (OR 20.04 WT PCT)
  LOADINGS OF LIQUID LEAVING STAGE -
          CO2 =   .031698 MOLE/MOLE AMINE(OR    159.09 GRAINS/GAL SOLUTION)
          H2S =   .025687 MOLE/MOLE AMINE(OR     99.62 GRAINS/GAL SOLUTION)
          H2O = 23.305140 MOLE/MOLE AMINE

  TOTAL LIQUID LEAVING =       1.000000 Lb Mole Amine/Min
                   (OR =      24.362530 Lb MOLE LIQUID/MIN)

  VAPOR ENTERING STAGE PER MOLE RICH AMINE FEED -
                       CO2 =   .000000 MOLE/MOLE AMINE FEED
                       H2S =   .000000 MOLE/MOLE AMINE FEED
                     STEAM =   .000000 MOLE/MOLE AMINE FEED

  VAPOR LEAVING STAGE PER MOLE RICH AMINE FEED -
                       CO2 =   .026229 MOLE/MOLE AMINE FEED
                       H2S =   .021953 MOLE/MOLE AMINE FEED
                     STEAM =  3.187376 MOLE/MOLE AMINE FEED

  TOTAL VAPOR LEAVING =       3.235559 Lb MOLE VAPOR/MIN

  ... REBOILER DUTY  =     3480442.00  BTU/HR
                 (OR =       58007.37  BTU/Lb MOLE AMINE FEED/MIN)
                 (OR =         945.24  BTU/GPM AMINE FEED)
        SATURATED STEAM TO REBOILER AT   250.00 DEG F(OR     29.82 PSIA)
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Problem Title: SAMPLE RUN OF FLASH CALCULATION
Calculation Option:
    0-Flash Calculation,
    1-Amine-to-Amine Heat Exchanger,
    2-Sour Gas Equilibrium Calculation? . . . . . . . . . . .   0
Amine Type:0-MEA,1-DEA,2-DGA,3-DIPA,4-MDEA?  . . . . . . . .   0
Amine Concentration Unit:0-Weight percent,1-Normality? . . .   0
Concentration of Amine Solution? . . . . . . . . . . . . .  15.00
Reaction Equilibrium Model:
    0-Kent & Eisenberg,         (For MEA,DEA)
    1-Improved Kent & Eisenberg,(For MEA,DEA,DGA,DIPA)
    2-Smoothed Data,            (For MEA,DEA,DGA,DIPA)
    3-MDEA? . . . . . . . . . . . . . . . . . . . . . . . .   0

Temperature Unit:0-F,1-R,2-C,3-K?  . . . . . . . . . . . . .   0
Pressure Unit:0-Psia,1-Atm,2-KPa,3-Bar,4-MPa,5-Kg/Cm2,6-MMHg?.  0
Energy Unit:0-BTU/Lb Mole Amine/F,1-KCal/Kg Mole Amine/C?  . .  0
Liquid Flow Rate Unit:0-Lb Mole Amine/Min,
    1-Kg Mole Amine/Min,2-Lb Amine Solution/Min,
    3-Kg Amine Solution/Min,4-GPM Amine Solution?  . . . . . .  0



Please enter data or press "ESC" key to accept all data.
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Flash Calculation Data:
    Specify either Feed Temperature(default)? F . . . . .    200.00
        Or Flash Temperature? F . . . . . . . . . . . . .      0.00
    Flash Pressure? Psia         . . . . . . . . . . . . .   25.0000
    Feed Rate? Lb Mole Amine/Min       . . . . . . . . . .    1.0000
    CO2 Loading, mole/mole amine? . . . . . . . . . . . .  0.300000
    H2S Loading, mole/mole amine? . . . . . . . . . . . .  0.100000
    CH4 Loading, mole/mole amine? . . . . . . . . . . . .  0.080000
    C2H6 Loading, mole/mole amine?  . . . . . . . . . . .  0.002000








Please enter data or press "ESC" key to accept all data.
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                        FLASH TANK

  TITLE -  SAMPLE RUN OF FLASH CALCULATION


  EQUILIBRIUM REACTION MODEL - Kent and Eisenberg Model

  AMINE - MEA

  TEMPERATURE OF FEED =   200.00 DEG F
  FEED FLOW RATE =     1.000000 Lb Mole Amine/Min

  CONCENTRATION OF FEED -  2.48 N (OR 15.00 WT PCT )
  FEED ENTERING FLASH TANK -
                 CO2 LOADING =    .300000 MOLE/MOLE AMINE
                 H2S LOADING =    .100000 MOLE/MOLE AMINE
                 CH4 LOADING =    .080000 MOLE/MOLE AMINE
                C2H6 LOADING =    .002000 MOLE/MOLE AMINE
                 H2O LOADING =  19.235190 MOLE/MOLE AMINE

  PRESSURE OF FLASH TANK =    25.00 Psia
  TEMPERATURE OF FLASH TANK =   199.91 DEG F

  CONCENTRATION OF LEAVING LIQUID -  2.48 N (OR 15.00 WT PCT )
  LIQUID LEAVING FLASH TANK -
                 CO2 LOADING =    .299672 MOLE/MOLE AMINE
                 H2S LOADING =    .099688 MOLE/MOLE AMINE
                 CH4 LOADING =    .000204 MOLE/MOLE AMINE
                C2H6 LOADING =    .000005 MOLE/MOLE AMINE
                 H2O LOADING =  19.232640 MOLE/MOLE AMINE

  VAPOR LEAVING FLASH TANK -
                 CO2 =    .001075 MOLE/MOLE AMINE FEED
                 H2S =    .001177 MOLE/MOLE AMINE FEED
                 CH4 =    .079796 MOLE/MOLE AMINE FEED
                C2H6 =    .001995 MOLE/MOLE AMINE FEED
                 H2O =    .002542 MOLE/MOLE AMINE FEED
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Problem Title: SAMPLE RUN OF AMINE-AMINE HEAT EXCHANGER
Calculation Option:
    0-Flash Calculation,
    1-Amine-to-Amine Heat Exchanger,
    2-Sour Gas Equilibrium Calculation? . . . . . . . . . . .   1
Amine Type:0-MEA,1-DEA,2-DGA,3-DIPA,4-MDEA? . . . . . . . . .   0
Amine Concentration Unit:0-Weight percent,1-Normality? . . . .  0
Concentration of Amine Solution? . . . . . . . . . . . . . . 15.00
Reaction Equilibrium Model:
    0-Kent & Eisenberg,          (For MEA,DEA)
    1-Improved Kent & Eisenberg,(For MEA,DEA,DGA,DIPA)
    2-Smoothed Data,             (For MEA,DEA,DGA,DIPA)
    3-MDEA? . . . . . . . . . . . . . . . . . . . . . . . . .   0

Temperature Unit:0-F,1-R,2-C,3-K? . . . . . . . . . . . . . .   0
Pressure Unit:0-Psia,1-Atm,2-KPa,3-Bar,4-MPa,5-Kg/Cm2,6-MMHg?.  0
Energy Unit:0-BTU/Lb Mole Amine/F,1-KCal/Kg Mole Amine/C?  . .  0
Liquid Flow Rate Unit:0-Lb Mole Amine/Min,
    1-Kg Mole Amine/Min,2-Lb Amine Solution/Min,
    3-Kg Amine Solution/Min,4-GPM Amine Solution?  . . . . . .  0


Please enter data or press "ESC" key to accept all data.
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Amine Concentration of Hot and Cool stream:0-Same,1-No?         0
    If 1, Amine Concentration of Hot stream? . . . . . .   0.0000
    If 1, Amine Concentration of Cool stream?  . . . . .   0.0000

Hot Stream Data:
    Inlet Temperature? F . . . . . . . . . . . . . . . .   240.00
    Flow Rate? Lb Mole Amine/Min       . . . . . . . . .   1.0000
    CO2 loading, mole/mole amine?  . . . . . . . . . . . 0.100000
    H2S loading, mole/mole amine?  . . . . . . . . . . . 0.020000

Cool Stream Data:
    Inlet Temperature? F . . . . . . . . . . . . . . . .   130.00
    Outlet Temperature? F  . . . . . . . . . . . . . . .   190.00
    Flow Rate? Lb Mole Amine/Min       . . . . . . . . .   1.0000
    CO2 loading, mole/mole amine?  . . . . . . . . . . . 0.300000
    H2S loading, mole/mole amine?  . . . . . . . . . . . 0.100000



Please enter data or press "ESC" key to accept all data.
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                   AMINE-AMINE HEAT EXCHANGER

  TITLE -  SAMPLE RUN OF AMINE-AMINE HEAT EXCHANGER


  AMINE - MEA

  HOT STREAM -

    INLET TEMPERATURE =   240.00 DEG F
    OUTLET TEMPERATURE =   180.79 DEG F

    CONCENTRATION OF AMINE SOLUTION =  2.48 N (OR 15.00 WT PCT )

    FLOW RATE =       1.000000 Lb Mole Amine/Min
    LOADINGS -
                 CO2 LOADING =    .100000 MOLE/MOLE AMINE
                 H2S LOADING =    .020000 MOLE/MOLE AMINE
                 H2O LOADING =  19.235190 MOLE/MOLE AMINE

  COOL STREAM -

    INLET TEMPERATURE =   130.00 DEG F
    OUTLET TEMPERATURE =   190.00 DEG F

    CONCENTRATION OF AMINE SOLUTION =  2.48 N (OR 15.00 WT PCT )

    FLOW RATE =       1.000000 Lb Mole Amine/Min
    LOADINGS -
                 CO2 LOADING =    .300000 MOLE/MOLE AMINE
                 H2S LOADING =    .100000 MOLE/MOLE AMINE
                 H2O LOADING =  19.235190 MOLE/MOLE AMINE

  HEAT EXCHANGER DUTY =    .1451E+07 BTU/HR
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Problem Title: SAMPLE RUN OF EQUILIBRIUM CALCULATION
Calculation Option:
    0-Flash Calculation,
    1-Amine-to-Amine Heat Exchanger,
    2-Sour Gas Equilibrium Calculation? . . . . . . . . . . .   2
Amine Type:0-MEA,1-DEA,2-DGA,3-DIPA,4-MDEA? . . . . . . . . .   0
Amine Concentration Unit:0-Weight percent,1-Normality? . . . .   0
Concentration of Amine Solution? . . . . . . . . . . . . .  20.00
Reaction Equilibrium Model:
    0-Kent & Eisenberg,         (For MEA,DEA)
    1-Improved Kent & Eisenberg,(For MEA,DEA,DGA,DIPA)
    2-Smoothed Data,            (For MEA,DEA,DGA,DIPA)
    3-MDEA? . . . . . . . . . . . . . . . . . . . . . . . . .   0

Temperature Unit:0-F,1-R,2-C,3-K? . . . . . . . . . . . . . .   0
Pressure Unit:0-Psia,1-Atm,2-KPa,3-Bar,4-MPa,5-Kg/Cm2,6-MMHg?.   6
Energy Unit:0-BTU/Lb Mole Amine/F,1-KCal/Kg Mole Amine/C?  . .   0
Liquid Flow Rate Unit:0-Lb Mole Amine/Min,
    1-Kg Mole Amine/Min,2-Lb Amine Solution/Min,
    3-Kg Amine Solution/Min,4-GPM Amine Solution? . . . . . .   0



Please enter data or press "ESC" key to accept all data.
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Equilibrium Calculation Data:
    Temperature? F . . . . . . . . . . . . . . . . . . . .      120.00
    Calculate Heat of Solution:0-No,1-Yes? . . . . . . . .           0
    Calculate Final Temperature:0-No,1-Yes?  . . . . . . .           0
    Calculate Option:
        0-From Partial Pressure to calculate Loading,
        1-From Loading to calculate Partial Pressure,
        2-Calculate First Guess on Amine Circulation Rate?           1
            If 0, CO2 Partial Pressure? MMHg      . . . . .     0.0000
                  H2S Partial Pressure? MMHg      . . . . .     0.0000
            If 1, CO2 Loading, mole/mole amine?   . . . . .   0.100000
                  H2S Loading, mole/mole amine?   . . . . .   0.010000
            If 2, Contactor Pressure Unit:0-Psia,1-Atm,
                      2-KPa,3-Bar,4-MPa,5-Kg/Cm2,6-MMHg?             0
                  Contactor Pressure?  . . . . . . . . . .      0.0000
                  CO2 percent in Sour Gas? . . . . . . . .        0.00
                  H2S percent in Sour Gas? . . . . . . . .        0.00
                  % Approach Equilibrium CO2 Loading?  . .        0.00
                  % Approach Equilibrium H2S Loading?  . .        0.00
    Output:0-Summary,1-With Ion Concentration? . . . . . .           0



Please enter data or press "ESC" key to accept all data.
```

```
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  TITLE -  SAMPLE RUN OF EQUILIBRIUM CALCULATION

  EQUILIBRIUM REACTION MODEL - Kent and Eisenberg Model

  AMINE - MEA

  AT SPECIFIED TEMPERATURE =   120.00 DEG F

       CONCENTRATION OF AMINE SOLUTION =  3.32 N (OR 20.00 WT PCT )

       EQUILIBRIUM PARTIAL PRESSURES OF SOUR GAS -
                CO2 =         .0266 MMHG
                H2S =         .1212 MMHG

       EQUILIBRIUM LOADINGS OF AMINE SOLUTION -
                CO2 =   .100000 MOLE/MOLE AMINE
                H2S =   .010000 MOLE/MOLE AMINE

*****************************************************************************

Stop - Program terminated.

A>
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2

VITA

Hsiao-Li Loh

Candidate for the Degree of

Doctor of Philosophy

Thesis: SIMULATION OF ALKANOLAMINE SWEETENING PROCESSES

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Taipei, Taiwan, Republic of China, May 30, 1954, the son of Mr. and Mrs. Kwang Loh.

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