1987

Enthalpies of Solution of CO_2 in Aqueous Methyldiethanolamine Solutions

Keith E. Merkley

1987

Enthalpies of Solution of CO_2 in Aqueous Methyldiethanolamine Solutions

Keith E. Merkley

ENTHALPIES OF SOLUTION OF CO_2 IN AQUEOUS METHYLDIETHANOLAMINE SOLUTIONS

A Thesis
Presented to the
Department of Chemical Engineering
Brigham Young University

In Partial Fulfillment
of the Requirements for the Degree
Master of Science

By
Keith Ellis Merkley
August 1987

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

ACKNOWLEDGEMENTS

I wish to express my appreciation to Dr. James J. Christensen, my thesis committee chairman, for his direction, enthusiasm, and advice in the preparation of this thesis and throughout my undergraduate and graduate work at Brigham Young University. I also acknowledge the help of Dr. Richard L. Rowley in the completion of this thesis. I wish to thank Dennis Cordray, Peter Faux, Teresa Walker, Greg Anderson, Paul Harding, Lyle Gunderson, Cheryl Orme, and Scott Christensen for their help in gathering the experimental data and in lending encouragement for the duration of my graduate work. Approximately 75% of the work in gathering the raw data (monitoring the calorimeter operation and calculating the enthalpy of solution [J/gmole solution] vs. mole fraction CO_2 from the steady-state heater pulse rates) was gathered by the colleagues listed above, while I performed 100% of the balance of the work reported upon in the thesis.

I gratefully acknowledge the financial support of the Gas Processors Association during the gathering of the data. This material is based upon work supported under a National Science Foundation Graduate Fellowship. Any opinions, findings, conclusions, or recommendations expressed in this publication are those of the author and do not necessarily reflect the views of the National Science Foundation.

Most importantly, I wish to express my sincere appreciation to my wife, Janet, and to my family for their encouragement and confidence in me through all of my studies.

INTRODUCTION

The purpose of this thesis is to report the results of a research project in which isothermal flow calorimeters were used to determine the enthalpies of solution of CO_2 in aqueous MDEA solutions over ranges of temperature, pressure, weight percent MDEA, and acid gas loading representative of conditions found in the gas processing industry. In addition to reporting on the experimental data, this thesis summarizes the development and validity of a preliminary computer model which predicts the enthalpies of solution over the range of conditions under which the experimental data were gathered using fundamental thermodynamic quantities (i.e. K, ΔH, and γ).

The thesis is divided into two parts. Part I includes a description of the experimental work, specifically a description of the experimental apparatus, followed by a discussion of the materials and the procedure used for data collection. It then presents experimental data, and concludes with a discussion and analysis of the experimental data. Part II describes the development of a computer model to predict the enthalpies of solution. Specifically, Part II begins by describing the development of the model, including a discussion of the reaction mechanism, the literature data used in the model, the model's logic, and the organization of the computer program. It then presents the results of the model's prediction of the enthalpy of solution and compares the prediction to the original experimental data. Finally, Part II concludes with an analysis of the validity of the preliminary computer model and suggests areas for further refinement and improvement of the model.

PART I. MEASUREMENT AND CORRELATION OF ENTHALPY OF SOLUTION DATA

I. INTRODUCTION

Aqueous solutions of methyldiethanolamine (2,2´-(methylimino) bis-ethanol, abbreviated MDEA) are finding increasing use in the gas processing industry for the selective removal of H_2S from gas mixtures containing both hydrogen sulfide and carbon dioxide (1). MDEA is more selective for H_2S removal than are the other "conventional" amine solvents such as monoethanolamine (MEA), diethanolamine (DEA), diglycolamine (DGA), and diisopropanolamine (DIPA).

All of the aforementioned alkanolamines are weakly basic and thus react directly with the acidic absorbed hydrogen sulfide producing a protonated amine and a hydrosulfide ion (HS^-). The rate of reaction for the direct proton transfer from the absorbed H_2S to the aqueous amine is very high for all of these alkanolamines.

MDEA's selectivity for absorption of H_2S in the presence of CO_2 arises from the kinetics of its reaction with absorbed CO_2. Both primary amines (such as DGA and MEA) and secondary amines (such as DEA and DIPA) react directly with absorbed carbon dioxide to form a carbamate (figure 1). For these primary and secondary amines, the rate of reaction for the carbamate reaction is nearly the same as the rate of reaction for the proton transfer reaction. Thus, primary and secondary amines are not selective for the removal of H_2S in the presence of CO_2. MDEA's selectivity for H_2S arises because MDEA is a tertiary amine which cannot react directly with the absorbed carbon dioxide molecule to form a carbamate (figure 1). Rather, the absorbed carbon dioxide (in the form of carbonic acid) undergoes

1. Primary Amine -- MEA

$$RNH_2 + CO_{2\,(aq)} \Leftrightarrow RNHCOO^- + H^+$$

(MEA) (Carbamate)

2. Secondary Amine -- DEA

$$R_2NH + CO_{2\,(aq)} \Leftrightarrow R_2NCOO^- + H^+$$

(DEA) (Carbamate)

3. Tertiary Amine -- MDEA

$$R_2NCH_3 + CO_{2\,(aq)} \Leftrightarrow \text{No Reaction}$$

(MDEA)

Figure 1. Direct reaction of absorbed CO_2 with the three types of amines (R = CH_2CH_2OH).

$$CO_{2\,(aq)} + H_2O \Leftrightarrow H^+ + HCO_3^-$$

$$H^+ + R_2R'N \Leftrightarrow R_2R'NH^+$$

Figure 2. Indirect reaction of absorbed CO_2 with methyldiethanolamine (MDEA), a representative tertiary amine (R = CH_2CH_2OH, R' = CH_3).

ionization followed by protonation of the basic amine (see figure 2). The first ionization of carbonic acid is a kinetically slow reaction in comparison to the reaction rate for the direct proton transfer from absorbed H_2S to MDEA (1). Thus, there is a kinetic rate advantage for the selective absorption by MDEA solutions of H_2S in gases containing both H_2S and CO_2.

Because of its selectivity, MDEA is finding increasing application for enriching the hydrogen sulfide content of the acid gas feed to Claus-type sulfur recovery units (thereby increasing sulfur conversion efficiency), for recovery of CO_2 in enhanced oil recovery processes, and, in general, for the removal of H_2S from gases rich in CO_2 (2). In addition to its selectivity, MDEA offers the following advantages over other amine solvents: (1) significant energy savings as a result of a smaller overall heat of solution and a lesser amount of absorbed CO_2 to regenerate in the acid gas stripper, (2) less corrosion, and (3) lower vapor loss because MDEA has a very low vapor pressure at normal operating conditions (1).

This research project was part of a multi-year experimental project sponsored by the Gas Processors Association (GPA) to determine enthalpies of solution of acid gases (CO_2, H_2S, SO_2, etc.) in various amine solutions. The long-range objective of this project is to provide a reliable data base for the modeling and design of gas treating facilities. In particular, the immediate aim of this thesis project was to measure the enthalpies of solution (H^S) of gaseous CO_2 in aqueous MDEA solutions. These data are not only essential for modeling the multi-stage, multi-component equilibria in acid gas absorption towers and stripping columns, but they are also necessary for accurate calculation of reboiler, condenser, and heat exchanger duties. The solvent systems investigated for this project include ranges of temperatures, pressures, solvent concentrations (MDEA weight percent), and carbon

dioxide loadings (gmole CO_2/gmole MDEA) representative of those found in the gas processing industry. Part I of this thesis reports on the measurement and correlation of enthalpy of solution data for the MDEA-CO_2-H_2O system.

II. EXPERIMENTAL WORK

Enthalpies of solution of carbon dioxide in MDEA-water solutions were measured under the following conditions:

Temperature (K):	288.7, 333.2, 388.7, 422.0
Concentration (weight percent):	20, 40, and 60 (except at 422.0 K)
Pressure (kPa):	156 at 288.7 K and 333.2 K
	1121 at 288.7, 333.2, and 388.7 K
	1466 at 422.0 K

These 17 systems are illustrated by the grid in figure 3. The enthalpies of solution for each system were measured from a loading (gmole CO_2/gmole MDEA) of 0 to loading values beyond the saturation loading point (the point at which the aqueous solution becomes saturated with carbon dioxide).

This section describes the apparatus used for gathering data, the materials used in the experimental runs, and the experimental procedure followed to obtain the data.

Description of Experimental Apparatus

The enthalpy of solution measurements were obtained from two isothermal flow calorimeters that were developed at Brigham Young University. The calorimeters used were moderate temperature (240 K to 550 K), high pressure (0 to 41.4 MPa) isothermal flow calorimeters. They have been described previously in the literature (3,4) and only an abbreviated discussion will be given here.

Isothermal calorimetry is based on maintaining the reaction vessel at a

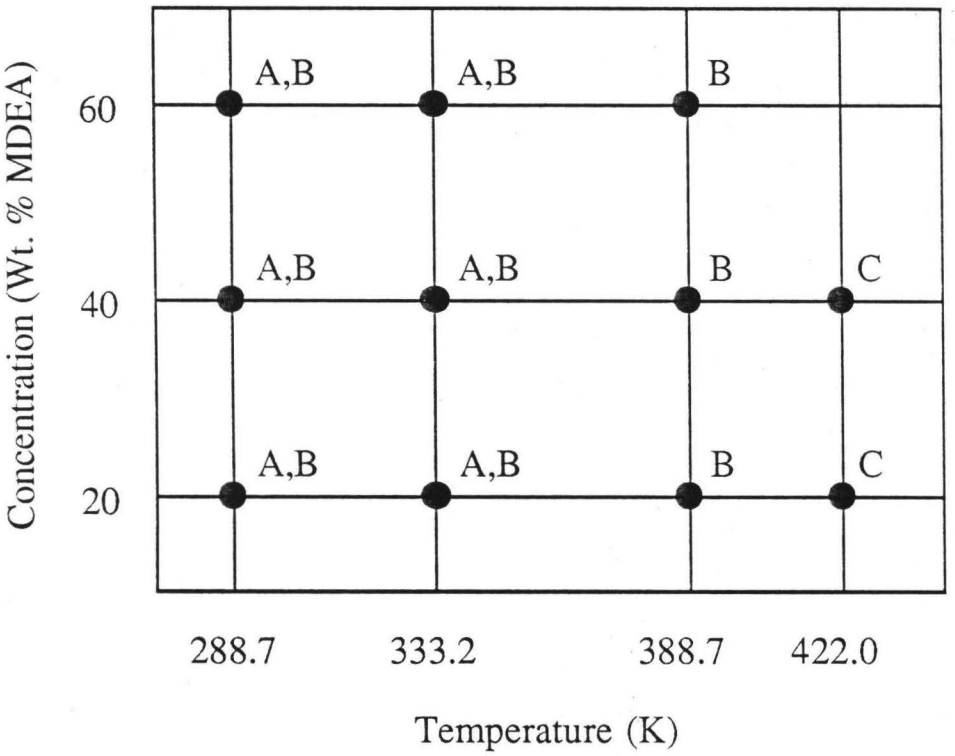


Figure 3. Grid representing the 17 systems investigated. The large dots indicate the combinations of temperature and MDEA concentration at which experimental runs were made. The letters represent the pressure(s) at which each run was performed (see the pressure key below).

Letter	Pressure
A	156 kPa
B	1121 kPa
C	1466 kPa

constant temperature (equal to the temperature of the vessel's surrounding container) during the course of the mixing of the two components within the reaction vessel. A simplified schematic of the reaction vessel is shown in figure 4. A variable pulsed heater is located directly beneath the plate upon which the reactants mix and equilibrate. A Peltier cooler is placed beneath the pulsed heater in contact with the heater above and the reaction vessel below. Isothermal conditions are achieved by adjusting the output of the variable heater to balance both the energy generated by the mixing or chemical reaction of the components and the energy removed from the system at a constant rate by the Peltier cooler. The method is equally applicable to endothermic and exothermic reactions. Because the temperature of the vessel is maintained at the temperature level of the immediate surroundings, no corrections for heat exchange with the environment are required. In addition, a knowledge of the heat capacity is not required for calculation of the heat of solution. Some specifications of the heat of mixing calorimeters are listed below:

Temperature Range :	240 to 550 K
Pressure Range :	0 to 41.4 MPa
Measurable Heats :	Exothermic and Endothermic 0.003 to 0.5 J/sec
Flow Rates :	0.0005 to 0.05 ml/sec
Materials of Construction :	Stainless Steel or Hastelloy C
Accuracy :	Better than 1% for Liquid-Liquid Test Systems
Type of Data :	Fixed Composition

The calorimeter reaction vessel (shown schematically in figure 5) contains the isothermal plate and equilibration coil. Directly beneath the plate are a 100 Ω wafer control heater and a high temperature model Peltier

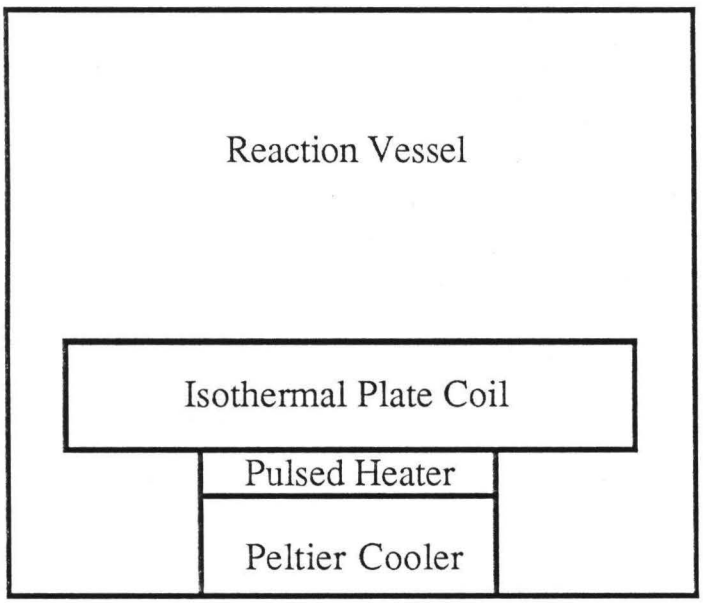


Figure 4. Schematic of the reaction vessel.

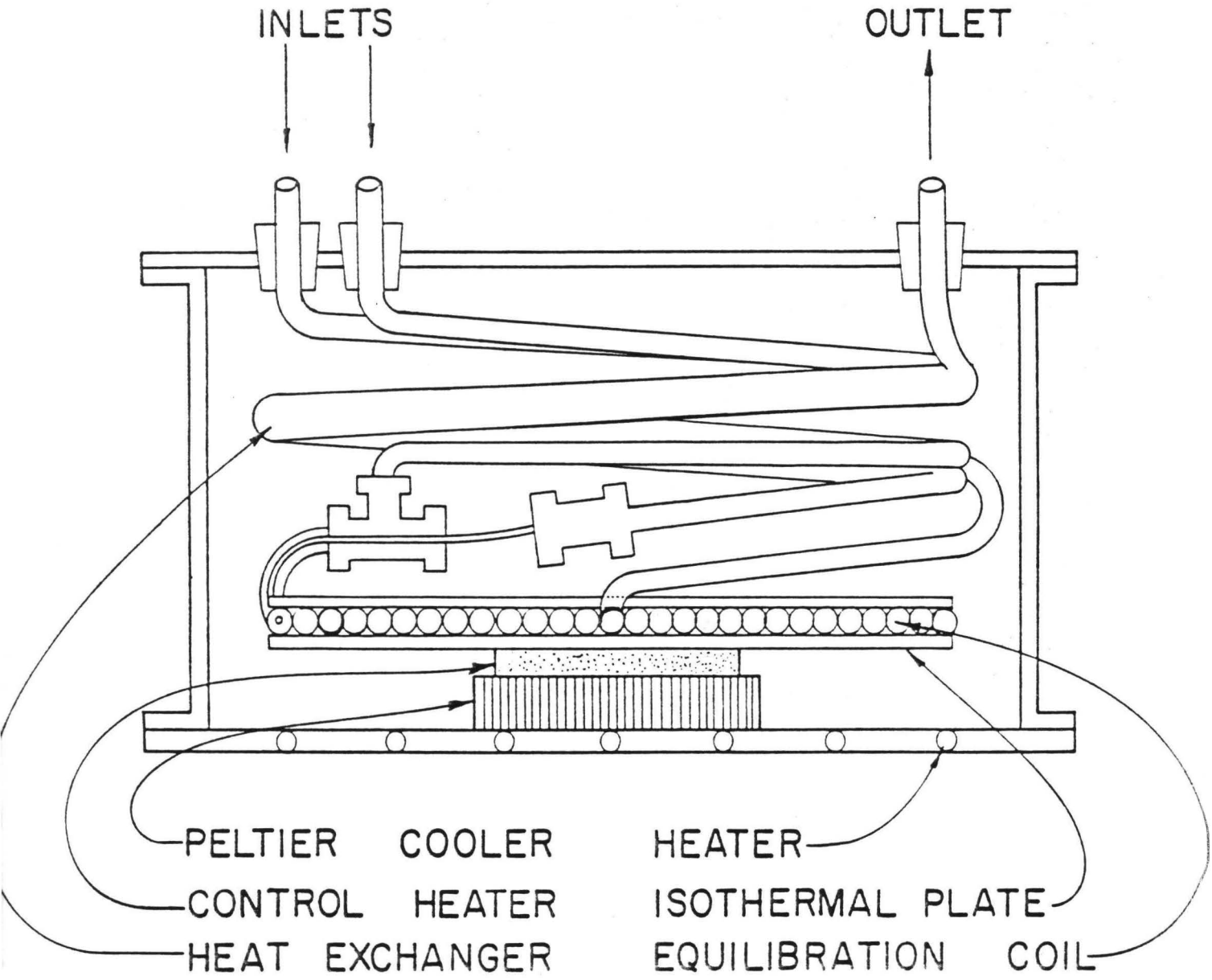


Figure 5. Detailed schematic of the reaction vessel (from reference 5).

thermoelectric cooler. The cooler is in direct contact with the heater above, and the vessel walls below, thus facilitating the transfer of heat from the reaction vessel. The isothermal plate consists of an equilibration coil soldered between two round brass plates. The equilibration coil is constructed of stainless steel tubing coiled in a flat helical shape and is filled with segments of fine crimped stainless steel wire. The wire promotes thorough mixing of the reactants as they flow through the coil. The reactants entering the reaction vessel and the products leaving the vessel are at all times contained within the stainless steel tubing. The reaction vessel is maintained at a constant temperature by: (1) removing heat from the reaction vessel at a constant rate with the Peltier cooler, and (2) varying the output of the pulsed heater to compensate for both the constant energy removal and the presence of any heat effects upon the mixing of the reactants. The heat of mixing (or in this case, the enthalpy or heat of solution of the gaseous component) is the difference between the power output of the heater during the mixing process, and the power output of the heater required to maintain a constant vessel temperature when no reaction is occurring.

Two calorimeters of the same design were used in order to cover the desired temperature range. The measurements at the two lower temperatures (288.7 and 333.2 K) were made with a calorimeter submerged in an isothermal water bath, while a calorimeter surrounded by a constant temperature air bath was used to collect data at the two higher temperatures (388.7 and 422.0 K). Two different pump systems (a Varian, Inc. 8700 series, and an ISCO Model 314 series) were used in the operation of the units.

A block diagram of the calorimeter, the fluid circuit, and the data

control and output components is shown in figure 6. The calorimeter or reaction vessel is fed by two pumps which have variable volumetric delivery rates. The back pressure regulator on the gaseous CO_2 inlet line from the pump maintains a constant high pressure (≈2700 kPa) gas feed to the calorimeter. The high pressure gas stream provides a constant, easily measured flow of gas into the calorimeter. Upon passing through the back pressure regulator, the high-pressure carbon dioxide rapidly expands until it reaches the system pressure. The calorimeter outlet stream empties into a collection vessel which traps the MDEA solution and prevents it from entering the outlet back pressure regulator, the device which maintains a constant pressure within the calorimeter. The waste MDEA solution is kept from entering the exit back pressure regulator in order to prevent the viscous MDEA solution from adhering to the walls and diaphragm of the regulator which can interfere with its ability to maintain a constant system pressure. The nitrogen tank connected to the system between the waste collection vessel and the exit back pressure regulator provides a constant flow of nitrogen through the outlet regulator to maintain the fixed total system pressure.

Materials

The chemicals employed for gathering the heats of solution data were carbon dioxide (Whitmore Oxygen Co., 99.98 mole percent pure), MDEA (Aldrich Chemical Company, 99 weight percent pure), and distilled, deionized water. The carbon dioxide was filtered through a Matheson gas purifier model 450 containing a molecular sieve desiccant. Prior to preparation of the aqueous MDEA solutions, the deionized, distilled water was boiled for 20 minutes to drive out any dissolved carbon dioxide. During

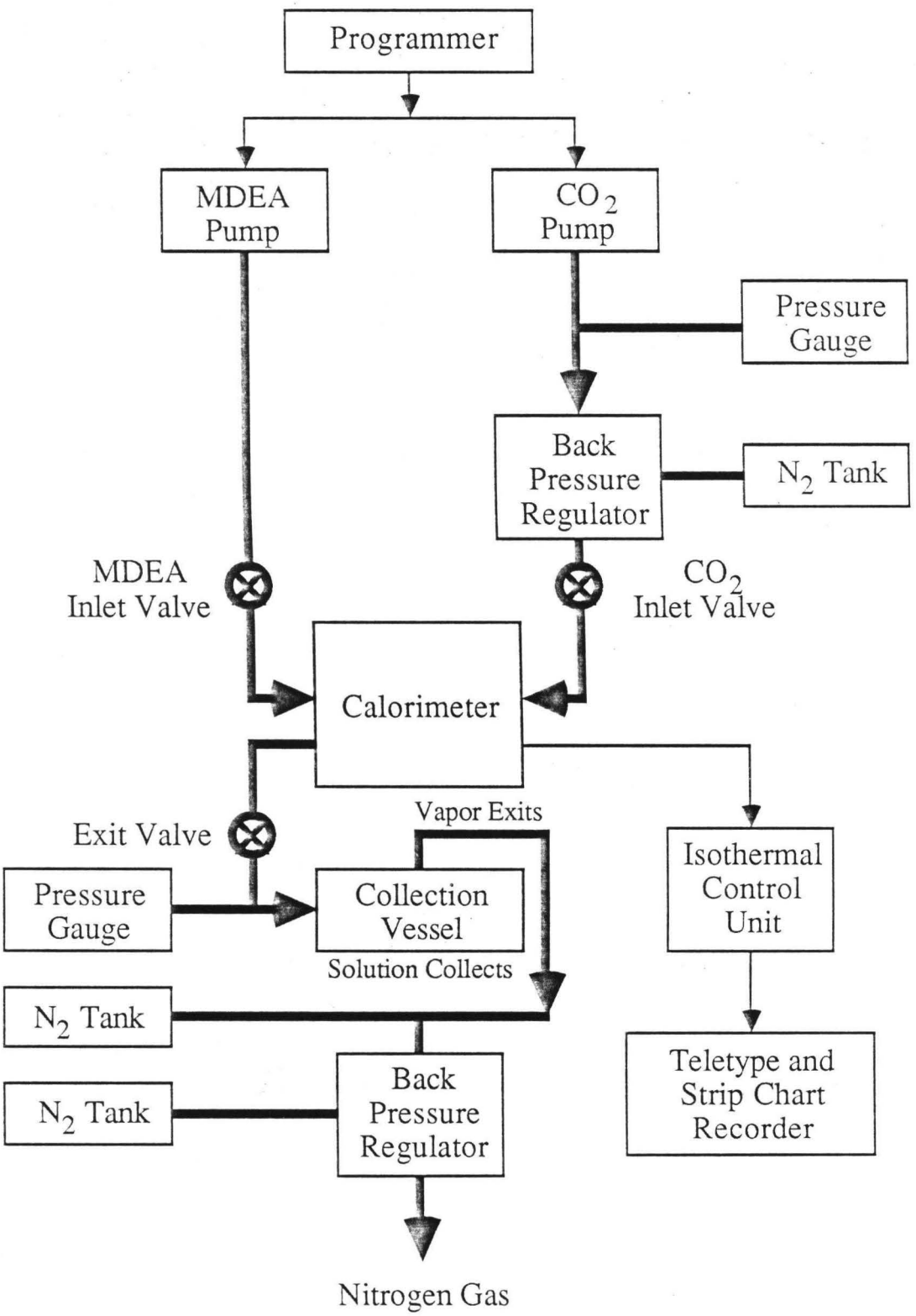


Figure 6. Block diagram of the isothermal flow calorimeter.

Fluid Lines

Electrical Lines

cooling, a carbon dioxide absorbing tube was attached to the top of the boiling flask with a one-hole stopper to prevent contamination of the water by atmospheric CO_2. The various weight percent MDEA solutions were kept from exposure to CO_2 in the air by mixing only one liter at a time. In addition , the solutions were not filtered in order to minimize exposure to the atmosphere. All of the aqueous solutions were degassed in an ultrasonic bath for ten minutes prior to use.

Procedure for Data Collection

Before taking data, the bath, the isothermal control unit, and the Peltier cooler were adjusted to maintain the reaction vessel at the temperature of interest. The pumps were then charged with carbon dioxide and the MDEA solution, respectively, after which the system operating pressure was set at the desired value. All experimental runs were made in the steady-state (fixed composition) mode. The total flow rate (both reactants combined) ranged from 0.0056 ml/sec to 0.0222 ml/sec with most runs being made at 0.0083 ml/sec.

The startup procedure prevented the contamination of either of the pure reactants with the waste products contained in the exit collection vessel. With the exit valve (between the calorimeter outlet line and the collection vessel) closed, the inlet CO_2 line and the calorimeter were pressurized to approximately 3450 kPa. The valves to the three nitrogen tanks which control the back-pressure regulators were then opened and adjusted to provide a high pressure inlet gas flow, and a constant system pressure on the outlet line. Once these pressures were set, the outlet valve was opened and the calorimeter was instantly flushed with pure carbon dioxide as the high pressure gas expanded to the lower system pressure. Once the system

pressure settled again on the desired value, the MDEA pump was pressurized to a pressure slightly higher (350 kPa higher) than the system pressure, at which time the MDEA inlet valve located between the MDEA pump and the calorimeter was opened and the mixing process began. Thereafter, whenever a single reactant baseline run was made, the pump for the other component was pressurized to 350 kPa above the system pressure before the inlet valve was opened and the component was again allowed to mix in the calorimeter.

The procedure used to measure the enthalpies of solution was as follows. First, each of the components (the aqueous MDEA solution and the gaseous CO_2) was fed individually to the calorimeter at the total flow rate chosen to determine baseline (i.e., no reaction) heater pulse rates. Then, both materials were fed to the calorimeter simultaneously (at flow rates required to obtain the desired CO_2 loading) and the reaction steady-state heater pulse rate was determined. The difference in the heater pulse rate during the reaction and the pulse rate for the baseline runs determined the enthalpy of solution. A calibration of the pulsed heater was performed to determine the energy equivalent of one pulse. This calibration may be carried out chemically, by carrying out a well characterized standard reaction, or electrically, by adding a measured amount of energy via the calorimeter's calibration heater and monitoring the change in pulse rate. For most experimental runs, only an electrical calibration was performed; a chemical calibration was conducted periodically to confirm the results of the electrical calibrations.

III. EXPERIMENTAL RESULTS AND DISCUSSION

Enthalpies of solution of carbon dioxide in aqueous MDEA solutions were measured under the conditions listed previously (figure 3). The experimental enthalpies of solution H^S (J/gmole solution) were determined at various values of mole fraction CO_2. These raw data were converted to H^S (kJ/gmole MDEA and kJ/gmole CO_2) versus loading (gmole CO_2/gmole MDEA) with a computer program utilizing simple conversion factors. A sample of the output from this program listing the raw data and converted data is shown in table 1. Included in appendix A is the computer program, a sample calculation, and the computer outputs for the rest of the sets of experimental data.

Figures 7, 8, 9, and 10 are sample plots of the experimentally determined enthalpies of solution as functions of the acid gas loading for runs 14 (40 wt. % MDEA, 388.7 K, 1121 kPa shown in figures 7 and 9) and 18 (40 wt. % MDEA, 422.0 K, 1466 kPa shown in figures 8 and 10). The negative enthalpy values indicate exothermic absorption reactions. Figures 7 and 8 are plots of the experimental enthalpies of solution in units of kJ/gmole MDEA as functions of loading, while figures 9 and 10 are plots of the identical enthalpy of solution data in units of kJ/gmole CO_2 as functions of loading. The plots of the experimental data (in units of kJ/gmole MDEA and kJ/gmole CO_2) for the other fifteen systems are included in appendix B.

All of the plots showing experimental enthalpies of solution in units of kJ/gmole MDEA (figures 7 and 8) have a positively sloped straight line portion from a loading value of 0 to loadings near the saturation loading

TABLE 1

Sample Computer Output Listing Raw and Converted Data for Run 18 (40 wt.% MDEA, 422.0 K,1466 kPa).

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 422.0 K AND 1465.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00258	-186.90	0.02825	-72.454	-2.047
0.00315	-209.75	0.03451	-66.598	-2.299
0.00405	-297.30	0.04442	-73.420	-3.260
0.00443	-295.00	0.04860	-66.602	-3.238
0.00506	-330.51	0.05555	-65.329	-3.629
0.00581	-386.86	0.06383	-66.596	-4.252
0.00650	-422.46	0.07146	-65.005	-4.645
0.00727	-474.85	0.07999	-65.327	-5.224
0.00733	-495.41	0.08065	-67.598	-5.451
0.00815	-541.71	0.08975	-66.479	-5.966
0.00815	-526.85	0.08975	-64.655	-5.803
0.00818	-532.41	0.09008	-65.098	-5.864
0.00894	-624.22	0.09853	-69.835	-6.880
0.00981	-642.79	0.10821	-65.534	-7.091
0.01079	-685.36	0.11914	-63.528	-7.567
0.01092	-686.32	0.12059	-62.860	-7.581
0.01162	-776.98	0.12841	-66.877	-8.587
0.01185	-766.18	0.13098	-64.667	-8.470
0.01195	-760.12	0.13210	-63.618	-8.404
0.01287	-789.85	0.14240	-61.381	-8.742
0.01295	-766.01	0.14330	-59.161	-8.479
0.01298	-766.30	0.14364	-59.047	-8.481
0.01401	-770.04	0.15520	-54.972	-8.531
0.01522	-767.37	0.16881	-50.427	-8.512
0.01658	-733.15	0.18415	-44.227	-8.143
0.01804	-731.45	0.20066	-40.553	-8.138
0.01945	-706.91	0.21665	-36.351	-7.875
0.02095	-673.50	0.23372	-32.153	-7.515
0.02275	-660.39	0.25427	-29.033	-7.382
0.02470	-620.06	0.27662	-25.108	-6.944
0.02660	-580.17	0.29848	-21.814	-6.512
0.02861	-542.28	0.32169	-18.957	-6.099
0.03127	-515.18	0.35257	-16.478	-5.808

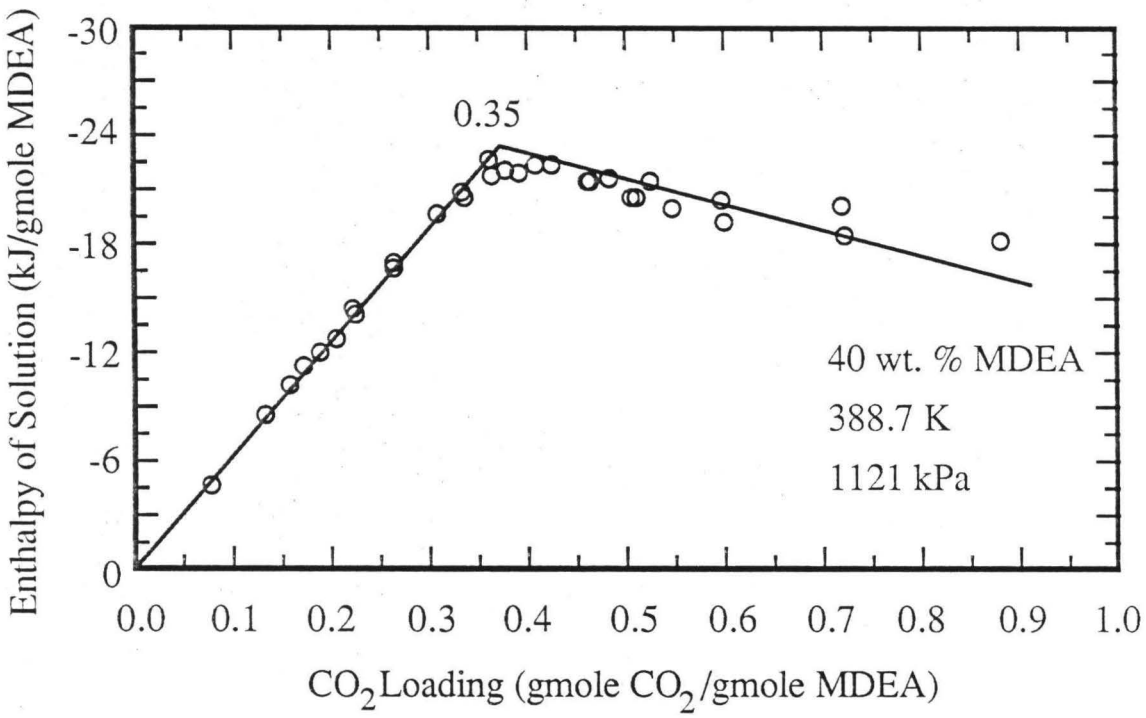


Figure 7. Plot of the experimental enthalpies of solution (kJ/gmole MDEA) for system 14.

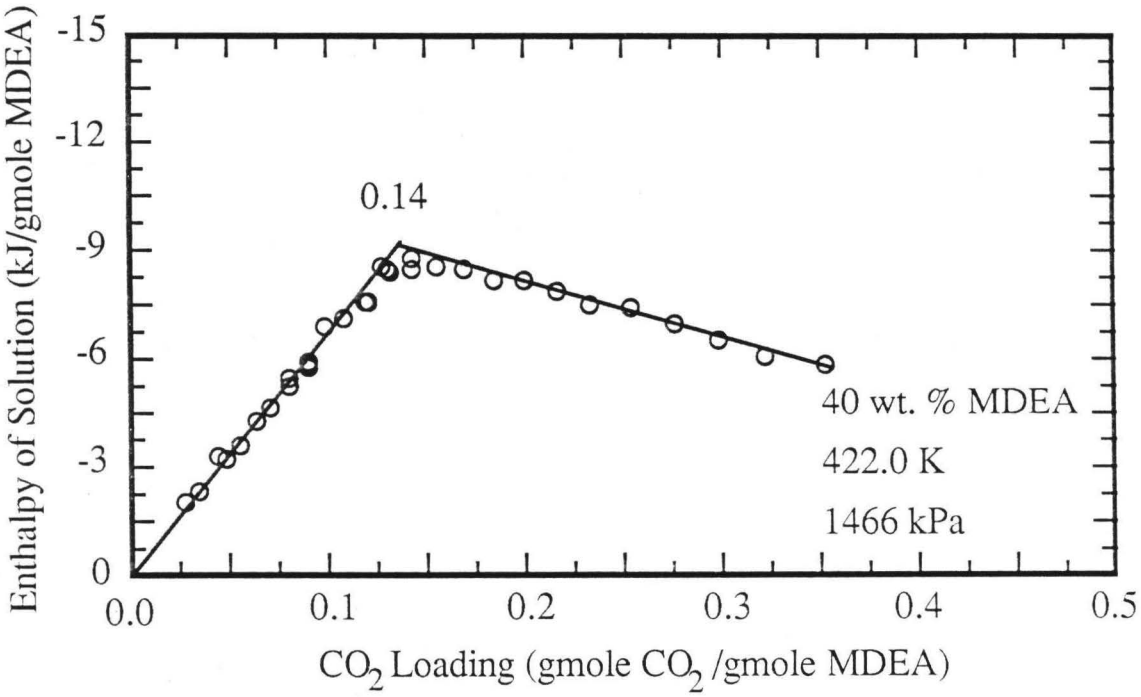


Figure 8. Plot of the experimental enthalpies of solution (kJ/gmole MDEA) for system 18.

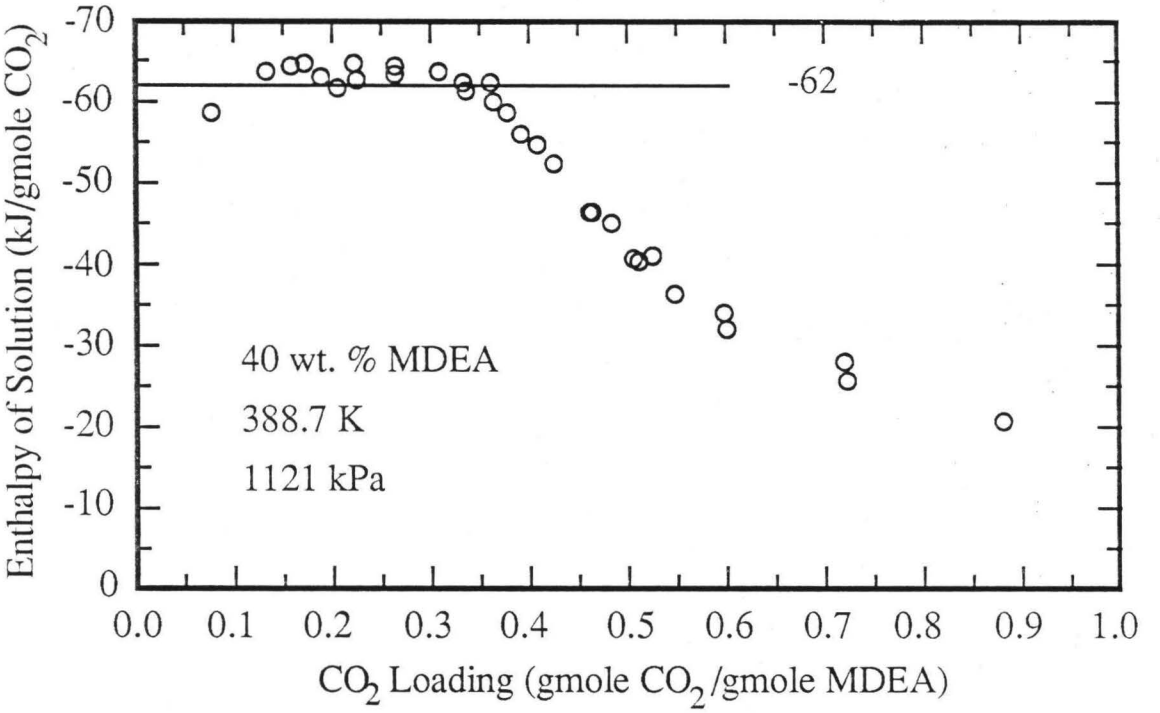


Figure 9. Plot of the experimental enthalpies of solution (kJ/gmole CO_2) for system 14.

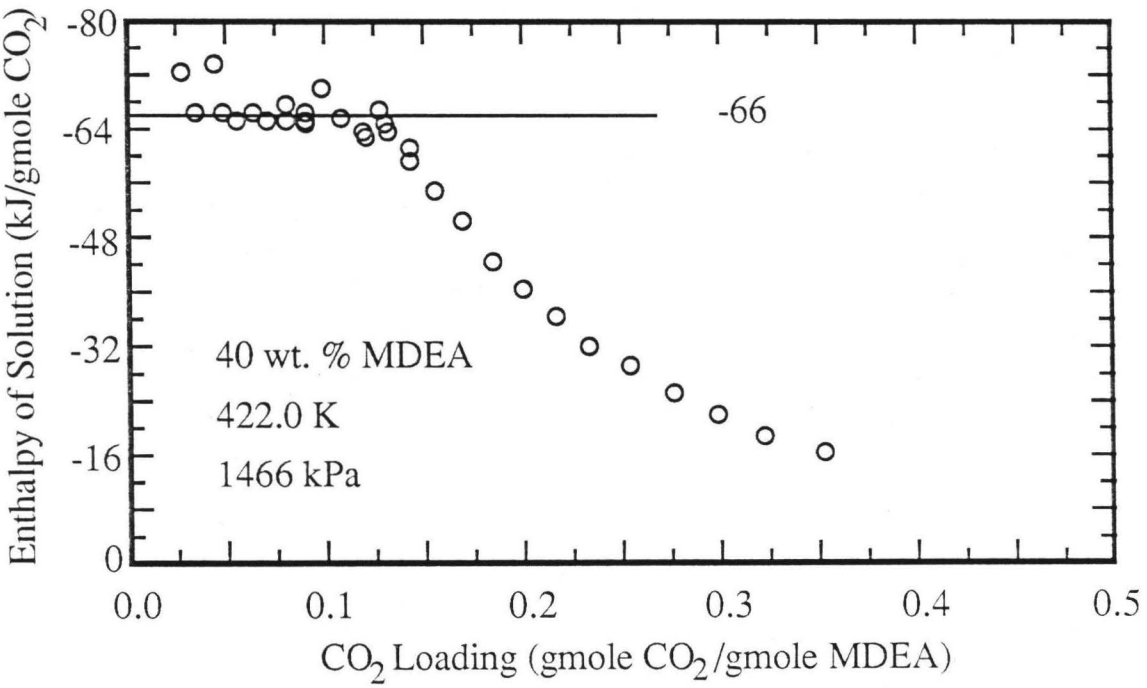


Figure 10. Plot of the experimental enthalpies of solution (kJ/gmole CO_2) for system 18.

point. Past the saturation loading point, the data show a negative linear relationship between the enthalpy of solution (per gmole MDEA) and the loading. A physical interpretation of these trends is that prior to the saturation loading point, all of the CO_2 fed to the calorimeter is completely absorbed, and the total heat released upon absorption is directly proportional to the amount of CO_2. Thus, as additional CO_2 is fed to the calorimeter (i.e., as the loading increases), the value of the numerator (total heat released) increases proportionally with the loading, while the value of the denominator (gmole MDEA) remains constant, giving a linearly increasing enthalpy of solution per gmole MDEA with increasing loading. Past the saturation loading point, the total heat measured is the heat required to just saturate the solution. Any CO_2 in excess of that required to saturate the solution has no contribution to the total heat of the system. Thus, beyond the saturation loading point, both the numerator (total heat) and the denominator (gmole MDEA) remain essentially constant with increasing loading, resulting in the enthalpy of solution per gmole MDEA remaining constant. Above the saturation loading point, especially at the two higher temperatures, evaporation of water and MDEA into the vapor phase cause the numerator (total heat) to be less negative (i.e., the constant exothermic heat of solution of the CO_2 is offset by the endothermic evaporation of the water and MDEA) while the denominator (gmole MDEA) remains constant. This causes the heat of solution per gmole MDEA to decrease with increasing loading. The evaporation of water and MDEA into the vapor phase is negligible at the two lower temperatures. Therefore, the enthalpy of solution per gmole MDEA remains constant at these two lower temperatures beyond the saturation loading point as described above. This trend is consistent with the results found in a similar study completed recently on

aqueous DGA systems (5).

An analysis of the experimental data plotted in units of kJ/gmole CO_2 (figures 9 and 10) revealed that in each of the systems studied, the enthalpy of solution (per gmole CO_2) was essentially independent of the amount of CO_2 absorbed up to the saturation loading point. Past the saturation loading point, the enthalpy of solution fell toward zero. A physical explanation of these trends is that before the saturation loading point, the numerator (total heat) increases approximately proportionally with increases in the denominator (gmole CO_2), resulting in the enthalpy of solution per gmole CO_2 remaining constant. Above the saturation loading point, the numerator (total heat) remains constant (as described previously) while the denominator (gmole CO_2) increases, giving a decreasing enthalpy of solution per gmole CO_2. This trend is also consistent with the results found in a similar study completed recently on aqueous DGA systems (5).

The numerical values of H^S (kJ/gmole CO_2) below the saturation loading point which are plotted as the horizontal lines on figures 9 and 10 (and in appendix B for the remaining systems) are fitted values obtained from an analysis of the experimental data plotted as H^S (kJ/gmole MDEA) in figures 7 and 8 (and in appendix B). The numerical value of the constant slope of this straight line portion has the units of kJ/gmole CO_2 and represents the desired constant value of the enthalpy of solution in units of kJ/gmole CO_2. The slope of the straight line portion below the saturation loading point was found by a modified least-squares linear regression which forces the line which best describes the experimental data below the saturation loading point to pass through the origin. The data were manipulated in this way because it was found that small deviations from linearity in the data plotted in units of kJ/gmole MDEA were greatly

magnified when the data were plotted in units of kJ/gmole CO_2. The computer program used to fit the data along with a summary of each linear regression is included in appendix C.

The numerical values of the constant enthalpy of solution (kJ/gmole CO_2) were determined for each system by the procedure just described. These enthalpies of solution (kJ/gmole CO_2) ranged from -47 kJ/gmole CO_2 for 20 wt. % MDEA solutions at 288.7 K to -66 kJ/gmole CO_2 for 40 wt. % MDEA solutions at 422.0 K. The numerical value of H^S (kJ/gmole CO_2) for loadings below the saturation loading point is reported in table 2 for each of the 17 systems.

Pressure was found to have virtually no effect on the values of H^S for a given MDEA concentration. At the two lower temperatures (288.7 K and 333.2 K) experimental runs were made at both 156 kPa and 1121 kPa for each of the three MDEA concentrations (a total of 12 runs, 6 at the lower pressure). In the case of 4 of the 6 lower pressure runs (see table 2), the calculated values of H^S below the saturation loading point differed by less than 2% from the results of the higher pressure runs. For the other 2 lower pressure systems, the higher pressure and lower pressure determinations agreed to within nine percent. Based upon these observations, it was decided to forego measurements at the lower pressure for all three of the MDEA solutions at 388.7 K and 422.0 K. In addition, it was observed that at 422.0 K, calorimeter operation at a system pressure of 1466 kPa lead to greater ease of measurement of the enthalpies of solution. Thus, the assumed pressure independence was extended to 1466 kPa. The enthalpies of solution (kJ/gmole CO_2) at loadings below the saturation loading point were found to be essentially independent of the total system pressure. This result is also consistent with the findings of the DGA study (5) which was referred to

TABLE 2

Experimental Enthalpies of Solution of CO_2 in MDEA Solutions Below the Saturation Loading Point Together with Saturation Loading Point Values.

System				
Wt. % MDEA	Temperature (K)	Pressure (kPa)	H^S (kJ/gmole CO_2)	Saturation Loading Point (gmole CO_2/ gmole MDEA)
20	288.7	1121	-47	1.28
20	288.7	156	-47	0.87
40	288.7	1121	-49	1.12
40	288.7	156	-48	1.00
60	288.7	1121	-51	1.10
60	288.7	156	-50	0.78
20	333.2	1121	-53	1.01
20	333.2	156	-56	0.71
40	333.2	1121	-55	0.94
40	333.2	156	-60	0.70
60	333.2	1121	-57	0.81
60	333.2	156	-57	0.36
20	388.7	1121	-59	0.58
40	388.7	1121	-62	0.35
60	388.7	1121	-63	0.17
20	422.0	1466	-63	0.27
40	422.0	1466	-66	0.14

previously.

Figure 11 is a plot of H^S versus MDEA concentration at the four temperatures investigated. It is apparent from this plot that H^S below the saturation loading point is a linear function of both MDEA concentration and temperature. This finding is in contrast to the results of the DGA study in which H^S was found to be dependent upon DGA concentration but independent of temperature over the same ranges of concentration and temperature as this study (5). However, as mentioned in the introduction, DGA is a primary amine which reacts directly with CO_2 to form a carbamate. Because MDEA does not form a carbamate, the differing trends with temperature are not unexpected.

A multiple linear regression of the experimental data shown in figure 11 gave the following equation:

$$H^S \text{ (kJ/gmole } CO_2) = -0.10070\ X_W - 0.12590\ T - 8.5955 \quad (1)$$

where X_W represents the weight percent of the MDEA in solution, and T is the temperature in K. This equation gives a very good fit of the experimental data as illustrated in figure 11. Equation 1 can be used to determine the enthalpy of solution of carbon dioxide in aqueous MDEA solutions below the saturation loading point within the temperature range 288.7 to 422.0 K and the total system pressure range of 156 to 1466 kPa for solutions between 20 and 60 weight percent MDEA. It is important to recognize that the H^S values reported in figure 11 and given by equation 1 are valid only for CO_2 loadings below the saturation concentration of CO_2 in the solution.

Few literature values of H^S for aqueous MDEA solutions are available for comparison. Dibble (6) reports a value of -49 kJ/gmole CO_2. His

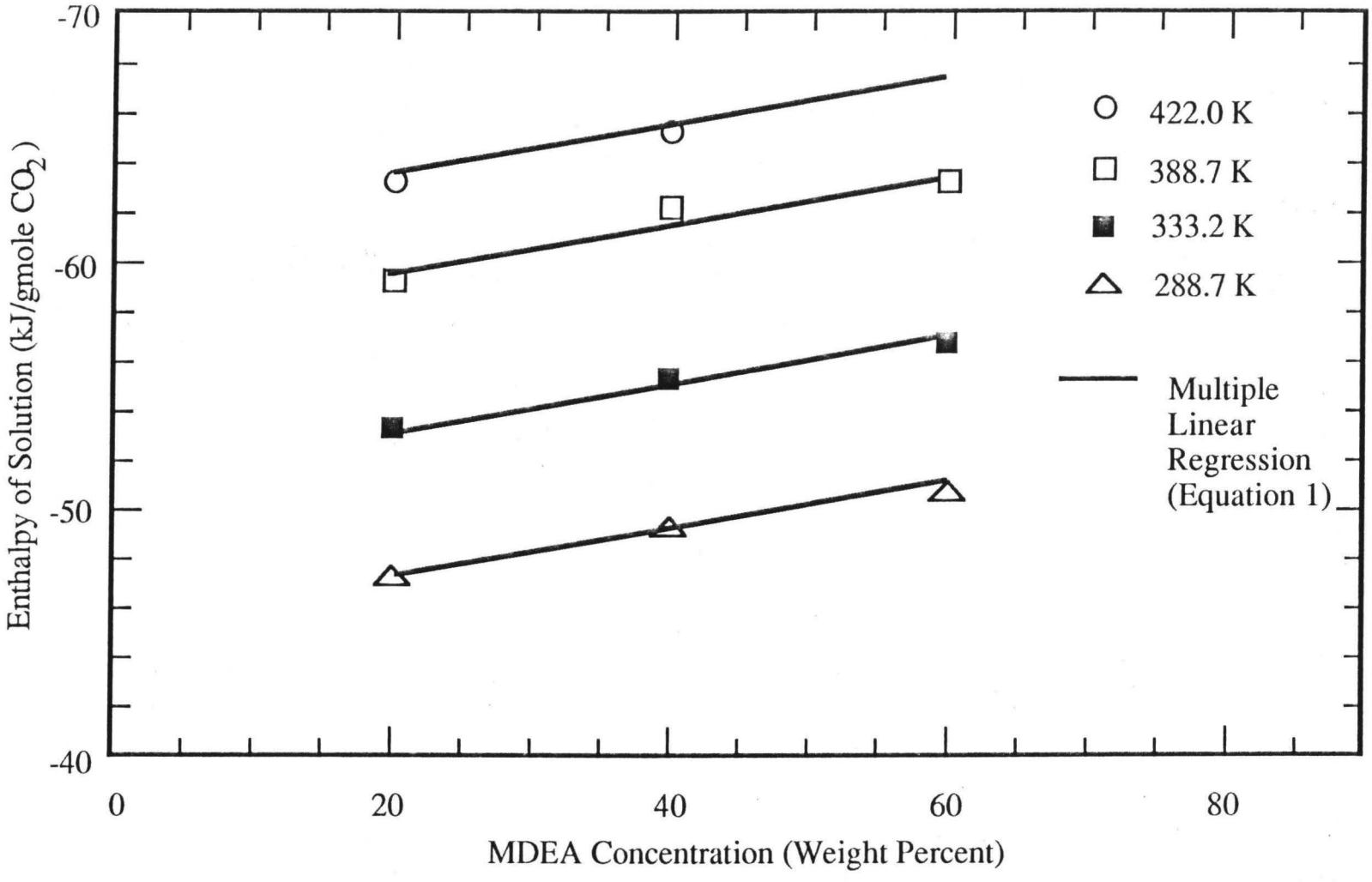


Figure 11. Enthalpy of solution (kJ/gmole CO_2) as a function of MDEA concentration (weight percent). Values of H^S applicable for CO_2 loadings below the saturation loading point and CO_2 partial pressures between 156 and 1466 kPa.

method of obtaining this value is unknown, as are the temperature, pressure, MDEA concentration, and loading for which the reported H^S value is valid. The values reported here range from -47 to -66 kJ/gmole CO_2 and enclose the single value of Dibble. Pearce (7) reports a value of -59 kJ/gmole CO_2 for unknown conditions of temperature, pressure, concentration, and loading. Again, the data of this study enclose this single value. Polasek and Bullin (8) report a value of -61 kJ/gmole CO_2 for an unknown temperature, a solution between 30 and 50 wt % MDEA and unlimited gas loadings. Using equation 1 and the range of temperatures encountered in this study, the values of this study range from -48 kJ/gmole CO_2 for 30 wt. % MDEA at 288.7 K to -68 kJ/gmole CO_2 for 50 wt. % MDEA at 422.0 K. Thus, the data of this study enclose the single value reported above, although this study shows a concentration dependency in contrast to Polasek's results.

Of the articles that have been published, only one (by Jou, Mather, and Otto (2)) reports data over a wide range of conditions of temperature, pressure, and concentration. They measured the solubility of carbon dioxide in two different MDEA solutions (23.5 wt. % MDEA and 52 wt. % MDEA) at temperatures from 298 to 393 K and pressures up to 6600 kPa. They found approximate values of the enthalpy of solution of CO_2 in MDEA solutions from the solubility data using the following form of the Gibbs-Helmholtz equation:

$$H^S / R = \left[\partial \ln p_1 / \partial (1/T) \right]_{x_1} \qquad (2)$$

where R is the universal gas constant, p is the partial pressure, x is the mole fraction, and the subscript 1 refers to CO_2. They reported that the heats of solution calculated in this manner are independent of temperature, but dependent upon the weight percent MDEA and upon the loading of the

solution at loadings greater than 0.3 gmole CO_2/gmole MDEA. The results reported here show that the enthalpies of solution are functions of concentration and temperature but independent of loading. However, Jou et al. found their value of H^S by plotting ln p_1 vs. 1/T for a constant mole fraction CO_2. The derivative of this plot is their reported value for the enthalpy of solution. The direct measurement of the enthalpy of solution is clearly the preferred method for examining the trends of the enthalpy data with variations in temperature, pressure, and concentration. Jou et al. reported H^S values below the saturation loading point ranging from -42 to -65 kJ/gmole CO_2 for the 23.5 wt. % MDEA solution (independent of temperature). The values of the present study (from equation 1), which ranged from -47 kJ/gmole CO_2 at 288.7 K to -64 kJ/gmole CO_2 at 422.0 K, compare favorably with Jou's results. Likewise, Jou et al. report H^S values below the saturation loading point ranging from -53 to -65 kJ/gmole CO_2 for the 52 wt. % MDEA solution. From equation 1, the values of this study (-50 kJ/gmole CO_2 at 288.7 K to -67 kJ/gmole CO_2 at 422.0 K) match well with the range of values reported by Jou.

From these comparisons (summarized in table 3), it is concluded that there is good agreement between the experimentally measured enthalpies of solution and those values found in the literature. Some of the trends shown by this experimental data contradict trends previously reported in the literature, but all of the trends and correlations reported in this thesis were found by analysis of actual experimental enthalpy of solution data, while the trends reported in the literature were found by analysis of partial pressure data. For this reason, the trends shown through analysis of these experimental enthalpy data are assumed to be more reliable than the reported trends in the literature.

TABLE 3

Comparison of Calorimetrically Determined Enthalpies of Solution (kJ/gmole CO_2) with Values from Literature Sources.

Reference	Literature Value(s)		Experimental Value(s)	
	H^S	Method/Conditions	H^S	Method/Conditions
Dibble (6)	-49	Unknown method; T, P, % MDEA, and loading ranges unknown.	-47 to -66	Experimental data; 20 wt. %, 288.7 K to 40 wt. %, 422.0 K
Pearce (7)	-59	Unknown method; T, P, % MDEA, and loading ranges unknown.	-47 to -66	Experimental data; 20 wt. %, 288.7 K to 40 wt. %, 422.0 K
Polasek and Bullin (8)	-61	Unknown method; Unknown T, 30-50 wt. % MDEA, all loadings.	-50 to -67	From Equation 1; 30 wt. %, 288.7 K to 50 wt. %, 422.0 K
Jou, Mather and Otto (2)	-42 to -65	Solubility measurement; 23.5 % MDEA, dependent on loading, independent of T.	-47 to -64	From Equation 1; 23.5 % MDEA from 288.7 to 422.0 K, ind. of loading.
Jou, Mather and Otto (2)	-53 to -65	Solubility measurement; 52 % MDEA, dependent on loading, independent of T.	-50 to -67	From Equation 1; 52 % MDEA from 288.7 to 422.0 K, ind. of loading.

In addition to providing the enthalpy of solution of CO_2 in aqueous MDEA solutions, the calorimetric data provided a means of determining the saturation concentration (or saturation loading point) of CO_2 in the solution. An examination of figures 7 and 8 reveals the enthalpy of solution (kJ/gmole MDEA) to be a linear function of loading both above and below the saturation loading point. The saturation loading point was taken to be the loading at which the data points started to deviate from the line representing the data beyond saturation. These saturation loading point values are summarized in table 2. The experimentally determined saturation loading points are approximately linear functions of temperature as can be seen in figure 12 which is a plot of these saturation loading points as functions of temperature and MDEA concentration at a constant pressure of 1121 kPa (except at 422.0 K where the system pressure was 1466 kPa).

A comparison of the experimental saturation loading points (determined as outlined above) and saturation loading points determined by the static cell method of measuring vapor-liquid equilibrium (as reported in the literature) is included in table 4. The values of this study show good agreement (within 9%) with the direct measurement of the loading. The values of the calorimetrically determined saturation loading points listed in table 4 for conditions not specifically investigated in this research were found by linear interpolation of the experimental saturation loading points.

The accuracy of the calorimeters has been shown to be better than ±1% for heat of mixing runs made with certain liquid-liquid test systems. However, in the determination of the enthalpies of solution of a gaseous reactant (CO_2) in an aqueous amine solution, the complexity of the experimental measurements is increased. The two major difficulties encountered in the experimental work were: (1) problems with the constant

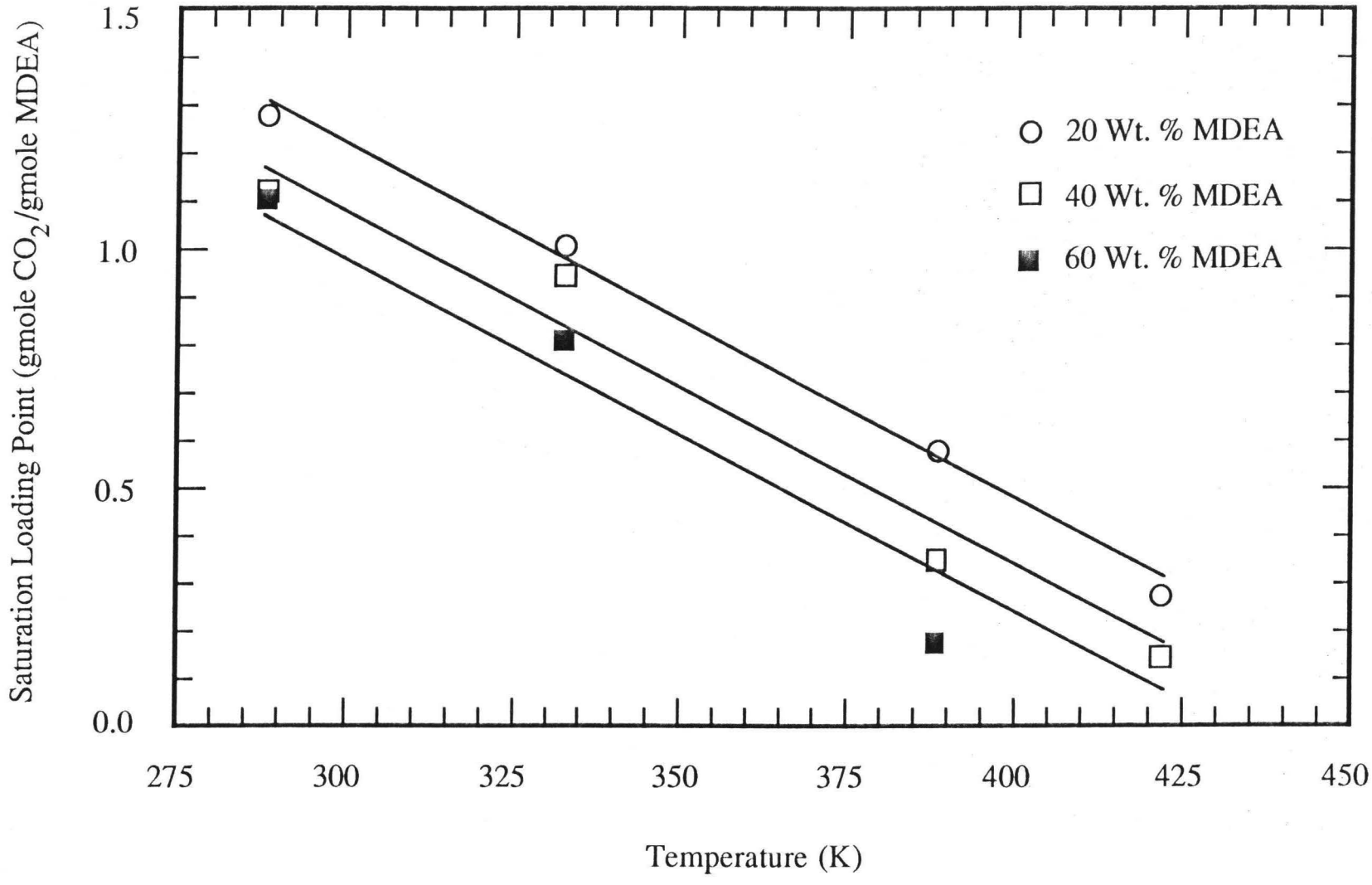


Figure 12. Calorimetrically determined saturation loading points as functions of temperature and MDEA concentration at a constant pressure of 1121 kPa (1466 kPa at 422.0 K).

TABLE 4

A Comparison of Seven Calorimetrically Determined Saturation Loading Points To Those Measured with a Static Equilibrium Cell.

System			Saturation Loading Point (gmole CO_2/gmole MDEA)		
Wt. % MDEA	Temperature (K)	Pressure (kPa)	Experimental Data*	Static Cell	Ref. for Static Cell
20	310.9	1121	1.14	1.11	(9)
20	338.7	1121	0.93	1.01	(9)
23.5	388.7	1121	0.58	0.54	(10)
23.5	298.2	1121	1.21	1.20	(2)
23.5	313.2	1121	1.10	1.12	(2)
23.5	373.2	1121	0.64	0.68	(2)
23.5	393.2	1121	0.49	0.49	(2)

* Those values not specifically measured in this study were obtained by interpolation of the experimental data.

delivery of the gas and (2) problems in the measurement of the heat released as a reacting gas is absorbed into an aqueous solution.

The problems with constant gas delivery were: (1) intermittent gas leakage caused by imperfect pump barrels and seals, and (2) inconsistent operation of the gas back pressure regulator which caused sporadic variation in the gas delivery rate. The gas leakage problem wasn't solved until after all of the experimental had been taken by placing a small layer (1 or 2 ml) of liquid mercury in the pump barrel to seal any imperfections in the barrel. The problem with the back pressure regulator was solved by frequent cleaning and replacement of the teflon diaphragm, the key component for the proper operation of the regulator.

The problems of measuring the enthalpy of solution of the very reactive gas in the aqueous solution were caused by the aqueous amine solution creeping up the input line containing the very reactive CO_2 gas. In order to collect data at loadings below the saturation loading point, only low gas flow rates ($\leq$20% of the total volumetric flow) could be used, and the MDEA solution not only reacted readily with the gas on the equilibration plate (figure 5) but also backed up the gas inlet line and reacted with the carbon dioxide before the CO_2 reached the isothermal plate. The fact that MDEA backed up the gas inlet line was first substantiated upon discovery of aqueous MDEA solution in the CO_2 inlet line near the CO_2 inlet valve. On several subsequent occasions, the same circumstance in which the MDEA had crept up the CO_2 line was observed during periodic cleaning of the system tubing. Because a portion of the reaction occurred at a point off of the equilibration plate, the measured heat of solution in these circumstances was less than the actual total heat of solution. This problem was overcome by flushing the calorimeter system with pure, high-pressure carbon dioxide (while the

MDEA flow was shut off) between each data point. As a result of these two problems, each data point often had to be retaken a number of times to properly characterize the true heat of solution curve.

Based on the complexities enumerated above, the accuracy of the calorimetric measurements reported here is estimated to be ±5% (appendix D contains a breakdown of this estimate). A better estimate is not possible due to the lack of extensive and reliable literature data for comparison to this study's results.

The precision of the enthalpy of solution measurements was estimated by examining the results of repeat runs which were made for 5 of the 17 experimental systems. Table 5 shows the results obtained when H^S below the saturation loading point was redetermined for these systems. Comparing the two results for each of the 5 systems shows that in each case, the two results agreed to within 4%. Thus, the precision is estimated to be ±4%.

Finally, the question of whether equilibrium is obtained in the calorimeter under flow conditions was raised. For the previously mentioned DGA study (5), the equilibrium question was investigated several times, and all indications were that conditions either at or close to equilibrium were present for all of the DGA experimental runs. For the DGA system, identical experimental points (i.e., measurement of the enthalpy of solution at a specified loading value) were taken over a wide range of flow rates (calorimeter residence times) and all H^S results were found to agree within the experimental error. Preliminary runs were made at very low flow rates giving residence times of 19, 38, 187, and 281 minutes (3-12 minutes is the normal residence time for most of the experimental data reported here). The H^S values for the runs with these long residence times matched a previously determined set of data (taken at residence times from 3-12

TABLE 5

Enthalpy of Solution Below the Saturation Loading Point for Five Repeated Runs Showing the Reproducibility of the H^S Determinations.

System			H^S (kJ/gmole CO_2)	
Wt. % MDEA	Temperature (K)	Pressure (kPa)	Initial Run (Month/Year)	Repeated Run (Month/Year)
20	288.7	1121	-47 (1/85)	-47 (2/85)
40	288.7	1121	-48 (4/84)	-49 (2/85)
60	288.7	1121	-49 (4/84)	-51 (2/85)
20	333.2	1121	-53 (3/84)	-53 (3/85)
40	422.0	1466	-63 (10/84)	-66 (2/85)

minutes) for the 20 wt. % DGA solution at 288.7 K and 156 kPa. This indicates that conditions at or very near equilibrium were present for the DGA system. In addition, a visual flow apparatus (transparent tubing) was constructed that had approximately the same configuration as the flow calorimeter. This apparatus was used to visually observe the absorption of carbon dioxide into the amine solution. Under conditions of temperature, pressure, and molar flow rates similar to actual calorimeter operating conditions, complete absorption of the gas was observed in less time (half or less) than the normal residence time of the components in the calorimeter.

In the case of this MDEA study, on several occasions a data point representing a certain CO_2 loading value was taken repeatedly at differing volumetric flow rates (giving residence times of 3-12 minutes) to see if the value of H^S changed with flow rate. Had equilibrium conditions not existed within the calorimeter, a volumetric flow rate dependent enthalpy of solution would have been observed. It was expected that this flow rate dependency would have indicated that conditions closer to equilibrium were present at the lower flow rates which gave longer residence times than at the higher flow rates which gave shorter residence times. However, no volumetric flow rate dependency was observed, leading to the conclusion that conditions at or close to equilibrium were present for all MDEA runs. Finally, the close agreement between the calorimetrically determined saturation loading points and the saturation loading points determined in a static-equilibrium cell (from literature sources as summarized in table 4) is taken as an indication that equilibrium was achieved (for all practical purposes) in the calorimeter.

IV. CONCLUSION, PART I

The enthalpies of solution of carbon dioxide in aqueous MDEA solutions were measured over ranges of temperature, pressure, weight percent MDEA, and loading representative of conditions found in the gas processing industry (table 2). The enthalpies of solution (per gmole CO_2) were found to be constant over the CO_2 loading range of 0 gmole CO_2/gmole MDEA to near the CO_2 saturation point for all 17 systems studied. In addition, the measurements showed that H^S was independent of the partial pressure of CO_2 above the MDEA solutions (between 156 and 1466 kPa), but dependent upon temperature (between 288.7 and 422.0 K), and concentration (between 20 and 60 wt. % MDEA). A correlation of H^S as a linear function of temperature and concentration was presented (equation 1).

In addition to determining the enthalpies of solution, the saturation loading point was found from the calorimetric data. The saturation loading point was seen to be dependent upon both temperature and concentration (figure 12).

The calorimetrically determined values of H^S and saturation loading point were compared to the existing literature data, and good agreement was shown (tables 3 and 4). Estimates of the experimental accuracy and precision were presented. Finally, the question of whether equilibrium is obtained in the flow calorimeter was examined, and it was concluded that conditions at or very near equilibrium existed for all of the experimental runs.

PART II. MODELING AND PREDICTION OF ENTHALPY OF SOLUTION AND VAPOR-LIQUID EQUILIBRIUM DATA

I. INTRODUCTION

Consistent with the goals of this research project was the objective of obtaining a thermodynamically consistent model of acid gas absorption that could be both extrapolated and interpolated with confidence as a result of a firm theoretical basis. This model was created and then used to predict the enthalpy of solution of CO_2 in MDEA solutions, the liquid-phase composition, and the equilibrium partial pressure of CO_2 over the solution for any acid gas loading. A preliminary model for the absorption of carbon dioxide into aqueous MDEA solutions was developed and it is described in this part of the thesis. The model is based upon fundamental thermodynamic quantities (equilibrium constants [K] and heats of reaction [ΔH]) and existing literature correlations for the calculation of activity coefficients. Where possible, all of these quantities were found in the literature. The main objective and chief emphasis of the computer model's development was the accurate prediction of the enthalpy of solution below the saturation loading point. In the model development, considerably less emphasis was placed upon the model's accurate prediction of the saturation loading points and the equilibrium partial pressures of CO_2.

The first section in Part II describes the development of the computer model. A discussion of the postulated reaction mechanism is given for the absorption of CO_2 into aqueous MDEA solutions and the corresponding set of equations that must be solved in order to calculate the solution composition and total heat of solution is presented. The assumptions of the model and the literature data that were incorporated in the computer

program are discussed. Then, a presentation of the logic behind the model's development is made. Finally, the computer program is introduced with a brief description of its operation.

The second section of Part II of this thesis presents the results of the modeling of the CO_2-H_2O-MDEA system. The development of a thermodynamically consistent set of values of K and ΔH for the MDEA protonation reaction is discussed. This is followed by a summary of the fit of the computer model's H^S to the experimental H^S values below the saturation loading point. Finally, a discussion of the prediction of compositions, CO_2 partial pressures, and overall enthalpies of solution is presented.

The third and final section of Part II discusses the existing weaknesses of this preliminary model and suggests future action for refinement of the model.

II. DEVELOPMENT OF COMPUTER MODEL

The absorption of CO_2 into aqueous MDEA was modeled in two steps. In the first step, the model was utilized to determine thermodynamically consistent values of K and ΔH for the MDEA protonation reaction over the temperature range of this study from the measured overall enthalpies of solution and literature values of K and ΔH for the four most common reactions in the chemical reaction scheme. In the second step, the model was used to calculate the enthalpies of solution, liquid phase composition, and equilibrium partial pressures of CO_2 over the MDEA solutions from the literature values of K and ΔH and the values of K and ΔH for the MDEA protonation reaction determined in the first step described above. This section describes the reaction mechanism, discusses the literature values used, introduces the logic of the model, and briefly describes the computer code.

Reaction Mechanism

The heat measured in the calorimeter when gaseous carbon dioxide contacts an aqueous solution of MDEA can be modeled by using the ΔH and K values of each reaction assumed to occur in the reaction vessel. In the case of the CO_2 absorption, the equilibrium is described by a Henry's law constant (H) as described later. The computer model is based upon the following chemical reaction scheme proposed by Jou, Mather, and Otto (2):

1. $H_2O \Leftrightarrow H^+ + OH^-$ $K_1, \Delta H_1$
2. $MDEAH^+ \Leftrightarrow MDEA + H^+$ $K_2, \Delta H_2$
3. $H_2O + CO_{2\,(aq)} \Leftrightarrow H^+ + HCO_3^-$ $K_3, \Delta H_3$
4. $HCO_3^- \Leftrightarrow H^+ + CO_3^=$ $K_4, \Delta H_4$
5. $CO_{2\,(g)} \Leftrightarrow CO_{2\,(aq)}$ $H, \Delta H_5$

Chemical reaction 1 is the water dissociation reaction, chemical reaction 2 is the dissociation of protonated MDEA (the reverse of the MDEA protonation reaction), chemical reaction 3 is the first ionization of carbonic acid, chemical reaction 4 is the second ionization of carbonic acid, and chemical reaction 5 is the absorption of the gaseous carbon dioxide into solution. The overall heat of solution (H^S) is the sum of the individual heat contributions ($\Delta n_i * \Delta H_i$) from each of the five reactions:

$$H^S = \sum \Delta n_i \Delta H_i \tag{3}$$

where Δn_i represents the change in the number of moles of a key component that is a product of chemical reaction i. The values of Δn_i for each of the chemical reactions are calculated from the following equations:

$$\Delta n_1 = [OH^-]_f - [OH^-]_i \tag{4}$$

$$\Delta n_2 = [MDEA]_f - [MDEA]_i \tag{5}$$

$$\Delta n_3 = [HCO_3^-]_f - [HCO_3^-]_i + [CO_3^=]_f - [CO_3^=]_i \tag{6}$$

$$\Delta n_4 = [CO_3^=]_f - [CO_3^=]_i \tag{7}$$

$$\Delta n_5 = (n_{CO2})_i - (n_{CO2})_f \tag{8}$$

where the terms enclosed in square brackets represent the molal concentrations (gmole/kg H_2O) of the chemical species, the subscripts f and i refer to final and initial concentrations in the solution, respectively, and

n_{CO2} refers to the gmole gaseous CO_2 mixed with the MDEA solution per kg H_2O in the aqueous phase. The above equations are simplified by the observation that $[HCO_3^-]_i$ and $[CO_3^=]_i$ are both zero because carbon dioxide is not present in the aqueous solution prior to mixing.

The composition (in molal concentrations) is calculated by considering the stoichiometric equilibria, the charge balance, and component mole balances. In the case of the composition of the initial solution (the aqueous MDEA solution prior to mixing with CO_2), only chemical reactions 1 and 2 need to be considered because carbon dioxide is absent. The equilibrium constant expressions for this case are:

$$K_1 = (\gamma_{H^+} [H^+]_i \gamma_{OH^-} [OH^-]_i) / (a_{H2O}) \quad (9)$$

$$K_2 = (\gamma_{H^+} [H^+]_i \gamma_{MDEA} [MDEA]_i) / (\gamma_{MDEAH^+} [MDEAH^+]_i) \quad (10)$$

where γ is the activity coefficient of the subscripted component and a_{H2O} is the activity of water. The other two equations needed to calculate the initial composition are the following charge balance and MDEA balance equations:

$$[MDEAH^+]_i + [H^+]_i = [OH^-]_i \quad (11)$$

$$[MDEA]_o = [MDEA]_i + [MDEAH^+]_i \quad (12)$$

where the subscript o represents the original stoichiometric composition in gmole/kg H_2O. The simultaneous solution of these four equations (9, 10, 11, and 12) gives the initial composition of the solution ($[H^+]_i$, $[OH^-]_i$, $[MDEA]_i$, and $[MDEAH^+]_i$).

The final composition (for the aqueous solution after mixing with CO_2) was calculated for each value of CO_2 loading. In the case of loadings below the saturation loading point, all of the carbon dioxide is absorbed, so the

equilibrium expressed by chemical reaction 5 is not applicable. The equilibrium expressions in this case are:

$$K_1 = (\gamma_{H^+}[H^+]_f \gamma_{OH^-}[OH^-]_f) / (a_{H2O}) \quad (13)$$

$$K_2 = (\gamma_{H^+}[H^+]_f \gamma_{MDEA}[MDEA]_f) / (\gamma_{MDEAH^+}[MDEAH^+]_f) \quad (14)$$

$$K_3 = (\gamma_{H^+}[H^+]_f \gamma_{HCO3^-}[HCO_3^-]_f) / (\gamma_{CO2}[CO_2]_f a_{H2O}) \quad (15)$$

$$K_4 = (\gamma_{H^+}[H^+]_f \gamma_{CO3=}[CO_3^=]_f) / (\gamma_{HCO3^-}[HCO_3^-]_f) \quad (16)$$

The other three equations needed to solve for the final composition are the charge balance, the MDEA component balance, and the CO_2 component balance:

$$[MDEAH^+]_f + [H^+]_f = [OH^-]_f + [HCO_3^-]_f + 2[CO_3^=]_f \quad (17)$$

$$[MDEA]_o = [MDEA]_f + [MDEAH^+]_f \quad (18)$$

$$(n_{CO2})_o = [CO_2]_f + [HCO_3^-]_f + [CO_3^=]_f \quad (19)$$

Simultaneous solution of equations 13-19 for known values of the equilibrium constants, activity coefficients, and original concentrations of MDEA and gaseous CO_2 yields the final composition ($[MDEA]_f$, $[MDEAH^+]_f$, $[H^+]_f$, $[OH^-]_f$, $[HCO_3^-]_f$, $[CO_3^=]_f$, and $[CO_2]_f$). Thus, by combining this final solution composition with the initial solution composition (calculated as described previously), the values of Δn_i for the 4 reactions that occur in solution upon mixing can be calculated (from equations 4-7).

The last case to be considered is the computation of the final solution composition for CO_2 loadings beyond the saturation loading point. The five equilibrium expressions in this case include the equilibrium expressions for the four chemical reactions just considered (given by equations 13-16) plus

the following expression for the carbon dioxide equilibrium:

$$H = (\gamma_{CO2}\,[CO_2]_f) / (p_{CO2}) \qquad (20)$$

where H represents the Henry's law coefficient for the absorption of carbon dioxide in pure water (gmole/kg H_2O*atm) and p_{CO2} is the equilibrium partial pressure of CO_2 over the aqueous solution. This equation ignores any gas phase nonidealities through the use of pressure rather than fugacity. The charge balance (equation 17) and the MDEA component balance (equation 18) remain unchanged, but the carbon dioxide balance (equation 19) becomes:

$$(n_{CO2})_o = (n_{CO2})_f + [CO_2]_f + [HCO_3^-]_f + [CO_3^=]_f \qquad (21)$$

Thus, simultaneous solution of equations 13-18, 20, and 21 for known values of K, γ, and the original concentrations of MDEA and CO_2 yields the final composition ($[MDEA]_f$, $[MDEAH^+]_f$, $[H^+]_f$, $[OH^-]_f$, $[HCO_3^-]_f$, $[CO_3^=]_f$, $[CO_2]_f$, and $(n_{CO2})_f$) for loadings beyond the saturation loading point. The values of Δn_i can then be calculated for each of the five chemical reactions.

To determine if the saturation loading point has been reached, first the final composition of the solution is calculated assuming that the saturation loading point has <u>not</u> been reached. From this final composition, the equilibrium partial pressure of CO_2 is determined by rearrangement of equation 20. The equilibrium partial pressures of MDEA and H_2O are determined by applying Raoult's law:

$$p_i = \gamma_i\, x_i\, P_i^{\bullet} \qquad (22)$$

where x_i is the mole fraction and $P_i^{\bullet}$ is the vapor pressure of the pure

component at the temperature investigated. The calculated total pressure is the sum of the partial pressures of CO_2, MDEA, and water. If this calculated total pressure is greater than the actual system pressure, then the saturation loading point has been exceeded and the final composition is recalculated (according to equations 13-18, 20, and 21) assuming gaseous CO_2 to be present.

Literature Data for Model

In order to calculate the composition and the enthalpy of solution with the model, a knowledge of K and ΔH values as functions of temperature for each of the 5 chemical reactions is essential. In addition, correlations for the activity coefficients are required for calculating the molal concentrations. Chemical reactions 1, 3, 4, and 5 (the water reaction, the first and second ionization of carbonic acid, and the absorption of gaseous carbon dioxide) are common reactions which have been studied and reported in the literature over wide ranges of temperature and pressure. On the other hand, the literature reports on chemical reaction 2 (the dissociation of the protonated MDEA) are limited to a single study performed by Schwabe in 1959 (11).

Thus, the proposed computer model was used to first find values of K and ΔH for the little studied protonation reaction (chemical reaction 2) which, when combined with the literature values of K and ΔH for chemical reactions 1, 3, 4, and 5, yielded the best match between the calculated heats of solution and the experimentally measured values.

Numerous literature references were found which report K and ΔH over widely varying conditions of temperature for chemical reactions 1 (12-19,29,51), 3 (18-26,29,51-53), 4 (19,23,24,27-29,51), and 5 (19,25,26,29-42). Most of these references reported the infinite dilution

equilibrium constant as a function of temperature. A fit of these K values as a function of temperature was made over the temperature range of interest (15.56 to 148.89°C). This fit took the following form:

$$- \ln K = A + B T + C/T + D \ln T + E/T^2 \qquad (23)$$

A plot of ln K versus T was made and those values of K which deviated significantly from the trend of the majority of the data (determined arbitrarily) were rejected. The remaining data points were fit to the above equation using a computer program included in appendix E. Table 6 is a tabulation of the curve fits for chemical reactions 1, 3, 4, and 5. The goodness of these curve fits is indicated by the value of the correlation coefficient, R^2, where a value of 1.00 means the data are perfectly represented by the curve. The values of R^2 for these data fits ranged from 0.9984 to 0.9999. The match between the curve fits and the literature data can also be seen by referring to table 7, a sample output from the multiple linear regression program which compares the literature values to the results of the curve fit. The remainder of the outputs are included in appendix E.

The numerical values of the heats of reaction can be determined from the multiple linear regression by the following form of the van't Hoff equation:

$$\partial \ln K / \partial T = \Delta H / R T^2 \qquad (24)$$

Thus, differentiating the equation obtained from the curve fit of - ln K vs. T with respect to temperature gives the following equation for the heats of reaction:

$$\Delta H = R (C - D T - B T^2 + 2 E/T) \qquad (25)$$

TABLE 6

Summary of Multiple Linear Regressions on the Literature Data.

$$-\ln K = A + B T + C/T + D \ln T + E/T^2$$

	Chemical Reaction Number				
Item	1	2	3	4	5
Number of Points in Fit	44	4	24	49	41
Fitting Parameters					
A	-3.3611E+3	3.0155E+0	3.6532E+3	-2.1341E+2	2.0802E+2
B	-5.1917E-1	3.7762E-3	5.9521E-1	-2.3301E-2	3.0346E-2
C	1.7969E+5	4.6106E+3	-1.9697E+5	8.0251E+3	-7.2797E+3
D	5.3452E+2	0	-5.7703E+2	3.7301E+1	-3.2595E+1
E	-8.8917E+6	0	1.1763E+7	4.1833E+6	-3.1630E+5
R^2	0.99997	1.00000	0.99838	0.99952	0.99988

TABLE 7

Sample Output (for Reaction 3) from Multiple Linear Regression Program. The Calculated Values and Literature Values Show Good Agreement.

MULTIPLE LINEAR REGRESSION FOR REACTION NUMBER 3

FORM OF THE EQUATION IS -Ln K = A + B*T + C/T + D*LnT + E/T**2

A = Ø.36531643E+Ø4 B = Ø.59521486E+ØØ

C = -Ø.19696531E+Ø6 D = -Ø.57703321E+Ø3

E = Ø.11762966E+Ø8

R2 = Ø.998375E+ØØ THE STANDARD DEVIATION = Ø.1ØØ722E-Ø2

N	T	-Ln K	REFERENCES	-Ln K CALC	DELTA
1	Ø.273150E+Ø3	Ø.151480E+Ø2	22	Ø.151477E+Ø2	-Ø.182337E-Ø4
2	Ø.273150E+Ø3	Ø.151576E+Ø2	52	Ø.151477E+Ø2	-Ø.651568E-Ø3
3	Ø.273150E+Ø3	Ø.151256E+Ø2	20	Ø.151477E+Ø2	Ø.146267E-Ø2
4	Ø.278150E+Ø3	Ø.150059E+Ø2	22	Ø.150018E+Ø2	-Ø.271058E-Ø3
5	Ø.283150E+Ø3	Ø.148839E+Ø2	22	Ø.148796E+Ø2	-Ø.290359E-Ø3
6	Ø.288150E+Ø3	Ø.147796E+Ø2	22	Ø.147780E+Ø2	-Ø.110253E-Ø3
7	Ø.288150E+Ø3	Ø.148038E+Ø2	52	Ø.147780E+Ø2	-Ø.174479E-Ø2
8	Ø.293150E+Ø3	Ø.146926E+Ø2	22	Ø.146944E+Ø2	Ø.125584E-Ø3
9	Ø.298150E+Ø3	Ø.146258E+Ø2	22	Ø.146268E+Ø2	Ø.688898E-Ø4
10	Ø.298150E+Ø3	Ø.146236E+Ø2	26	Ø.146268E+Ø2	Ø.219342E-Ø3
11	Ø.298150E+Ø3	Ø.146207E+Ø2	53	Ø.146268E+Ø2	Ø.417734E-Ø3
12	Ø.298150E+Ø3	Ø.146191E+Ø2	20	Ø.146268E+Ø2	Ø.527226E-Ø3
13	Ø.303150E+Ø3	Ø.145680E+Ø2	22	Ø.145732E+Ø2	Ø.355747E-Ø3
14	Ø.308150E+Ø3	Ø.145279E+Ø2	22	Ø.145320E+Ø2	Ø.280258E-Ø3
15	Ø.313150E+Ø3	Ø.145012E+Ø2	22	Ø.145018E+Ø2	Ø.424748E-Ø4
16	Ø.318150E+Ø3	Ø.144837E+Ø2	22	Ø.144816E+Ø2	-Ø.147430E-Ø3
17	Ø.323150E+Ø3	Ø.144720E+Ø2	22	Ø.144702E+Ø2	-Ø.121142E-Ø3
18	Ø.348150E+Ø3	Ø.145177E+Ø2	20	Ø.145235E+Ø2	Ø.399990E-Ø3
19	Ø.373150E+Ø3	Ø.147318E+Ø2	53	Ø.147237E+Ø2	-Ø.551773E-Ø3
20	Ø.373150E+Ø3	Ø.147296E+Ø2	20	Ø.147237E+Ø2	-Ø.402497E-Ø3
21	Ø.398150E+Ø3	Ø.150565E+Ø2	20	Ø.150521E+Ø2	-Ø.292710E-Ø3
22	Ø.423150E+Ø3	Ø.154964E+Ø2	29	Ø.155107E+Ø2	Ø.921959E-Ø3
23	Ø.423150E+Ø3	Ø.154757E+Ø2	20	Ø.155107E+Ø2	Ø.226077E-Ø2
24	Ø.429150E+Ø3	Ø.156798E+Ø2	23	Ø.156412E+Ø2	-Ø.246156E-Ø2

The values of the heats of reaction calculated in this manner were compared to the limited number of experimentally determined heats of reaction reported in the literature. This comparison, included in table 8, shows that the differentiation of the curve fits gives ΔH values in close agreement to those measured calorimetrically.

In addition to these correlations of K and ΔH as a function of temperature, equations from which the activity coefficients could be calculated were required before the system of equations describing the solution composition could be solved.

For chemical reaction 1, a correlation for the activity coefficient ratio ($\gamma_{H^+} \gamma_{OH^-} / a_{H2O}$) as a function of temperature (between 273 and 573 K) and solution ionic strength (up to 5.0 molal) was used (16). Similarly, a correlation for the activity coefficient ratio of chemical reaction 3 ($\gamma_{H^+}\gamma_{HCO3^-} / \gamma_{CO2}\, a_{H2O}$) as a function of temperature (between 323 and 573 K) and solution ionic strength (up to 5.0 molal) was located in the literature and incorporated into the model (20). A similar correlation (27) was used in the program to calculate the activity coefficient ratio of chemical reaction 4 ($\gamma_{H^+} \gamma_{CO3=} / \gamma_{HCO3^-}$) as a function of temperature (between 323 and 523 K) and solution ionic strength (up to 5.0 molal). A summary of the activity coefficient correlations used in the model is included in appendix F.

For chemical reaction 5, the activity coefficient of the aqueous carbon dioxide (γ_{CO2}) was calculated as a function of temperature (between 273 and 323 K) and solution ionic strength (up to 3.0 molal) from a literature correlation (19,25).

For chemical reaction 2, the activity coefficient of the hydrogen ion (γ_{H^+}) was calculated as a function of ionic strength (up to 6.0 molal) at 298.2

TABLE 8

Comparison of Calorimetrically Determined Heats of Reaction from the Literature with Heats of Reaction Calculated from Curve Fits (Equation 25).

Reaction Number	Temperature (K)	Curve Fit ΔH_{rxn} (kJ/gmole)	Literature Values: Calorimetric ΔH_{rxn} (kJ/gmole)	Literature Values: Reference
1	298.2	56.78	55.92	17
1	323.4	51.02	50.92	17
1	347.6	45.41	46.67	17
1	373.6	40.40	42.07	17
1	398.5	37.45	34.59	17
1	417.8	36.82	33.45	17
3	298.2	8.92	9.15	26
4	298.2	14.82	14.70	26
5	298.2	-19.79	-19.74	26
5	298.2	-19.79	-19.41	26

K from the Pitzer equation (43). An attempt to account for the temperature dependence of the activity coefficient was made by including the temperature dependence of the Debye-Hückel term of the Pitzer equation (44). Also for chemical reaction 2, the activity coefficient of the unprotonated MDEA (γ_{MDEA}) was assumed to be unity. Finally, no models for the activity coefficient of the protonated MDEA (γ_{MDEAH^+}) were found in the literature. However, an activity coefficient correlation for a similar protonated amine (monoethanolamine [MEA]) was located (45). For lack of an activity coefficient correlation specific to the protonated MDEA, the correlation for the protonated MEA was applied to the protonated MDEA species. The activity coefficient model is the extended Debye-Hückel expression as proposed by Guggenheim (see appendix F for the form of the equation). This equation requires knowledge of the interaction parameters between the component of interest (protonated amine) and all other species in solution. It was claimed that these parameters showed only a weak dependence on ionic strength and temperature (45), and, because this "weak" dependency was not specifically quantified, the parameters were assumed constant over the range of temperatures and ionic strengths of this study. The only interaction parameter reported in the publication is for the protonated MEA-bicarbonate ion interaction. However, because a better literature model was not located, the Guggenheim form of the extended Debye-Hückel equation with only one interaction parameter was used to estimate the activity coefficient of the protonated MDEA. The temperature dependency of the activity coefficient was taken into account by applying the temperature dependence of the Debye-Hückel limiting slope term.

With a knowledge of the equilibrium constants, heats of reaction, and activity coefficients as functions of temperature and composition (or ionic

strength), the equations describing the equilibrium can be solved and the solution composition can be calculated for any loading value. From this determination of composition, the values of Δn_i and the theoretical total heat of solution can be determined.

Model Logic

As noted previously, the first step in the modeling procedure is using the measured overall enthalpies of solution and literature values of the equilibrium constants and heats of reaction for chemical reactions 1, 3, 4, and 5 along with the activity coefficient correlations to determine a thermodynamically consistent set of K and ΔH values for the MDEA protonation reaction (chemical reaction 2).

The procedure for finding the "best" values of K and ΔH for one reaction in a sequence of reactions for which the total heat is known has been described by Christensen et al. (46). An overview is presented here. The mixing of carbon dioxide and an aqueous MDEA solution results in the occurrence of the five chemical reactions where the extent of reaction and the energy produced are related to the corresponding equilibrium constants and enthalpy changes for the reactions. The mathematical relationship between the total heat produced, the equilibrium constants, and the enthalpy changes for each reaction is very complex. The relationship between the measured heat and these quantities was given earlier by:

$$H^S = \sum \Delta n_i \, \Delta H_i \qquad (3)$$

The summation is over all 5 chemical reactions and the values of Δn_i are calculated by equations 4-8. Then, the energy released by the MDEA protonation reaction alone ($Q_{c,j}$) for which reaction both K and ΔH are

unknown is calculated by subtracting the heat contributed by each of the four reactions for which K and ΔH are known from the total measured heat:

$$Q_{c,j} = H^S_{,j} - \sum_{i \neq 2} \Delta n_{i,j} \Delta H_i \qquad (26)$$

where the subscript j refers to a single data point (a single loading value). This corrected heat value is calculated for each datum point. The summation term refers to all reactions other than the protonation reaction (chemical reaction 2) for which the values of K and ΔH are to be determined.

Because this corrected heat represents the net effect of the MDEA protonation reaction alone, $Q_{c,j}$ may be expressed as follows:

$$Q_{c,j} = \Delta H_2 \Delta n_{2,j} \qquad (27)$$

The best values of K_2 and ΔH_2 at each temperature were calculated by a least squares analysis of equation 27. The normalized error square (u_j) for a single data point is given by:

$$u_j = (Q_{c,j} - \Delta H_2 \Delta n_{2,j})^2 / \text{npts} \qquad (28)$$

where npts refers to the number of data points in the set of data from which the data point j was obtained. Because K_2 and ΔH_2 are functions of temperature only, all of the sets of experimental data taken at a single temperature were combined to determine a single best value of K_2 and a single best value of ΔH_2 at that temperature. In order to give equal weight to each experimental data set (as opposed to equal weight for each experimental datum point) the error square was normalized as in equation 28 by dividing the error term by the number of experimental data points in the data set from which the data point j was taken. With this definition of normalized error

square, the normalized error square sum (U) is simply the summation of the normalized error square (u_j) over all of the data sets at the temperature studied, and over each data point of each data set:

$$U(K_2, \Delta H_2) = \sum_L \sum_j u_{j,L} = \sum_L \sum_j [(Q_{c,j,L} - \Delta n_{2,j,L}\, \Delta H_2)^2 / npts(L)] \quad (29)$$

where the subscripts L and j on Q_c and Δn_2 refer to the data set number and data point number, respectively. The limits on the first summation are from 1 to the number of the data sets used at the temperature being studied (L=1, nsets), and the limits on the second summation are from 1 to the number of points in the current data set (j=1, npts(L)).

The best values for K_2 and ΔH_2 for a given temperature are those which minimize $U(K_2, \Delta H_2)$, that is those values which satisfy the following equations:

$$\partial U(K_2, \Delta H_2) / \partial \Delta H_2 = 0 \quad (30)$$

$$\partial U(K_2, \Delta H_2) / \partial K_2 = 0 \quad (31)$$

Since $U(K_2, \Delta H_2)$ is explicit and linear in ΔH_2, the partial derivative given by equation 30 can be evaluated explicitly and solved for ΔH_2, giving:

$$\Delta H_2 = \{\sum_L \sum_j [Q_{c,j,L}\, \Delta n_{2,j,L}/npts(L)]\} / \{\sum_L \sum_j [(\Delta n_{2,j,L})^2/npts(L)]\} \quad (32)$$

However, because $U(K_2, \Delta H_2)$ is implicit in K_2 (through the calculation of Δn_2), equation 31 cannot be solved explicitly for the equilibrium constant. Instead, the following trial and error procedure is followed: (1) guess a value of K_2, (2) calculate the initial concentration and final concentration as outlined in the previous section ("Reaction Mechanism"), find the five Δn values (equations 4-8), and determine the values of $Q_{c,j}$ (equation 26) for

each data point of each data set, (3) calculate the "best" value of ΔH_2 for this guess of K_2 (from equation 32), (4) evaluate the normalized error square sum (equation 29) for this guess of K_2, and (5) guess new values of K_2 and iterate on steps 2, 3, and 4 using these K_2 values until the value of K_2 is found which produces the minimum error in step 4.

An efficient method (in terms of computer time) of iterating on K_2 in order to find the minimum error was proposed by Mullens et al.(47, 48), a modification of which was used in the development of the computer program. After the initial guess for ln K_2 is made (this initial guess is called the central point), steps 2, 3, and 4 of the above procedure are completed, giving the first iteration on ln K_2. Ten subsequent iterations on ln K_2 are completed after which a determination of the best value of ln K_2 from among the eleven iterates (based upon minimum normalized error square sum) for the next set of iterations is made. Five of these ln K_2 values are successive increments of 0.20 greater than the central point, and the other five are successive increments of 0.20 less than the central point. Thus, the range of ln K_2 values considered in this set of eleven iterations is 2.0, almost one order of magnitude. After completing these 11 iterations, the value of ln K_2 which produces the smallest normalized error sum square is determined, and that ln K_2 value becomes the new first guess (or central point) for the next set of 11 iterations. If this new central point lies on either extreme of the 11 ln K_2 values considered in the iterations, then the value of ln K_2 producing the minimum error may still lie outside of the range of the eleven ln K_2 values examined, and the same increment for the ln K_2 values (0.20) is used with the new central point. This procedure is followed until the K_2 value which produces the smallest error of the eleven iterates is no longer on the extremes, but falls somewhere within the extreme values of ln K_2 of the

eleven iterates. Then, after setting the central point to be that value of K_2 with the smallest calculated error, the increment is decreased by a factor of 5 (to 0.04) and the series of 11 iterations is repeated. This process continues until the minimum is found with the increment being less than 0.0005, at which time the iteration procedure is terminated, and those values of K_2 and ΔH_2 which produced this minimum error are output along with a summary of the agreement between the experimental data and the model's predictions.

In this procedure to determine the best K and ΔH values for the protonation reaction, only the experimental data points below the saturation loading point were used. The chief objective of this endeavor was to model the enthalpy of solution below the saturation loading point. Thus, only loading values below the saturation loading point (where H^S is constant) were used in the determination of K_2 and ΔH_2.

After determining the best values of K_2 and ΔH_2 at each of the four temperatures (288.7, 333.2, 388.7, and 422.0 K), a set of thermodynamically consistent values of K and ΔH were determined. Thermodynamic consistency was tested by the van't Hoff equation introduced previously:

$$\partial \ln K / \partial T = \Delta H / R T^2 \qquad (24)$$

Equation 24 was integrated with Simpson's rule to calculate K_2 at 333.2, 388.7, and 422.0 K based upon a fixed value of K_2 at 288.7 K and assumed values of ΔH_2 at the various discrete temperature values used in the Simpson's rule integration. The temperatures at which the values of ΔH_2 must be known are dependent upon the size of the increment on temperature used to approximate the integral. The method used to determine the required numerical values of ΔH_2 was a simple linear interpolation of the

known ΔH_2 values at the four temperatures examined.

The application of this integration method was as follows: (1) using the computer model, determine the value of ΔH_2 and the normalized error sum square (from equation 29) that corresponds to each of a wide range of values of ln K_2 (centered about the "best" value of ln K_2) at each temperature, (2) fix the values of ln K_2 and ΔH_2 at 288.7 K and apply the Simpson's rule integration (equation 24) to determine the value of ln K_2 at 333.2 K using an estimate for the value of ΔH_2 at 333.2 K and linear interpolation to determine the value(s) of ΔH_2 at the intermediate temperature(s) dictated by the temperature increment chosen for the Simpson's rule calculation, (3) update the estimated value of ΔH_2 at 333.2 K by finding the value of ΔH_2 (from the data base gathered in step 1) which corresponds to the value of ln K_2 at 333.2 K calculated in step 2, (4) repeat steps 2 and 3 until the difference between the estimate of ΔH_2 used in step 2 and the updated value of ΔH_2 calculated in step 3 is negligibly small, (5) using these thermodynamically consistent values of K_2 and ΔH_2 at 288.7 and 333.2 K, repeat steps 2, 3, and 4 to find thermodynamically consistent values first at 388.7 K, and finally at 422.0 K, (6) using the thermodynamically consistent values of ln K_2 and ΔH_2 determined in steps 1 through 5, calculate the overall average relative error between the experimental enthalpies of solution and the enthalpies of solution calculated by the computer model.

It is apparent that the calculated set of thermodynamically consistent values of K_2 and ΔH_2 is dependent upon the initially fixed value of ln K_2 at 288.7 K. Several sets of thermodynamically consistent values of K_2 and ΔH_2 were determined using the procedure outlined above by choosing different starting values of ln K_2 at 288.7 K, and the overall average relative error was calculated for each set of thermodynamically consistent values. The set

of thermodynamically consistent K and ΔH values which minimized this error became the optimum set of K_2 and ΔH_2 values.

After finding this set of thermodynamically consistent values for K_2 and ΔH_2, all values of K and ΔH were fixed (at a fixed temperature), and the entire loading curve (enthalpy of solution as a function of loading) was calculated by the computer model and compared to the experimental data to determine how well the model predicted enthalpies of solution, equilibrium partial pressures of carbon dioxide, and saturation loading points.

Computer Program Description

The computer program which was developed has three main options: -1, 0, and +1. Option -1 determines values of ln K_2 and ΔH_2 which give the minimum error between the measured and predicted enthalpies of solution. Program option 0 fixes ln K_2 and finds the best value of ΔH_2 (equation 32) for the value of ln K_2 chosen and the average relative error. It was this option that was used to gather the data base of ln K_2 and ΔH_2 values used in the procedure for determining the best set of thermodynamically consistent values of ln K_2 and ΔH_2. Program option 1 fixes both ln K_2 and ΔH_2 and generates the entire loading curve. These latter two options are somewhat less complex than the first and no further description is given here. The program description that follows is for program option -1. The documented computer program is given in its entirety in appendix G.

After reading in (from external data files) the experimental data (in the form of H^S (Btu/lb MDEA) vs. loading (mole CO_2/mole MDEA)) and the constants used in the calculation of the activity coefficients, the equilibrium constants, the heats of reaction, etc.(sample input files are included and described in appendix G), the data are converted to total heat (cal/kg H_2O)

vs. concentration ($[MDEA]_o$ and $(n_{CO2})_o$). In addition, the input data are converted back to the form of the raw data (i.e., total heat (J/mole solution) vs. x_{CO2}) to double-check the calculation procedure against the original data.

In solving the required system of equations (as presented previously) that describe the aqueous solution composition, the unknown variables (whose values are to be found by solving the system of equations) used in the computer program are the natural logarithms of the molal concentrations (i.e., X(1) = ln $[H^+]$, X(2) = ln $[OH^-]$, X(3) = ln [MDEA], X(4) = ln $[MDEA^+]$, X(5) = ln $[CO_2]$, X(6) = ln $[HCO_3^-]$, and X(7) = ln $[CO_3^=]$). With these definitions of the unknown variables, and upon rearrangement of equations 13-19, the system of equations solved for in the case of this program option are shown in figure 13. Broyden's method (49), a quasi-Newton method for solution of systems of nonlinear equations, was used to determine each value of X(i) which satisfy the system of equations. Broyden's method requires an initial guess for each value of X(i) and the determination of the Jacobian matrix ($J(i,j) = \partial F(i) / \partial X(j)$) for this set of initial guesses. Broyden's algorithm iterates upon X(i) to find the solution within a specified tolerance (1×10^{-5} for all computer runs reported here).

Figure 14 is a flow sheet representing the organization of the computer program. After the entry and conversion of the data, the corrected heat of solution (Q_{corr}, cal/kg H_2O) is calculated by subtracting from the total heat (H^S) the enthalpy of absorption of the gaseous carbon dioxide:

$$Q_{corr} = H^S - (n_{CO2})_o \Delta H_5 \qquad (33)$$

The corrected heat of solution is used rather than the total heat of solution because in modeling the total heat of solution for loadings <u>below</u> the saturation loading point, all of the carbon dioxide is absorbed and, by

Definition of Variables for Substitution into the System of Equations

$X(1) = \ln [H^+]$ $X(2) = \ln [OH^-]$ $X(3) = \ln [MDEA]$

$X(4) = \ln [MDEAH^+]$ $X(5) = \ln [CO_2]$ $X(6) = \ln [HCO_3^-]$

$X(7) = \ln [CO_3^=]$

$K_1 = K_{1,\gamma} [H^+] [OH^-]$ $K_{1,\gamma} = \gamma_{H^+} \gamma_{OH^-} / a_{H2O}$

$K_2 = K_{2,\gamma} [H^+] [MDEA] / [MDEAH^+]$ $K_{2,\gamma} = \gamma_{H^+} \gamma_{MDEA} / \gamma_{MDEAH^+}$

$K_3 = K_{3,\gamma} [H^+] [HCO_3^-] / [CO_2]$ $K_{3,\gamma} = \gamma_{H^+} \gamma_{HCO3-} / \gamma_{CO2}\, a_{H2O}$

$K_4 = K_{4,\gamma} [H^+] [CO_3^=] / [HCO_3^-]$ $K_{4,\gamma} = \gamma_{H^+} \gamma_{CO3=} / \gamma_{HCO3-}$

Final System of Equations Used in Computer Program

1. Charge Balance $F(1) = 0 = e^{X(1)} + e^{X(4)} - e^{X(2)} - e^{X(6)} - 2e^{X(7)}$
2. MDEA Balance $F(2) = 0 = [MDEA]_o - e^{X(3)} - e^{X(4)}$
3. Water Reaction $F(3) = 0 = [\ln K_1 - \ln K_{1,\gamma}] - X(1) - X(2)$
4. MDEA Proton. $F(4) = 0 = [\ln K_2 - \ln K_{2,\gamma}] - X(1) - X(3) + X(4)$
5. First Ionization $F(5) = 0 = (n_{CO2})_o - e^{X(5)} - e^{X(6)} - e^{X(7)}$
6. Second Ionization $F(6) = 0 = [\ln K_3 - \ln K_{3,\gamma}] - X(1) - X(6) + X(5)$
7. CO_2 Absorption $F(7) = 0 = [\ln K_4 - \ln K_{4,\gamma}] - X(1) - X(7) + X(6)$

Figure 13. Final system of equations solved by the computer program. Equations 1-7 above were formed upon rearrangement of equations 13-19 (defined in the text) with substitution of the variables X(i) as defined above.

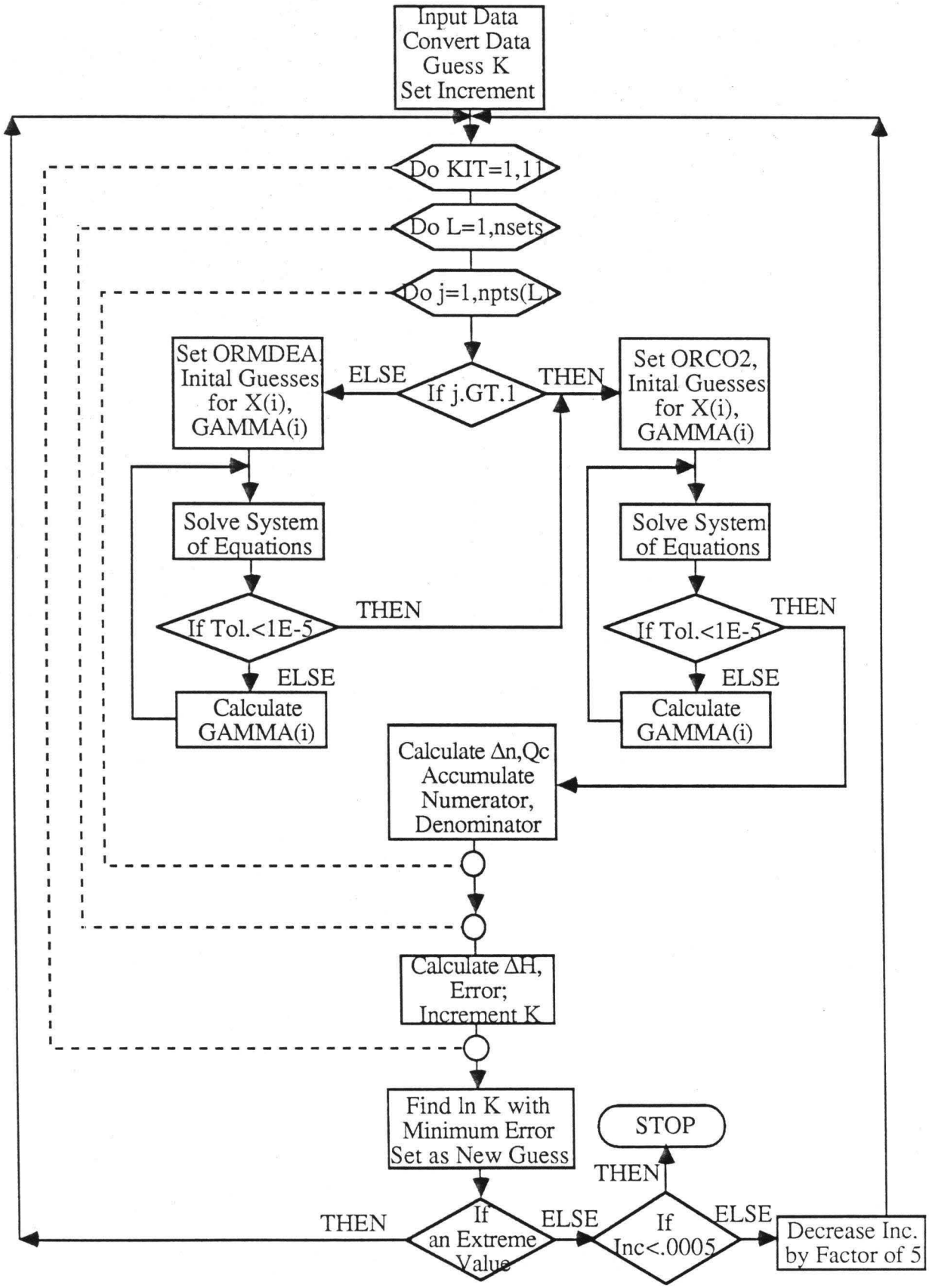


Figure 14. Flow sheet of computer program

subtracting out the effect of this absorption prior to applying the method described in the previous section, one less equilibrium expression is considered in the determination of the final solution composition, and the computation procedure is simplified.

After calculating the corrected heat of solution, the fixed values of K and ΔH (for chemical reactions 1, 3, 4, and 5) are calculated from the correlations. Next, the initial guess for $\ln K_2$ is entered and the starting value of the increment on $\ln K_2$ is chosen (the default is 0.2). Once the initial guess for $\ln K_2$ has been entered, the procedure is as follows (refer to figure 14):

(1) Set the value of of $[MDEA]_o$ for the data set being investigated. This is only a function of the weight percent MDEA in the solution.

(2) Guess values of X(i), i=1,7 (as defined in figure 13) and the activity coefficient ratios $K_{i,\gamma}$ to approximate the actual solution.

(3) Solve the system of equations by Broyden's method for the initial composition only.

(4) Check the tolerance (compare values of X(i) from the previous solution by Broyden's method to the current values of X(i)) to see if convergence has been achieved. If it has, continue with step 6.

(5) Calculate the activity coefficient ratios from the temperature and solution composition calculated in step 3. Return to step 3.

(6) Set the value of $(n_{CO2})_o$ for the data point being investigated. This is only a function of the loading value of the specific data point examined.

(7) Repeat steps 2-5 to calculate the final solution composition with the following exception: in step 4, when convergence is achieved, execution is to continue with step 8, rather than with step 6.

(8) Calculate the values of Δn for each of the five reactions using equations 4-7 introduced earlier.

(9) Calculate Q_c for this data point from equation 26.

(10) Accumulate the numerical values that form the numerator and denominator of equation 32 (used to calculate ΔH_2) as given in the following expressions:

$$\text{Numerator:} \quad Q_c \, \Delta n_2 \, / \, \text{npts(L)} \tag{34}$$

$$\text{Denominator:} \quad (\Delta n_2)^2 \, / \, \text{npts(L)} \tag{35}$$

(11) Repeat steps 6 through 10 for each data point in the data set.

(12) Repeat steps 1 through 11 for each data set at the temperature being examined.

(13) Calculate the numerical value of ΔH_2 as given in equation 32 by taking the ratio of the numerator and the denominator given in equations 34 and 35 and accumulated in step 10.

(14) Calculate the normalized error as given in equation 29.

(15) Increment the current guess of ln K_2 by: the current increment value for iterations 2-6, -6*increment for the 7th iteration, or -1*increment for iterations 8 -11.

(16) Repeat steps 1-15 until the 11th iteration is completed.

(17) Find the value of ln K_2 from among the 11 ln K_2 iterates which gives the minimum error as evaluated in step 14.

(18) Set this value to be the initial guess for the next set of 11 iterations.

(19) If this value of ln K_2 is from the 6th or the 11th iteration (one of the two extreme values of 11 ln K_2 values considered) do not change the increment. Return to step 1 and begin the iterative procedure again with the new value of ln K_2 and the old value of the increment. Otherwise, continue with step 20

(20) If the value of the increment is less than 0.0005, the procedure is complete and the "best" values of ln K_2 and ΔH_2 have been determined. If the increment exceeds 0.0005, decrease the increment value by a factor of 5 and return to step 1 to begin the iterative procedure again with the new value of ln K_2 and the new value of the increment.

(21) Repeat steps 1-20 for each of the four temperatures to find the "best" values of K_2 and ΔH_2 at each temperature.

III. RESULTS OF THE MODEL'S PREDICTIONS OF H^S AND VLE

The computer model was first used to determine the "best" values of K and ΔH for the MDEA protonation reaction which gave the minimum error between the predicted and measured enthalpies of solution below the saturation loading point at each temperature. These "best" values of K and ΔH are the values found by considering each temperature independently. The "best" values of K_2 and ΔH_2 along with their average relative errors are shown in table 9 for each of the 4 temperatures. Figure 15 is a plot of the experimental and calculated values of H^S below the saturation loading point for system 18 (40 wt. % MDEA, 422.0 K, and 1466 kPa) which shows the excellent match between the experimental and predicted values, a match typical of those obtained from these "best" fits. When tested with the van't Hoff equation (equation 29), however, these "best" values of ΔH_2 and ln K_2 at 288.7, 333.2, 388.7, and 422.0 K were not thermodynamically consistent.

The best thermodynamically consistent set of values of ΔH_2 and ln K_2 were calculated according to the procedure outlined previously and are shown in table 10. Figure 16 shows the match between the experimental and calculated values of the total heat below the saturation loading point using the thermodynamically consistent values of ΔH_2 and ln K_2 for the same system (system 18) which is plotted in figure 15. For both the "best" values of K and ΔH and the best thermodynamically consistent set of K and ΔH values, the average relative error was determined. This average relative error is the average of the relative errors between the experimental H^S values and the model's predicted H^S values over all of the data points. By comparing both

TABLE 9

Results of Determination of K_2 and ΔH_2 At Each Temperature Independently ("Best Fits").

Temperature (K)	Number of Data Points	ln K_2 (unitless)	ΔH_2 (kJ/gmole)	Avg. Relative Error (%)
288.7	159	-17.627	41.63	8.57
333.2	89	-16.361	42.11	4.86
388.7	44	-15.804	37.88	3.68
422.0	35	-16.086	29.73	2.71

Overall Average Relative Error: 6.28%

TABLE 10

Results of Determination of Thermodynamically Consistent Values of K_2 and ΔH_2

Temperature (K)	Number of Data Points	ln K_2 (unitless)	ΔH_2 (kJ/gmole)	Avg. Relative Error (%)
288.7	159	-20.000	39.74	13.72
333.2	89	-17.800	39.32	6.12
388.7	44	-15.810	37.85	3.68
422.0	35	-14.930	34.37	3.25

Overall Average Relative Error: 9.18%

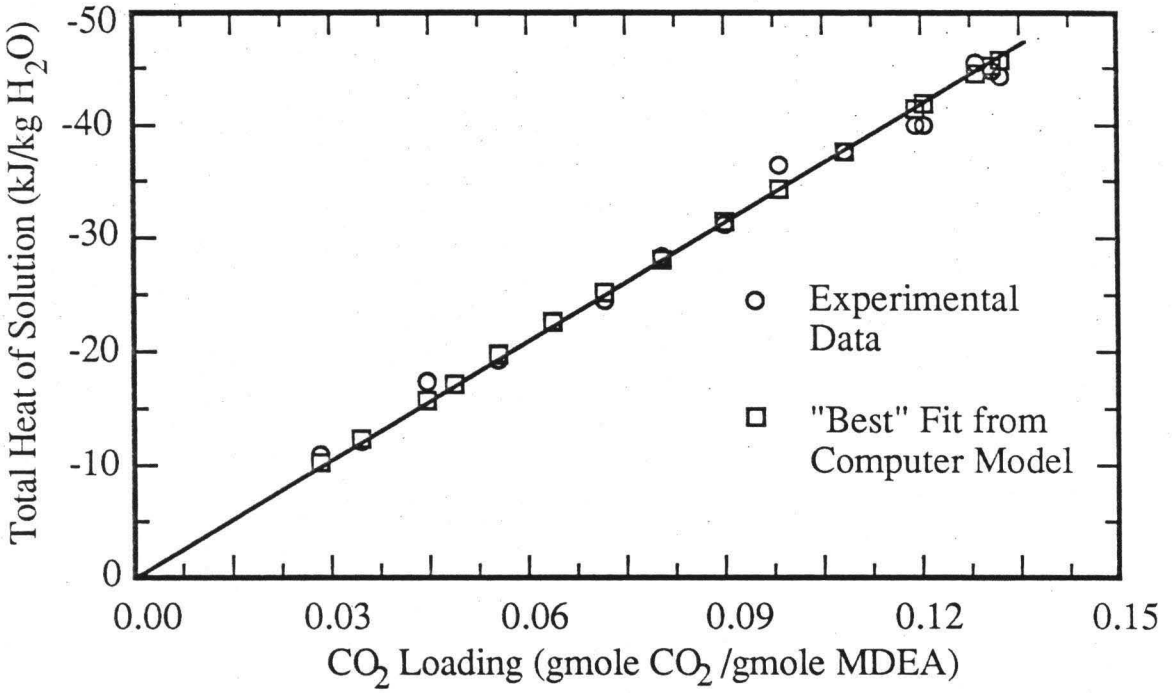


Figure 15. Plot of the experimental enthalpies of solution below the saturation loading point and the "best" fit from the model for system 18.

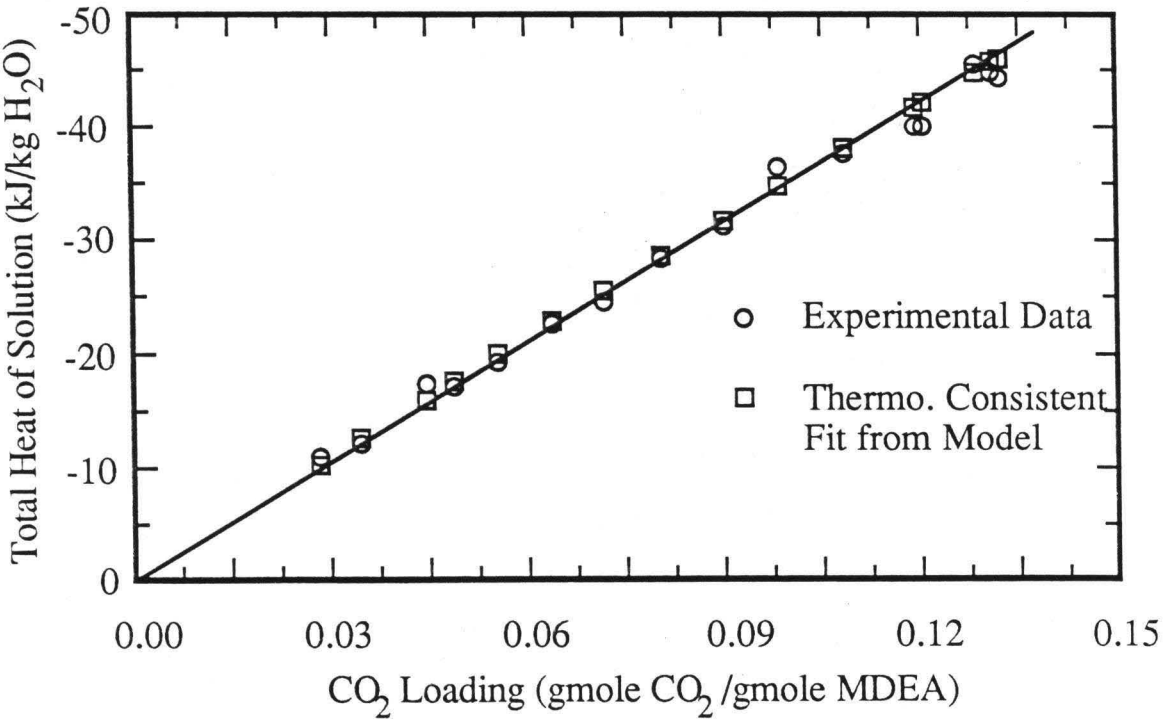


Figure 16. Plot of the experimental enthalpies of solution below the saturation loading point and the thermodynamically consistent fit from the model for system 18.

figures 15 and 16 and the overall average relative errors listed in tables 9 and 10, it is concluded that the closeness of the match between the predicted enthalpies of solution and the experimental data is somewhat worse for the best thermodynamically consistent fit than for the "best" individual fits. This is especially true for the fit at 288.7 K (See tables 9 and 10). In addition, based upon the average relative error listed in table 10, it is concluded that the thermodynamically consistent model predicts the actual heats of solution below the saturation loading point to within 9%.

One of the objectives of this determination of ΔH_2 and ln K_2 was to compare the literature values of ΔH_2 and ln K_2 to the values found from the computer model. However, only one literature study (by Schwabe) was found (11) which reports potentiometrically determined values of the equilibrium constant at 298.2, 308.2, 318.2, and 333.2 K. These values (shown in table 11) were fit with the multiple linear regression program (using only three parameters) described previously for the purposes of extrapolation to the temperatures of this study. The results of this curve fit are summarized and compared to Schwabe's experimental data in table 11. Using the results of this multiple linear regression, Schwabe's K_2 data were extrapolated to the temperatures of this investigation. A comparison of this extrapolation of Schwabe's K_2 data to the thermodynamically consistent values of K_2 determined by the model is summarized in table 12 and plotted in figure 17. While the match between the extrapolation of Schwabe's K_2 data and the thermodynamically consistent values of K_2 found with the model is by no means exact, both sets of results do show the same general trends with temperature and the agreement between the numerical values of K_2 is not bad. Because the extrapolation of Schwabe's data to the highest temperature of this study is an extrapolation of 90 K, the value attributed to

TABLE 11

Values of ln K_2 Measured by Schwabe (11). Also Listed Are the Predictions and Summary of a Curve Fit (Equation 23) of the Experimental Data.

Temperature (K)	Schwabe's Experimental ln K_2	Curve Fit Predicted ln K_2	Relative Error (%)
298.2	-19.605	-19.605	0.00
308.2	-19.142	-19.141	0.00
318.2	-18.708	-18.709	0.00
333.2	-18.113	-18.113	0.00

Regression Results

A = 3.01548 E+00

B = 3.77620 E-03

C = 4.61057 E+03

D = 0

E = 0

R^2 = 1.00000

TABLE 12

Comparison of the Extrapolation of Schwabe's K_2 Data (by Equation 23) and the Thermodynamically Consistent Values of ln K_2 (from Table 10).

Temperature (K)	Schwabe's Data Extrapolated ln K_2	Thermodynamically Consistent ln K_2	Relative Error (%)
288.7	-20.075	-20.000	-0.37
333.2	-18.113	-17.800	-1.73
388.7	-16.345	-15.810	-3.27
422.0	-15.534	-14.930	-3.89

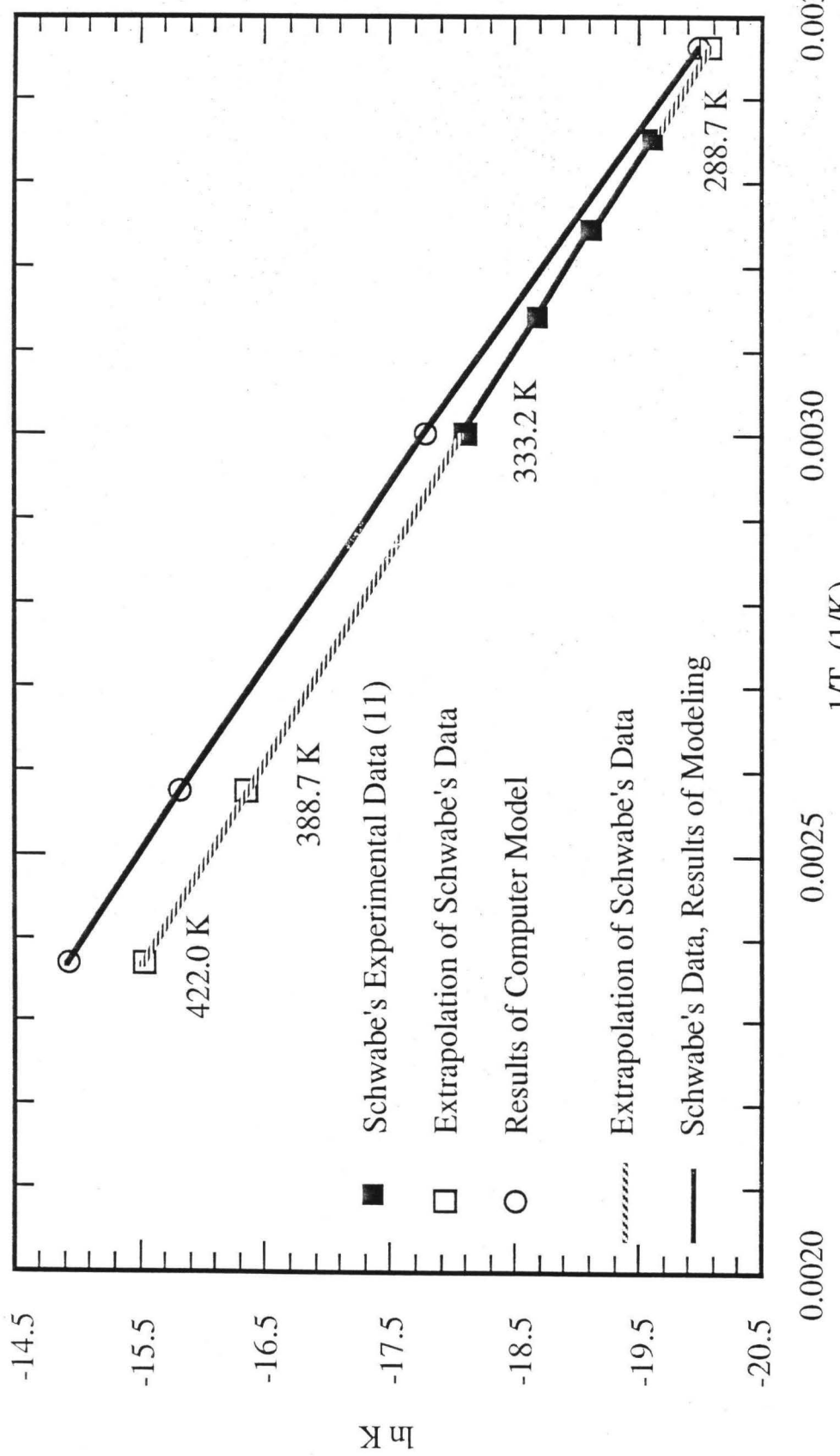


Figure 17. Comparison of the equilibrium constants for the MDEA protonation reaction as a function of temperature. The plot compares the following three sets of data: Schwabe's original experimental data, the extrapolation of Schwabe's data to the temperatures of this research (by equation 23; a summary of this fit is in table 11), and the results of the computer modeling (thermodynamically consistent K_2 values).

Schwabe cannot be assumed to be more than a "ballpark" estimate of the equilibrium constant.

The theoretically sound model predicts values of K_2 that rise more sharply with temperature than do the experimental values of K_2 from Schwabe's study. The following form of the van't Hoff equation directly relates the slope of the plot of ln K_2 vs. 1/T to the value of the heat of reaction:

$$\partial \ln K_2 / \partial (1/T) = - \Delta H_2 / R \qquad (36)$$

Thus, since the computer model predicted values of K_2 that rose more sharply with temperature than do Schwabe's experimental K_2 values (exhibited by a steeper slope on the plot of ln K_2 vs. 1/T in figure 17), the computer model predicts higher values of ΔH_2 than did Schwabe's experimental data. Schwabe applied equation 36 to his own experimental data and claimed that the value of ΔH_2 at 298.2 K was 38.5 kJ/gmole. Upon plotting ln K_2 vs. 1/T and finding the derivative (i.e., slope of the tangent line) at 298.2 K, the value of ΔH_2 was determined to be 35.4 kJ/gmole. In addition, the multiple linear regression on Schwabe's data predicted the value of ΔH_2 (by equation 25) to be 35.5 kJ/gmole at 298.2 K. See figure 18 for a graphical illustration of this inconsistency in the results reported by Schwabe. A comparison of Schwabe's "predicted" ΔH_2 values and the ΔH_2 values predicted by the model is shown in table 13 and plotted in figure 19. Schwabe's "predicted" ΔH_2 values were found from the regression on Schwabe's data described previously (given by equation 25; the curve fit is summarized in table 11) to extrapolate Schwabe's values of ΔH_2 to cover the whole range of temperatures of this study. The agreement between the two sets of ΔH_2 values is not good, but this is to be expected because, as explained

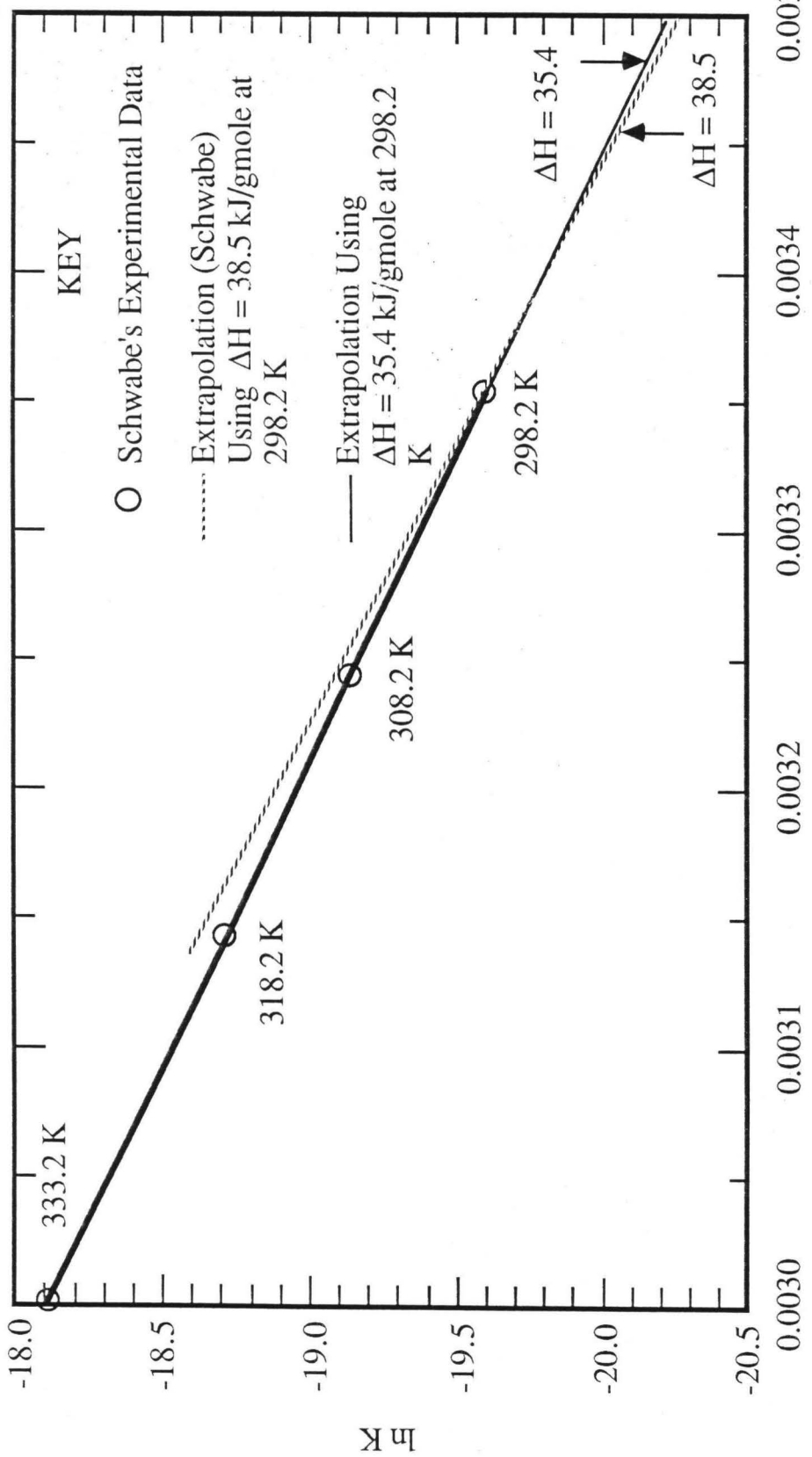


Figure 18. An illustration of the inconsistency of the data reported by Schwabe (11). Schwabe's value of ΔH (38.5 kJ/gmole) at 298.2 K does not represent the true slope (derivative) of the ln K vs. 1/T curve and thus does not represent a thermodynamically consistent value of ΔH at 298.2 K.

TABLE 13

Comparison of the Extrapolation of Schwabe's Data (by Equation 25) and the Thermodynamically Consistent Values of ΔH_2 (from Table 10).

Temperature (K)	Schwabe's Data Extrapolated ΔH_2 (kJ/gmole)	Thermodynamically Consistent ΔH_2 (kJ/gmole)	Relative Error
288.7	35.72	39.74	11.25%
333.2	34.85	39.32	12.83%
388.7	33.59	37.85	12.69%
422.0	32.74	34.37	4.97%

Calorimetric Determination of ΔH_2 at 360.9 K (Ref. 54): 38.66 kJ/gmole

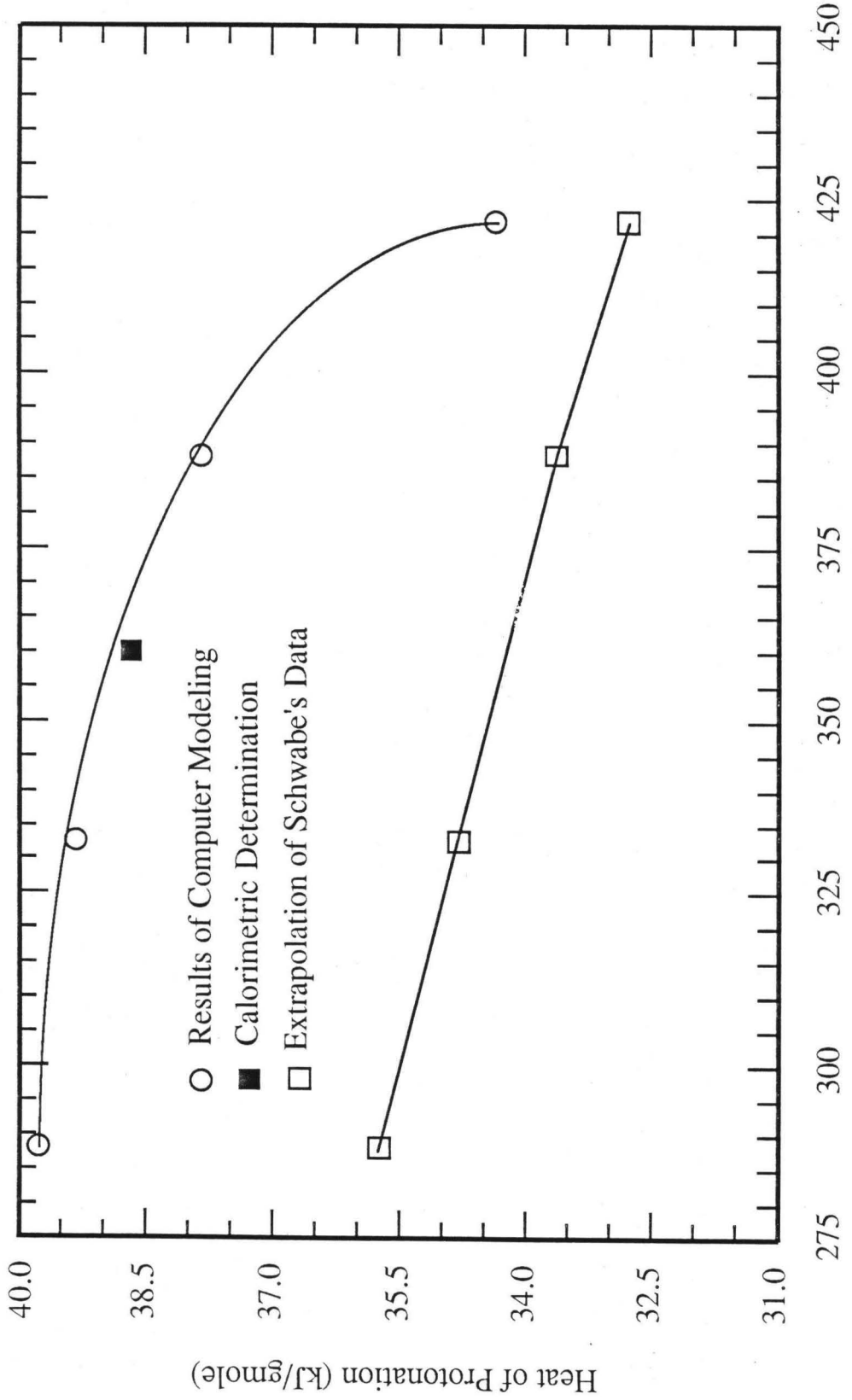


Figure 19. Graphical comparison of the thermodynamically consistent ΔH_2 values as a function of temperature determined with the computer model to the results of a recent calorimetric determination (54) and to the extrapolation of the curve fit of Schwabe's data (11).

above, the model's predicted equilibrium constants showed a significantly steeper slope (∂ [ln K_2]/∂ [1/T]) than did Schwabe's experimental data, thus indicating much higher values of ΔH_2. In addition, the values of ΔH_2 credited to Schwabe in this comparison are actually from the differentiation of the extrapolation of a curve fit of data taken over a very limited range of temperatures, and thus closer agreement is not expected. To validate the computer model's predictions of ΔH_2, the heat of protonation of the MDEA at 360.9 K was measured calorimetrically, and found to be 38.7 kJ/gmole (54). This value is also included in table 13 and plotted in figure 19 for comparison. The agreement between this single value and the computer model's predictions is very good (see figure 19).

Using the thermodynamically consistent set of ln K_2 and ΔH_2 values, the computer program was used to reproduce the entire loading curve. This included computing H^S, the partial pressure of carbon dioxide, and the solution composition for each value of the loading. In addition, the model was used to predict the saturation loading point. The computer outputs from the model for all four temperatures are included in appendix H.

Figures 20 and 21 are sample plots comparing the experimental enthalpies of solution and the model's calculated values (thermodynamically consistent) for the enthalpies of solution (in kJ/gmole MDEA) for the same sample systems as those shown previously in figures 7 and 8. Similarly, figures 22 and 23 compare the experimental H^S values in kJ/gmole CO_2 to the H^S values calculated by the computer model for these same two systems. Similar plots for the remaining systems are included in appendix I.

An examination of these sample plots shows three major differences between the computer model's predictions and the experimental data. The first of these differences is that the model predicts the value of the enthalpy

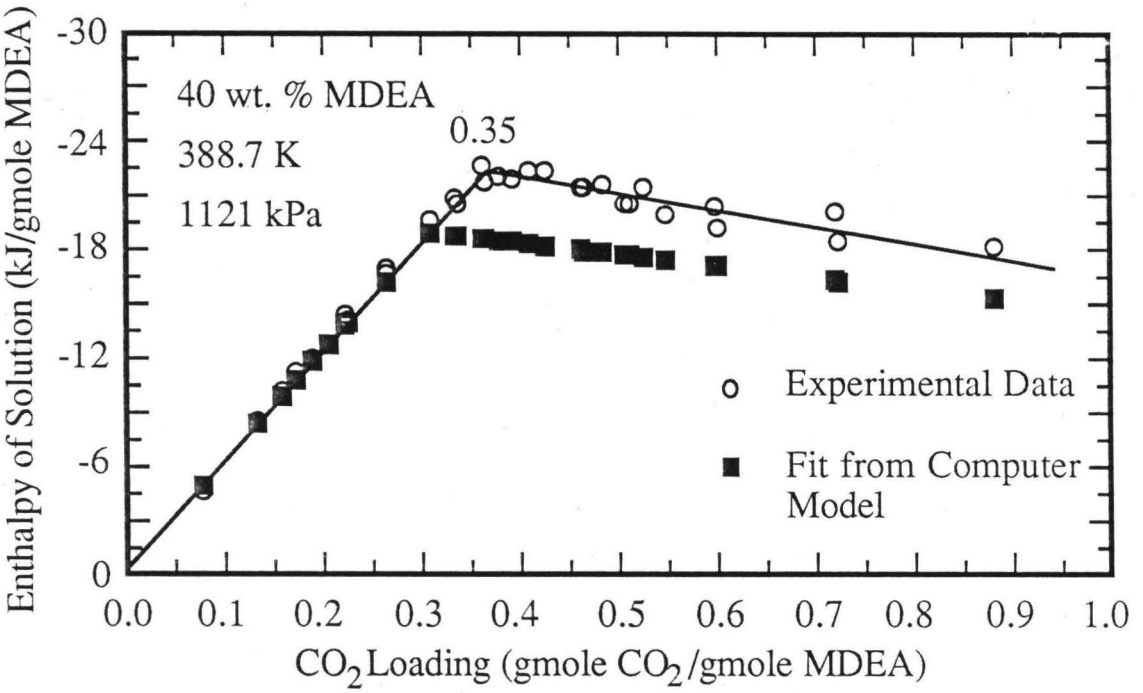


Figure 20. Plot of the experimental enthalpies of solution (kJ/gmole MDEA) and the thermodynamically consistent fit from the model for system 14.

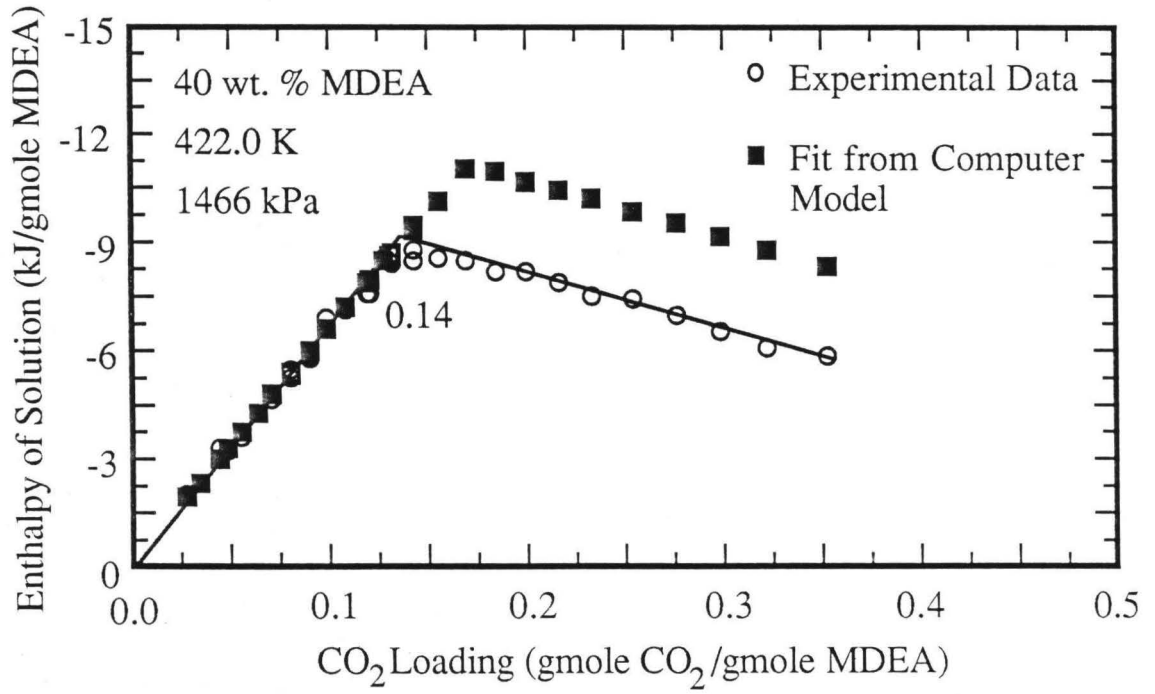


Figure 21. Plot of the experimental enthalpies of solution (kJ/gmole MDEA) and the thermodynamically consistent fit from the model for system 18.

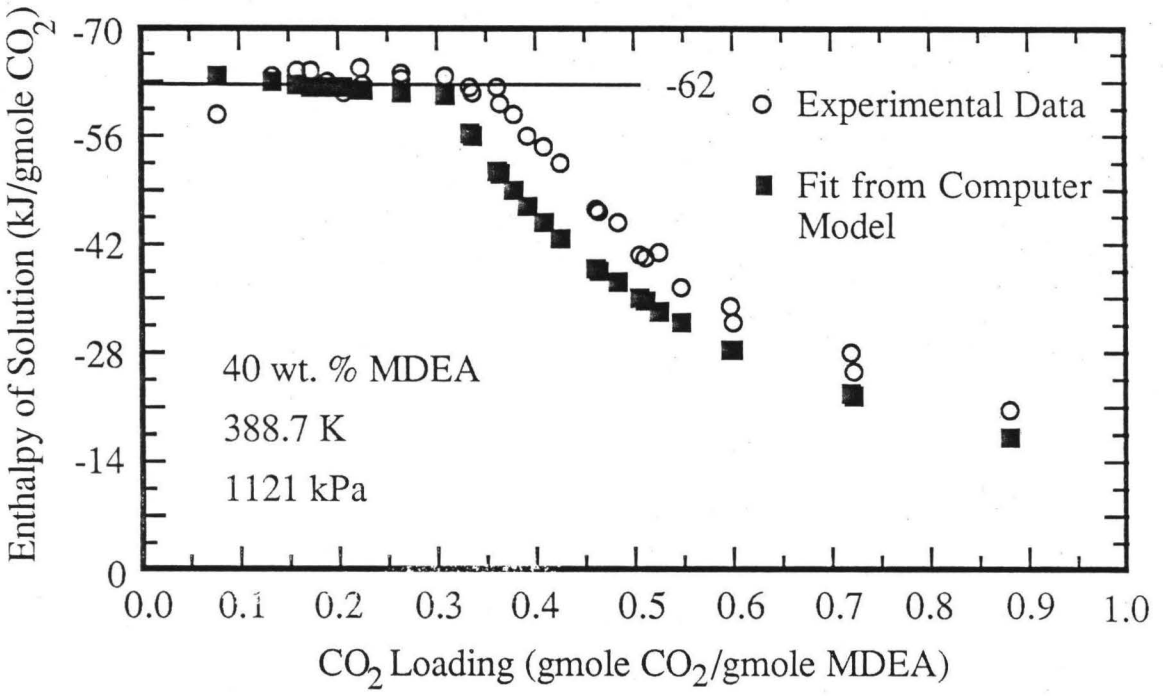


Figure 22. Plot of the experimental enthalpies of solution (kJ/gmole CO_2) and the thermodynamically consistent fit from the model for system 14

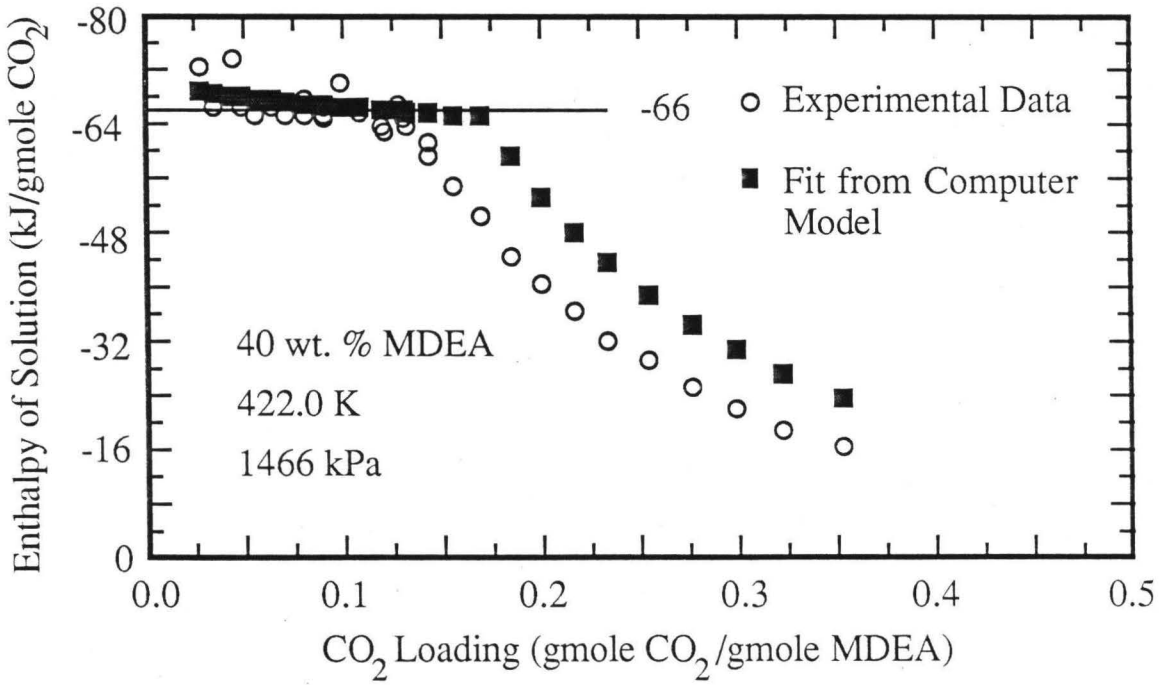


Figure 23. Plot of the experimental enthalpies of solution (kJ/gmole CO_2) and the thermodynamically consistent fit from the model for system 18.

of solution (kJ/gmole CO_2) before the saturation loading point to decrease slightly with loading up to the saturation loading point (see figures 22 and 23), while the experimental data were analyzed with a linear regression program which required the data to conform to a straight line on the MDEA-basis plots (figures 7, 8, 20, and 21). Thus, the analysis of the data artificially forced the enthalpy of solution to remain constant up to the saturation loading point by applying a linear regression to the data. Upon closer examination of the plots of the experimental data (per gmole CO_2) in figures 20, 21, and in appendix I, it is concluded that many of the systems studied exhibited behavior similar to that predicted by the model (within the uncertainty of the experimental data). Those systems exhibiting this behavior are: system 2 (appendix I), system 7 (appendix I), system 10 (appendix I), system 11 (appendix I), system 12 (appendix I), system 15 (appendix I), system 16 (appendix I), and system 18 (figure 23). Thus, by comparing the experimental data to the model and to the analysis of the experimental data itself, and in consideration of the experimental uncertainty, it is concluded that the experimental data are not accurate enough to substantiate the correctness of either the straight-line analysis applied to the data or the trend predicted by the model as just described.

The second difference between the data and the model is in the prediction of the saturation loading point. While the model generally matches the experimental data in the numerical values of the slopes of the two straight line portions (see figures 20 and 21), the model does not accurately predict the numerical value of the saturation loading point itself. The saturation loading points predicted by the model show both positive and negative deviations from the experimentally determined saturation loading points. From the previously presented comparison of the experimental and the

literature values of the saturation loading points (table 4), it is clear that the experimental data closely match the literature values of the saturation loading points. Thus, the difference is most likely the result of inaccurate modeling of the vapor-liquid equilibrium of this complex system.

In addition to these two differences, a comparison of the partial pressures of CO_2 predicted by the model and experimentally determined values from the literature (9,10) shows that the computer model predicts partial pressures higher than those measured experimentally (see figure 24).

Upon consideration of these differences, it was concluded that they are the result of several weaknesses in the preliminary computer model. The first of these weaknesses comes in the calculation of the activity coefficients. The correlations for the activity coefficient ratios of chemical reactions 1, 3, and 4 are valid over the temperature range of this study, but are only valid to an ionic strength of 5 molal. The solution ionic strengths of the concentrated (60 wt. %) MDEA solutions can exceed 12 molal, in which case the application of these correlations represents a significant extrapolation of the fitted correlation. The activity coefficient model for the hydrogen ion was valid to an ionic strength of 6.0 molal but was only valid at 298.2 K. An attempt to account for the temperature dependence was made, but an improved correlation which gives the activity coefficient over the whole range of temperatures and ionic strengths needs to be incorporated. The activity coefficient correlation for aqueous carbon dioxide is valid up to an ionic strength of 3.0 molal only and temperatures between 273.2 and 323.2 K. A correlation extending over a much wider range of temperatures and ionic strengths must be found or estimated. This activity coefficient is especially critical in the prediction of the saturation loading point of CO_2 in the MDEA solution and in the calculation of the equilibrium partial pressure

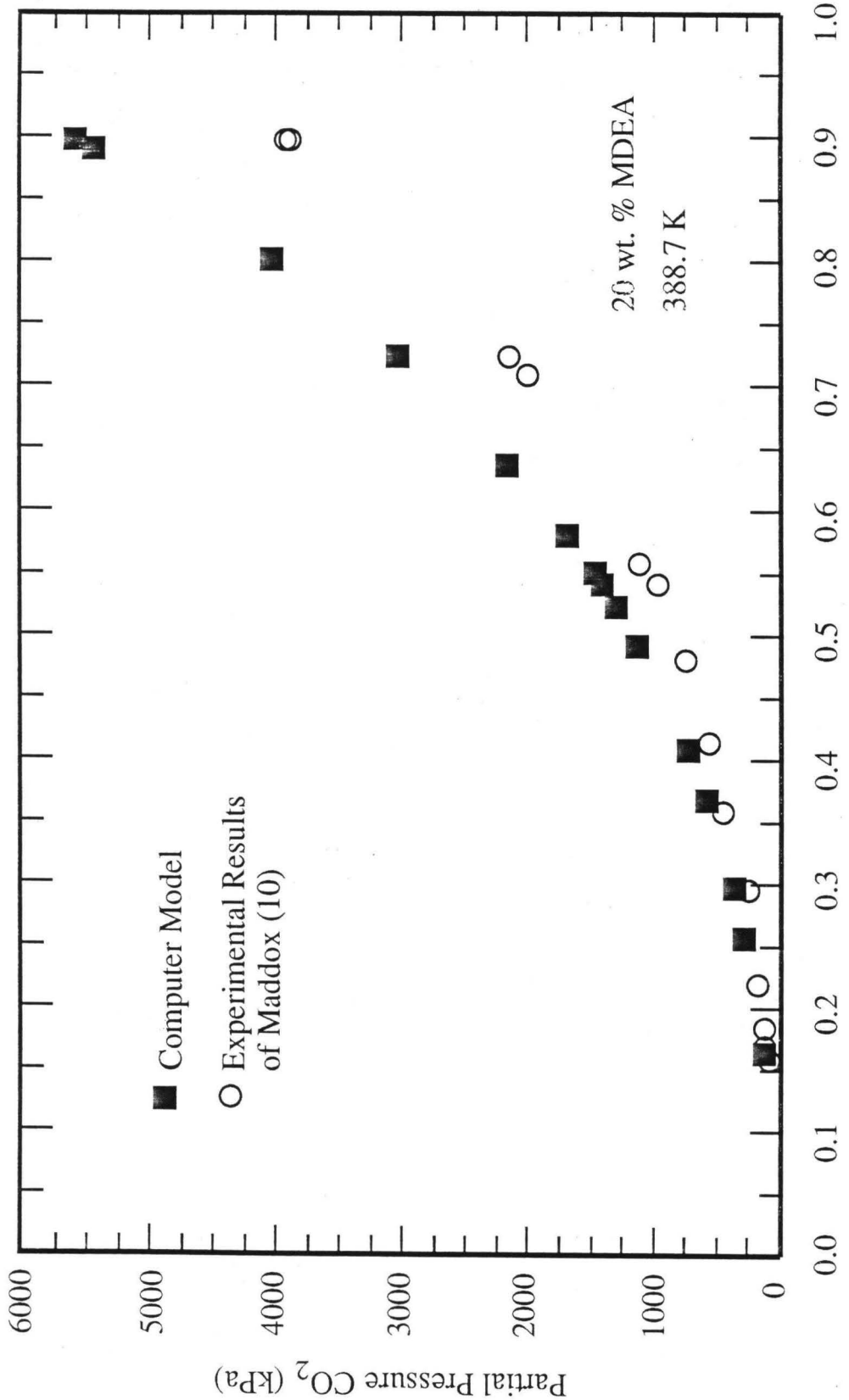


Figure 24. Comparison of equilibrium partial pressures CO_2 predicted by the model with the experimental values of Maddox et al. (10).

of CO_2 over the solution. The activity coefficient for the unprotonated amine was assumed to be unity. A correlation to calculate this activity coefficient should be found. Finally, the correlation which was used to estimate the activity coefficient of the protonated MDEA was actually an activity coefficient correlation for protonated MEA over a temperature range from 298.2 to 393.2 K and ionic strengths to 5 molal. The computer model needs to incorporate an improved correlation for the $MDEAH^+$ activity coefficient. If correlations for activity coefficients that are valid up to 12 molal cannot be found or formulated, a method for extrapolating activity coefficient correlations valid at low ionic strength to higher ionic strengths must be found and incorporated in the model.

The second weakness of the preliminary computer model is the assumption that the vapor-liquid equilibrium of the carbon dioxide (i.e., the equilibrium partial pressure of CO_2) in these concentrated MDEA solutions can be modeled with the Henry's law constant of carbon dioxide in pure water corrected by an activity coefficient which is a function of the ionic strength (charged species only). There is some evidence that the free gas solubility (Henry's law constant) of carbon dioxide in aqueous MDEA solutions may vary significantly from the value for pure water (50).

The third weakness of the model is found in the modeling of the vapor phase for determining saturation loading points, calculating vapor-phase compositions, and predicting the equilibrium partial pressure of carbon dioxide. In the determination of the vapor-phase composition (i.e., partial pressures), Raoult's law (equation 22) was utilized to determine the partial pressures of H_2O and MDEA, and the Henry's law equation (equation 20) was used to calculate the partial pressure of CO_2. In the Raoult's law calculation, it was assumed that the vapor phase was ideal, which is a

reasonable assumption at the pressures of this study. But, a fugacity coefficient model for all three species in the gas phase (MDEA, water, CO_2) should be used for a more thermodynamically sound model. In addition, in the Raoult's law calculation, the activity coefficients (based upon mole fraction) were assumed to be unity for both MDEA and H_2O. This was justified because, under the conditions of temperature and pressure of this study, the partial pressures of water and MDEA over the aqueous solution are relatively insignificant (at the two lower temperatures) when compared to the partial pressures of CO_2. But, improvement in the model could be realized at a future time by incorporating activity coefficient correlations for both water and MDEA in the aqueous phase.

The fourth weakness of the computer model is the assumption that the literature values of the equilibrium constants incorporated in the curve fits used in the computer model are accurate over the temperature range of this experimental study. In conjunction with this, another weakness is assuming the heats of reaction calculated by taking the temperature derivative of the curve fits of the equilibrium constant values are accurate representations of the actual heats of reaction.

Finally, the fifth weakness of the computer model is the validity or accuracy of the experimental data itself. Because of the unique problems encountered in the delivery of the gaseous component to the calorimeter, the experimental data was estimated to be no more accurate than ±5%. Thus, as noted previously, the uncertainties in the experimental data may explain any observed differences between the experimental data and the trends in the enthalpy of solution below the saturation loading point as predicted by the model.

IV. CONCLUSION, PART II

A computer program based on fundamental thermodynamic quantities (equilibrium constants, heats of reaction, and activity coefficients) was developed to model the absorption of carbon dioxide into aqueous MDEA solutions. The model was based upon the reaction scheme proposed by Jou et al.(2) with the corresponding equilibrium relationships, and mass and charge balances.

The values of K and ΔH for each reaction (except the MDEA protonation reaction) were determined by fitting the numerous literature data for equilibrium constant vs. temperature to a five constant nonlinear function of temperature. Activity coefficient correlations were found in the literature for all species except the protonated MDEA, in which case a correlation for protonated MEA was used.

The logic of the program was presented. The equations used to determine the best values of K and ΔH for the protonation reaction based upon a knowledge of the overall heat of solution and the values of K and ΔH for the remaining reactions were developed. In addition, a procedure for finding the minimum normalized error sum square was described.

The results of applying the computer model to the experimental data were summarized. The best set of thermodynamically consistent values of K and ΔH for the protonation reaction were determined, after which these values were compared to the available literature values and independent laboratory measurements. All comparisons showed good agreement. Then, using the thermodynamically consistent values of K and ΔH, loading curves

were generated for each experimental system, and values of the enthalpies of solution, the partial pressures of CO_2, and the solution composition at each loading value were determined. The saturation loading points were also found. Comparison of these results to the original data showed three differences: (1) the value of H^S below the saturation loading point was measured to be constant, but was predicted to decrease slightly as the saturation loading point is approached, (2) the predicted saturation loading points showed both positive and negative deviations from the experimentally measured values, and (3) the predicted values of the equilibrium partial pressure of carbon dioxide were higher than the literature values. In considering difference number 1 identified above, it was concluded that the experimental data are not accurate enough to substantiate either the straight-line analysis which forced the data to fit a straight line giving a constant enthalpy of solution (per gmole CO_2) or the trend shown by the model in which the enthalpy of solution decreased slightly with increasing loading up to the saturation loading point.

The discovery of these differences helps to point out the preliminary nature of the computer model. Specifically, there are five weaknesses that were pointed out which need to be examined and rectified for improvement of the model: (1) the use of activity coefficient models outside their range of applicability, and the use of an activity coefficient correlation for protonated MEA in the place of the protonated MDEA, (2) the assumption that the vapor-liquid equilibrium for the carbon dioxide can be adequately described by the Henry's law constant for CO_2 in pure water corrected by an activity coefficient, (3) the modeling of the vapor phase as an ideal gas and the liquid phase as an ideal solution by applying Raoult's law for MDEA and water, (4) the assumption that the K values incorporated in the curve fits used in the

computer program are accurate, and the assumption that the ΔH values determined by differentiating these curve fits of K vs. T are accurate, and (5) the inaccuracies of the original data.

The preliminary computer model developed matches the experimental data well. Future work on the five weaknesses listed above may lead to rectification of the differences and a refined model for more accurate prediction of the enthalpies of solution, saturation loading points, and partial pressures of CO_2 for the absorption of CO_2 by aqueous MDEA solutions.

CONCLUSION

The enthalpies of solution of CO_2 in aqueous MDEA solutions were measured with an isothermal flow calorimeter over ranges of temperature, pressure, weight percent MDEA, and acid gas loading. The experimental measurements showed that the enthalpies of solution (per mole CO_2) are essentially independent of acid gas loading up to the saturation loading point. An analysis of the data also indicated that H^S is independent of pressure, but linearly dependent upon both the temperature and the weight percent MDEA. A correlation to predict H^S as a function of temperature and weight percent MDEA was given. The experimental data showed that the saturation loading point was dependent upon both the temperature and pressure. A review of the appropriate literature showed good agreement between the experimental results and the literature values.

A computer program based on fundamental thermodynamic quantities (K, ΔH, and γ) was developed to model the absorption of CO_2 into aqueous MDEA. The model was based on a reaction scheme from the literature, and the corresponding equilibrium relationships, mass balances, and charge balance. The numerical values of the various thermodynamic quantities (with the exception of K and ΔH for the MDEA protonation reaction) were found by curve-fitting literature data or by using existing literature correlations that are based upon experimental data. A discussion of how the model is used to find the set of thermodynamically consistent values of K and ΔH for the MDEA protonation reaction which minimizes the difference between the experimental values and the model's predictions was included.

The results of the application of the model were presented. The thermodynamically consistent values of K and ΔH for the protonation reaction compared favorably with the limited literature data and with an independent laboratory determination of ΔH. The model was then used to predict the enthalpies of solution, the partial pressures of CO_2, the solution composition at each loading value, and the saturation loading points based upon fundamental thermodynamic quantities. Comparison of the model's predictions with the experimental data showed three major differences: (1) the value of H^S below the saturation loading point was measured to be constant, but the model predicted it to decrease slightly as the saturation loading point is approached, (2) the predicted values of the saturation loading points are significantly different than the experimental saturation loading points, and (3) the predicted values of the equilibrium partial pressure of CO_2 were higher than the values published in the literature. Upon closer examination of difference 1 presented above, it was concluded that the uncertainty in the experimental data precludes substantiation of either the constant H^S found by a linear regression on the experimental data or the computer model's prediction of H^S decreasing with increasing loading up to the saturation loading point.

The differences between the experimental data and the predicted heats of solution are evidence of the preliminary nature of the computer model. The following weaknesses of the computer model were identified and addressed: (1) the use of correlations for predicting activity coefficients beyond their range of applicability, (2) the modeling of CO_2 vapor-liquid equilibrium with a Henry's law constant for CO_2 in water corrected only by an activity coefficient for absorbed CO_2 , (3) the modeling of the vapor phase as an ideal gas and the liquid phase an an ideal solution by applying Raoult's law to

describe the vapor phase composition (for MDEA and water only), (4) the assumption that the literature values of the thermodynamic quantities and the curve fits of these quantities are accurate, and (5) the accuracy or inaccuracy of the calorimetric experimental data reported upon here. Resolution of these weaknesses in modeling should lead to a computer model that more closely matches the experimental data.

Thus, it may be possible in the future to accurately describe the complexities of the absorption of CO_2 into aqueous MDEA solutions by a relatively simple reaction scheme and values of K and ΔH for each reaction of the sequence.

LITERATURE CITED

(1) Blanc, Claude J., Jean Eluge, and Francois J. Lallemand. *Hydrocarbon Processing.* **60** (8), 111(1981).

(2) Jou, Fang-yuan, Alan E. Mather, and Frederick D. Otto. *Industrial Engineering Chemistry Process Design and Development.* **21**, 539(1982).

(3) Christensen, J. J., L. D. Hansen, D. J. Eatough, R. M. Izatt, and R. M. Hart. *Review of Scientific Instrumentation.* **47**, 730(1976).

(4) Christensen, J. J., L. D. Hansen, D. J. Eatough, R. M. Izatt, and R. M. Hart. *Review of Scientific Instrumentation.* **52**, 1226(1981).

(5) Christensen, Scott P., James J. Christensen, and Reed M. Izatt. RR-85: "Enthalpies of Solution of CO_2 in Aqueous Diglycolamine Solutions". Gas Processors Association, May 1985.

(6) Dibble, J. H. "UCARSOL Solvents for Acid Gas Removal". Paper presented at Petroenergy '83, Houston, Texas, September 1983. Quoted in Arthur Kohl and Fred Riesenfeld. Gas Purification. 4th Ed. Houston: Gulf Publishing, 1985.

(7) Pearce, R. L. *Oil and Gas Journal.* **76** (30), 46(1978).

(8) Polasek, John, and Jerry Bullin. "Process Considerations in Selecting Amines", in Acid and Sour Gas Treating Processes. Stephen A. Newman, Ed. Houston: Gulf Publishing, 1985.

(9) Maddox, R. N., G. J. Mains, and S. Bhairi. Progress Report Project 841: "Acid Gases in Solvents". Gas Processors Association, February 15, 1984.

(10) Maddox, R. N., G. J. Mains, and S. Bhairi. Progress Report Project 841: "Acid Gases in Solvents". Gas Processors Association, May 15, 1984.

(11) Schwabe, K., W. Graichen, and D. Spiethoff. *Zeitschrift fur Physikalische Chemie Neue Folge.* **20**, 68(1959).

(12) Grenthe, Ingmar, Heikki Ots, and Olle Ginstrup. *Acta Chemica Scandinavica.* **24**, 21(1970).

(13) Olofsson, Gerd, and Loren G. Hepler. *Journal of Solution Chemistry.* **4**(2), 127(1975).

(14) Marshall, William L., and E. U. Franck. *Journal of Physical*

Chemistry Reference Data. **10**, 295(1981).

(15) Olofsson, Gerd, and Inger Olofsson. *Journal of Chemical Thermodynamics.* **5**, 533(1973).

(16) Busey, Richard H., and Robert E. Mesmer. *Journal of Chemical and Engineering Data.* **23**(2), 175(1978).

(17) Harned, Herbert S., and Walter J. Hamer. *Journal of the American Chemical Society.* **55**, 2194(1933).

(18) Pitzer, Kenneth S. *Journal of the American Chemical Society.* **59**, 2365(1937).

(19) Peiper, J. Christopher, and Kenneth S. Pitzer. *Journal of Chemical Thermodynamics.* **14**, 613(1982).

(20) Patterson, C. S., G. H. Slocum, R. H. Busey, and R. E. Mesmer. *Geochimica et Cosmochimica Acta.* **46**, 1653(1982).

(21) Read, A. J. *Journal of Solution Chemistry.* **4**, 53(1975).

(22) Harned, Herbert S., and Francis T. Bonner. *Journal of the American Chemical Society.* **67**, 1026(1945).

(23) Ryzhenko, R. H. *Geochemistry.* **2**, 151(1963).

(24) MacInnes, Duncan A., and Donald Belcher. *Journal of the American Chemical Society.* **55**, 2630(1933).

(25) Harned, Herbert S., and Raymond Davis, Jr. *Journal of the American Chemical Society.* **65**, 2030(1943).

(26) Berg, Robert L., and Cecil E. Vanderzee. *Journal of Chemical Thermodynamics.* **10**, 1113(1978).

(27) Patterson, C. S., R. H. Busey, and R. E. Mesmer. *Journal of Solution Chemistry.* **13**, 647(1984).

(28) Harned, Herbert S., and Samuel R. Scholes, Jr. *Journal of the American Chemical Society.* **63**, 1706(1941).

(29) Butler, James N. Carbon Dioxide Equilibria and Their Applications. Menlo Park, California: Addison-Wesley Publishing Co., 1982.

(30) Haimor, Noman, Ali Bidarian, and Orville C. Sandall. "Simultaneous Absorption of H_2S and CO_2 into Aqueous Methyldiethanolamine". Paper presented at the 4th Symposium on Separation Science and Technology for Energy Applications, Knoxville, Tennessee, Oct. 20-24, 1985.

(31) Wiebe, R., and V. L. Gaddy. *Journal of the American Chemical Society.* **61**, 315(1939).

(32) Ellis, A. J. *American Journal of Science.* **257**, 217(1959).

(33) Ellis, A. J., and R. M. Golding. *American Journal of Science*. **261**, 47(1963).

(34) Wiebe, R., and V. L. Gaddy. *Journal of the American Chemical Society*. **62**, 815(1940).

(35) Zambonin, Giorgio, and Joseph Jordan. *Analytical Chemistry*. **41**, 437(1969).

(36) Zawisza, Andrzej, and BogusVawa Malesinska. *Journal of Chemical and Engineering Data*. **26**, 388(1981).

(37) Dodds, W. S., L. F. Stutzman, and B. J. Sollami. *Industrial and Engineering Chemistry*. **1**, 92(1956).

(38) Nilsson, Gerhard, Torsten Rengemo, and Lars Gunnar Sillen. *Acta Chemica Scandinavica*. **12**, 868(1958).

(39) Malinin, S. D. *Geokhimiya*. **10**, 1523(1974).

(40) Wilhelm, Emmerich, Rubin Battino, and Robert J. Wilcock. *Chemical Reviews*. **77**, 219(1977).

(41) Markham, Aaron E., and Kenneth A. Kobe. *Journal of the American Chemical Society*. **63**, 1165(1941).

(42) Markham, Aaron E., and Kenneth A. Kobe. *Journal of the American Chemical Society*. **63**, 449(1941).

(43) Pitzer, Kenneth S. *The Journal of Physical Chemistry*. **77**, 268(1973).

(44) Liu, Chia-tsun, and W. T. Lindsay, Jr. *Journal of Solution Chemistry*. **1**, 45(1972).

(45) Deshmukh, R. D., and A. E. Mather. *Chemical Engineering Science*. **36**, 355(1981).

(46) Eatough, Delbert J., James J. Christensen, and Reed M. Izatt. Experiments in Thermometric Titrimetry and Titration Calorimetry. Provo: Brigham Young University Press, 1974.

(47) Mullens, J., J. Yperman, J. P. Francois, and L. C. Poucke. *The Journal of Physical Chemistry*. **89**, 2937(1985).

(48) Mullens, J., J. Yperman, J. P. Francois, and L. C. Poucke. *The Journal of Physical Chemistry*. **89**, 2941(1985).

(49) Burden, Richard L., and J. Douglas Faires. Numerical Analysis. Third Edition. Boston: Prindle, Weber & Schmidt, 1985.

(50) Haimour, Noman, and Orville C. Sandall. *Chemical Engineering Science*. **39**, 1791(1984).

(51) Christensen, James J., Lee D. Hansen, and Reed M. Izatt. Handbook of Proton Ionization Heats and Related Thermodynamic Quantities. New York: John Wiley & Sons, 1976.

(52) Shedlovsky, Theodore, and D. A. MacInnes. *Journal of the American Chemical Society*. **57**, 1705(1935).

(53) Mesmer, R. E., and B. F. Hitch. *Journal of Solution Chemistry*. **6**, 251(1977).

(54) Christensen, James J. Unpublished Data, Brigham Young University, 1986.

APPENDIX A

RAW AND CONVERTED DATA

Description of Data Conversion Program

The following program accepts data entered interactively in the form of total heat of solution (J/gmole solution) vs. mole fraction CO_2. The program as originally written converted these units to total heat (expressed in units of Btu/lb CO_2 and Btu/lb MDEA) as a function of acid gas loading (gmole CO_2/gmole MDEA). These units were especially useful for the purposes of the Gas Processors Association (GPA) who sponsored and supported the research. All of the programs which utilized the experimental data were written to accept and process data in English units for the GPA. However, for the purposes of this thesis, all of the reported data are in SI units. Thus, all of the numbers reported in this appendix and in the body of the thesis have been converted from the English units actually used in the computer programs as written to SI units of total heat (kJ/gmole CO_2 and kJ/gmole MDEA) as a function of acid gas loading (gmole CO_2/gmole MDEA).

Thus, the outputs immediately following the computer program in this appendix A were not directly generated by the following Fortran code. Rather, the program as written converts the raw data to the English units described above. The computer outputs actually included in this appendix were generated by applying simple conversion factors and molecular weights to the output generated by the Fortran program to convert from Btu to kJ, from pound to gram, and from gram to gram-mole. The sample calculation sheet immediately following the listing of the computer program shows the conversion of the raw data to the SI units summarized on the computer outputs.

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C       THIS PROGRAM IS ENTITLED MDEA.FOR AND IT READ IN THE RAW DATA          C
C       IN J/MOLE VS. XCO2 AND CONVERTS IT TO THE FORM BTU/LB CO2 AND          C
C       BTU/LB MDEA VS. LOADING (MOLE CO2/MOLE MDEA).                          C
C                                                                              C
C       WRITTEN BY KEITH MERKLEY  MAY 1985                                     C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                     VARIABLE IDENTIFICATION AND DESCRIPTION                  C
C                                                                              C
C       ANSWER=CHARACTER STRING TO HOLD Y/N FOR QUESTIONS                      C
C       CO2PD=ARRAY STORING LOADING IN LBMOLE CO2/LBMOLE MDEA                  C
C       HE=ARRAY STORING RAW DATA OF HEAT OF MIXING IN J/MOLE                  C
C       HTMIX=NEGATIVE OF HEAT OF MIXING (POSITIVE QUANTITY                    C
C       HTPCO2=ARRAY STORING HEAT OF MIXING IN BTU/LB CO2                      C
C       HTPDGA=ARRAY STORING HEAT OF MIXING IN BTU/LB MDEA                     C
C       I=COUNTER FOR DATA POINT BEING CONVERTED                               C
C       NPTS=NUMBERJ OF POINTS                                                 C
C       PERCENT=WEIGHT PERCENT AMINE                                           C
C       PRESS=PRESSURE IN PSIA                                                 C
C       PUREMW=MOLECULAR WEIGHT OF AMINE COMPONENT                             C
C       SACO2P=TEMPORARY STORAGE FOR LOADING IN SORT ROUTINE                   C
C       SAVECO=TEMPORARY STORAGE FOR MOLE FRACTION CO2 IN SORT ROUTINE         C
C       SAVEHE=TEMPORARY STORAGE FOR HEAT OF MIXING (J/MOLE) IN SORT           C
C              ROUTINE                                                         C
C       SHTPCO=TEMPORARY STORAGE FOR HEAT OF MIXING (BTU/LB CO2) IN            C
C              SORT ROUTINE                                                    C
C       SHTPDG=TEMPORARY STORAGE FOR HEAT OF MIXING (BTU/LB MDEA) IN           C
C              SORT ROUTINE                                                    C
C       SYSTEM=AMINE COMPONENT (MDEA)                                          C
C       TEMP=TEMPERATURE IN FARENHEIT                                          C
C       WTMOL=MOLECULAR WEIGHT OF AQUEOUS SOLUTION                             C
C       XCO2=ARRAY STORING RAW DATA OF MOLE FRACTION CO2 FOR EACH POINT        C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

CCCCCCCCCCCC
C               1A. DIMENSION VARIABLES
CCCCCCCCCCCC

      DIMENSION XCO2(100),HE(100),HTPCO2(100),HTPDGA(100),CO2PD(100)

CCCCCCCCCCCC
C               1B. UNIT 7 IS THE OUTPUT SUMMARY; UNIT 8 HOLDS DATA
C                       IN BTU/LB MDEA VS. LOADING FOR LINEAR
C                       REGRESSION PROGRAM (LSQ.FOR)
CCCCCCCCCCCC

      OPEN( UNIT=7,STATUS='NEW',FILE='OUT')
      OPEN( UNIT=8,STATUS='NEW',FILE='SLOPE')

CCCCCCCCCCCC
C               2. READ IN DATA FROM SCREEN
CCCCCCCCCCCC

  14  WRITE(6,*)' ENTER PHYSICAL CONDITIONS'
      WRITE(6,*) ' SYSTEM'
      READ(5,1) SYSTEM
    1 FORMAT(A4)
      WRITE(6,*)' PERCENT, TEMP(FARENHEIT), PRESS(PSIA)'
      READ(5,*) PERCEN, TEMP, PRESS
```

```
CCCCCCCCCCCC
C               3. CALCULATE MOLECULAR WEIGHT
CCCCCCCCCCCC

      PUREMW = 119.17
      WTMOL = (100.)/((PERCEN/PUREMW) + ((100.-PERCEN)/18.0153))
      WRITE(6,*) ' MOL. WT. OF SOLN. = ',WTMOL
      WRITE(6,*)' STARTING TO ENTER DATA'
      I = 1
      GOTO 17

CCCCCCCCCCCC
C               4. DECIDE IF ANOTHER DATA POINT IS TO BE ENTERED
CCCCCCCCCCCC

   15 I = I + 1
      WRITE(6,*) ' DO YOU WISH TO ENTER ANOTHER DATA POINT?(<CR>/N)'
      READ(5,2) ANSWER
    2 FORMAT(A1)
      IF(ANSWER.EQ.'N') GOTO 50
      GOTO 17

CCCCCCCCCCCC
C               5. ENTER DATA POINT FROM SCREEN
CCCCCCCCCCCC

   17 WRITE(6,*) ' ENTER MOLE FRACTION CO2, NEGATIVE HEAT OF MIXING'
      READ(5,*) XCO2(I), HTMIX
      HE(I) = -1 * HTMIX
      NPTS = NPTS + 1

CCCCCCCCCCCC
C               6. CONVERT DATA TO NEW UNITS
CCCCCCCCCCCC

      CO2PD(I) = (100.*PUREMW)/(WTMOL*PERCEN*((1.0/XCO2(I))-1.))
      HTPCO2(I)= (HE(I)*453.593)/(XCO2(I)*44.0098*1054.18)
      HTPDGA(I)=(HE(I)*100.*453.593)/((1.-XCO2(I))*WTMOL*PERCEN*1054.18)
      WRITE(6,*) ' MOLE CO2/MOLE DGA = ',CO2PD(I)
      WRITE(6,*) ' BTU/LB CO2 = ', HTPCO2(I)
      WRITE(6,*) ' BTU/LB DGA = ', HTPDGA(I)
      GOTO 15

CCCCCCCCCCCC
C               7. PRINT OUTPUT LABELS
CCCCCCCCCCCC

   50 WRITE(7,51) PERCEN,SYSTEM,TEMP,PRESS
   51 FORMAT(/,15X,'HEAT OF MIXING DATA FOR A ',F4.1,'% ',A4,
     1       ' IN WATER',/,16X,'SOLUTION AND CO2 AT ',F5.1,' F AND ',
     2       F5.1,' PSIA')
      WRITE(7,52) SYSTEM,SYSTEM
   52 FORMAT(//,4X,'MOLE',9X,'HEAT OF',7X,'MOLE CO2',10X,'BTU',12X,
     1       'BTU',/,2X,'FRACTION',8X,'MIXING',7X,'---------',8X,
     2       '------',8X,'-------',/,4X,'CO2',10X,'(J/MOLE)',6X,
     3       'MOLE ',A4,8X,'LB CO2',8X,'LB ',A4,//)

CCCCCCCCCCCC
C                8. SORT ROUTINE TO ORDER DATA IN ORDER OF INCREASING XCO2
CCCCCCCCCCCC

      DO 100 JJ=2,NPTS
          DO 60 KK=JJ-1,1,-1
              IF( XCO2(KK+1).LT.XCO2(KK) ) THEN
```

```
                    SAVECO = XCO2(KK+1)
                    SAVEHE = HE(KK+1)
                    SHTPCO = HTPCO2(KK+1)
                    SACO2P = CO2PD(KK+1)
                    SHTPDG = HTPDGA(KK+1)
                    XCO2(KK+1) = XCO2(KK)
                    HE(KK+1) = HE(KK)
                    CO2PD(KK+1) = CO2PD(KK)
                    HTPCO2(KK+1) = HTPCO2(KK)
                    HTPDGA(KK+1) = HTPDGA(KK)
                    XCO2(KK) = SAVECO
                    HE(KK) = SAVEHE
                    CO2PD(KK) = SACO2P
                    HTPCO2(KK) = SHTPCO
                    HTPDGA(KK) = SHTPDG
                ELSE
                    GOTO 61
                ENDIF
   60       CONTINUE
   61       ITCNT=JJ
  100 CONTINUE

CCCCCCCCCCCC
C               9.  OUTPUT SUMMARY OF RAW AND CONVERTED DATA TO FILE
CCCCCCCCCCCC

      WRITE(7,53)(XCO2(J),HE(J),CO2PD(J),HTPCO2(J),HTPDGA(J),J=1,NPTS)
   53 FORMAT(2X,F7.5,7X,F9.2,7X,F7.5,8X,F8.2,7X,F7.2)
      WRITE(8,54) SYSTEM,PERCEN,TEMP,PRESS
   54 FORMAT(1X,A4,2X,F7.3,2X,F8.2,2X,F10.4)
      WRITE(8,55) NPTS,PUREMW,WTMOL
   55 FORMAT(1X,I3,2X,F15.7,2X,F15.7)
      WRITE(8,56) ( CO2PD(K),HTPDGA(K),K=1,NPTS)
   56 FORMAT(2X,F15.7,2X,F15.7)
      WRITE(6,*) ' DONE ENTERING DATA'
      STOP
      END
```

Sample Calculations

1. Molecular Weight of Aqueous MDEA Solution (MW Soln)

   a. g Soln = g (H_2O + MDEA)

   b. $\frac{\text{Wt. \% MDEA}}{100} \times \frac{1}{\text{MW MDEA}} = \frac{\text{g MDEA}}{\text{g Soln}} \times \frac{\text{mol MDEA}}{\text{g MDEA}} = \frac{\text{mol MDEA}}{\text{g Soln}}$

   c. $\frac{100 - \text{Wt. \% MDEA}}{100} \times \frac{1}{\text{MW } H_2O} = \frac{\text{g } H_2O}{\text{g Soln}} \times \frac{\text{mol } H_2O}{\text{g } H_2O} = \frac{\text{mol } H_2O}{\text{g Soln}}$

   d. $\text{MW Soln} = \frac{\text{g Soln}}{\text{mol Soln}} = \frac{1}{(\text{mol MDEA/g Soln}) + (\text{mol } H_2O/\text{g Soln})} = \frac{1}{b + c}$

2. Loading

   a. $\text{MW Soln} \times \frac{\text{Wt. \% MDEA}}{100} = \frac{\text{g Soln}}{\text{mol Soln}} \times \frac{\text{g MDEA}}{\text{g Soln}} = \frac{\text{g MDEA}}{\text{mol Soln}}$

   b. $\frac{1}{x_{CO2}} - 1 = \frac{1}{[\text{mol } CO_2/\text{mol (Soln + } CO_2)]} - 1 = \frac{\text{mol Soln}}{\text{mol } CO_2}$

   c. $\text{Loading} = \frac{\text{MW MDEA}}{a \times b} = \frac{(\text{g MDEA/mol MDEA})}{(\text{g MDEA/mol Soln}) \times (\text{mol Soln/mol } CO_2)}$

   $= \frac{\text{mol } CO_2}{\text{mol MDEA}}$

3. Heat of Solution (kJ/gmole CO_2)

   a. $H^S = \frac{H^E}{1000\, x_{CO2}} = \frac{\text{J/mol Total Soln}}{\text{mol } CO_2/\text{mol Total Soln}} \times \frac{1\text{ kJ}}{1000\text{ J}} = \frac{\text{kJ}}{\text{mol } CO_2}$

4. Heat of Solution (kJ/gmole MDEA)

   a. $H^S \times \text{Loading} = \frac{\text{kJ}}{\text{mol } CO_2} \times \frac{\text{mol } CO_2}{\text{mol MDEA}} = \frac{\text{kJ}}{\text{mol MDEA}}$

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00708	-319.87	0.19580	-45.187	-8.847
0.00916	-431.97	0.25386	-47.166	-11.971
0.00916	-444.34	0.25386	-48.517	-12.315
0.01141	-554.39	0.31693	-48.596	-15.401
0.01413	-695.98	0.39357	-49.264	-19.386
0.02109	-969.50	0.59160	-45.977	-27.197
0.03124	-1466.32	0.88551	-46.945	-41.568
0.03846	-1781.80	1.09834	-46.336	-50.891
0.04013	-1822.02	1.14803	-45.410	-52.129
0.04190	-1831.29	1.20088	-43.713	-52.492
0.04377	-1833.90	1.25693	-41.906	-52.669
0.04793	-1839.09	1.38240	-38.376	-53.049
0.07920	-1777.96	2.36187	-22.452	-53.027
0.10861	-1751.32	3.34579	-16.127	-53.957
0.19825	-1594.97	6.79001	-8.047	-54.633

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00624	-288.74	0.17242	-46.280	-7.980
0.01523	-697.86	0.42468	-45.829	-19.461
0.01863	-909.96	0.52129	-48.852	-25.463
0.02277	-1095.65	0.63983	-48.126	-30.790
0.02435	-1158.03	0.68533	-47.566	-32.596
0.02769	-1337.07	0.78201	-48.295	-37.765
0.03107	-1467.20	0.88053	-47.230	-41.584
0.03379	-1562.54	0.96031	-46.250	-44.412
0.03406	-1621.70	0.96826	-47.621	-46.107
0.03683	-1692.48	1.05001	-45.962	-48.257
0.03937	-1766.61	1.12540	-44.879	-50.503
0.04299	-1830.47	1.23352	-42.586	-52.528
0.05235	-1832.21	1.51693	-35.005	-53.096
0.07150	-1795.35	2.11456	-25.114	-53.101
0.09642	-1687.44	2.93020	-17.504	-51.287
0.09642	-1687.44	2.93020	-17.504	-51.287
0.14492	-1576.29	4.65391	-10.878	-50.625

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 155.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00209	-125.19	0.05751	-59.909	-3.446
0.00471	-157.35	0.12995	-33.413	-4.340
0.00808	-394.39	0.22368	-48.819	-10.919
0.01251	-613.74	0.34787	-49.069	-17.068
0.01872	-883.63	0.52385	-47.210	-24.729
0.02288	-1024.84	0.64299	-44.800	-28.804
0.02780	-1091.36	0.78521	-39.264	-30.829
0.03031	-1122.20	0.85832	-37.030	-31.782
0.03422	-1163.01	0.97297	-33.992	-33.070
0.03912	-1180.17	1.11796	-30.173	-33.729
0.04262	-1198.51	1.22243	-28.126	-34.380
0.04663	-1250.04	1.34307	-26.812	-36.008
0.04695	-1234.26	1.35275	-26.293	-35.565
0.05171	-1239.96	1.49737	-23.983	-35.909
0.05435	-1228.70	1.57821	-22.611	-35.682
0.05633	-1253.49	1.63914	-22.256	-36.479
0.06027	-1266.75	1.76114	-21.021	-37.019
0.06336	-1246.97	1.85754	-19.684	-36.562
0.06360	-1276.08	1.86506	-20.068	-37.424
0.06722	-1283.34	1.97886	-19.095	-37.784
0.07091	-1327.59	2.09578	-18.726	-39.241
0.07550	-1308.56	2.24252	-17.334	-38.872
0.08027	-1323.07	2.39656	-16.485	-39.507
0.08553	-1314.31	2.56830	-15.369	-39.471
0.09138	-1354.58	2.76163	-14.826	-40.942
0.09757	-1351.79	2.96892	-13.857	-41.138
0.11364	-1331.63	3.52061	-11.720	-41.257
0.12318	-1371.30	3.85768	-11.134	-42.950
0.14656	-1345.32	4.71562	-9.181	-43.290
0.16227	-1325.29	5.31901	-8.169	-43.446
0.18050	-1327.00	6.04818	-7.353	-44.470

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00266	-234.15	0.02913	-88.041	-2.565
0.01032	-537.95	0.11389	-52.135	-5.939
0.01596	-723.87	0.17715	-45.362	-8.035
0.02375	-1134.90	0.26572	-47.793	-12.700
0.03521	-1718.72	0.39861	-48.821	-19.458
0.04935	-2330.53	0.56700	-47.232	-26.779
0.05138	-2598.98	0.59159	-50.592	-29.929
0.05373	-2830.85	0.62018	-52.695	-32.679
0.05392	-2707.44	0.62250	-50.220	-31.261
0.05392	-2877.37	0.62250	-53.372	-33.222
0.06195	-3052.07	0.72133	-49.275	-35.540
0.06853	-3242.44	0.80358	-47.322	-38.025
0.07180	-3332.59	0.84489	-46.422	-39.219
0.07533	-3748.45	0.88981	-49.768	-44.282
0.07560	-3822.31	0.89326	-50.568	-45.168
0.07560	-3622.24	0.89326	-47.921	-42.803
0.07971	-3707.18	0.94603	-46.516	-44.002
0.08933	-4127.78	1.07141	-46.215	-49.512
0.09432	-4363.14	1.13749	-46.267	-52.625
0.09432	-4344.32	1.13749	-46.067	-52.398
0.10014	-4380.73	1.21549	-43.753	-53.179
0.10656	-4360.59	1.30271	-40.929	-53.315
0.11328	-4323.15	1.39536	-38.170	-53.256
0.12200	-4348.87	1.51769	-35.652	-54.107
0.14051	-4236.85	1.78560	-30.159	-53.846
0.16449	-4119.77	2.15033	-25.050	-53.863
0.18080	-4013.00	2.41061	-22.200	-53.511

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00960	-483.54	0.10587	-50.377	-5.332
0.01188	-603.63	0.13132	-50.819	-6.673
0.01238	-582.66	0.13691	-47.073	-6.446
0.01486	-754.36	0.16476	-50.773	-8.365
0.01852	-983.96	0.20610	-53.138	-10.952
0.01857	-904.41	0.20667	-48.710	-10.066
0.02212	-1097.04	0.24707	-49.604	-12.254
0.02481	-1177.76	0.27788	-47.479	-13.193
0.02636	-1316.47	0.29571	-49.950	-14.769
0.02988	-1443.83	0.33641	-48.329	-16.256
0.03004	-1418.36	0.33827	-47.223	-15.974
0.03122	-1471.68	0.35199	-47.146	-16.594
0.03175	-1504.64	0.35816	-47.398	-16.974
0.03179	-1519.56	0.35862	-47.808	-17.143
0.03444	-1654.81	0.38958	-48.057	-18.722
0.03548	-1732.53	0.40178	-48.839	-19.622
0.04002	-1959.80	0.45534	-48.978	-22.300
0.04071	-2005.34	0.46352	-49.267	-22.835
0.04153	-2116.87	0.47326	-50.980	-24.126
0.04170	-1981.46	0.47528	-47.525	-22.586
0.04321	-2251.61	0.49327	-52.117	-25.707
0.04536	-2167.74	0.51898	-47.798	-24.804
0.04761	-2405.76	0.54601	-50.539	-27.594
0.04854	-2354.38	0.55722	-48.512	-27.031
0.04990	-2473.82	0.57365	-49.584	-28.441
0.05081	-2486.78	0.58467	-48.951	-28.618
0.05452	-2689.89	0.62983	-49.346	-31.078
0.05455	-2803.63	0.63019	-51.404	-32.394
0.05541	-2671.17	0.64071	-48.215	-30.890
0.05617	-2705.14	0.65002	-48.168	-31.308
0.05741	-2816.22	0.66525	-49.062	-32.637
0.05802	-2920.64	0.67275	-50.347	-33.870
0.05810	-2858.33	0.67374	-49.205	-33.150
0.06211	-3031.67	0.72332	-48.819	-35.310
0.06241	-3073.28	0.72704	-49.252	-35.806
0.06548	-3289.50	0.76531	-50.245	-38.451
0.06785	-3419.51	0.79503	-50.407	-40.072
0.06834	-3303.82	0.80119	-48.351	-38.737
0.07194	-3423.00	0.84667	-47.589	-40.291
0.07293	-3549.13	0.85923	-48.673	-41.820
0.07599	-3751.29	0.89825	-49.373	-44.349
0.08000	-3887.65	0.94977	-48.604	-46.160
0.08042	-3947.01	0.95520	-49.088	-46.886
0.08394	-4013.87	1.00084	-47.827	-47.863
0.08698	-4102.10	1.04054	-47.169	-49.079
0.08953	-4254.11	1.07404	-47.524	-51.041
0.09200	-4525.14	1.10667	-49.194	-54.439
0.09226	-4331.54	1.11012	-46.957	-52.124
0.09644	-4492.36	1.16578	-46.590	-54.309
0.09909	-4494.41	1.20134	-45.364	-54.495
0.10236	-4516.82	1.24551	-44.134	-54.965
0.11320	-4398.81	1.39424	-38.865	-54.184
0.16857	-4105.82	2.21448	-24.360	-53.943

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 155.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.01623	-756.93	0.18020	-46.645	-8.404
0.03605	-1712.69	0.40848	-47.517	-19.409
0.04489	-2204.37	0.51335	-49.115	-25.211
0.04683	-2310.70	0.53663	-49.351	-26.480
0.05104	-2485.44	0.58746	-48.704	-28.610
0.05333	-2579.12	0.61531	-48.370	-29.760
0.05497	-2616.10	0.63533	-47.600	-30.239
0.05773	-2663.37	0.66918	-46.143	-30.876
0.06003	-2673.99	0.69755	-44.552	-31.075
0.06111	-2926.43	0.71091	-47.896	-34.047
0.06625	-2917.31	0.77495	-44.043	-34.128
0.06959	-2956.97	0.81694	-42.498	-34.718
0.07033	-3031.66	0.82628	-43.114	-35.621
0.07343	-3055.17	0.86559	-41.613	-36.017
0.07676	-3132.34	0.90811	-40.814	-37.061
0.08121	-3008.21	0.96541	-37.048	-35.765
0.08121	-3100.97	0.96541	-38.191	-36.867
0.08235	-3175.89	0.98018	-38.570	-37.803
0.08235	-3181.91	0.98018	-38.645	-37.878
0.08574	-3158.48	1.02431	-36.844	-37.737
0.08574	-3040.04	1.02431	-35.463	-36.321
0.08574	-3158.68	1.02431	-36.846	-37.740
0.08694	-3235.93	1.04001	-37.226	-38.715
0.09068	-3220.07	1.08921	-35.516	-38.681
0.09068	-3144.29	1.08921	-34.680	-37.773
0.09193	-3291.01	1.10575	-35.804	-39.590
0.09640	-3272.40	1.16525	-33.952	-39.559
0.09739	-3322.40	1.17851	-34.120	-40.208
0.10164	-3381.87	1.23575	-33.279	-41.122
0.10851	-3401.19	1.32945	-31.349	-41.676
0.10962	-3382.91	1.34472	-30.866	-41.504
0.11534	-3457.70	1.42404	-29.984	-42.695
0.12378	-3356.47	1.54296	-27.121	-41.845
0.12544	-3510.84	1.56662	-27.993	-43.853
0.13280	-3429.11	1.67262	-25.826	-43.193
0.14298	-3441.96	1.82223	-24.077	-43.872
0.15406	-3506.42	1.98915	-22.763	-45.279
0.16998	-3601.88	2.23680	-21.193	-47.404
0.18380	-3528.78	2.45961	-19.202	-47.226
0.20377	-3578.30	2.79524	-17.564	-49.091

HEAT OF MIXING DATA FOR A 60.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00378	-179.77	0.02053	-47.566	-0.975
0.01442	-588.88	0.07915	-40.845	-3.232
0.03301	-1559.79	0.18468	-47.260	-8.728
0.04906	-2369.95	0.27911	-48.316	-13.484
0.06003	-2861.57	0.34550	-47.677	-16.472
0.07428	-3691.12	0.43410	-49.700	-21.575
0.09352	-4585.00	0.55814	-49.035	-27.366
0.09854	-4895.00	0.59137	-49.683	-29.380
0.10617	-5292.36	0.64260	-49.856	-32.036
0.12050	-5887.55	0.74122	-48.867	-36.219
0.12413	-6320.48	0.76671	-50.926	-39.044
0.12830	-6423.23	0.79626	-50.072	-39.867
0.13590	-6836.67	0.85084	-50.315	-42.808
0.13672	-6771.68	0.85679	-49.538	-42.440
0.13750	-6835.14	0.86246	-49.718	-42.878
0.14420	-7168.29	0.91156	-49.719	-45.318
0.14600	-7393.99	0.92489	-50.652	-46.844
0.15340	-7582.74	0.98026	-49.439	-48.459
0.15364	-7562.26	0.98207	-49.229	-48.343
0.16199	-7971.55	1.04576	-49.218	-51.467
0.16290	-8099.96	1.05278	-49.731	-52.353
0.16310	-8023.66	1.05432	-49.203	-51.871
0.17392	-8419.78	1.13899	-48.420	-55.145
0.17490	-8501.59	1.14677	-48.616	-55.749
0.18421	-8398.76	1.22160	-45.601	-55.702
0.18690	-8209.47	1.24354	-43.932	-54.628
0.18770	-8656.78	1.25009	-46.127	-57.661
0.19564	-8303.41	1.31583	-42.449	-55.852
0.19920	-8224.80	1.34573	-41.296	-55.569
0.20110	-8203.94	1.36180	-40.802	-55.561
0.20200	-8387.88	1.36944	-41.531	-56.871
0.20947	-8086.84	1.43350	-38.613	-55.348
0.21159	-8094.45	1.45190	-38.262	-55.550
0.22100	-7957.94	1.53479	-36.015	-55.273
0.22502	-7925.88	1.57081	-35.229	-55.334
0.22660	-7927.74	1.58507	-34.991	-55.461
0.22910	-7882.22	1.60776	-34.411	-55.320
0.23570	-7972.99	1.66836	-33.832	-56.442
0.26272	-7543.72	1.92777	-28.718	-55.359
0.28670	-7459.81	2.17445	-26.024	-56.583
0.30450	-7140.04	2.36856	-23.452	-55.544
0.31561	-7060.70	2.49483	-22.376	-55.819
0.38283	-6285.01	3.35579	-16.420	-55.098
0.48644	-5157.57	5.12427	-10.604	-54.337

HEAT OF MIXING DATA FOR A 60.0% MDEA IN WATER SOLUTION AND CO2 AT 288.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.01245	-593.20	0.06820	-47.655	-3.249
0.01928	-919.95	0.10635	-47.723	-5.074
0.02858	-1426.22	0.15917	-49.911	-7.944
0.03325	-1673.38	0.18607	-50.336	-9.365
0.03904	-1901.30	0.21979	-48.709	-10.706
0.04252	-2274.94	0.24025	-53.511	-12.855
0.04770	-2325.63	0.27098	-48.764	-13.212
0.05139	-2523.36	0.29308	-49.110	-14.392
0.05211	-2735.12	0.29741	-52.497	-15.611
0.05861	-2867.12	0.33682	-48.926	-16.478
0.06424	-3178.67	0.37139	-49.489	-18.378
0.07060	-3633.80	0.41096	-51.479	-21.154
0.07726	-4082.00	0.45297	-52.843	-23.935
0.07741	-3818.18	0.45392	-49.332	-22.392
0.08157	-4360.98	0.48048	-53.471	-25.691
0.08490	-4280.45	0.50192	-50.426	-25.308
0.08522	-4366.94	0.50399	-51.252	-25.829
0.08915	-4506.01	0.52950	-50.553	-26.765
0.08932	-4469.38	0.53061	-50.046	-26.552
0.09000	-4747.23	0.53505	-52.755	-28.225
0.09481	-4710.22	0.56664	-49.688	-28.153
0.09947	-4957.31	0.59754	-49.847	-29.784
0.09983	-5017.56	0.59997	-50.270	-30.158
0.10489	-5221.75	0.63394	-49.792	-31.563
0.10568	-5497.89	0.63928	-52.032	-33.261
0.11124	-5783.38	0.67713	-51.998	-35.208
0.11165	-5395.66	0.67994	-48.334	-32.862
0.11780	-5939.46	0.72239	-50.428	-36.427
0.11905	-6230.01	0.73109	-52.340	-38.263
0.12540	-6334.57	0.77568	-50.523	-39.188
0.12606	-6287.03	0.78035	-49.882	-38.922
0.13379	-6624.81	0.83559	-49.525	-41.379
0.13452	-6812.56	0.84086	-50.652	-42.590
0.14238	-7255.46	0.89815	-50.967	-45.772
0.14289	-6998.77	0.90190	-48.988	-44.180
0.14340	-7415.67	0.90566	-51.722	-46.839
0.15306	-7598.34	0.97769	-49.651	-48.539
0.15414	-8017.21	0.98585	-52.021	-51.282
0.16536	-8255.08	1.07183	-49.930	-53.514
0.17868	-8359.52	1.17695	-46.792	-55.068

HEAT OF MIXING DATA FOR A 60.0% MDEA IN WATER
SOLUTION AND CO2 AT 288.7 K AND 155.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00373	-150.97	0.02025	-40.482	-0.820
0.01438	-623.40	0.07893	-43.359	-3.421
0.02228	-1056.95	0.12328	-47.447	-5.850
0.03304	-1570.30	0.18485	-47.535	-8.786
0.04876	-2372.12	0.27731	-48.657	-13.492
0.07410	-3702.35	0.43296	-49.973	-21.636
0.07747	-3904.40	0.45430	-50.408	-22.899
0.08924	-4488.24	0.53009	-50.302	-26.663
0.09830	-4970.37	0.58977	-50.571	-29.823
0.10335	-5197.23	0.62356	-50.296	-31.361
0.10810	-5424.16	0.65570	-50.186	-32.903
0.11470	-5747.19	0.70092	-50.115	-35.125
0.12065	-5932.64	0.74227	-49.180	-36.501
0.12070	-6063.37	0.74262	-50.243	-37.310
0.12070	-6092.48	0.74262	-50.484	-37.488
0.12799	-6204.11	0.79405	-48.481	-38.493
0.13514	-6225.36	0.84534	-46.073	-38.944
0.13560	-6276.37	0.84867	-46.293	-39.285
0.14250	-6279.55	0.89903	-44.074	-39.620
0.14390	-6318.82	0.90935	-43.919	-39.933
0.15260	-6390.67	0.97423	-41.885	-40.803
0.16173	-6336.16	1.04376	-39.183	-40.897
0.17404	-6545.82	1.13994	-37.617	-42.878
0.17457	-6456.51	1.14415	-36.991	-42.321
0.18560	-6369.94	1.23292	-34.326	-42.318
0.20158	-6537.90	1.36587	-32.439	-44.304
0.23655	-6433.57	1.67624	-27.202	-45.595

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 333.1 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00218	-122.08	0.05999	-56.009	-3.360
0.00489	-280.76	0.13494	-57.424	-7.747
0.00836	-479.37	0.23150	-57.351	-13.276
0.01294	-729.22	0.35999	-56.363	-20.289
0.01936	-1047.98	0.54212	-54.140	-29.350
0.02401	-1256.82	0.67553	-52.354	-35.366
0.02877	-1529.80	0.81342	-53.182	-43.257
0.03265	-1671.42	0.92682	-51.200	-47.451
0.03314	-1741.21	0.94121	-52.550	-49.456
0.03551	-1782.05	1.01100	-50.193	-50.741
0.03603	-1814.36	1.02635	-50.366	-51.689
0.03760	-1842.69	1.07282	-49.015	-52.583
0.03926	-1831.04	1.12212	-46.646	-52.340
0.04042	-1801.46	1.15667	-44.576	-51.556
0.04288	-1812.80	1.23023	-42.283	-52.016
0.04421	-1803.77	1.27015	-40.807	-51.827
0.04486	-1824.72	1.28970	-40.682	-52.464
0.04921	-1820.31	1.42123	-36.996	-52.578
0.05612	-1731.40	1.63267	-30.857	-50.376
0.05694	-1813.75	1.65796	-31.859	-52.819
0.06313	-1776.67	1.85034	-28.147	-52.079
0.07347	-1700.84	2.17744	-23.154	-50.415
0.08399	-1697.49	2.51781	-20.214	-50.891
0.10238	-1700.58	3.13198	-16.613	-52.029
0.12862	-1606.86	4.05319	-12.495	-50.642
0.15337	-1481.85	4.97443	-9.663	-48.068

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 333.1 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00765	-410.08	0.21169	-53.614	-11.348
0.00968	-520.74	0.26841	-53.804	-14.439
0.01190	-617.54	0.33071	-51.902	-17.162
0.01297	-697.25	0.36083	-53.767	-19.400
0.01577	-874.06	0.43998	-55.435	-24.389
0.01779	-913.57	0.49736	-51.361	-25.544
0.01928	-1052.65	0.53983	-54.607	-29.477
0.02069	-1102.74	0.58015	-53.307	-30.923
0.02170	-1156.33	0.60909	-53.295	-32.460
0.02339	-1236.89	0.65767	-52.889	-34.781
0.02425	-1282.23	0.68245	-52.884	-36.089
0.02628	-1363.90	0.74112	-51.907	-38.468
0.02650	-1423.75	0.74749	-53.735	-40.163
0.02876	-1541.56	0.81313	-53.610	-43.590
0.03234	-1675.77	0.91773	-51.825	-47.559
0.03260	-1723.03	0.92535	-52.863	-48.913
0.04030	-1884.73	1.15310	-46.775	-53.932
0.05122	-1867.32	1.48242	-36.463	-54.049
0.06715	-1835.48	1.97665	-27.338	-54.035
0.09253	-1774.36	2.79993	-19.179	-53.697

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER
SOLUTION AND CO2 AT 333.1 K AND 155.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00213	-114.70	0.05870	-53.782	-3.158
0.00824	-505.08	0.22815	-61.306	-13.985
0.01281	-735.07	0.35632	-57.392	-20.450
0.01902	-1071.49	0.53241	-56.344	-29.998
0.02078	-1201.93	0.58272	-57.850	-33.709
0.02148	-1226.30	0.60278	-57.100	-34.416
0.02315	-1276.16	0.65076	-55.135	-35.878
0.02417	-1309.78	0.68014	-54.199	-36.862
0.02617	-1347.60	0.73793	-51.502	-38.003
0.02826	-1354.94	0.79858	-47.953	-38.294
0.02847	-1350.33	0.80469	-47.438	-38.169
0.02999	-1331.79	0.84898	-44.415	-37.706
0.03078	-1384.96	0.87205	-45.003	-39.244
0.03244	-1336.88	0.92066	-41.218	-37.945
0.03344	-1382.58	0.95002	-41.352	-39.282
0.03475	-1397.81	0.98858	-40.231	-39.770
0.03791	-1374.17	1.08202	-36.255	-39.224
0.03801	-1399.67	1.08498	-36.830	-39.958
0.03956	-1376.48	1.13105	-34.801	-39.360
0.04344	-1379.70	1.24702	-31.767	-39.612
0.04717	-1363.52	1.35940	-28.912	-39.299
0.05496	-1332.59	1.59696	-24.251	-38.726
0.07196	-1210.46	2.12922	-16.824	-35.820
0.09933	-938.33	3.02838	-9.448	-28.610
0.14905	-674.48	4.80977	-4.526	-21.768

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 333.1 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00303	-162.85	0.03322	-53.719	-1.784
0.00369	-204.10	0.04045	-55.321	-2.238
0.00597	-336.70	0.06560	-56.408	-3.701
0.00827	-468.74	0.09108	-56.689	-5.163
0.00953	-533.68	0.10509	-56.009	-5.886
0.01410	-794.57	0.15621	-56.361	-8.803
0.01650	-923.33	0.18324	-55.969	-10.254
0.03270	-1870.67	0.36924	-57.217	-21.126
0.03853	-2055.49	0.43770	-53.357	-23.353
0.05490	-2899.32	0.63447	-52.820	-33.510
0.06316	-3564.90	0.73637	-56.451	-41.568
0.06627	-3730.94	0.77520	-56.308	-43.648
0.06937	-3837.27	0.81417	-55.325	-45.041
0.07268	-3996.68	0.85606	-54.999	-47.080
0.07290	-4080.96	0.85885	-55.989	-48.085
0.07622	-4218.19	0.90119	-55.352	-49.880
0.07645	-4120.09	0.90414	-53.901	-48.730
0.08001	-4170.91	0.94990	-52.138	-49.523
0.08025	-4207.68	0.95300	-52.441	-49.974
0.08408	-4210.81	1.00266	-50.089	-50.221
0.08459	-4265.07	1.00930	-50.429	-50.894
0.08873	-4304.72	1.06351	-48.523	-51.600
0.09293	-4236.22	1.11901	-45.592	-51.016
0.09891	-4287.28	1.19892	-43.352	-51.974
0.10390	-4193.57	1.26642	-40.368	-51.121
0.11733	-4219.37	1.45187	-35.967	-52.218
0.11770	-4183.35	1.45706	-35.549	-51.794
0.13280	-4133.40	1.67262	-31.130	-52.065
0.14950	-3998.74	1.91993	-26.752	-51.359
0.16340	-3995.11	2.13330	-24.453	-52.165
0.17620	-3980.18	2.33616	-22.593	-52.777
0.19100	-3895.22	2.57871	-20.397	-52.594
0.20640	-3652.75	2.84070	-17.701	-50.279
0.32370	-1883.29	5.22783	-5.819	-30.419

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 333.1 K AND 155.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.01691	-1033.70	0.18787	-61.140	-11.487
0.02487	-1551.61	0.27857	-62.399	-17.381
0.03427	-2059.35	0.38759	-60.101	-23.295
0.03760	-2234.90	0.42673	-59.449	-25.367
0.03995	-2419.60	0.45451	-60.576	-27.530
0.04168	-2562.91	0.47505	-61.500	-29.214
0.04272	-2685.20	0.48743	-62.867	-30.640
0.04595	-2609.81	0.52606	-56.806	-29.881
0.04700	-2617.78	0.53867	-55.707	-30.006
0.05084	-2739.88	0.58504	-53.901	-31.532
0.05299	-2798.86	0.61116	-52.827	-32.283
0.05542	-2820.80	0.64083	-50.907	-32.621
0.05782	-2837.96	0.67029	-49.091	-32.903
0.06017	-2837.97	0.69928	-47.174	-32.986
0.06285	-2831.48	0.73251	-45.058	-33.003
0.07011	-2713.35	0.82351	-38.708	-31.873
0.07031	-2766.86	0.82603	-39.358	-32.510
0.08309	-2615.52	0.98978	-31.483	-31.161
0.09135	-2642.06	1.09807	-28.927	-31.762
0.09633	-2598.33	1.16431	-26.978	-31.408
0.12670	-2441.29	1.58464	-19.271	-30.535
0.13420	-2547.78	1.69298	-18.988	-32.144
0.16070	-2344.00	2.09130	-14.589	-30.507
0.17044	-2371.66	2.24410	-13.918	-31.230
0.18380	-2257.54	2.45961	-12.285	-30.214

HEAT OF MIXING DATA FOR A 60.0% MDEA IN WATER SOLUTION AND CO2 AT 333.1 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00540	-338.28	0.02937	-62.666	-1.839
0.01207	-762.74	0.06608	-63.219	-4.177
0.01610	-919.43	0.08853	-57.117	-5.055
0.02046	-1232.24	0.11300	-60.236	-6.806
0.02266	-1264.65	0.12543	-55.819	-7.002
0.03110	-1735.79	0.17365	-55.822	-9.692
0.03146	-1923.72	0.17573	-61.158	-10.747
0.04238	-2326.92	0.23942	-54.915	-13.146
0.05146	-2942.28	0.29350	-57.186	-16.783
0.05822	-3335.85	0.33444	-57.307	-19.165
0.07114	-4058.42	0.41433	-57.059	-23.641
0.07782	-4460.78	0.45653	-57.331	-26.173
0.08207	-4656.31	0.48369	-56.745	-27.447
0.09333	-5351.86	0.55689	-57.353	-31.937
0.10240	-5800.12	0.61718	-56.651	-34.961
0.10800	-6169.20	0.65502	-57.132	-37.421
0.11370	-6446.34	0.69402	-56.705	-39.352
0.11900	-6811.60	0.73074	-57.249	-41.833
0.11940	-6683.94	0.73353	-55.989	-41.066
0.12210	-6805.40	0.75243	-55.746	-41.941
0.12310	-7057.52	0.75945	-57.341	-43.545
0.12340	-6981.76	0.76157	-56.587	-43.094
0.12632	-7036.40	0.78219	-55.712	-43.576
0.12960	-7116.31	0.80553	-54.919	-44.235
0.13360	-7142.64	0.83422	-53.471	-44.603
0.13630	-7139.25	0.85374	-52.387	-44.722
0.14150	-7109.36	0.89168	-50.251	-44.806
0.14583	-7129.85	0.92363	-48.900	-45.163
0.15320	-7071.53	0.97875	-46.166	-45.182
0.15620	-7036.40	1.00146	-45.054	-45.119
0.16240	-7026.69	1.04892	-43.275	-45.390
0.17010	-6970.68	1.10885	-40.987	-45.445
0.17210	-6991.21	1.12460	-40.630	-45.689
0.18330	-6951.76	1.21421	-37.932	-46.055
0.19560	-6877.81	1.31550	-35.168	-46.262
0.24560	-6204.96	1.76125	-25.269	-44.501

HEAT OF MIXING DATA FOR A 60.0% MDEA IN WATER
SOLUTION AND CO2 AT 333.1 K AND 155.8 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00315	-227.03	0.01710	-72.085	-1.233
0.00706	-465.74	0.03847	-65.979	-2.537
0.01205	-716.59	0.06599	-59.477	-3.925
0.01862	-1175.81	0.10264	-63.158	-6.482
0.02533	-1500.93	0.14060	-59.265	-8.332
0.02767	-1644.78	0.15395	-59.453	-9.152
0.04111	-2437.87	0.23194	-59.311	-13.755
0.04339	-2452.40	0.24539	-56.529	-13.872
0.04945	-2809.47	0.28144	-56.824	-15.990
0.05062	-3011.69	0.28845	-59.506	-17.165
0.05610	-3208.97	0.32154	-57.210	-18.395
0.06109	-3444.60	0.35200	-56.395	-19.849
0.06227	-3468.91	0.35925	-55.717	-20.015
0.06322	-3548.28	0.36510	-56.135	-20.494
0.06602	-3543.29	0.38241	-53.679	-20.525
0.06899	-3553.90	0.40089	-51.522	-20.652
0.07215	-3542.18	0.42068	-49.102	-20.655
0.07326	-3552.46	0.42766	-48.499	-20.741
0.07550	-3462.45	0.44181	-45.868	-20.264
0.08412	-3481.67	0.49688	-41.396	-20.569
0.08699	-3417.48	0.51545	-39.293	-20.253
0.09829	-3317.77	0.58971	-33.761	-19.907
0.10220	-3260.49	0.61584	-31.908	-19.650
0.11312	-3227.08	0.69003	-28.533	-19.688
0.13425	-3052.14	0.83891	-22.739	-19.073
0.13993	-2891.42	0.88018	-20.666	-18.190
0.16380	-2917.98	1.05974	-17.817	-18.879
0.18336	-2655.25	1.21470	-14.483	-17.591

HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 388.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00590	-325.64	0.16297	-55.202	-8.997
0.00926	-587.48	0.25665	-63.454	-16.284
0.00929	-531.07	0.25749	-57.176	-14.722
0.01066	-589.52	0.29587	-55.311	-16.364
0.01066	-658.15	0.29587	-61.750	-18.270
0.01317	-742.74	0.36647	-56.405	-20.669
0.01334	-771.05	0.37127	-57.809	-21.461
0.01466	-816.53	0.40855	-55.707	-22.757
0.01761	-1056.30	0.49223	-59.993	-29.530
0.01866	-1076.12	0.52214	-57.679	-30.114
0.01872	-1210.71	0.52385	-64.685	-33.884
0.01935	-1119.15	0.54183	-57.847	-31.341
0.01961	-1177.17	0.54926	-60.039	-32.975
0.01972	-1208.36	0.55240	-61.286	-33.853
0.02071	-1201.85	0.58072	-58.042	-33.704
0.02268	-1184.34	0.63724	-52.229	-33.280
0.02563	-1184.38	0.72231	-46.218	-33.383
0.02832	-1142.06	0.80032	-40.333	-32.277
0.03139	-1095.28	0.88989	-34.898	-31.053
0.03167	-1162.63	0.89809	-36.717	-32.973
0.03549	-1098.30	1.01041	-30.951	-31.272
0.04040	-1067.41	1.15608	-26.426	-30.549
0.04190	-1021.79	1.20088	-24.390	-29.289
0.04330	-1085.25	1.24282	-25.067	-31.153
0.04523	-1049.43	1.30084	-23.205	-30.186
0.04946	-970.95	1.42883	-19.634	-28.053
0.05493	-946.24	1.59603	-17.229	-27.497
0.07068	-813.74	2.08847	-11.515	-24.048
0.08678	-684.50	2.60940	-7.889	-20.586
0.10220	-495.59	3.12585	-4.850	-15.160

HEAT OF MIXING DATA FOR A 40.0% MDEA IN WATER SOLUTION AND CO2 AT 388.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00713	-417.97	0.07844	-58.631	-4.598
0.01211	-770.87	0.13389	-63.667	-8.523
0.01433	-920.92	0.15879	-64.276	-10.207
0.01563	-1008.24	0.17343	-64.518	-11.188
0.01707	-1076.08	0.18968	-63.050	-11.958
0.01853	-1141.40	0.20621	-61.607	-12.703
0.02003	-1297.06	0.22325	-64.766	-14.459
0.02016	-1265.28	0.22473	-62.772	-14.107
0.02348	-1487.09	0.26262	-63.344	-16.636
0.02356	-1512.40	0.26354	-64.205	-16.918
0.02754	-1751.45	0.30932	-63.607	-19.674
0.02967	-1849.02	0.33398	-62.329	-20.816
0.02977	-1828.69	0.33514	-61.437	-20.588
0.03208	-2002.43	0.36200	-62.430	-22.599
0.03218	-1931.44	0.36317	-60.030	-21.799
0.03335	-1956.87	0.37683	-58.687	-22.115
0.03468	-1941.32	0.39240	-55.987	-21.968
0.03607	-1971.64	0.40871	-54.670	-22.342
0.03752	-1965.91	0.42578	-52.404	-22.311
0.04062	-1887.17	0.46245	-46.467	-21.489
0.04076	-1883.50	0.46411	-46.217	-21.450
0.04229	-1897.69	0.48230	-44.880	-21.644
0.04417	-1799.59	0.50474	-40.749	-20.566
0.04460	-1801.08	0.50988	-40.390	-20.591
0.04586	-1877.66	0.52498	-40.950	-21.497
0.04779	-1737.28	0.54818	-36.358	-19.929
0.05195	-1770.52	0.59851	-34.087	-20.400
0.05212	-1667.34	0.60058	-31.996	-19.215
0.06180	-1722.80	0.71947	-27.881	-20.059
0.06199	-1582.94	0.72183	-25.540	-18.434
0.07460	-1537.25	0.88050	-20.610	-18.145
0.09098	-1759.02	1.09318	-19.337	-21.137

HEAT OF MIXING DATA FOR A 60.0% MDEA IN WATER SOLUTION AND CO2 AT 388.7 K AND 1121.1 KPA

MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00693	-473.51	0.03775	-68.338	-2.579
0.00901	-639.75	0.04919	-71.016	-3.493
0.01145	-704.79	0.06266	-61.564	-3.858
0.01246	-790.90	0.06826	-63.485	-4.332
0.01401	-887.31	0.07687	-63.344	-4.869
0.01532	-1018.75	0.08417	-66.509	-5.598
0.01694	-1052.99	0.09322	-62.170	-5.795
0.01839	-1217.55	0.10135	-66.218	-6.711
0.01980	-1278.89	0.10928	-64.602	-7.060
0.02014	-1302.51	0.11120	-64.683	-7.193
0.02184	-1357.40	0.12079	-62.163	-7.509
0.02198	-1341.43	0.12158	-61.039	-7.421
0.02371	-1522.94	0.13139	-64.242	-8.440
0.02427	-1626.36	0.13457	-67.022	-9.019
0.02570	-1573.01	0.14270	-61.216	-8.736
0.02587	-1568.29	0.14367	-60.632	-8.711
0.02782	-1733.01	0.15481	-62.304	-9.645
0.02894	-1851.29	0.16123	-63.981	-10.315
0.03070	-1945.78	0.17135	-63.391	-10.861
0.03129	-1924.48	0.17475	-61.515	-10.750
0.03253	-1862.31	0.18190	-57.259	-10.415
0.03381	-1882.05	0.18931	-55.675	-10.539
0.03591	-1899.60	0.20151	-52.908	-10.661
0.04189	-1790.57	0.23653	-42.752	-10.113
0.04821	-1753.13	0.27402	-36.370	-9.966
0.05291	-1707.73	0.30223	-32.281	-9.756
0.06061	-1721.65	0.34905	-28.410	-9.916
0.07996	-1427.21	0.47018	-17.852	-8.393
0.12967	-988.39	0.80603	-7.623	-6.144

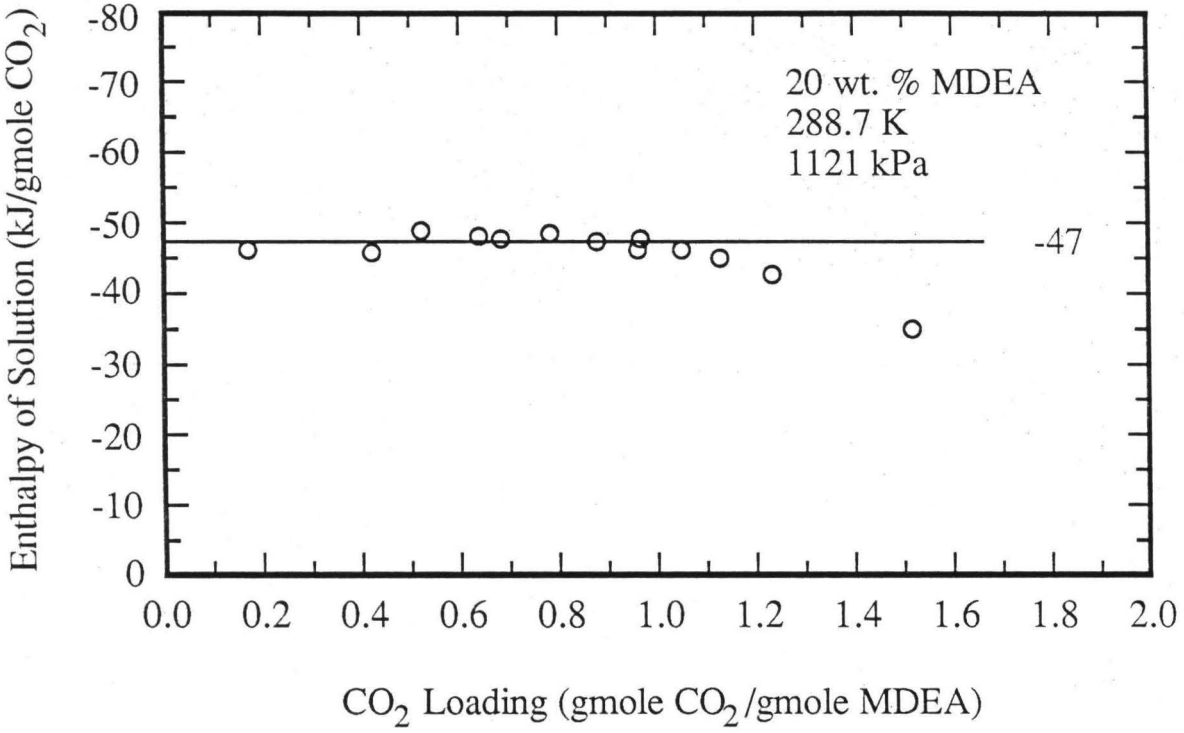
HEAT OF MIXING DATA FOR A 20.0% MDEA IN WATER SOLUTION AND CO2 AT 422.0 K AND 1465.8 KPA

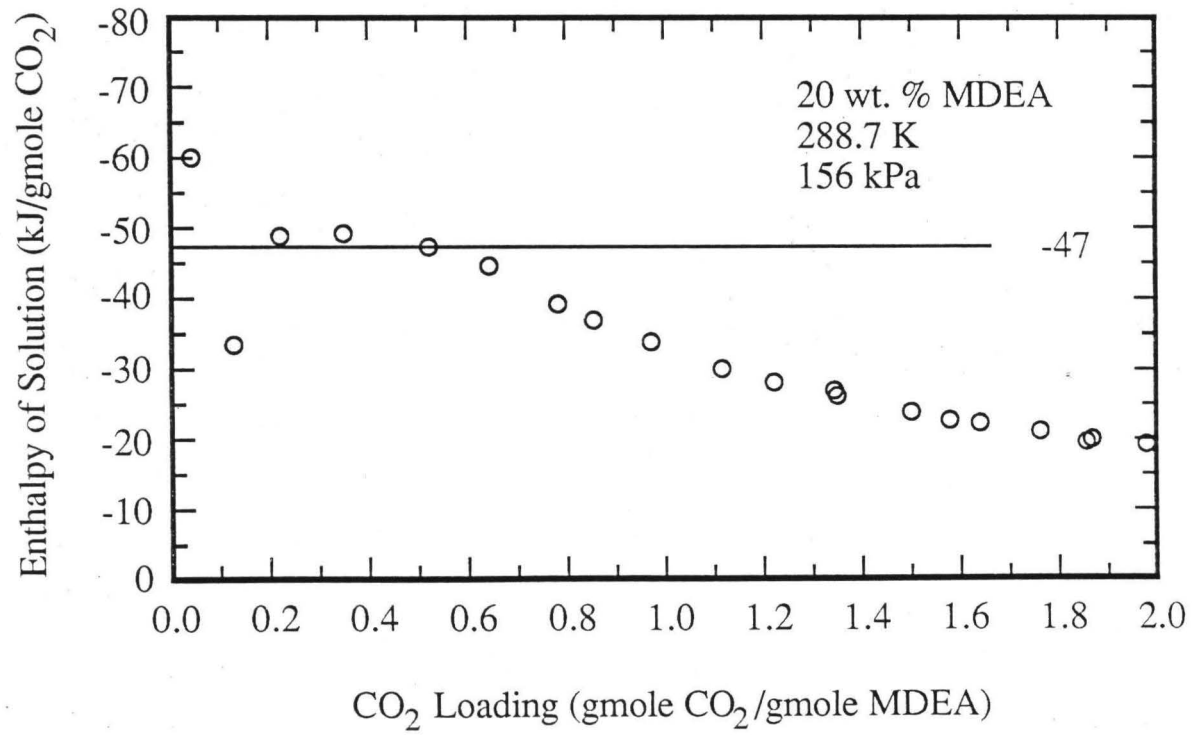
MOLE FRACTION CO2	HEAT OF MIXING (J/GMOLE)	GMOLE CO2 / GMOLE MDEA	KJ / GMOLE CO2	KJ / GMOLE MDEA
0.00189	-129.02	0.05200	-68.276	-3.551
0.00299	-194.21	0.08235	-64.964	-5.349
0.00350	-213.06	0.09645	-60.884	-5.872
0.00418	-282.03	0.11526	-67.482	-7.778
0.00418	-255.76	0.11526	-61.197	-7.052
0.00459	-295.81	0.12662	-64.457	-8.160
0.00505	-317.93	0.13938	-62.967	-8.775
0.00520	-347.86	0.14354	-66.907	-9.603
0.00543	-337.46	0.14992	-62.158	-9.318
0.00587	-371.52	0.16214	-63.301	-10.262
0.00588	-378.50	0.16242	-64.382	-10.456
0.00649	-422.51	0.17938	-65.112	-11.678
0.00689	-459.64	0.19051	-66.722	-12.711
0.00747	-470.15	0.20667	-62.948	-13.007
0.00784	-511.40	0.21699	-65.240	-14.154
0.00829	-534.45	0.22954	-64.480	-14.799
0.00874	-544.47	0.24211	-62.307	-15.085
0.00887	-551.88	0.24575	-62.229	-15.292
0.00941	-578.17	0.26085	-61.452	-16.029
0.00947	-563.79	0.26253	-59.544	-15.630
0.00953	-618.70	0.26421	-64.932	-17.154
0.01042	-588.55	0.28914	-56.492	-16.334
0.01104	-587.88	0.30654	-53.259	-16.326
0.01134	-582.35	0.31497	-51.362	-16.176
0.01155	-555.56	0.32087	-48.108	-15.437
0.01215	-544.03	0.33774	-44.783	-15.124
0.01274	-534.25	0.35435	-41.941	-14.860
0.01318	-540.74	0.36675	-41.034	-15.049
0.01471	-526.74	0.40996	-35.814	-14.680
0.01566	-518.24	0.43686	-33.099	-14.459
0.01723	-466.96	0.48143	-27.106	-13.049
0.01816	-460.17	0.50789	-25.343	-12.872

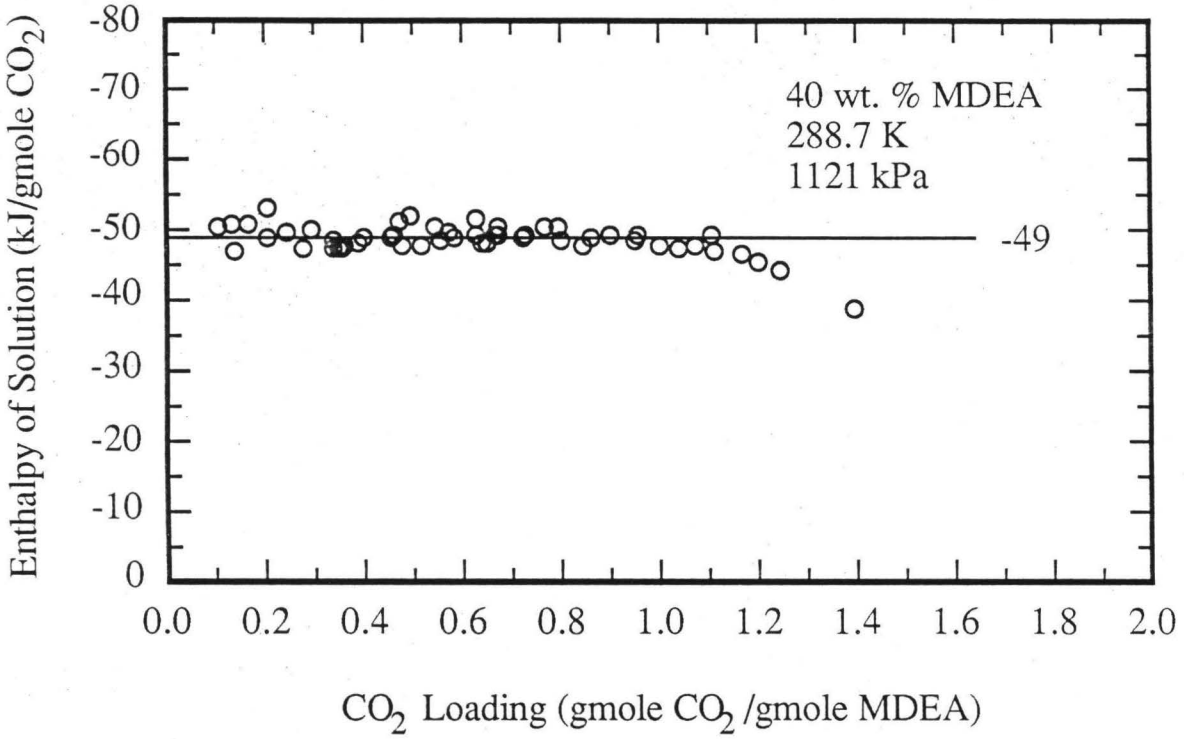
APPENDIX B

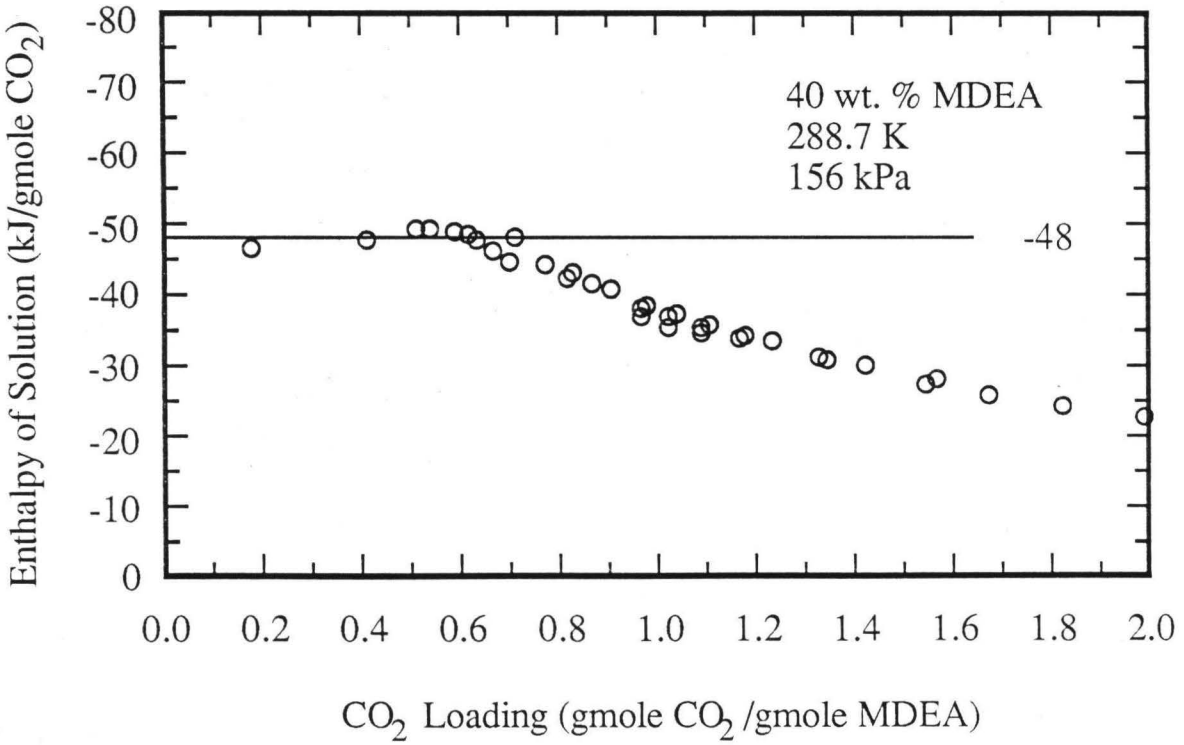
PLOTS OF EXPERIMENTAL DATA:

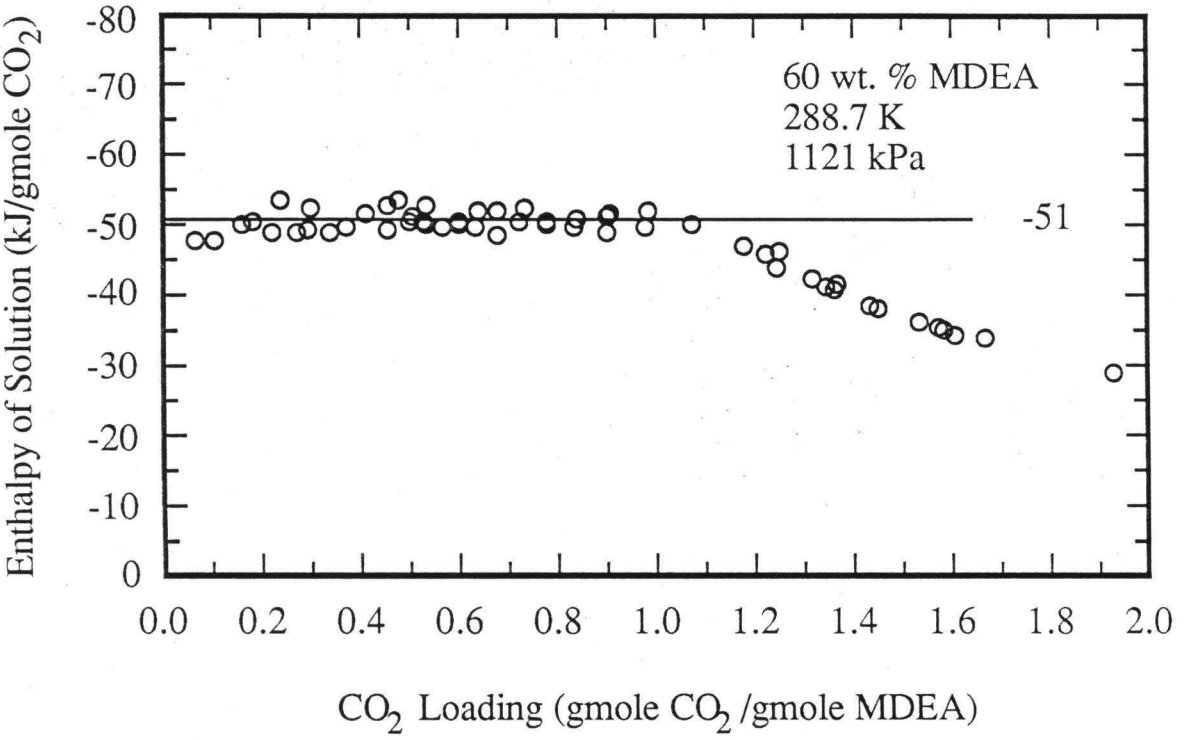
Enthalpy of Solution (kJ/gmole CO_2 and kJ/gmole MDEA) as a Function of Loading (gmole CO_2/gmole MDEA)

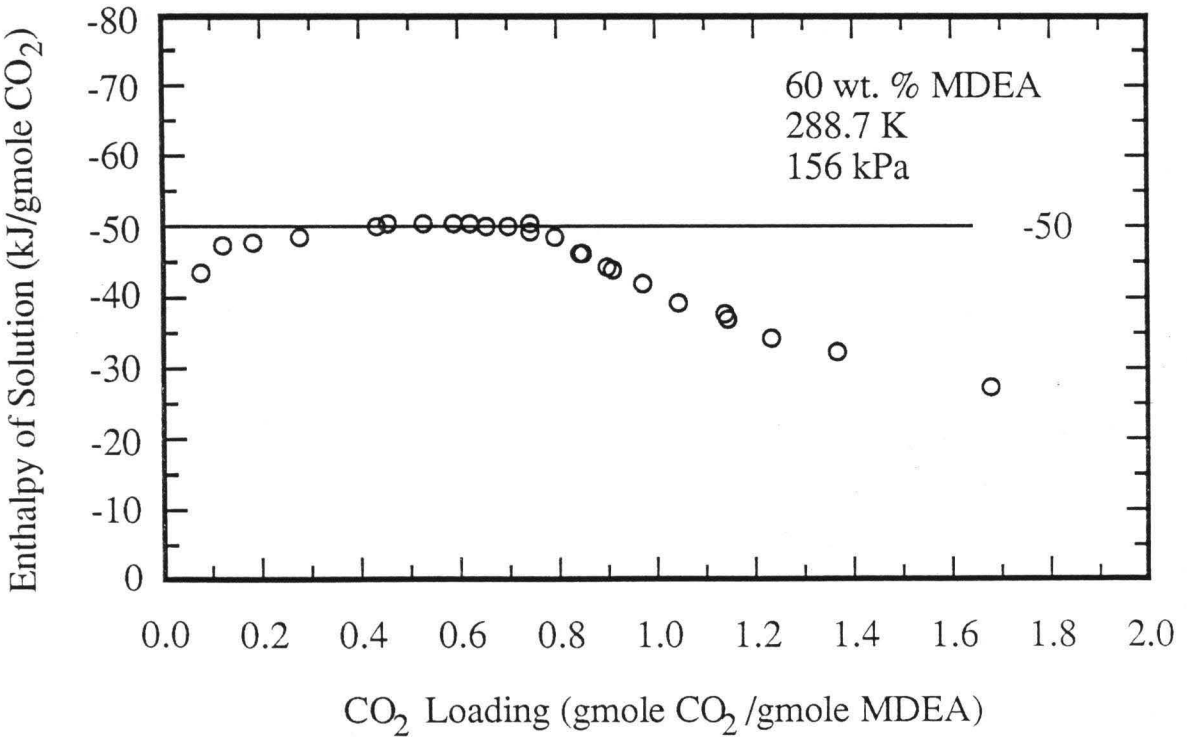

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
20 wt. % MDEA
288.7 K
1121 kPa
-47
CO_2 Loading (gmole CO_2/gmole MDEA)

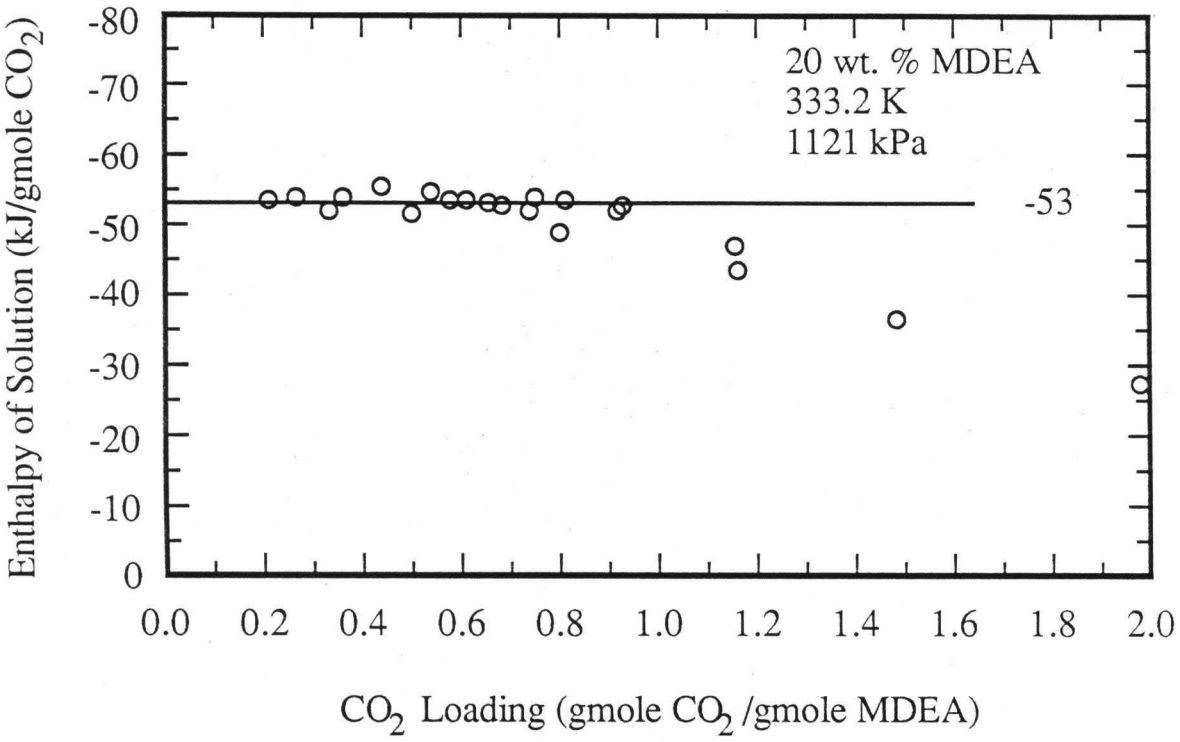

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
20 wt. % MDEA
288.7 K
156 kPa
-47
CO_2 Loading (gmole CO_2/gmole MDEA)

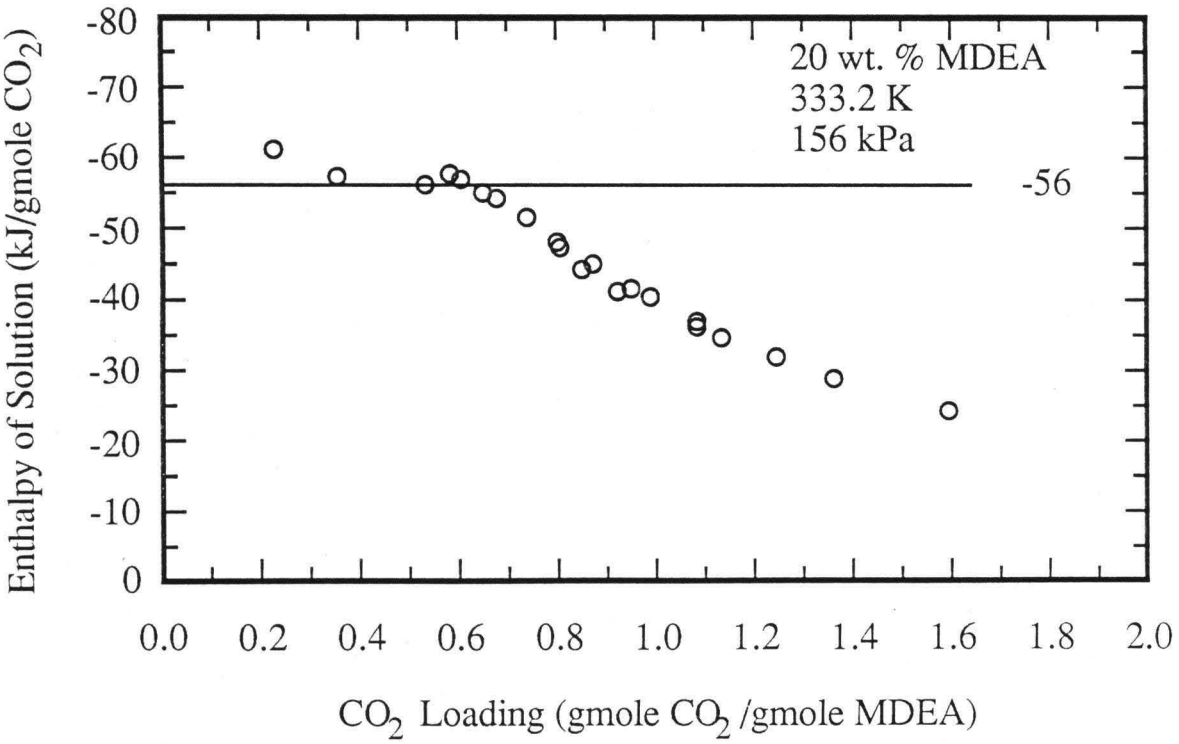

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
40 wt. % MDEA
288.7 K
1121 kPa
-49
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

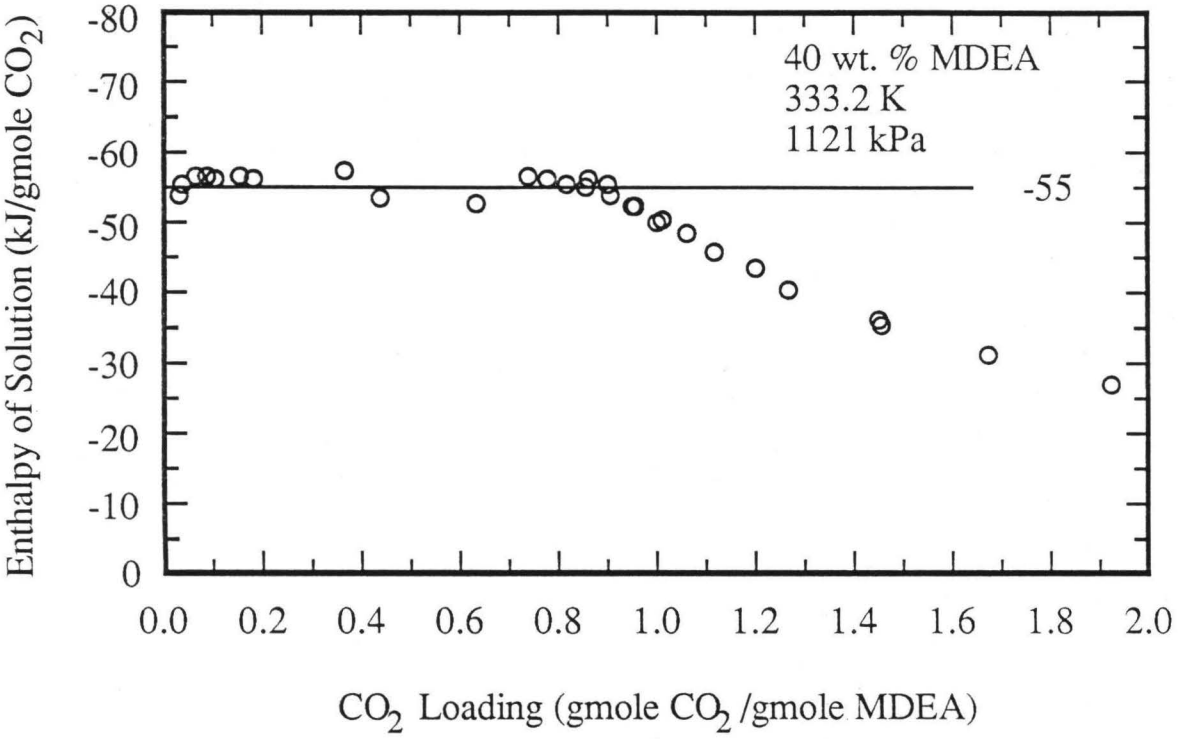

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
40 wt. % MDEA
288.7 K
156 kPa
-48
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

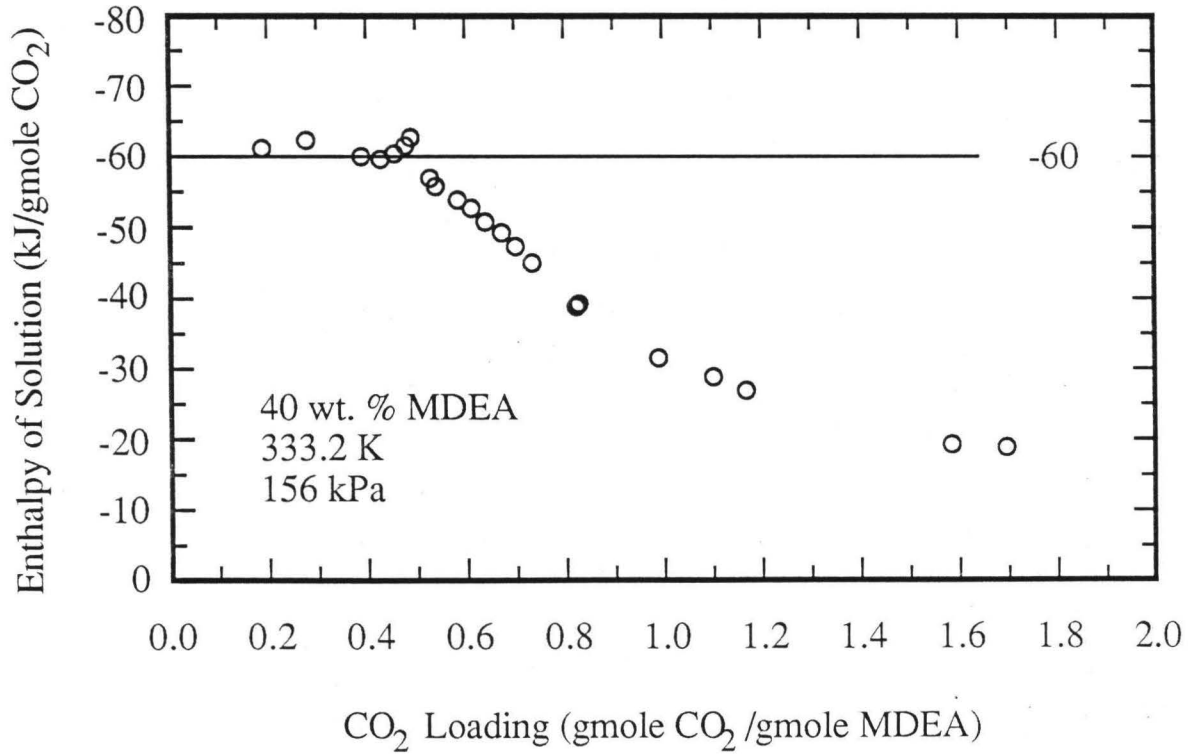

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
60 wt. % MDEA
288.7 K
1121 kPa
-51
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

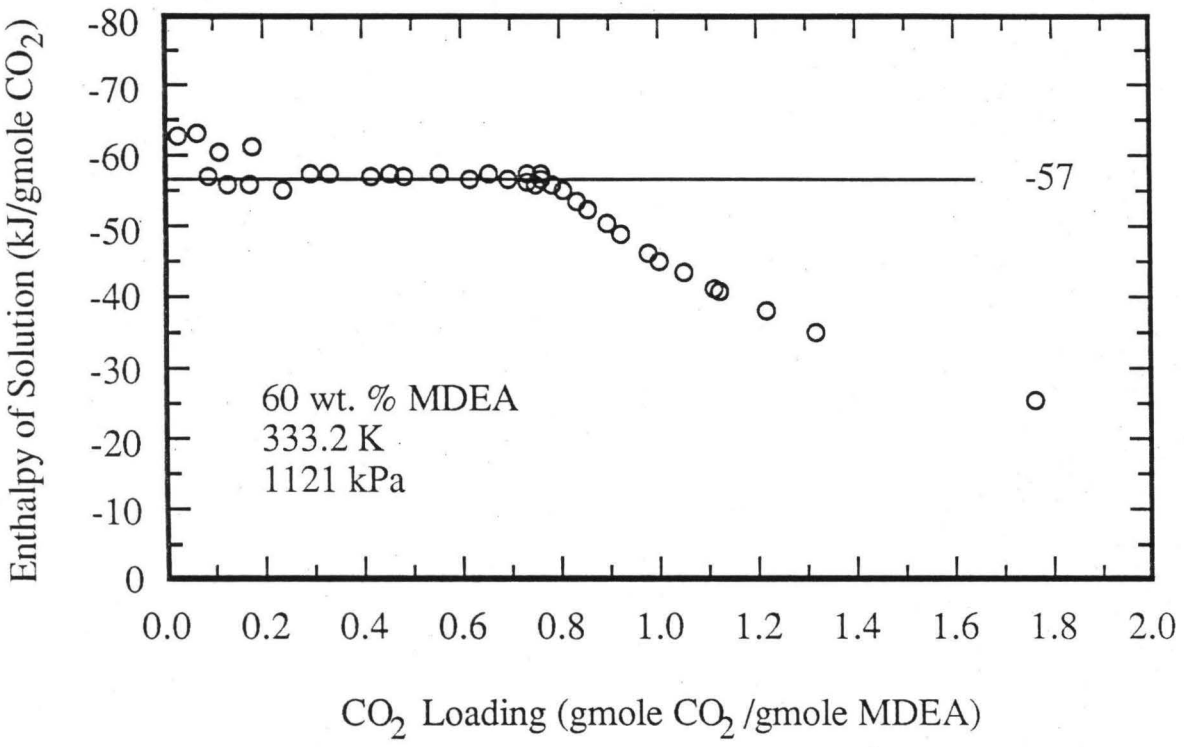

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
60 wt. % MDEA
288.7 K
156 kPa
-50
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

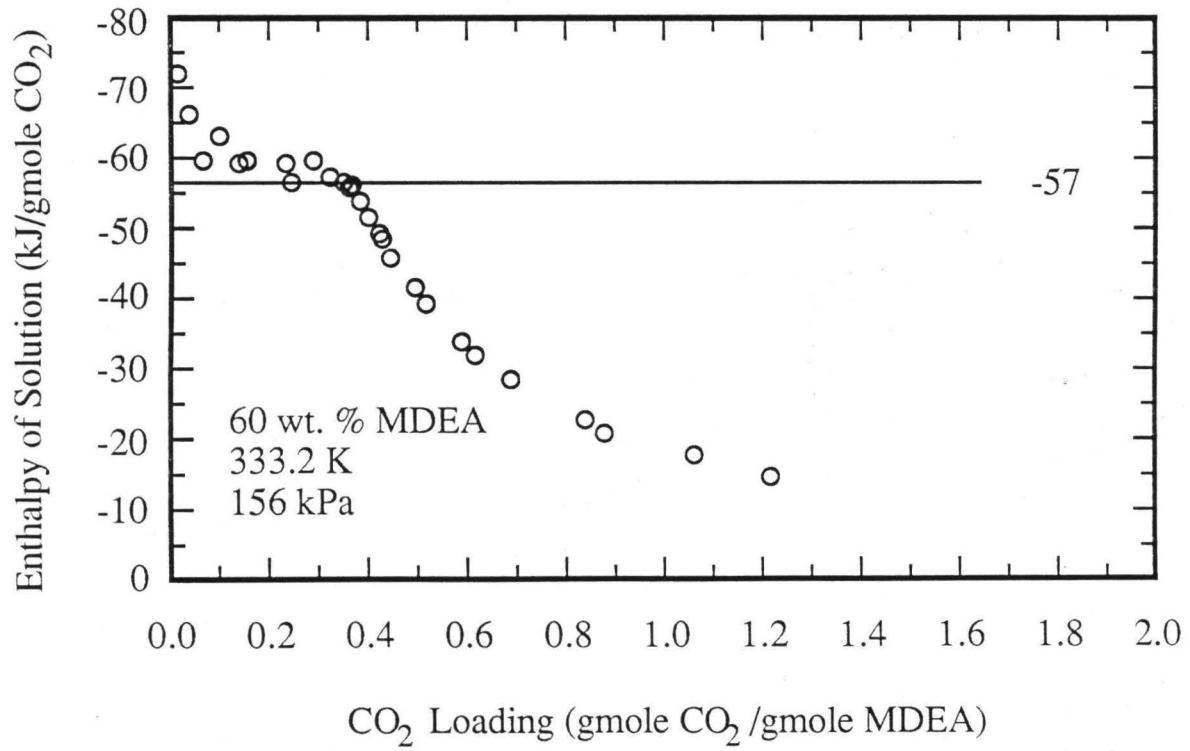

20 wt. % MDEA
333.2 K
1121 kPa
-53
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)

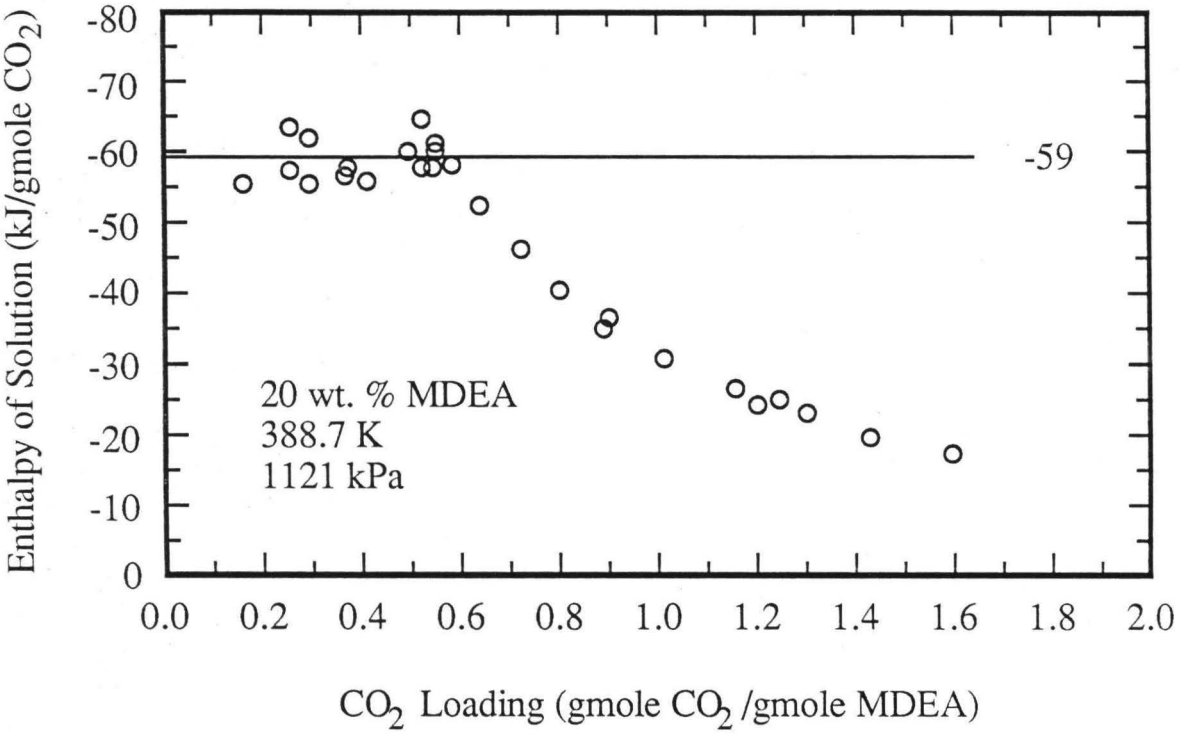

20 wt. % MDEA
333.2 K
156 kPa
-56
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)

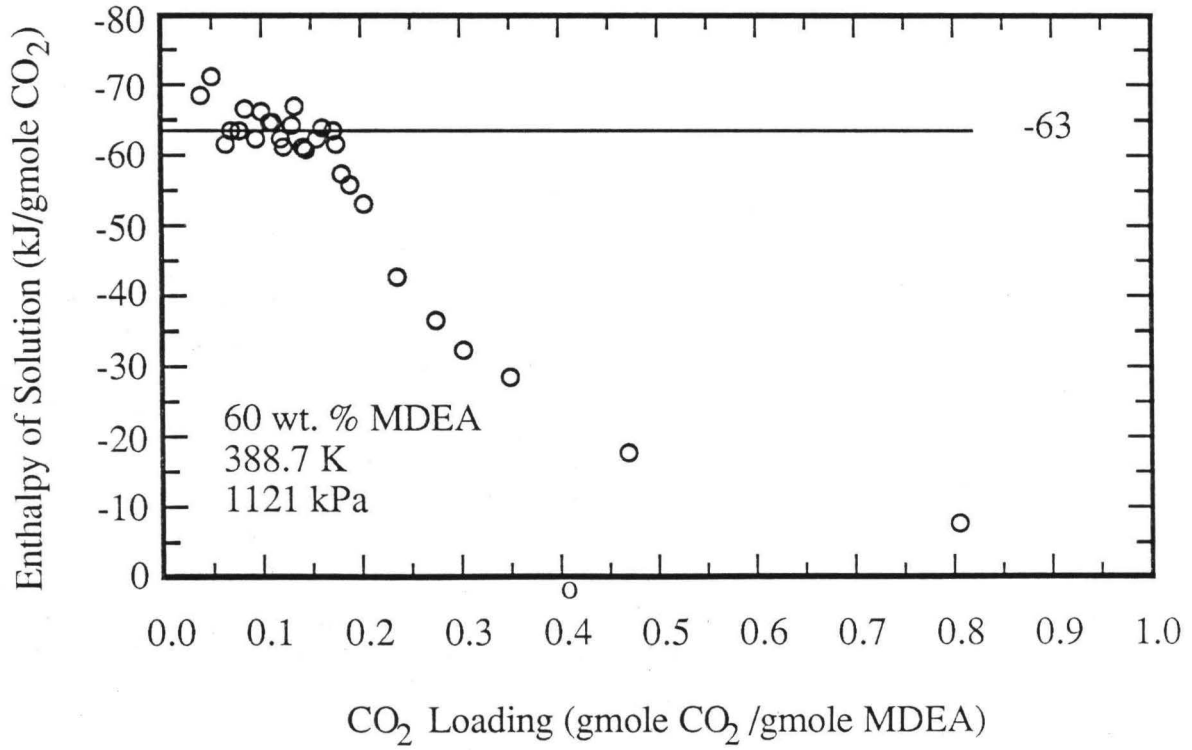

40 wt. % MDEA
333.2 K
1121 kPa
-55
Enthalpy of Solution (kJ/gmole CO_2)
CO_2 Loading (gmole CO_2 /gmole MDEA)

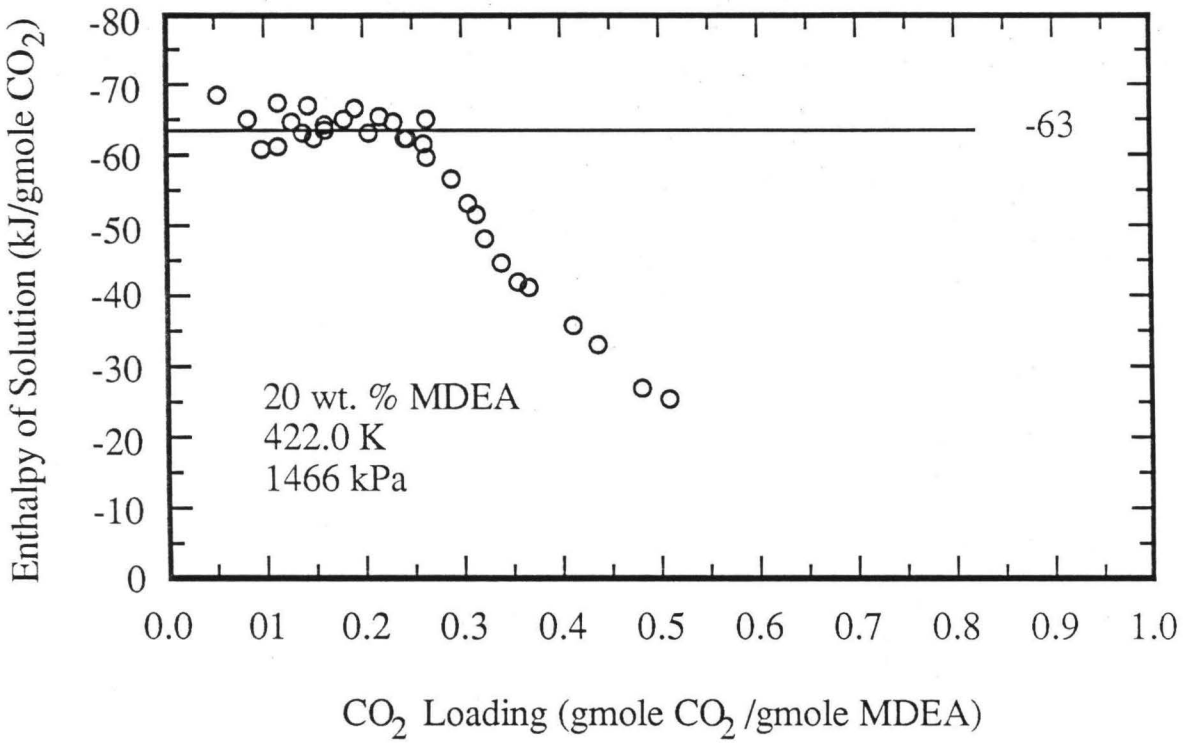

40 wt. % MDEA
333.2 K
156 kPa
-60
Enthalpy of Solution (kJ/gmole CO_2)
CO_2 Loading (gmole CO_2 /gmole MDEA)

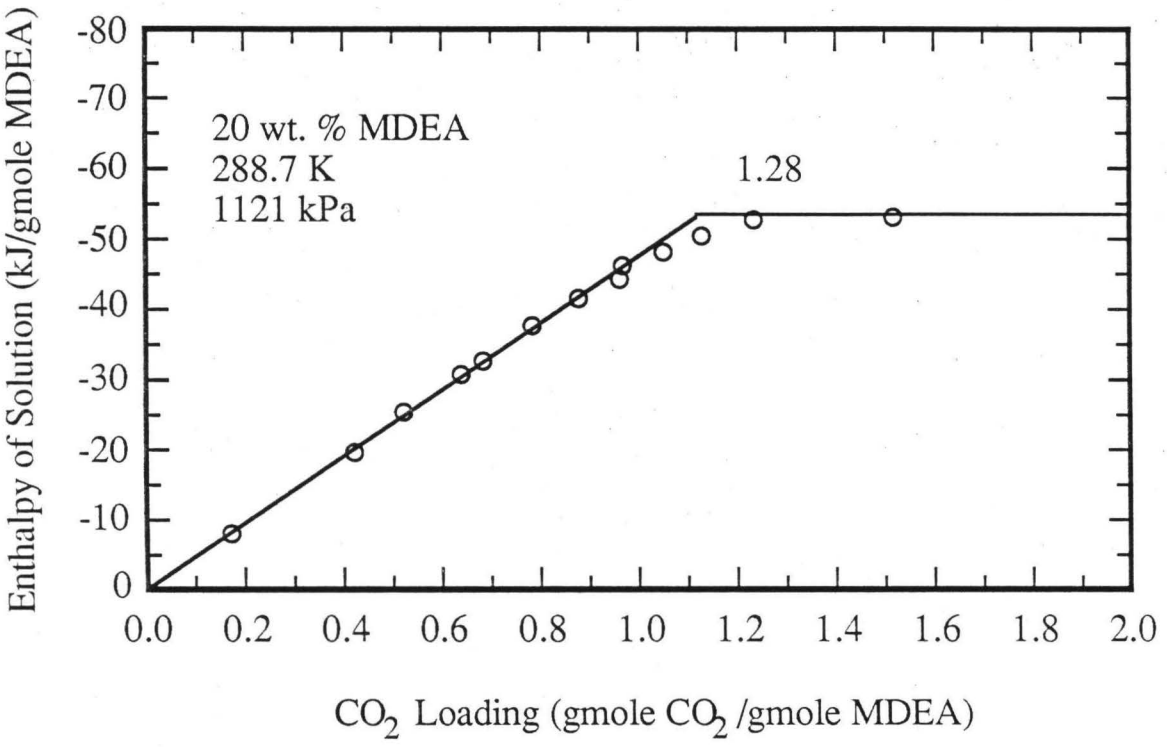

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-57
60 wt. % MDEA
333.2 K
1121 kPa
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

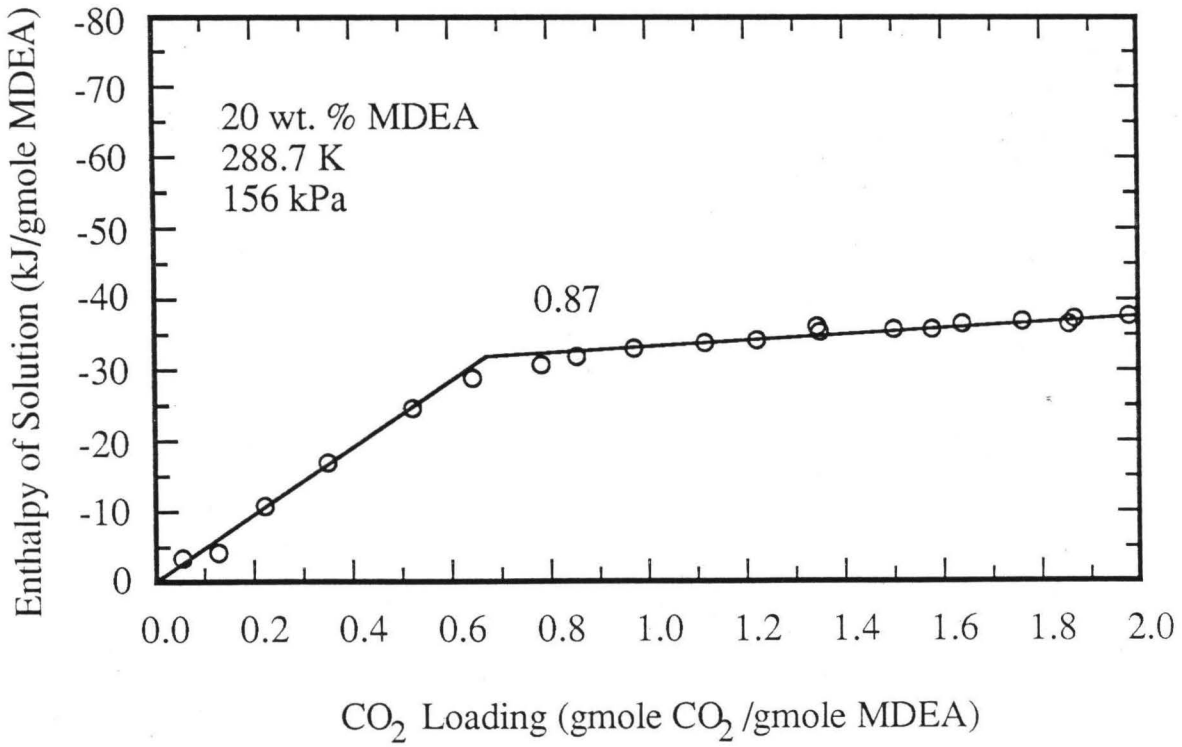

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-57
60 wt. % MDEA
333.2 K
156 kPa
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

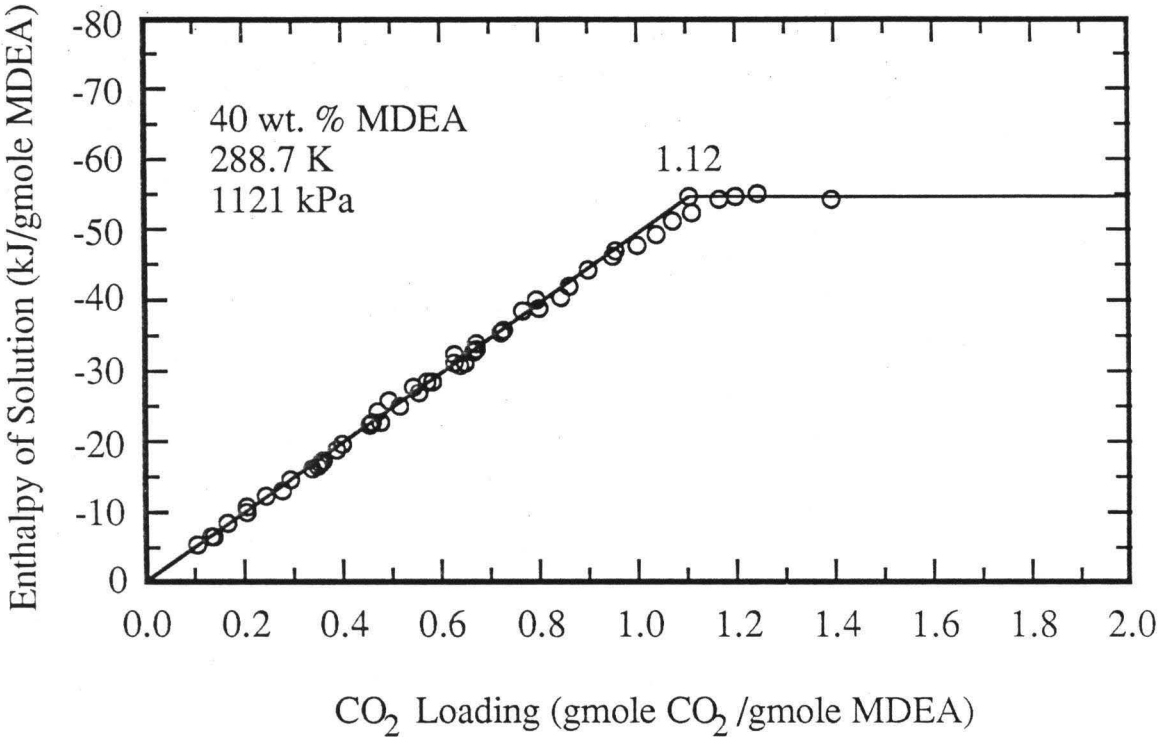

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-59
20 wt. % MDEA
388.7 K
1121 kPa
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

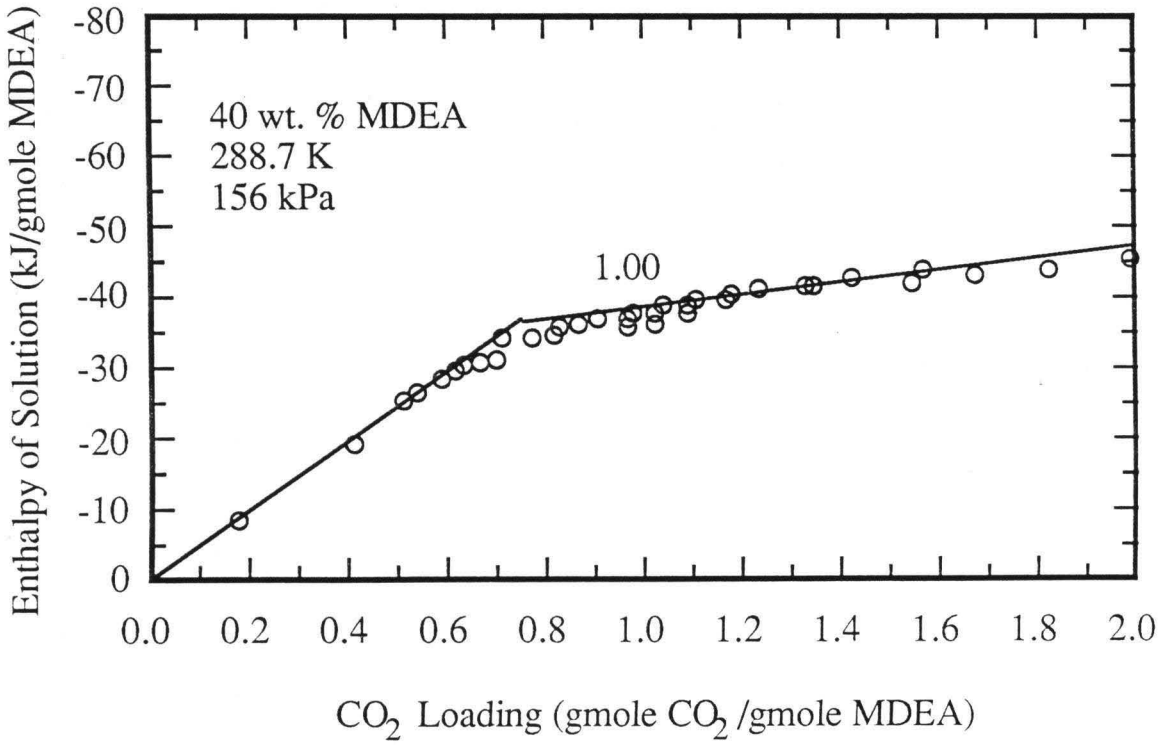

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-63
60 wt. % MDEA
388.7 K
1121 kPa
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

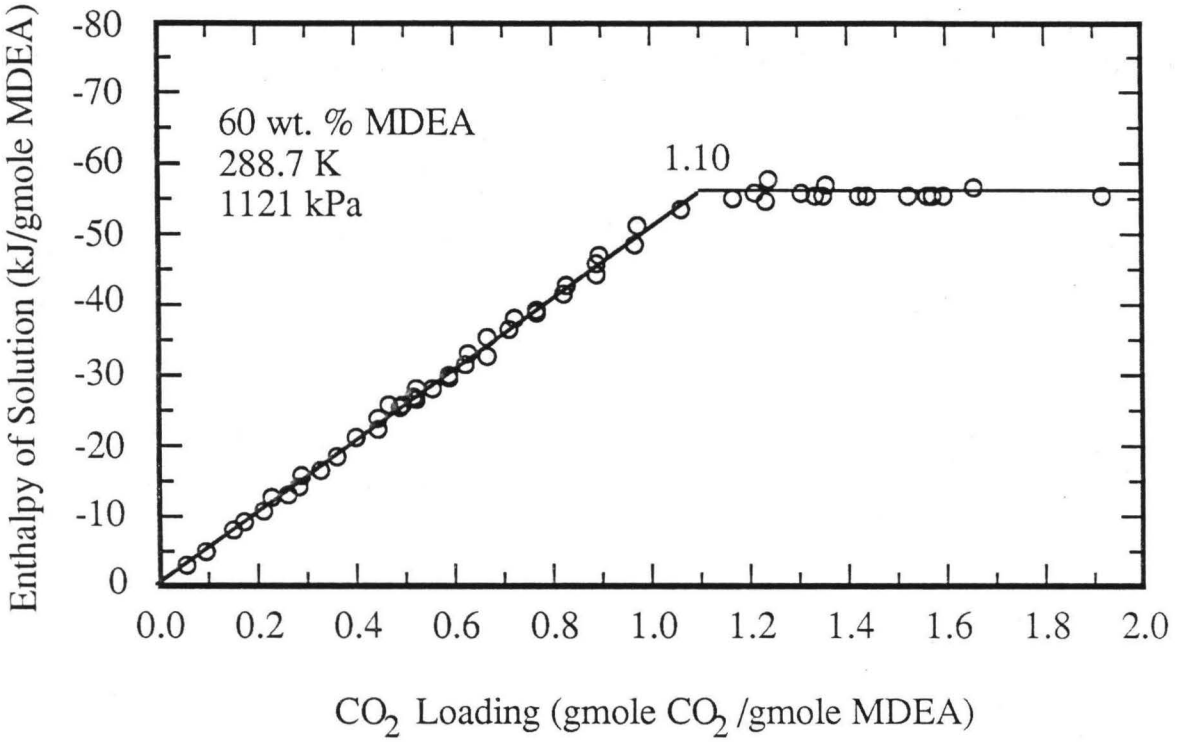

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-63
20 wt. % MDEA
422.0 K
1466 kPa
0.0
01
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

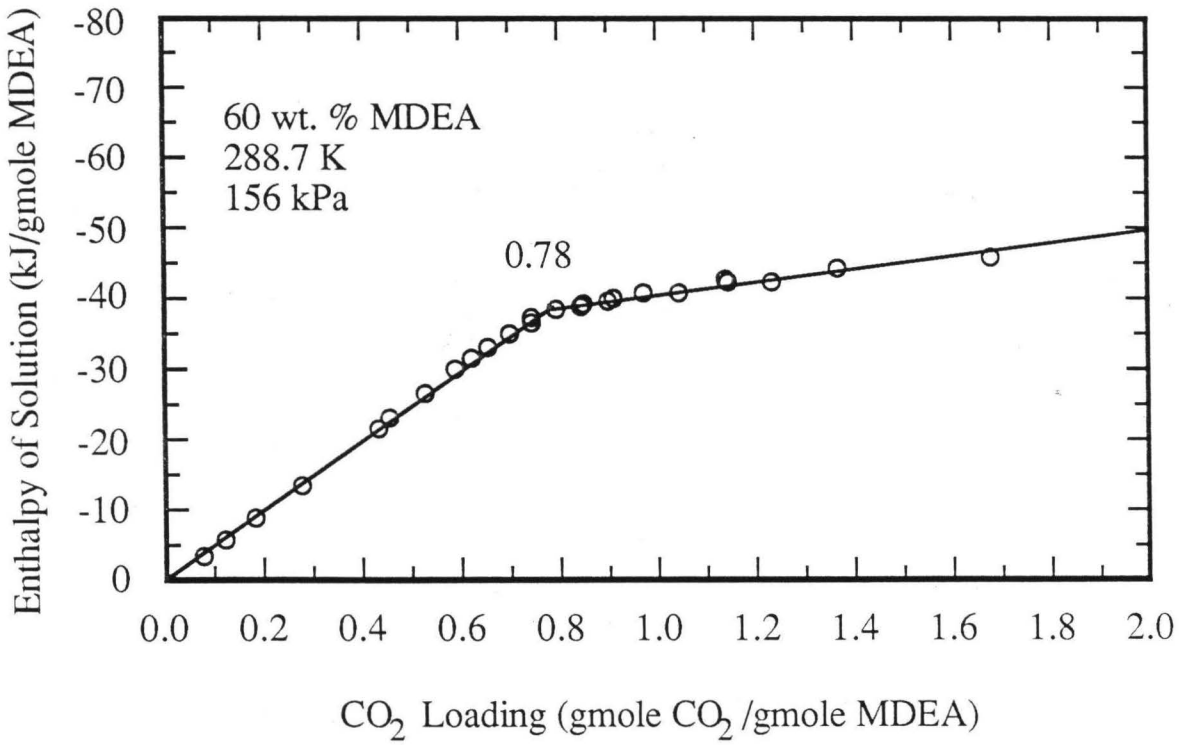

20 wt. % MDEA
288.7 K
1121 kPa
1.28
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

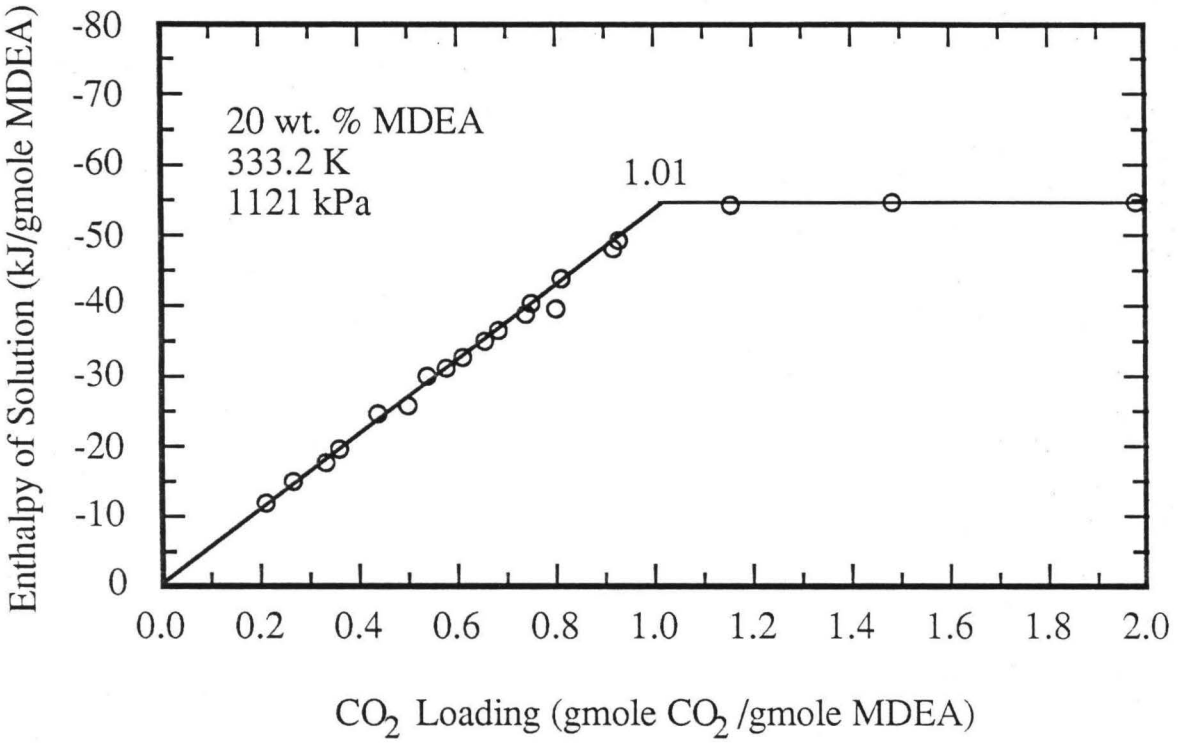

20 wt. % MDEA
288.7 K
156 kPa
0.87
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

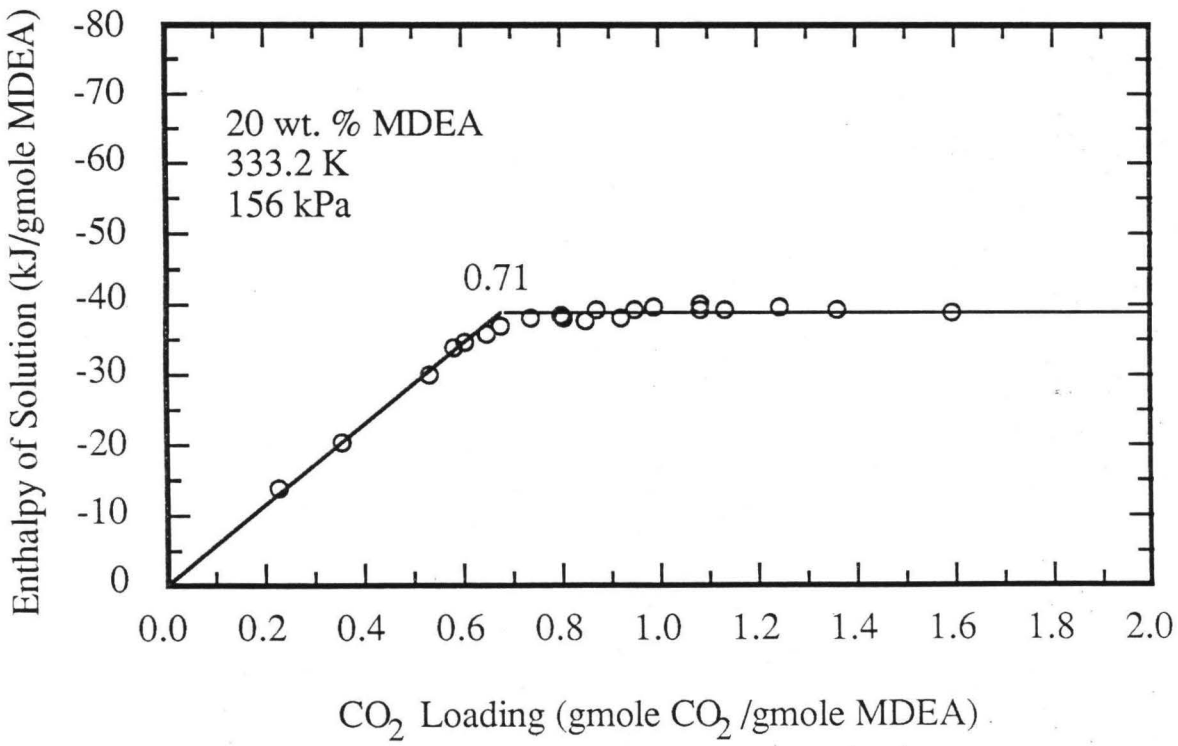

40 wt. % MDEA
288.7 K
1121 kPa
1.12
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

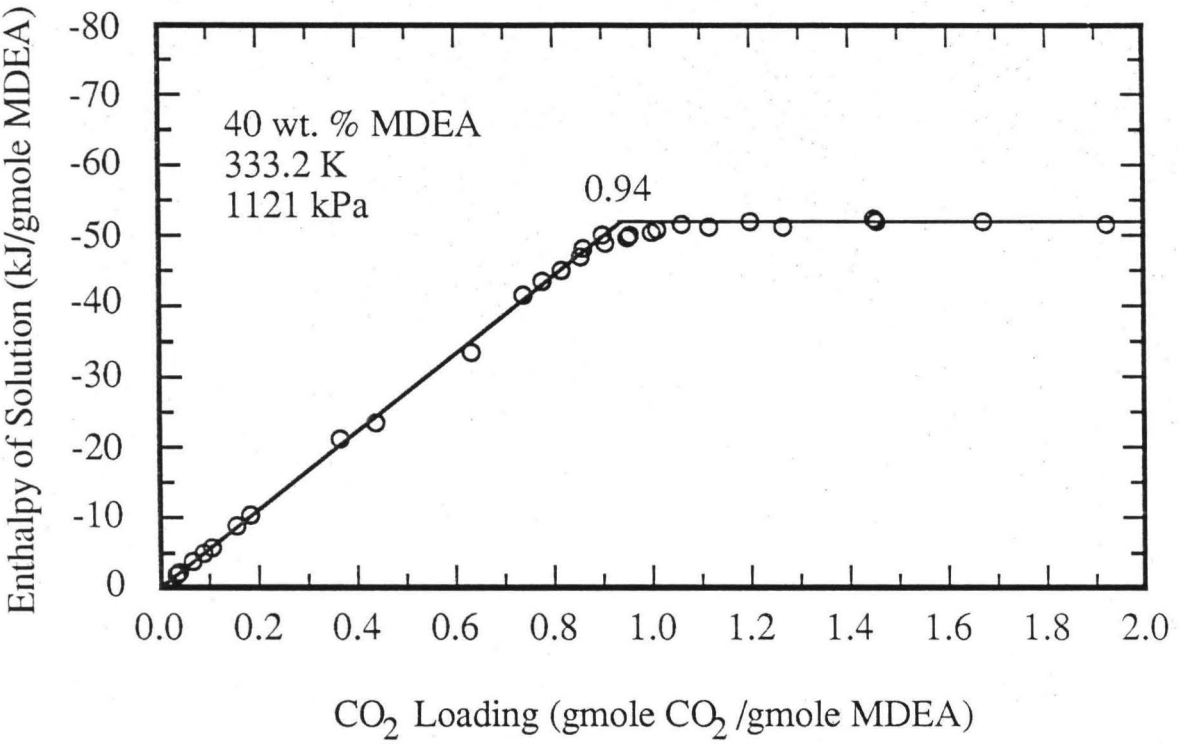

40 wt. % MDEA
288.7 K
156 kPa
1.00
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

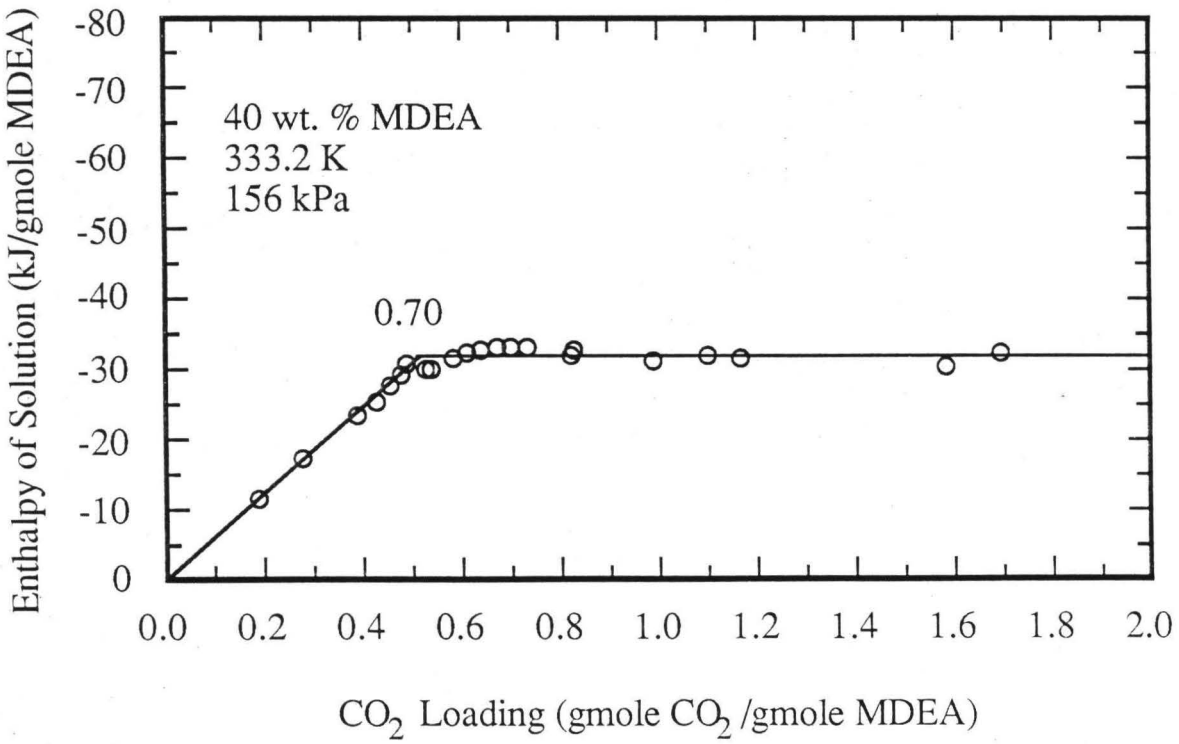

60 wt. % MDEA
288.7 K
1121 kPa
1.10
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

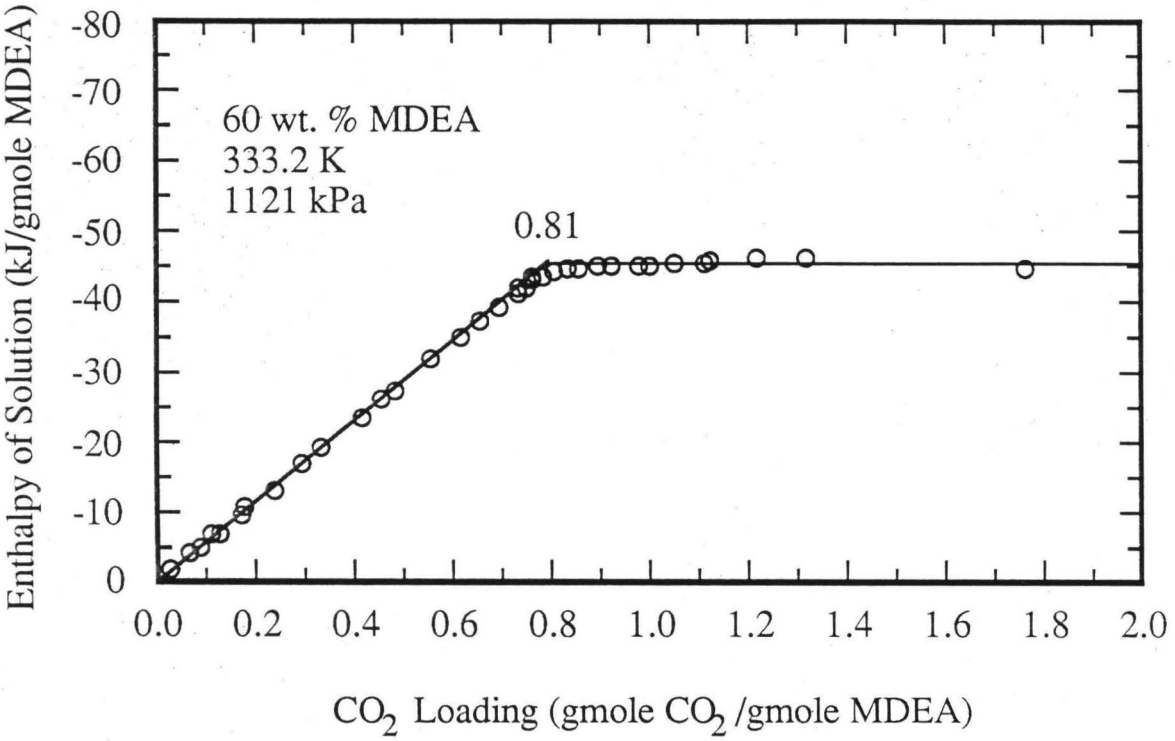

60 wt. % MDEA
288.7 K
156 kPa
0.78
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

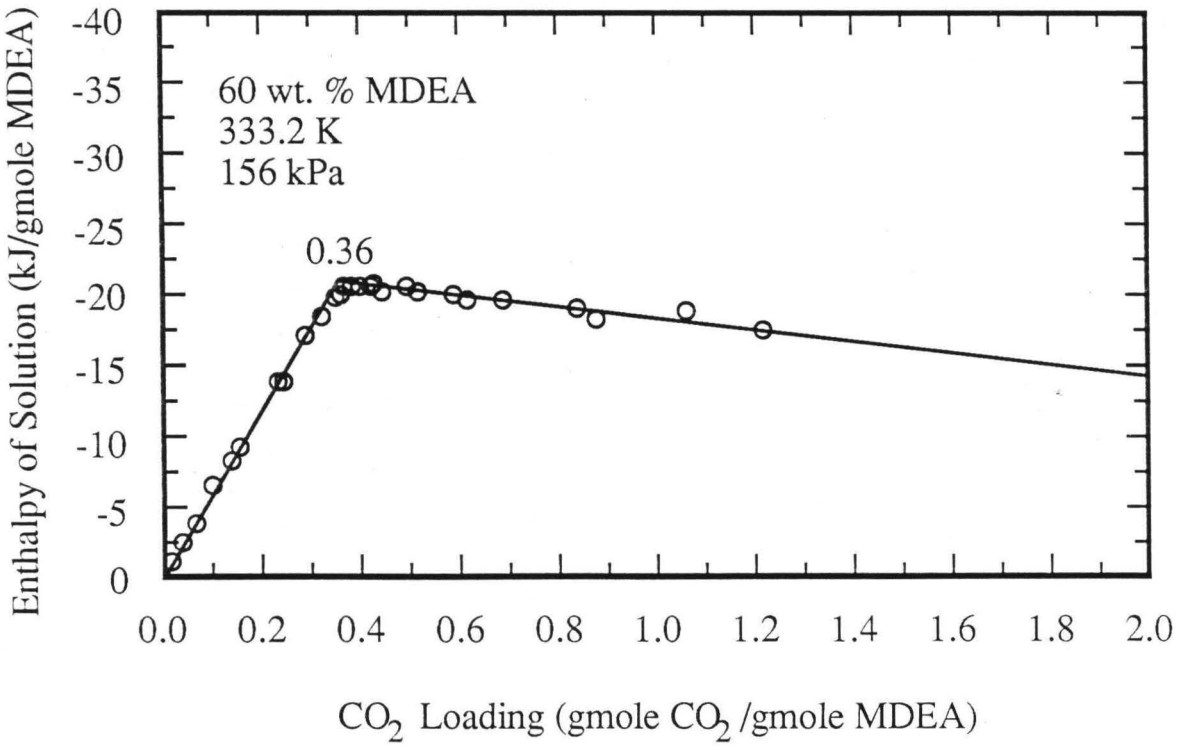

20 wt. % MDEA
333.2 K
1121 kPa
1.01
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

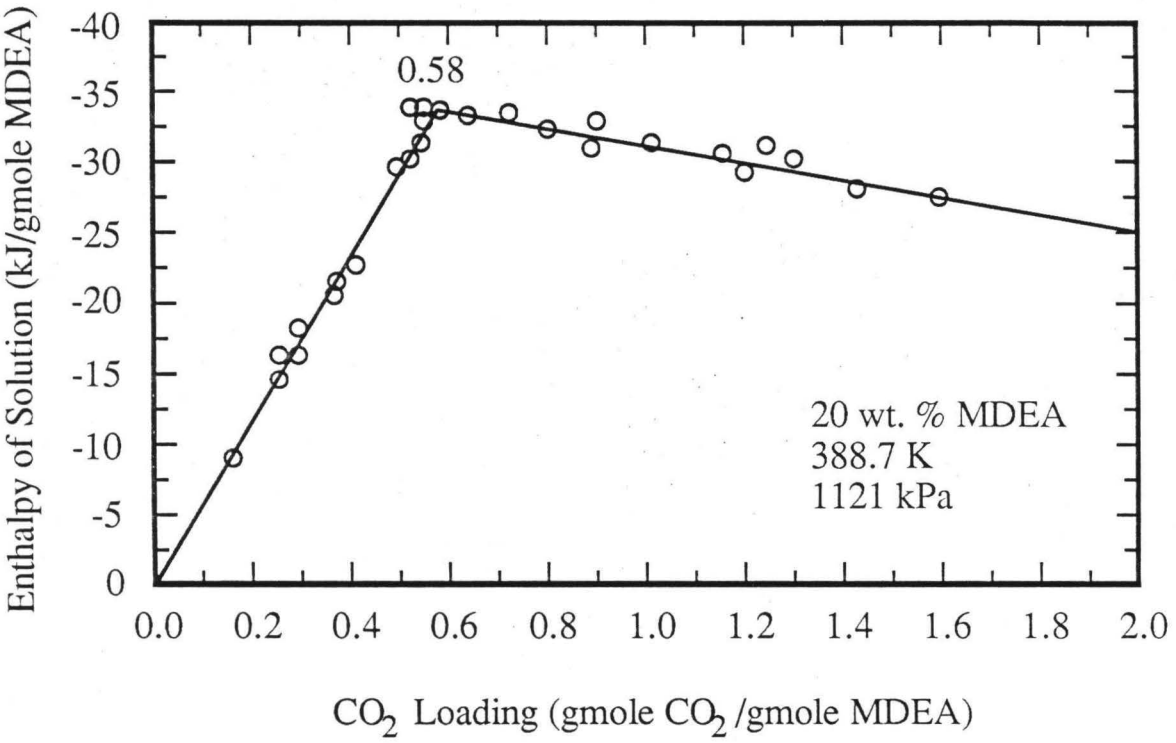

20 wt. % MDEA
333.2 K
156 kPa
0.71
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

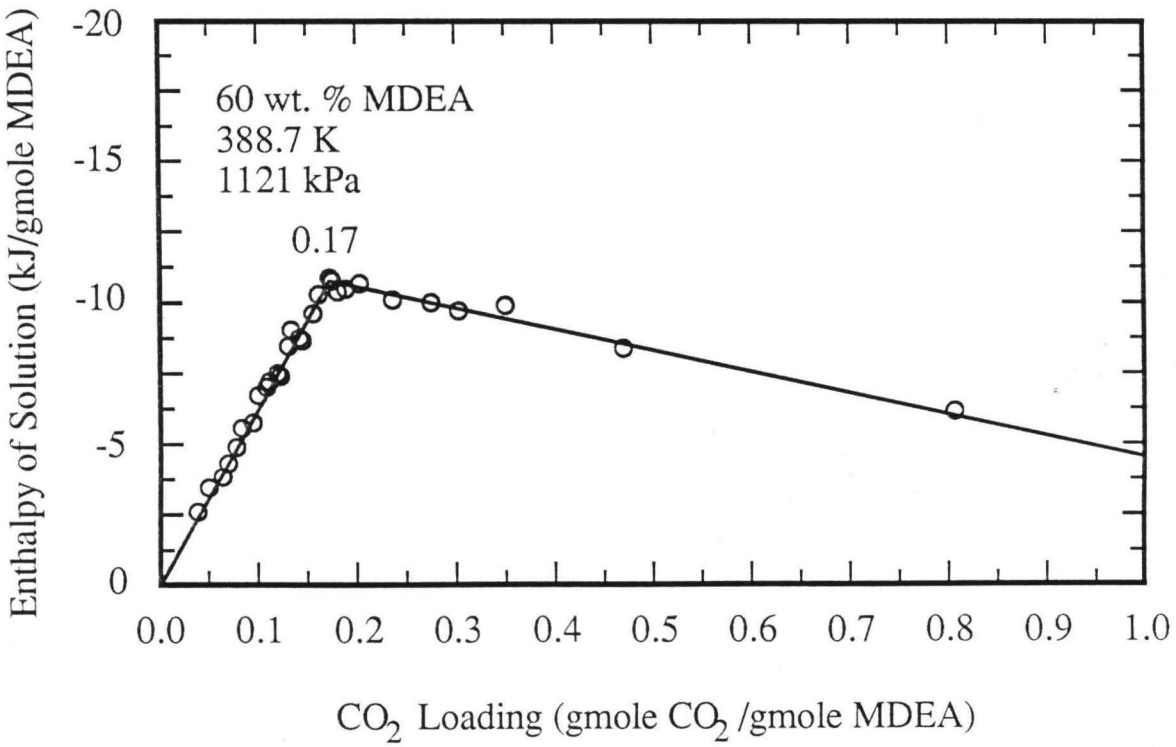

40 wt. % MDEA
333.2 K
1121 kPa
0.94
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

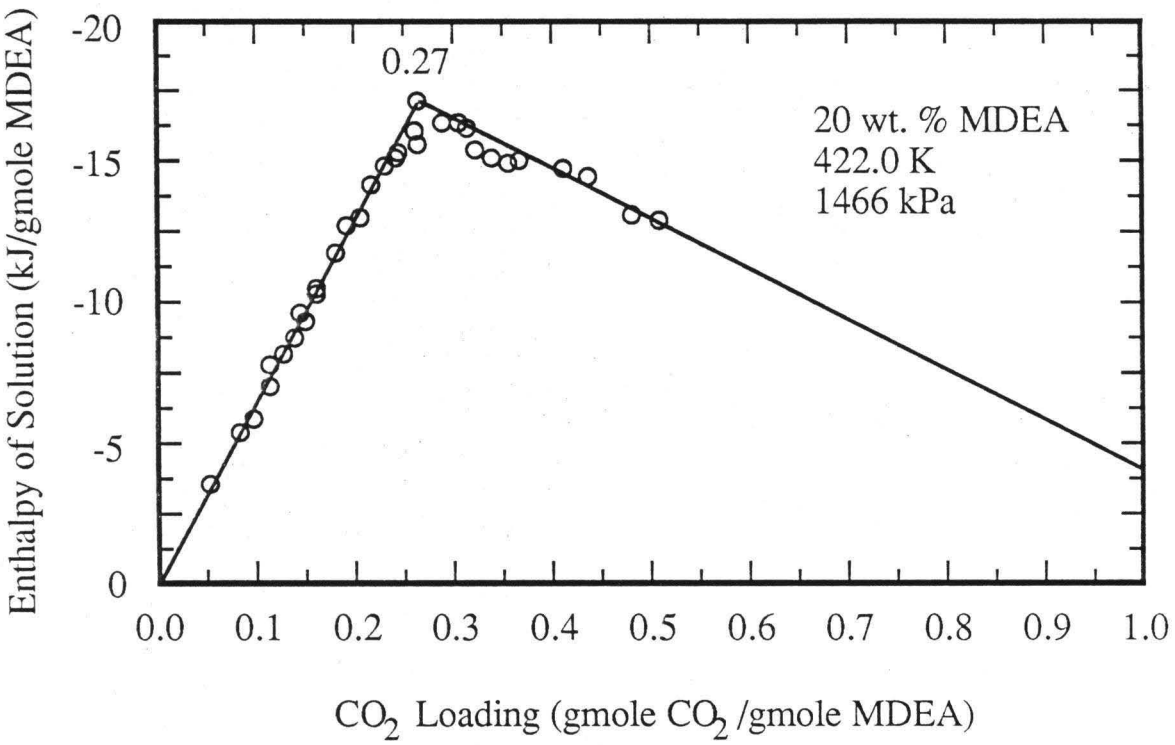

40 wt. % MDEA
333.2 K
156 kPa
0.70
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


60 wt. % MDEA
333.2 K
1121 kPa
0.81
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


60 wt. % MDEA
333.2 K
156 kPa
0.36
Enthalpy of Solution (kJ/gmole MDEA)
-40
-35
-30
-25
-20
-15
-10
-5
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


Enthalpy of Solution (kJ/gmole MDEA)
-40
-35
-30
-25
-20
-15
-10
-5
0
0.58
20 wt. % MDEA
388.7 K
1121 kPa
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


Enthalpy of Solution (kJ/gmole MDEA)
-20
-15
-10
-5
0
60 wt. % MDEA
388.7 K
1121 kPa
0.17
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
CO2 Loading (gmole CO2 /gmole MDEA)


-20
-15
-10
-5
0
0.27
20 wt. % MDEA
422.0 K
1466 kPa
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Enthalpy of Solution (kJ/gmole MDEA)
CO2 Loading (gmole CO2 /gmole MDEA)

APPENDIX C

LINEAR REGRESSION TO DETERMINE H^S FROM EXPERIMENTAL DATA

Description of Linear Regression Program

The experimental heat of solution data below the loading point is read in from an external data file in the form of total heat (Btu/lb MDEA) as a function of loading (gmole CO_2/gmole MDEA). As explained in appendix A, the data was manipulated in these English units at the request of the Gas Processors Association, the research sponsor. The results of the linear regression program were converted to the appropriate SI units for the slope (kJ/gmole CO_2).

Following are the linear regression program and a summary of the linear regression results.

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                             C
C       THIS PROGRAM IS ENTITLED LSQ.FOR AND IT MAKES A LINEAR                C
C       REGRESSION ON THE DATA IN THE UNITS BTU/LB MDEA AS A FUNCTION         C
C       OF LOADING (MOLE CO2/MOLE MDEA).  THIS LINEAR REGRESSION FORCES       C
C       THE LINE TO PASS THROUGH THE ORIGIN AND THEN FINDS THE VALUE          C
C       OF THE SLOPE WHICH MINIMZES THE ERROR BETWEEN THE CALCULATED          C
C       HEAT OF SOLUTION AND THE EXPERIMENTAL VALUES                          C
C                                                                             C
C       WRITTEN BY KEITH MERKLEY  MAY 1985                                    C
C                                                                             C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                             C
C                    VARIABLE IDENTIFICATION AND DESCRIPTION                  C
C                                                                             C
C       AN2=CHARACTER STRING TO HOLD Y/N FOR QUESTIONS                        C
C       BTU=BTU/LB CO2 VALUE DETERMINED FROM LINEAR REGRESSION SLOPE          C
C       CO2=ARRAY STORING LOADING (LBMOLE CO2/LBMOLE MDEA) VALUES USED        C
C               IN THE LINEAR REGRESSION                                      C
C       DELY=SUM OF SQUARE OF DEVIATION OF LINEAR REGRESSION FROM             C
C               EXPERIMENTAL DATA                                             C
C       DEVNEW=CURRENT VALUE OF DELY                                          C
C       DEVOLD=VALUE OF DELY FROM PREVIOUS ITERATION                          C
C       HEAT=ARRAY STORING HEAT OF MIXING (BTU/LB MDEA) VALUES USED IN        C
C               THE LINEAR REGRESSION                                         C
C       JCNT=COUNTER FOR NUMBER OF DATA POINTS INCLUDED IN REGRESSION         C
C       NCNT=NUMBER OF POINTS USED IN REGRESSION                              C
C       NPTS=NUMBERJ OF POINTS                                                C
C       PERCENT=WEIGHT PERCENT AMINE                                          C
C       PRESS=PRESSURE IN PSIA                                                C
C       PUREMW=MOLECULAR WEIGHT OF AMINE COMPONENT                            C
C               SORT ROUTINE                                                  C
C       SLINCR=INCREMENT FOR SLOPE DETERMINATION                              C
C       SLOPE=SLOPE OF LINEAR REGRESSION LINE                                 C
C       SYSTEM=AMINE COMPONENT (MDEA)                                         C
C       TEMP=TEMPERATURE IN FARENHEIT                                         C
C       TEMPX=ARRAY STORING ALL VALUES OF LOADING                             C
C       TEMPHT=ARRAY STORING ALL VALUES OF HEAT OF MIXING (BTU/LB MDEA)       C
C       WTMOL=MOLECULAR WEIGHT OF AQUEOUS SOLUTION                            C
C                                                                             C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

CCCCCCCCCCCC
C               1. DIMENSION VARIABLES
CCCCCCCCCCCC

      DIMENSION CO2(100),HEAT(100),TEMPX(100),TEMPHT(100)
      OPEN(UNIT=10,STATUS='OLD',FILE='SLOPE')

CCCCCCCCCCCC
C               2. READ IN SYSTEM, T, P, ETC.
CCCCCCCCCCCC

      READ(10,11) SYSTEM,PERCEN,TEMP,PRESS
   11 FORMAT(1X,A4,2X,F7.3,2X,F8.2,2X,F10.4)
      READ(10,*)NPTS,PUREMW,WTMOL
      JCNT=1
      DO 50 I=1,NPTS

CCCCCCCCCCCC
C               3. READ IN VALUE OF LOADING, BTU/LB MDEA FOR THIS POINT
CCCCCCCCCCCC

            READ(10,*) TEMPX(I),TEMPHT(I)
```

```
            WRITE(6,12) TEMPX(I),TEMPHT(I)

CCCCCCCCCCCC
C                4. KEY IN ANSWER TO QUESTION: "DO YOU WANT THIS POINT
C                       INCLUDED IN THE LINEAR REGRESSION"
CCCCCCCCCCCC

   12       FORMAT(1X,'DO YOU WANT TO INCLUDE THE POINT (',
     1              F6.4,',',F8.2,')?')
            WRITE(6,*) ' <CR> = YES, N = NO, S = NO FOR REST OF POINTS'
            READ(5,1)AN2
    1       FORMAT(A1)

CCCCCCCCCCCC
C                4A. IF THE ANSWER IS "N", RETURN AND READ THE NEXT POINT
CCCCCCCCCCCC

            IF(AN2.EQ.'N') THEN
                 GOTO 49

CCCCCCCCCCCC
C                4B. IF THE ANSWER IS "S", STOP READING DATA AND PERFORM
C                       REGRESSION TO FIND THE VALUE OF THE SLOPE
CCCCCCCCCCCC

            ELSEIF (AN2.EQ.'S') THEN
                 GOTO 52
            ELSE

CCCCCCCCCCCC
C                4C. IF ANSWER IS NEITHER "N" NOR "S" ADD THIS POINT TO
C                       THE ARRAY CONTAINING THE POINTS TO BE REGRESSED
CCCCCCCCCCCC

                 CO2(JCNT)=TEMPX(I)
                 HEAT(JCNT)=TEMPHT(I)
                 JCNT=JCNT+1
   49       ENDIF
   50 CONTINUE

CCCCCCCCCCCC
C                5. DATA ENTRY COMPLETED; PERFORM REGRESSION
CCCCCCCCCCCC

   52 NCOUNT=JCNT-1
      WRITE(6,*) ' JCNT=',NCOUNT
      SLINCR=100.

CCCCCCCCCCCC
C                5A. INITIAL GUESS FOR SLOPE IS THAT GIVEN CONSIDERING
C                       FIRST DATA POINT ONLY
CCCCCCCCCCCC

      SLOPE=HEAT(1)/CO2(1)
      DO 100 I=1,100
   51    DELY=0.0

CCCCCCCCCCCC
C                5B. CALCULATE SUM OF SQUARE OF DEVIATION BETWEEN
C                       EXPERIMENTAL HEAT OF SOLUTION AND CALCULATED
C                       HEAT OF MIXING
CCCCCCCCCCCC

         DO 75 J=1,JCNT-1
```

```
               DELY=DELY+((SLOPE*CO2(J)-HEAT(J))**2.0)
   75     CONTINUE
          DEVNEW=DELY

CCCCCCCCCCCC
C                 5C. IF THIS IS FIRST ITERATION, SET THIS DELY EQUAL TO
C                         DEVOLD, INCREMENT THE SLOPE FOR THE NEXT
C                         ITERATION AND RETURN TO PERFORM THE SECOND
C                         ITERATION
CCCCCCCCCCCC

          IF(I.EQ.1) THEN
             DEVOLD=DELY
             SLOPE=SLOPE+SLINCR
             GOTO 100
          ENDIF

CCCCCCCCCCCC
C                 5D. COMPARE THIS VALUE OF DELY TO VALUE FROM PREVIOUS
C                         ITERATION.  IF THE NEW VALUE IS LOWER, CONTINUE
C                         TO INCREMENT SLOPE IN THE SAME DIRECTION WITH
C                         THE SAME INCREMENT VALUE
CCCCCCCCCCCC

          IF(DEVNEW.LE.DEVOLD) THEN
               DEVOLD=DEVNEW
               SLOPE=SLOPE+SLINCR
               GOTO 100

CCCCCCCCCCCC
C                 5E. IF THE NEW VALUE OF DELY IS NOT AS LOW AS THE
C                         PREVIOUS VALUE THEN:
C                                 (1) IF ABSOLUTE VALUE OF THE CURRENT
C                                         SLOPE INCREMENT IS <.0001 THEN
C                                         CEASE THE ITERATION PROCEDURE
C                                 (2) IF THE CURRENT SLOPE VALUE IS <0.0
C                                         THEN DECREASE THE INCREMENT BY
C                                         A FACTOR OF 10
C                                 (3) SET INCREMENT TO BE NEGATIVE OF
C                                         CURRENT VALUE
C                                 (4) INCREMENT SLOPE AND DO ANOTHER
C                                         ITERATION
CCCCCCCCCCCC

          ELSE
               SLOPE=SLOPE-SLINCR
               IF(ABS(SLINCR).LT.0.0001) GOTO 101
               IF(SLINCR.LT.0.00000) SLINCR=SLINCR/10.0
               SLINCR=SLINCR*(-1.0)
               SLOPE=SLOPE+SLINCR
          ENDIF
  100 CONTINUE

CCCCCCCCCCCC
C                 6. CALCULATE VALUE OF HEAT OF SOLUTION IN BTU/LB CO2
CCCCCCCCCCCC

  101 BTU=SLOPE*PUREMW/44.0098

CCCCCCCCCCCC
C                 7. OUTPUT RESULTS TO SCREEN
CCCCCCCCCCCC

       WRITE(6,*) ' DEL Y = ',DEVOLD
```

```
      WRITE(6,*)  ' SLOPE = ',SLOPE
      WRITE(6,*)  ' INCREM=',SLINCR
      WRITE(6,*)  ' BTU/LB CO2 = ',BTU
      STOP
      END
```

Summary of Curve Fits of the Experimental Data by LSQ.FOR

System						
ID #	Wt. % MDEA	T (K)	P (kPa)	# Data Points	Slope (kJ/ gmole CO_2)	σ (kJ/ gmole MDEA)
1.2	20	288.7	1121	8	-46.8	0.54
1.3	20	288.7	1121	10	-47.1	0.74
2.1	20	288.7	156	6	-47.5	0.92
3.1	40	288.7	1121	20	-48.0	1.64
3.3	40	288.7	1121	47	-48.8	0.70
4.1	40	288.7	156	9	-48.0	0.59
5.1	60	288.7	1121	24	-49.4	0.57
5.3	60	288.7	1121	39	-50.6	0.54
6.1	60	288.7	156	16	-49.9	0.44
7.1	20	333.2	1121	9	-52.7	0.87
7.2	20	333.2	1121	16	-53.0	0.59
8.1	20	333.2	156	8	-56.2	0.85
9.1	40	333.2	1121	17	-55.2	0.66
10.1	40	333.2	156	8	-60.3	0.91
11.1	60	333.2	1121	22	-56.8	0.36
12.1	60	333.2	156	14	-57.2	0.39
13.1	20	388.7	1121	15	-59.3	1.16
14.1	40	388.7	1121	15	-62.5	0.37
15.1	60	388.7	1121	19	-63.4	0.24
16.1	20	422.0	1466	21	-63.4	0.39
18.1	40	422.0	1466	19	-65.4	0.19

APPENDIX D

ESTIMATION OF EXPERIMENTAL ACCURACY

The experimental accuracy was estimated to be ±5% for the data reported in the thesis. Listed below are the components which make up this ±5% uncertainty in the experimental results.*

Uncertainty Item	Description	Percent Uncertainty
1. Accuracy of Calorimeter for Test Systems	With standard systems (such as ethanol-water systems), the calorimeter has been shown to exhibit an accuracy of ±1%.	±1%
2. Effect of MDEA Impurities	The MDEA is only 99 wt. % pure. The ±1% uncertainty is an estimation of the most probable uncertainty caused by the impurities of the MDEA solvent.	±1%
3. Gas Leakage/ Gas Delivery Problems	As discussed in the text, problems with the inlet CO_2 back-pressure regulator and with the leakage of inlet CO_2 were encountered. The uncertainty is again an estimate of the most probable error.	±3%
	TOTAL UNCERTAINTY	±5%

* The text describes the experimental difficulties resulting from MDEA creeping up the CO_2 inlet line which caused a portion of the reaction and heat release to occur at a point removed from the reaction plate. In this circumstance, the measured heat was less than the actual heat generated by the mixing. The raw data reported in this thesis were free from this experimental problem and thus there is no contribution to the estimated experimental uncertainty from this item.

APPENDIX E

MULTIPLE LINEAR REGRESSION ON LITERATURE DATA--LN K VS. T

Description of Multiple Linear Regression Program

The following computer code reads input data from an external data file or, alternately, the data may be entered interactively. The data is entered in the form of discrete data points ln K vs. T (K). The computer program then performs the multiple linear regression fitting the data with up to 5 adjustable parameters. The exact form of the equation to which the literature data was fitted is as follows:

$$-\ln K = A + B * T + C/T + D \ln T + E/T^2$$

The program and the program output for chemical reactions 1, 2, 4, and 5 follow. The program output for reaction 3 is included in the body of the thesis as table 7.

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C       THIS IS A PROGRAM TO COMPUTE A MULTIPLE LINEAR REGRESSION              C
C       OF THE FORM T = A + BW + CX + DY + EZ FOR                              C
C       A SYSTEM OF POINTS.                                                    C
C       WRITTEN BY K.E. MERKLEY MAY 1986                                       C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C               VARIABLE IDENTIFICATION AND DESCRIPTION                        C
C                                                                              C
C       A,B,C,D,AND E=COEFFICIENTS FOR EQUATION                                C
C       AIJ=NxN MATRIX WHOSE ELEMENTS ARE THE FINAL VALUES OF THE              C
C       COEFF=ONE DIMENSIONAL MATRIX HOLDING LEAST SQUARES VALUES OF           C
C               A,B,C,D,AND E                                                  C
C       EQK=ONE DIMENSIONAL ARRAY TO STORE ALL -lnK VALUES                     C
C       IADD=FLAG FOR BRANCHING IN POINT DELETION/ADDITION SECTION             C
C       ICHECK=FLAG FOR BRANCHING IN DATA CHECKING/CORRECTING SECTION          C
C       LCOUNT=COUNTER FOR DATA POINTS ENTERED INTERACTIVELY                   C
C       LOOP=NUMBER OF DATA POINTS INCLUDED IN REGRESSION                      C
C       N=DIMENSION OF MATRIX                                                  C
C               ACCUMULATION VARIABLES                                         C
C       NTRIAL=COUNTER FOR TRIAL NUMBER WITH A PARTICULAR SET OF DATA          C
C       NPARAM=NUMBER OF PARAMETERS FIT BY MULTIPLE LINEAR                     C
C               REGRESSION (MAXIMUM IS 5).                                     C
C       R2=CORRELATION COEFFICIENT                                             C
C       SIGMA=STANDARD DEVIATION OF CURVE FIT                                  C
C       SUM*=ACCUMULATION VARIABLES FOR SUMMATIONS IN LEAST SQUARES            C
C               REGRESSION                                                     C
C       T=-ln K FOR ACCUMULATION IN REGRESSION                                 C
C       TEMP=ONE DIMENSIONAL ARRAY TO STORE ALL VALUES OF TEMPERATURE          C
C       W=TEMPERATURE FOR ACCUMULATION IN REGRESSION                           C
C       X=1.Ø/W FOR ACCUMULATION IN REGRESSION                                 C
C       Y=LN W FOR ACCUMULATION IN REGRESSION                                  C
C       Z=1.Ø/W**2                                                             C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C               1. DIMENSION VARIABLES
CCCCCCCCCC

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AIJ(5,6),EQK(2ØØ),TNEW(2ØØ),DELTA(2ØØ),TEMP(2ØØ),
     1          NROW(5),COEFF(5)
      OPEN(UNIT=1Ø,STATUS='OLD',FILE='MLRIN.DAT')
      OPEN(UNIT=11,STATUS='NEW',FILE='MLROUT.MAS')
      OPEN(UNIT=12,STATUS='NEW',FILE='MLROUT.TRY')
    1 FORMAT(A1)
      NTRIAL = Ø

CCCCCCCCCC
C               2.  READ IN DATA FROM FILE OR FROM SCREEN
CCCCCCCCCC

    4 TYPE 5
    5 FORMAT (1ØX,'INPUT NUMBER OF PARAMETERS TO BE FITTED')
      ACCEPT*,NPARAM
   1Ø TYPE 15
   15 FORMAT (5X, 'THIS IS A PROGRAM TO COMPUTE A MULTIPLE LINEAR ',
     1 'REGRESSION FOR'/5X,'Ln K VS. T.  THE FORM OF THE EQUATION ',
     2 'IS:'///5X,'           -Ln K = A + BT + C/T +D LnT + E/T2.'/
     3 5X,'DOES AN INPUT FILE ALREADY EXIST FOR THE POINTS TO BE ',
     4 'FITTED?')
      READ(6,1) ANS
      IF(ANS.EQ.'N'.OR.ANS.EQ.'n') GOTO 3Ø
```

```
CCCCCCCCCC
C                2 A.  READ FROM DATA FILE
CCCCCCCCCC

        READ(10,*) LOOP
        READ(10,*) (EQK(I),TEMP(I),I=1,LOOP)
        GOTO 100

CCCCCCCCCC
C                2 B.  READ FROM SCREEN
CCCCCCCCCC

   30   TYPE 35
   35   FORMAT (5X,'  INPUT ALL THE POINTS TO BE FIT IN THE FORM',
     1  ' "-Ln K"<CR>, "T"<CR>.')
        LCOUNT=1
   40   WRITE(6,45) LCOUNT
   45   FORMAT(15X,'POINT NUMBER ',I3,/
     1  2X,'ENTER -Ln K <CR>, T <CR> (-Ln K = 0 STOPS PROGRAM)')
        ACCEPT*,EQK(LCOUNT)
        IF (EQK(LCOUNT).EQ.0.0) GOTO 50
        ACCEPT*,TEMP(LCOUNT)
        LCOUNT = LCOUNT + 1
        GOTO 40
  50    LOOP = LCOUNT - 1

CCCCCCCCCC
C                3. DATA ECHO--EDIT INPUT POINTS BY MENU BEFORE FIT.
CCCCCCCCCC

 100    TYPE 125
 125    FORMAT(5X,'THIS IS A LISTING OF THE DATA YOU HAVE INPUT.  IF',
     *  ' THERE ARE ANY '/5X,'MISTAKES, INPUT THE NUMBER OF THE DATA ',
     *  'POINT THAT IS INCORRECT '/5X,'FOLLOWED BY A SINGLE ZERO FOR ',
     *  'AN INCORRECT -Ln K VALUE OR 3 ZEROES '/5X,'FOR AN INCORRECT ',
     *  ' T VALUE. IF THERE ARE NO MISTAKES INPUT -1.  IF '/5X,'YOU ',
     *  ' WISH TO ADD OR DELETE POINTS INPUT A DIGIT GREATER THAN 0')

CCCCCCCCCC
C                3 A.  ECHO DATA TO SCREEN
CCCCCCCCCC

 130    TYPE 135
 135    FORMAT(11X,'N',8X,'-Ln K',9X,'T')
        WRITE(6,140)(N,EQK(N),TEMP(N),N=1,LOOP)
 140    FORMAT(9X,I3,6X,F8.4,4X,F8.2)
 145    TYPE 150
 150    FORMAT(/10X,'INPUT NUMBER OF MISTAKE (*10 FOR -Ln K, ',
     1  '*1000 FOR T)'/10X,'TO EXIT ENTER -1.  TO SEE LISTING AGAIN ',
     2  'ENTER 0.'/10X,'TO ADD OR DELETE POINTS ENTER SINGLE DIGIT >0')

CCCCCCCCCC
C                3 B. ENTER CORRECTION INTERACIVELY FROM OPTION FROM MENU
CCCCCCCCCC

        ACCEPT*,ICHECK
        IF(ICHECK.EQ.0) GOTO 100
        IF(ICHECK.LT.0) GOTO 200
        IF(ICHECK.GT.0.AND.ICHECK.LT.10)GOTO 170
        IF(ICHECK.GE.1000)GOTO 160

CCCCCCCCCC
C                3 C.  CORRECT -lnK VALUE
CCCCCCCCCC
```

```
        I=ICHECK/10
        WRITE(6,155) I
 155    FORMAT(10X,'INPUT THE CORRECT -Ln K VALUE FOR POINT ',I3)
        ACCEPT*,EQK(I)
        GOTO 145

CCCCCCCCCC
C               3 D.  CORRECT TEMP VALUE
CCCCCCCCCC

 160    I=ICHECK/1000
        WRITE(6,165) I
 165    FORMAT(10X,'INPUT THE CORRECT T VALUE FOR POINT ',I3)
        ACCEPT*,TEMP(I)
        GOTO 145

CCCCCCCCCC
C               3E.  ADD/DELETE DATA POINTS
CCCCCCCCCC

 170    TYPE 175
 175    FORMAT(5X,'IF YOU WANT TO ADD POINTS, ENTER A POSITIVE NUMBER',
     *  ' EQUAL TO THE NUMBER'/5X,'OF POINTS YOU WANT TO ADD. IF YOU',
     *  '  WANT TO DELETE POINTS ENTER A'/5X,'NEGATIVE NUMBER.  YOU ',
     *  'WILL KEEP LOOPING HERE UNTIL YOU HAVE ADDED OR'/5X,'DELETED',
     *  ' ALL THE POINTS YOU CHOOSE.  TO RETURN TO THE MAIN MENU, ',
     *  'ENTER 0.')
        ACCEPT*,IADD
        IF(IADD.EQ.0)GOTO 100

CCCCCCCCCC
C               3 F.  ADD DATA POINTS
CCCCCCCCCC

        IF(IADD.GT.0)THEN
                LLOOP=LOOP+1
                LOOP=LOOP+IADD
                TYPE 180
 180          FORMAT(5X,'INPUT ADDITIONAL VALUE(S) -Ln K <CR>, T<CR>'/)
                DO 185 I=LLOOP,LOOP
                        ACCEPT*,EQK(I)
                        ACCEPT*,TEMP(I)
  185           CONTINUE
                GOTO 170

CCCCCCCCCC
C               3 G.  DELETE DATA POINTS
CCCCCCCCCC

        ELSE
  187           TYPE 190
  190           FORMAT(5X,'ENTER THE NUMBER OF THE POINT YOU WISH',
     1          ' TO DELETE.  TO EXIT ENTER -1.')
                ACCEPT*,IDEL
                IF(IDEL.LT.0) GOTO 170
                LOOP=LOOP-1
                DO 195 I=IDEL,LOOP
                        EQK(I)=EQK(I+1)
                        TEMP(I)=TEMP(I+1)
  195           CONTINUE
        ENDIF
        GOTO 187
 200    NTRIAL=NTRIAL+1
```

```
CCCCCCCCCC
C               4.  OUTPUT CORRECTED DATA TO FILE
CCCCCCCCCC

        DO 250 LL=1,LOOP
                WRITE(11,265) EQK(LL),TEMP(LL)
  250   CONTINUE
  260   FORMAT(5X,I3)
  265   FORMAT(3X,E15.8,5X,E15.8)
        WRITE(12,270) NTRIAL
  270   FORMAT(///,19X,'MULTIPLE LINEAR REGRESSION FOR TRIAL NUMBER ',
     1  I3,///10X,' FORM OF THE EQUATION IS -Ln K = A + B*T + C/T ',
     2  '+ D*LnT + E/T**2'///)

CCCCCCCCCC
C               5.  INITIALIZE ACCUMULATION VARIABLES AT 0
CCCCCCCCCC

        SUMT=0.0
        SUMW=0.0
        SUMX=0.0
        SUMY=0.0
        SUMZ=0.0
        SUMTW=0.0
        SUMTX=0.0
        SUMTY=0.0
        SUMTZ=0.0
        SUMWX=0.0
        SUMWY=0.0
        SUMWZ=0.0
        SUMXY=0.0
        SUMXZ=0.0
        SUMYZ=0.0
        SUMT2=0.0
        SUMW2=0.0
        SUMX2=0.0
        SUMY2=0.0
        SUMZ2=0.0
        SUMDEL=0.0
        SUMDL2=0.0
        ALOOP=FLOAT(LOOP)

CCCCCCCCCC
C               6.  ACCUMULATE SUMMATION VARIABLES FOR EACH POINT
CCCCCCCCCC

        DO 300 NNN=1,LOOP
                T=EQK(NNN)
                W=TEMP(NNN)
                X=1.0/W
                Y=DLOG(W)
                Z=1.0/(W*W)
                SUMT=SUMT+T
                SUMW=SUMW+W
                SUMX=SUMX+X
                SUMY=SUMY+Y
                SUMZ=SUMZ+Z
                SUMTW=SUMTW+(T*W)
                SUMTX=SUMTX+(T*X)
                SUMTY=SUMTY+(T*Y)
                SUMTZ=SUMTZ+(T*Z)
                SUMWX=SUMWX+(W*X)
                SUMWY=SUMWY+(W*Y)
                SUMWZ=SUMWZ+(W*Z)
```

```
                SUMXY=SUMXY+(X*Y)
                SUMXZ=SUMXZ+(X*Z)
                SUMYZ=SUMYZ+(Y*Z)
                SUMT2=SUMT2+(T*T)
                SUMW2=SUMW2+(W*W)
                SUMX2=SUMX2+(X*X)
                SUMY2=SUMY2+(Y*Y)
                SUMZ2=SUMZ2+(Z*Z)
  300   CONTINUE

CCCCCCCCCC
C               SET ACCUMULATION VARIABLES IN MATRIX IN PROPER LOCATION
CCCCCCCCCC

        N=NPARAM
        AIJ(1,1)=ALOOP
        AIJ(1,2)=SUMW
        AIJ(1,3)=SUMX
        AIJ(1,4)=SUMY
        AIJ(1,5)=SUMZ
        AIJ(2,1)=SUMW
        AIJ(2,2)=SUMW2
        AIJ(2,3)=SUMWX
        AIJ(2,4)=SUMWY
        AIJ(2,5)=SUMWZ
        AIJ(3,1)=SUMX
        AIJ(3,2)=SUMWX
        AIJ(3,3)=SUMX2
        AIJ(3,4)=SUMXY
        AIJ(3,5)=SUMXZ
        AIJ(4,1)=SUMY
        AIJ(4,2)=SUMWY
        AIJ(4,3)=SUMXY
        AIJ(4,4)=SUMY2
        AIJ(4,5)=SUMYZ
        AIJ(5,1)=SUMZ
        AIJ(5,2)=SUMWZ
        AIJ(5,3)=SUMXZ
        AIJ(5,4)=SUMYZ
        AIJ(5,5)=SUMZ2
        AIJ(1,N+1)=SUMT
        AIJ(2,N+1)=SUMTW
        AIJ(3,N+1)=SUMTX
        AIJ(4,N+1)=SUMTY
        AIJ(5,N+1)=SUMTZ

CCCCCCCCCC
C               7.  SOLVE MATRIX SYSTEM
CCCCCCCCCC

        M=N+1
        ICHG=0

CCCCCCCCCC
C               7 A.  NROW KEEPS TRACK OF ROW INTERCHANGES
CCCCCCCCCC

        DO 310 I=1,N
                NROW(I) = I
  310   CONTINUE
        NN = N-1

CCCCCCCCCC
C               7 B.  MATRIX SOLVING ROUTINE--PRTIAL PIVOTING
```

```
CCCCCCCCCC

        DO 370 I=1,NN
                IMAX=NROW(I)
                AMAX=ABS(AIJ(IMAX,I))
                JJ=I+1
                DO 330 IP=JJ,N
                        JP=NROW(IP)
                        IF(ABS(AIJ(JP,I)).GT.AMAX) THEN
                                AMAX = ABS(AIJ(JP,I))
                                IMAX = IP
                        ELSE
                        ENDIF
  330           CONTINUE
                IF(NROW(I).NE.IMAX) THEN
                        ICHG=ICHG+1
                        NCOPY=NROW(I)
                        NROW(I)=NROW(IMAX)
                        NROW(IMAX)=NCOPY
                ELSE
                ENDIF
                II=NROW(I)
                DO 350 J = JJ,N
                        JI=NROW(J)
                        XM=AIJ(JI,I)/AIJ(II,I)
                        DO 340 K=JJ,M
                                AIJ(JI,K)=AIJ(JI,K)-XM*AIJ(II,K)
  340                   CONTINUE
                        AIJ(JI,I) = 0.0
  350           CONTINUE
  370   CONTINUE
        WRITE(6,394)
        DO 374 I=1,N
                WRITE(6,392) (AIJ(NROW(I),J),J=1,M)
  374   CONTINUE
        WRITE(6,396) ICHG
        WRITE(6,397) (NROW(I),I=1,N)
        WRITE(6,399)
        NI=NROW(N)

CCCCCCCCCC
C               7 C.  CALCULATE VALUES OF COEFFICIENTS
CCCCCCCCCC

        COEFF(N)=AIJ(NI,N+1)/AIJ(NI,N)
        DO 390 I=N-1,1,-1
                JJ=I+1
                N2=NROW(I)
                SUM=AIJ(N2,N+1)
                DO 380 KK=JJ,N
                        SUM = SUM-AIJ(N2,KK)*COEFF(KK)
  380           CONTINUE
                COEFF(I)= SUM/AIJ(N2,I)
  390   CONTINUE

CCCCCCCCCC
C               8. OUTPUT
CCCCCCCCCC

  391   FORMAT(/////,38X,'GAUSSIAN SOLUTION OF MLR EQUATIONS'///,
     1  48X,' ORIGINAL SYSTEM: ',//)
  392   FORMAT(/,6(3X,E15.8))
  393   FORMAT(5X,' THE PRECEEDING SYSTEM HAS NO SOLUTION')
  394   FORMAT(///,47X,'THE REDUCED SYSTEM:  '///)
```

```
  395   FORMAT(//,' HAS SOLUTION VECTOR',5(3X,E15.8))
  396   FORMAT(//,' NUMBER OF INTERCHANGES = ',3X,I2)
  397   FORMAT(1X,5I5)
  399   FORMAT(/////)
        A=COEFF(1)
        B=COEFF(2)
        C=COEFF(3)
        D=COEFF(4)
        E=COEFF(5)

CCCCCCCCCC
C               9. CALCULTE R2, AND STANDARD DEVIATION
CCCCCCCCCC

        R2=(A*SUMT+B*SUMTW+C*SUMTX+D*SUMTY+E*SUMTZ-(SUMT*SUMT/ALOOP))/
     1         (SUMT2 - (SUMT*SUMT/ALOOP))
        DO 400 NN=1,LOOP
               TNEW(NN)=A + B*TEMP(NN) + C/TEMP(NN) +
     1                  D*DLOG( TEMP(NN) ) + E/(TEMP(NN)*TEMP(NN))
               DELTA(NN)=(TNEW(NN) - EQK(NN))/EQK(NN)
               DELTA2=DELTA(NN)*DELTA(NN)
               SUMDL2=SUMDL2+DELTA2
  400   CONTINUE
        SIGMA=SQRT((SUMDL2)/(ALOOP-NPARAM))

CCCCCCCCCC
C               10.  FINAL OUTPUT
CCCCCCCCCC

        WRITE(6,410) A,B,C,D,E,R2,SIGMA
        WRITE (6,420)(N,TEMP(N),EQK(N),TNEW(N),DELTA(N),N=1,LOOP)
        WRITE(12,410) A,B,C,D,E,R2,SIGMA
        WRITE (12,420)(N,TEMP(N),EQK(N),TNEW(N),DELTA(N),N=1,LOOP)
  410   FORMAT(23X,'A = ',E15.8,'    B = ',E15.8//
     1   23X,'C = ',E15.8,'    D = ',E15.8//
     2   35X,'E = ',E15.8//
     3   14X,'R2 = ',E13.6,'    THE STANDARD DEVIATION = ',E13.6///
     4   1X,7X,'N',10X,'T',12X,'-Ln K',6X,'REFERENCES',3X,'-Ln K CALC',
     5   10X,'DELTA'//)
  420   FORMAT(7X,I2,3X,E13.6,3X,E13.6,14X,E13.6,4X,E13.6)

CCCCCCCCCC
C               11. OPTION TO DO ANOTHER RUN WITHOUT REREADING DATA
CCCCCCCCCC

        TYPE 430
  430   FORMAT(5X,'IF YOU WOULD LIKE TO CHANGE VALUES (INCLUDING ',
     1   'ADDING OR DELETING'/5X,'POINTS) FOR THIS REGRESSION INPUT',
     2   ' -1.  IF YOU WOULD LIKE TO DO '/5X,'ANOTHER REGRESSION ',
     3   'INPUT ZERO, OTHERWISE INPUT 1.')
        ACCEPT*,G
        IF(G.EQ.0.0)GOTO 4
        IF(G.LT.0.0)GOTO 100
        IF(G.EQ.1.)GOTO 999
  999   STOP
        END
```

MULTIPLE LINEAR REGRESSION FOR REACTION 1

FORM OF THE EQUATION IS -Ln K = A + B*T + C/T + D*LnT + E/T**2

A = -Ø.33611189E+Ø4 B = -Ø.51917065E+ØØ

C = Ø.17969018E+Ø6 D = Ø.53451952E+Ø3

E = -Ø.88916639E+Ø7

R2 = Ø.999973E+ØØ THE STANDARD DEVIATION = Ø.357651E-Ø3

N	T	-Ln K	REFERENCES	-Ln K CALC	DELTA
1	Ø.273150E+Ø3	Ø.343990E+Ø2	17	Ø.344060E+Ø2	Ø.204313E-Ø3
2	Ø.273150E+Ø3	Ø.344350E+Ø2	29	Ø.344060E+Ø2	-Ø.841348E-Ø3
3	Ø.278150E+Ø3	Ø.339180E+Ø2	17	Ø.339267E+Ø2	Ø.256907E-Ø3
4	Ø.278150E+Ø3	Ø.339260E+Ø2	25	Ø.339267E+Ø2	Ø.210387E-Ø4
5	Ø.283150E+Ø3	Ø.334640E+Ø2	17	Ø.334693E+Ø2	Ø.159690E-Ø3
6	Ø.283150E+Ø3	Ø.334660E+Ø2	29	Ø.334693E+Ø2	Ø.999183E-Ø4
7	Ø.283150E+Ø3	Ø.334680E+Ø2	51	Ø.334693E+Ø2	Ø.401538E-Ø4
8	Ø.288150E+Ø3	Ø.330300E+Ø2	17	Ø.330336E+Ø2	Ø.107932E-Ø3
9	Ø.288150E+Ø3	Ø.330120E+Ø2	29	Ø.330336E+Ø2	Ø.653247E-Ø3
10	Ø.288150E+Ø3	Ø.330320E+Ø2	51	Ø.330336E+Ø2	Ø.473777E-Ø4
11	Ø.293150E+Ø3	Ø.326200E+Ø2	17	Ø.326189E+Ø2	-Ø.337893E-Ø4
12	Ø.293150E+Ø3	Ø.326070E+Ø2	29	Ø.326189E+Ø2	Ø.364885E-Ø3
13	Ø.293150E+Ø3	Ø.326160E+Ø2	51	Ø.326189E+Ø2	Ø.888458E-Ø4
14	Ø.298150E+Ø3	Ø.322280E+Ø2	17	Ø.322248E+Ø2	-Ø.100429E-Ø3
15	Ø.298150E+Ø3	Ø.322340E+Ø2	29	Ø.322248E+Ø2	-Ø.286550E-Ø3
16	Ø.298150E+Ø3	Ø.322290E+Ø2	51	Ø.322248E+Ø2	-Ø.131454E-Ø3
17	Ø.303150E+Ø3	Ø.318500E+Ø2	17	Ø.318505E+Ø2	Ø.158536E-Ø4
18	Ø.303150E+Ø3	Ø.318520E+Ø2	29	Ø.318505E+Ø2	-Ø.469378E-Ø4
19	Ø.303150E+Ø3	Ø.318540E+Ø2	51	Ø.318505E+Ø2	-Ø.109721E-Ø3
20	Ø.308150E+Ø3	Ø.315000E+Ø2	17	Ø.314954E+Ø2	-Ø.145832E-Ø3
21	Ø.308150E+Ø3	Ø.314900E+Ø2	29	Ø.314954E+Ø2	Ø.171683E-Ø3
22	Ø.308150E+Ø3	Ø.315020E+Ø2	51	Ø.314954E+Ø2	-Ø.209310E-Ø3
23	Ø.313150E+Ø3	Ø.311660E+Ø2	17	Ø.311587E+Ø2	-Ø.234004E-Ø3
24	Ø.313150E+Ø3	Ø.311610E+Ø2	29	Ø.311587E+Ø2	-Ø.735848E-Ø4
25	Ø.313150E+Ø3	Ø.311650E+Ø2	51	Ø.311587E+Ø2	-Ø.201924E-Ø3
26	Ø.318150E+Ø3	Ø.308460E+Ø2	17	Ø.308396E+Ø2	-Ø.206990E-Ø3
27	Ø.318150E+Ø3	Ø.308410E+Ø2	29	Ø.308396E+Ø2	-Ø.449015E-Ø4
28	Ø.318150E+Ø3	Ø.308480E+Ø2	51	Ø.308396E+Ø2	-Ø.271810E-Ø3
29	Ø.323150E+Ø3	Ø.305360E+Ø2	17	Ø.305373E+Ø2	Ø.431639E-Ø4
30	Ø.323150E+Ø3	Ø.305390E+Ø2	29	Ø.305373E+Ø2	-Ø.550754E-Ø4
31	Ø.323150E+Ø3	Ø.305440E+Ø2	51	Ø.305373E+Ø2	-Ø.218765E-Ø3
32	Ø.328150E+Ø3	Ø.302490E+Ø2	17	Ø.302510E+Ø2	Ø.658134E-Ø4
33	Ø.328150E+Ø3	Ø.302610E+Ø2	51	Ø.302510E+Ø2	-Ø.330763E-Ø3
34	Ø.333150E+Ø3	Ø.299730E+Ø2	17	Ø.299798E+Ø2	Ø.226999E-Ø3
35	Ø.333150E+Ø3	Ø.299700E+Ø2	51	Ø.299798E+Ø2	Ø.327121E-Ø3
36	Ø.343150E+Ø3	Ø.294730E+Ø2	51	Ø.294795E+Ø2	Ø.222018E-Ø3
37	Ø.353150E+Ø3	Ø.290080E+Ø2	51	Ø.290300E+Ø2	Ø.758665E-Ø3
38	Ø.363150E+Ø3	Ø.286030E+Ø2	51	Ø.286249E+Ø2	Ø.764751E-Ø3
39	Ø.373150E+Ø3	Ø.282530E+Ø2	29	Ø.282581E+Ø2	Ø.180746E-Ø3
40	Ø.373150E+Ø3	Ø.282850E+Ø2	51	Ø.282581E+Ø2	-Ø.950800E-Ø3
41	Ø.383150E+Ø3	Ø.279210E+Ø2	51	Ø.279240E+Ø2	Ø.107300E-Ø3
42	Ø.393150E+Ø3	Ø.276360E+Ø2	51	Ø.276172E+Ø2	-Ø.680806E-Ø3
43	Ø.423150E+Ø3	Ø.268020E+Ø2	29	Ø.268124E+Ø2	Ø.386964E-Ø3
44	Ø.423150E+Ø3	Ø.268160E+Ø2	51	Ø.268124E+Ø2	-Ø.135314E-Ø3

MULTIPLE LINEAR REGRESSION FOR REACTION NUMBER 2

FORM OF THE EQUATION IS -Ln K = A + B*T + C/T + D*LnT + E/T**2

A = Ø.30154811E+Ø1 B = Ø.37761995E-Ø2

C = Ø.46105676E+Ø4 D = Ø.00000000E+Ø0

E = Ø.00000000E+Ø0

R2 = Ø.999999E+Ø0 THE STANDARD DEVIATION = Ø.577470E-Ø4

N	T	-Ln K	REFERENCES	-Ln K CALC	DELTA
1	Ø.298150E+Ø3	Ø.196050E+Ø2	11	Ø.196053E+Ø2	Ø.140020E-Ø4
2	Ø.308150E+Ø3	Ø.191420E+Ø2	11	Ø.191412E+Ø2	-Ø.415007E-Ø4
3	Ø.318150E+Ø3	Ø.187080E+Ø2	11	Ø.187087E+Ø2	Ø.365346E-Ø4
4	Ø.333150E+Ø3	Ø.181130E+Ø2	11	Ø.181128E+Ø2	-Ø.903173E-Ø5

MULTIPLE LINEAR REGRESSION FOR REACTION NUMBER 4

FORM OF THE EQUATION IS -Ln K = A + B*T + C/T + D*LnT + E/T**2

A = -0.21340693E+03 B = -0.23309934E-01

C = 0.80250613E+04 D = 0.37300950E+02

E = 0.41833361E+06

R2 = 0.999515E+00 THE STANDARD DEVIATION = 0.346186E-03

N	T	-Ln K	REFERENCES	-Ln K CALC	DELTA
1	0.273150E+03	0.244700E+02	28	0.244716E+02	0.666764E-04
2	0.273150E+03	0.244700E+02	27	0.244716E+02	0.666764E-04
3	0.273150E+03	0.244670E+02	27	0.244716E+02	0.189299E-03
4	0.273150E+03	0.244760E+02	27	0.244716E+02	-0.178478E-03
5	0.273150E+03	0.244650E+02	29	0.244716E+02	0.271064E-03
6	0.273150E+03	0.244680E+02	19	0.244716E+02	0.148421E-03
7	0.278150E+03	0.243100E+02	28	0.243038E+02	-0.254699E-03
8	0.278150E+03	0.243090E+02	29	0.243038E+02	-0.213572E-03
9	0.278150E+03	0.243050E+02	19	0.243038E+02	-0.490323E-04
10	0.283150E+03	0.241530E+02	28	0.241531E+02	0.292349E-05
11	0.283150E+03	0.241540E+02	29	0.241531E+02	-0.384776E-04
12	0.283150E+03	0.241580E+02	19	0.241531E+02	-0.204048E-03
13	0.288150E+03	0.240170E+02	28	0.240181E+02	0.478014E-04
14	0.288150E+03	0.240160E+02	29	0.240181E+02	0.894423E-04
15	0.288150E+03	0.240260E+02	19	0.240181E+02	-0.326811E-03
16	0.293150E+03	0.238930E+02	28	0.238979E+02	0.204055E-03
17	0.293150E+03	0.238940E+02	29	0.238979E+02	0.162195E-03
18	0.293150E+03	0.239070E+02	19	0.238979E+02	-0.381667E-03
19	0.298150E+03	0.237830E+02	26	0.237912E+02	0.344077E-03
20	0.298150E+03	0.237830E+02	26	0.237912E+02	0.344077E-03
21	0.298150E+03	0.238020E+02	23	0.237912E+02	-0.454450E-03
22	0.298150E+03	0.237790E+02	23	0.237912E+02	0.512350E-03
23	0.298150E+03	0.238020E+02	29	0.237912E+02	-0.454450E-03
24	0.298150E+03	0.238040E+02	27	0.237912E+02	-0.538431E-03
25	0.298150E+03	0.237830E+02	28	0.237912E+02	0.344077E-03
26	0.298150E+03	0.237830E+02	29	0.237912E+02	0.344077E-03
27	0.298150E+03	0.238020E+02	19	0.237912E+02	-0.454450E-03
28	0.303150E+03	0.236930E+02	28	0.236971E+02	0.172523E-03
29	0.303150E+03	0.236940E+02	29	0.236971E+02	0.130311E-03
30	0.303150E+03	0.237080E+02	19	0.236971E+02	-0.460284E-03
31	0.308150E+03	0.236020E+02	28	0.236147E+02	0.537387E-03
32	0.308150E+03	0.236020E+02	29	0.236147E+02	0.537387E-03
33	0.308150E+03	0.236260E+02	19	0.236147E+02	-0.478989E-03
34	0.313150E+03	0.235320E+02	28	0.235431E+02	0.473243E-03
35	0.313150E+03	0.235320E+02	29	0.235431E+02	0.473243E-03
36	0.313150E+03	0.235550E+02	19	0.235431E+02	-0.503658E-03
37	0.318150E+03	0.234750E+02	28	0.234817E+02	0.284415E-03
38	0.318150E+03	0.234750E+02	29	0.234817E+02	0.284415E-03
39	0.318150E+03	0.234930E+02	19	0.234817E+02	-0.481989E-03
40	0.323150E+03	0.234400E+02	27	0.234296E+02	-0.443970E-03
41	0.323150E+03	0.234220E+02	28	0.234296E+02	0.324197E-03
42	0.323150E+03	0.234220E+02	29	0.234296E+02	0.324197E-03
43	0.323150E+03	0.234420E+02	19	0.234296E+02	-0.529249E-03
44	0.348150E+03	0.232950E+02	27	0.232884E+02	-0.281379E-03
45	0.373150E+03	0.233020E+02	27	0.233011E+02	-0.380564E-04
46	0.373150E+03	0.233020E+02	27	0.233011E+02	-0.380564E-04
47	0.398150E+03	0.234200E+02	27	0.234214E+02	0.612450E-04
48	0.423150E+03	0.236130E+02	27	0.236168E+02	0.161061E-03
49	0.448150E+03	0.238660E+02	27	0.238638E+02	-0.913361E-04

MULTIPLE LINEAR REGRESSION FOR REACTION NUMBER 5

FORM OF THE EQUATION IS -Ln K = A + B*T + C/T + D*LnT + E/T**2

A = Ø.20802296E+Ø3 B = Ø.30346171E-Ø1

C = -Ø.72797036E+Ø4 D = -Ø.32595034E+Ø2

E = -Ø.31630520E+Ø6

R2 = Ø.999883E+ØØ THE STANDARD DEVIATION = Ø.199011E-Ø2

N	T	-Ln K	REFERENCES	-Ln K CALC	DELTA
1	Ø.273150E+Ø3	Ø.256600E+Ø1	25	Ø.256285E+Ø1	-Ø.122706E-Ø2
2	Ø.278150E+Ø3	Ø.275479E+Ø1	37	Ø.275345E+Ø1	-Ø.488047E-Ø3
3	Ø.278150E+Ø3	Ø.274883E+Ø1	25	Ø.275345E+Ø1	Ø.167909E-Ø2
4	Ø.283150E+Ø3	Ø.293426E+Ø1	37	Ø.292972E+Ø1	-Ø.154598E-Ø2
5	Ø.283150E+Ø3	Ø.292313E+Ø1	25	Ø.292972E+Ø1	Ø.225570E-Ø2
6	Ø.285650E+Ø3	Ø.300510E+Ø1	37	Ø.301283E+Ø1	Ø.257173E-Ø2
7	Ø.288150E+Ø3	Ø.309127E+Ø1	37	Ø.309274E+Ø1	Ø.476658E-Ø3
8	Ø.288150E+Ø3	Ø.308628E+Ø1	37	Ø.309274E+Ø1	Ø.209426E-Ø2
9	Ø.288150E+Ø3	Ø.308823E+Ø1	25	Ø.309274E+Ø1	Ø.146151E-Ø2
10	Ø.288150E+Ø3	Ø.309986E+Ø1	39	Ø.309274E+Ø1	-Ø.229576E-Ø2
11	Ø.293150E+Ø3	Ø.324209E+Ø1	37	Ø.324348E+Ø1	Ø.427285E-Ø3
12	Ø.293150E+Ø3	Ø.323813E+Ø1	25	Ø.324348E+Ø1	Ø.165074E-Ø2
13	Ø.293150E+Ø3	Ø.324959E+Ø1	39	Ø.324348E+Ø1	-Ø.188168E-Ø2
14	Ø.296150E+Ø3	Ø.333334E+Ø1	37	Ø.332839E+Ø1	-Ø.148496E-Ø2
15	Ø.297150E+Ø3	Ø.336570E+Ø1	37	Ø.335582E+Ø1	-Ø.293698E-Ø2
16	Ø.298150E+Ø3	Ø.338530E+Ø1	32	Ø.338281E+Ø1	-Ø.735314E-Ø3
17	Ø.298150E+Ø3	Ø.338564E+Ø1	37	Ø.338281E+Ø1	-Ø.835665E-Ø3
18	Ø.298150E+Ø3	Ø.339237E+Ø1	37	Ø.338281E+Ø1	-Ø.281787E-Ø2
19	Ø.298150E+Ø3	Ø.338564E+Ø1	37	Ø.338281E+Ø1	-Ø.835665E-Ø3
20	Ø.298150E+Ø3	Ø.339237E+Ø1	37	Ø.338281E+Ø1	-Ø.281787E-Ø2
21	Ø.298150E+Ø3	Ø.338103E+Ø1	39	Ø.338281E+Ø1	Ø.526686E-Ø3
22	Ø.298150E+Ø3	Ø.338564E+Ø1	37	Ø.338281E+Ø1	-Ø.835665E-Ø3
23	Ø.303150E+Ø3	Ø.351439E+Ø1	37	Ø.351157E+Ø1	-Ø.802416E-Ø3
24	Ø.303150E+Ø3	Ø.350200E+Ø1	25	Ø.351157E+Ø1	Ø.273272E-Ø2
25	Ø.308150E+Ø3	Ø.362012E+Ø1	25	Ø.363051E+Ø1	Ø.286965E-Ø2
26	Ø.308150E+Ø3	Ø.363173E+Ø1	39	Ø.363051E+Ø1	-Ø.336344E-Ø3
27	Ø.313150E+Ø3	Ø.373562E+Ø1	37	Ø.374032E+Ø1	Ø.125890E-Ø2
28	Ø.313150E+Ø3	Ø.373019E+Ø1	25	Ø.374032E+Ø1	Ø.271643E-Ø2
29	Ø.323150E+Ø3	Ø.394518E+Ø1	32	Ø.393510E+Ø1	-Ø.255447E-Ø2
30	Ø.323150E+Ø3	Ø.392367E+Ø1	37	Ø.393510E+Ø1	Ø.291364E-Ø2
31	Ø.323150E+Ø3	Ø.392660E+Ø1	25	Ø.393510E+Ø1	Ø.216527E-Ø2
32	Ø.333150E+Ø3	Ø.411292E+Ø1	37	Ø.410049E+Ø1	-Ø.302167E-Ø2
33	Ø.373150E+Ø3	Ø.453002E+Ø1	32	Ø.453905E+Ø1	Ø.199307E-Ø2
34	Ø.373150E+Ø3	Ø.455306E+Ø1	32	Ø.453905E+Ø1	-Ø.307735E-Ø2
35	Ø.373150E+Ø3	Ø.453969E+Ø1	33	Ø.453905E+Ø1	-Ø.141281E-Ø3
36	Ø.373150E+Ø3	Ø.453724E+Ø1	35	Ø.453905E+Ø1	Ø.398619E-Ø3
37	Ø.398150E+Ø3	Ø.468281E+Ø1	33	Ø.468525E+Ø1	Ø.521466E-Ø3
38	Ø.423150E+Ø3	Ø.477814E+Ø1	33	Ø.476796E+Ø1	-Ø.212987E-Ø2
39	Ø.423150E+Ø3	Ø.476285E+Ø1	35	Ø.476796E+Ø1	Ø.107355E-Ø2
40	Ø.423150E+Ø3	Ø.476133E+Ø1	39	Ø.476796E+Ø1	Ø.139314E-Ø2
41	Ø.448150E+Ø3	Ø.480800E+Ø1	33	Ø.480691E+Ø1	-Ø.225747E-Ø3

APPENDIX F

ACTIVITY COEFFICIENT CORRELATIONS FROM LITERATURE USED IN COMPUTER MODEL

I. CHEMICAL REACTION 1: Water Reaction

$$K_{1,\gamma} = \frac{\gamma_{H^+}\,\gamma_{OH^-}}{a_{H_2O}}$$

The correlation for the activity coefficient ratio was obtained from Reference 16:

$$-\mathrm{Log}_{10}K_{1,\gamma} = \frac{2S\sqrt{I}}{1+\sqrt{I}} + \left[P_{10} + \frac{P_{11}}{T} + P_{12}T^2 + P_{13}F(I) \right] I - 0.157\phi I$$

Where,

P_{10} = Fitted Constant
= -0.61139

P_{11} = Fitted Constant
= 87.645

P_{12} = Fitted Constant
= 1.6698×10^{-6}

P_{13} = Fitted Constant
= -0.24456

I = Ionic Strength (gmole/kg H_2O)
= $0.5 \Sigma m_i z_i$

Where,

m_i = Molality of component i

z_i = Ionic charge of component i

S = Debye-Hückel Coefficient
= $-2.97627 + 4.80688 \times 10^{-2} T - 2.69280 \times 10^{-4} T^2 + 7.49524 \times 10^{-7} T^3 - 1.02352 \times 10^{-9} T^4 + 5.58004 \times 10^{-13} T^5$

T = Temperature (K)

$F(I) = [\, 1 - (1 + 2 I^{1/2} - 2 I) \exp (-2 I^{1/2}) \,] / 4 I$

ϕ = Osmotic Coefficient given in Reference 44

$= 1 - DH (ß\, m^{1/2}) + B\, m + C\, m^2$

Where,

B $= 4.43570 \times 10^{-2} + 2.14240 \times 10^{-4}\, t - 1.21582 \times 10^{-6}\, t^2$

Where,

t = Temperature (°C)

C $= 4.86989 \times 10^{-3} - 6.65184 \times 10^{-5}\, t + 1.69534 \times 10^{-7}\, t^2$

m = Ionic Strength (defined as "I" above)

$DH (ß\, m^{1/2}) = (\alpha / ß^3\, m) [(1 + ß\, m^{1/2}) - 2 \ln (1 + ß\, m^{1/2}) - (1 + ß\, m^{1/2})^{-1}]$

Where,

ß = Ion-Size Parameter

$= 1.64801 - 2.83246 \times 10^{-3}\, t + 4.67896 \times 10^{-6}\, t^2$ (t > 107.7 °C)

$= 0.980075 + 7.07654 \times 10^{-3}\, t - 2.97433 \times 10^{-5}\, t^2$ (t < 107.7 °C)

α = Debye-Hückel Limiting Slope

$= 1.17202\, \rho^{1/2} (2.33752 \times 10^4 / D\, T)^{3/2}$

Where,

D = Dielectric Constant of Pure Water

$= 5321 / T + 233.76 - 0.9297\, T + 1.417 \times 10^{-3}\, T^2 - 8.292 \times 10^{-7}\, T^3$

ρ = Density of Pure Water

$= 1.00157 - 1.56096 \times 10^{-4}\, t - 2.69491 \times 10^{-6}\, t^2$

II. CHEMICAL REACTION 2: Dissociation Reaction of Protonated MDEA

$$K_{2,\gamma} = \frac{\gamma_{MDEA}\,\gamma_{H^+}}{\gamma_{MDEAH^+}}$$

A. γ_{MDEA}

This was assumed to be unity because: (1) unionized molecules have activity coefficients near unity in most solutions, and (2) no activity coefficient model was found in the literature

B. γ_{H^+}

The correlation was obtained from Reference 43.

$$\ln \gamma_{H^+} = f + m\,B + m^2\,C$$

Where,

$f = -A_\phi [\, I^{1/2} / (1 + b\, I^{1/2}) \,]$

Where,

$b = 1.20$

I = Ionic Strength (See Reaction 1)

$A_\phi = \alpha$

= Debye-Hückel Limiting Slope (See Reaction 1)

$B = \beta^{(0)} - \beta^{(1)} \exp (-\alpha\, I^{1/2})$

Where,

$\beta^{(0)} = 0.18352$

$\beta^{(1)} = 0.25503$

$\alpha = 2.00$

$C = -0.00059$

C. γ_{MDEAH^+}

It was assumed that $\gamma_{MDEAH^+} = \gamma_{MEAH^+}$. The correlation for γ_{MEAH^+} was obtained from Reference 45.

$$\ln \gamma_{MEAH^+} = \frac{- A I^{1/2}}{1 + b B I^{1/2}} - 0.0750 [HCO_3^-]$$

Where,

A $= \alpha$

= Debye-Hückel Limiting Slope (See Reaction 1)

b $= 4.5 \times 10^{-8}$

B $= 50.3 \times 10^8 (D T)^{-1/2}$

Where,

D = Dielectric Constant of Pure Water (See Reaction 1)

T = Temperature (K)

III. CHEMICAL REACTION 3: 1st Ionization of Carbonic Acid

$$K_{3,\gamma} = \frac{\gamma_{H^+}\,\gamma_{HCO_3^-}}{\gamma_{CO_2}\,a_{H_2O}}$$

The correlation for the activity coefficient ratio was obtained from Reference 20.

$$-\mathrm{Log}_{10}K_{3,\gamma} = \frac{2S\sqrt{I}}{1+\sqrt{I}} + \left[P_{10} + \frac{P_{11}}{T} + P_{12}T^2 + P_{13}F(I) \right] I - 0.157\phi I$$

Where,

P_{10} = Fitted Constant
= -0.688379

P_{11} = Fitted Constant
= 136.722

P_{12} = Fitted Constant
= 1.93521×10^{-6}

P_{13} = Fitted Constant
= -0.124789

I = Ionic Strength (Defined in Reaction 1)

S = Debye-Hückel Coefficient (Defined in Reaction 1)

T = Temperature (K)

$F(I) = [\, 1 - (1 + 2\, I^{1/2} - 2\, I)\, \exp(-2\, I^{1/2})\,] \,/\, 4\, I$ (Defined in Reaction 1)

ϕ = Osmotic Coefficient (Defined in Reaction 1)

IV. CHEMICAL REACTION 4: 2nd Ionization of Carbonic Acid

$$K_{4,\gamma} = \frac{\gamma_{H^+}\,\gamma_{CO_3^=}}{\gamma_{HCO_3^-}}$$

The correlation for the activity coefficient ratio was obtained from Reference 27.

$$-\mathrm{Log}_{10}K_{4,\gamma} = \frac{4\,S\,\sqrt{I}}{1+\sqrt{I}} + \left[P_{10} + \frac{P_{11}}{T} + P_{12}T^2 + P_{13}F(I) \right] I$$

Where,

P_{10} = Fitted Constant
= 9.56741×10^{-3}

P_{11} = Fitted Constant
= -47.4028

P_{12} = Fitted Constant
= 2.30264×10^{-7}

P_{13} = Fitted Constant
= -0.159489

I = Ionic Strength (See Reaction 1)

S = Debye-Hückel Coefficient (See Reaction 1)

T = Temperature (K)

$F(I) = [\, 1 - (1 + 2\,I^{1/2} - 2\,I)\, \exp(-2\,I^{1/2})\,] \,/\, 4\,I$ (See Reaction 1)

V. CHEMICAL REACTION 5: Absorption of CO_2 into Solution

$$K_{5,\gamma} = \gamma_{CO_2}$$

The correlation for this activity coefficient was obtained from Reference 19.

$$\text{Ln } K_{5,\gamma} = \frac{Q_1}{T} + Q_2 + Q_3 T$$

Where,

T = Temperature (K)

$Q_i = - b_i I + c_i [1 - \exp (d_i I^{1.3})]$

Where,

I = Ionic Strength (See Reaction 1)

$b_1 = -653.3$

$b_2 = 3.9398$

$b_3 = -0.006491$

$c_1 = -155.3$

$c_2 = 1.1695$

$c_3 = -0.001981$

$d_1 = -2.504$

$d_2 = -2.276$

$d_3 = -2.163$

APPENDIX G

COMPUTER MODEL--PROGRAM REACTIONS.FOR

Description of REACTIONS.FOR Computer Program

The following program reads data from files INPUT.PAR and INPUT.DAT. The experimental data is read as heat of solution (Btu/lb MDEA) vs. loading (gmole CO_2/gmole MDEA). All of the experimental data for a single temperature (with varying conditions of pressure and weight percent MDEA) are read in. After reading in the data, the user can interactively modify the data set by adding or deleting data points from existing data sets, adding or deleting data sets, or correcting existing data points.

After establishment of the desired set of data, all of the experimental data is converted from Btu/lb MDEA to cal/gmole MDEA and program execution continues as outlined in the main body of the thesis.

The output compares the experimental data to the calculated overall heat of solution (see appendix I).

```
'CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C       THIS PROGRAM IS REACTIONS.FOR AND IS THE FULL BLOWN COMPUTER           C
C       MODEL FOR THE ABSORPTION OF THE CO2 INTO AQUEOUS MDEA SOLUTIONS        C
C       THE PROGRAM IS INTENDED TO BE PRETTY USER FRIENDLY DURING              C
C       OPERATION.  IT WAS ALSO WRITTEN TO BE QUITE GENERAL FOR ACID           C
C       GAS ABSORPTION INTO AMINE SOLUTIONS.                                   C
C                                                                              C
C       WRITTEN BY KEITH E. MERKLEY APRIL 1986 TO AUGUST 1986                  C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                ARRAY IDENTIFICATION AND DESCRIPTION                          C
C                                                                              C
C       A=FIRST COEFFICIENT IN FIT OF -ln K VS. T FOR EACH RXN (10)            C
C       B=SECOND COEFFICIENT IN FIT OF -ln K VS. T FOR EACH RXN (10)           C
C       BTU=EXP HT OF SOLN (BTU/LB MDEA) FOR SET #, POINT # (10,60)            C
C       BTU1=CALCULATED HT OF SOLN (BTU/LB MDEA) FOR SET #, POINT #            C
C               DETERMINED FOR PROGRAM OPTION 1 ONLY (10,60)                   C
C       BTU2=CALCULATED HT OF SOLN (BTU/LB CO2) FOR SET #, POINT #             C
C               DETERMINED FOR PROGRAM OPTION 1 ONLY (10,60)                   C
C       C=THIRD COEFFICIENT IN FIT OF -ln K VS. T FOR EACH RXN (10)            C
C       CC=MOLALITY (GMOLE/KG H2O) FOR EACH COMPONENT--FINAL CONCENTN          C
C               NOT STORED FOR EACH ITERATION (10)                             C
C       CC0=MOLALITY (GMOLE/KG H2O) FOR EACH COMPONENT--INITIAL                C
C               CONCENTRATION (BEFORE CO2 ADDITION) ONLY (10)                  C
C       CHARGE=ELECTRICAL CHARGE FOR EACH COMPONENT: I.E., FOR I=3,            C
C               THE COMPONENT IS MDEA WHICH HAS A CHARGE OF 0 (10)             C
C       CHEAT=TOTAL MOLAL HT OF SOLN (CAL/KG H2O) LESS THE HT OF               C
C               ABSORPTION OF CO2 GAS--THE CORRECTED HT OF SOLN (10)           C
C       CNAME=CHARACTER STRING--CHEMICAL FORMULA (OR NAME) OF EACH             C
C               COMPONENT (10)                                                 C
C       CO2=LOADING (GMOLE CO2/GMOLE MDEA) FOR SET #, POINT # (10,60)          C
C       CONCO2=STOICHIOMETRIC MOLALITY OF CO2 (MOLE CO2/KG H2O): I.E.,         C
C               [CO2] IN SOLN ASSUMING COMPLETE ABSORPTION FOR SET #,          C
C               POINT # (10,60)                                                C
C       CONMDE=STOICHIOMETRIC MOLALITY OF MDEA (GMOLE MDEA/KG H2O):            C
C               I.E., [MDEA] ASSUMING NO PROTONATION FOR SET # (10)            C
C       CONST=CONSTANT TERMS IN SYSTEM OF EQUATIONS SOLVED TO FIND COMP        C
C               OF SOLN--THESE INVOLVE GAMMA'S AND K'S (10)                    C
C       D=FOURTH COEFFICIENT IN FIT OF -ln K VS. T FOR EACH RXN (10)           C
C       DEBYE=COEFFICIENT ON DEBYE-HUCKEL CONTRIBUTION TO GAMMA FOR            C
C               EACH REACTION (10)                                             C
C       DELH=HT OF RXN FOR EACH REACTION (10)                                  C
C       DELHS=HT OF RXN FOR KEY RXN--THAT RXN WHOSE HEAT IS UNKNOWN AND        C
C               AND BEING SOLVED FOR. USED IN PROGRAM OPTIONS -1 AND 0         C
C               ONLY. SAVED FOR EACH OF THE 11 ITERATIONS(11)                  C
C       DELN=DELTA N FOR EACH REACTION (10)                                    C
C       DELNS=DELTA N FOR THE KEY RXN--THAT RXN WHOSE HT AND/OR K ARE          C
C               UNKNOWN AND BEING SOLVED FOR.  USED IN PROGRAM OPTIONS         C
C               -1 AND 0 ONLY.  SAVED FOR EACH SET #, POINT # (10,60)          C
C       DIFF=DIFFERENCE BETWEEN THE K WHICH GIVES MINIMUM ERROR AND THE        C
C               OTHER 10 K'S TRIED IN THE 11 ITERATIONS (11)                   C
C       E=FIFTH COEFFICIENT IN FIT OF -ln K VS. T FOR EACH RXN (10)            C
C       EQKLN=ln K FOR EACH REACTION (10)                                      C
C       EQKLNS=ln K FOR THE KEY REACTION. USED ONLY FOR PROGRAM OPTION         C
C               -1 IN WHICH K IS FOUND (11)                                    C
C       EQPCO2=EQ. PARTIAL PRESSURE OF CO2 FOR SET #, POINT # (10,60)          C
C       ERR=NORMALIZED SUM SQUARE ERROR FOR EACH ITERATION (11)                C
C       GAM=GAMMA FOR FINAL COMP USED ONLY IN PROGRAM OPTION 1                 C
C               FOR SET #, COMP #, PT # (1,10,10,60)                           C
C       GAM0=GAMMA FOR INITIAL COMP USED IN PROGRAM OPTION 1 ONLY              C
C               FOR SET #, COMP # (1,10,10,1)                                  C
C       GAMMA=ACTIVITY COEFFICIENT RATIO FOR EACH REACTION (10)                C
```

```
C       GSAVE=GAMMA FOR FINAL COMP FOR IT #, SET #, COMP #, PT #          C
C             (11,10,10,60)                                               C
C       GSAVE0=GAMMA FOR INITIAL COMP FOR IT #, SET #, COMP #             C
C             (11,10,10,1)                                                C
C       NPTS=NUMBER OF DATA POINTS IN EACH DATA SET (10)                  C
C       P10=COEFFICIENT IN ACTIVITY COEFF RATIO FOR EACH REACTION (10)    C
C       P11=COEFFICIENT IN ACTIVITY COEFF RATIO FOR EACH REACTION (10)    C
C       P12=COEFFICIENT IN ACTIVITY COEFF RATIO FOR EACH REACTION (10)    C
C       P13=COEFFICIENT IN ACTIVITY COEFF RATIO FOR EACH REACTION (10)    C
C       PERCEN=WT. % MDEA FOR EACH DATA SET (10)                          C
C       PHI=COEFFICIENT OF OSMOTIC COEFF USED IN CALCULATION OF ACTIVITYC
C             COEFF RATIO FOR EACH REACTION (10)                          C
C       PRESS=PRESSURE AT WHICH EACH DATA SET WAS TAKEN (10)              C
C       QB=CONSTANT USED IN CALCULATION OF ACT COEFF OF CO2 (3)           C
C       QC=CONSTANT USED IN CALCULATION OF ACT COEFF OF CO2 (3)           C
C       QD=CONSTANT USED IN CALCULATION OF ACT COEFF OF CO2 (3)           C
C       QCORR=HEAT CONTRIBUTION FROM KEY REACTION ONLY: I.E., TOTAL HT    C
C             LESS HT FROM EACH KNOWN RXN FOR EACH SET #, PT # (10,60)C
C       SOLNMW=MOLECULAR WEIGHT OF MDEA SOLN FOR EACH DATA SET (10)       C
C       SYSID=CHARACTER--IDENTIFICATION FOR EACH SET (10)                 C
C       X=BASE 10 LOG OF THE MOLALITY OF EACH COMPONENT (10)              C
C       XCO2=MOLE FRACTION OF CO2 IN SOLN ASSUMING COMPLETE ABSORPTION    C
C             FOR EACH SET #, PT #                                        C
C       XOLD=BASE 10 LOG OF THE FINAL COMP MOLALITY OF EACH COMPONENT     C
C             FOR EACH IT #, SET #, COMP #, PT # (11,10,10,60)            C
C       XOLD0=BASE 10 LOG OF THE INIT COMP MOLALITY OF EACH COMPONENT     C
C             FOR EACH IT#, SET #, COMP # (11,10,10,1)                    C
C       XSAV=BASE 10 LOG OF THE FINAL COMP MOLALITY OF EACH COMPONENT.    C
C             USED IN PROGRAM OPTION 1 FOR EACH SET #, COMP #, PT #       C
C             (1,10,10,60)                                                C
C       XSAV0=BASE 10 LOG OF THE INIT COMP MOLALITY OF EACH COMPONENT.    C
C             USED IN PROGRAM OPTION 1 FOR EACH SET #, COMP #             C
C             (1,10,10,1)                                                 C
C                                                                         C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                         C
C             VARIABLE IDENTIFICATION AND DESCRIPTION                     C
C                                                                         C
C       ANS=HOLD "Y" OR "N" AS ANSWER TO QUESTION                         C
C       CO2MW=MOLECULAR WEIGHT OF CO2                                     C
C       DELHC=HEAT OF REACTION FOR THE PROTONIZATION OF MDEA GIVEN        C
C             BY EQUATION 37 IN THE THESIS                                C
C       DELMD=HEAT OF VAPORIZATION FOR PURE MDEA                          C
C       DELH2O=HEAT OF VAPORIZATION FOR PURE H2O                          C
C       DELINC=INCREMENT OF VALUE OF ln K2                                C
C       DIFMIN=MINIMUM DIFFERENCE BETWEEN AN ARBITRARY VALUE OF           C
C             ln K2 AND THE 11 VALUES OF ln K2 MAKING UP ONE              C
C             PASS THROUGH THE PROGRAM                                    C
C       ERRMIN=MINIMUM VALUE OF THE NORMALIZED ERROR SQUARE               C
C             SUM (EQUATION 34)                                           C
C       ERNORM=NORMALIZED ERROR SQUARE FOR A SINGLE DATA                  C
C             POINT (EQUATION 33)                                         C
C       ERRO=ERROR SQUARE FOR A SINGLE DATA POINT                         C
C       FLAGD=FLAG TO INDICATE IF A USER SUPPLIED INITIAL VALUE           C
C             OF DELINC (FLAGD=1) IS TO BE USED IN PLACE OF               C
C             THE DEFAULT VALUE OF 0.20 (FLAGD=0)                         C
C       FLAGK=FLAG TO INDICATE IF A USER SUPPLIED INITIAL VALUE OF        C
C             THE EQUILIBRIUM CONSTANT FOR THE MDEA PROTONATION           C
C             REACTION (FLAGK=1) IS TO BE USED IN PLACE OF                C
C             THE DEFAULT VALUE OF K CALCULATED BY THE COR-               C
C             RELATION (FLAGK=0)                                          C
C       GUES=INITIAL GUESSES FOR THE MOLALITY OF EACH COMPONENT           C
C             IN SOLUTION                                                 C
C       HE=OVERALL HEAT OF SOLUTION (KJ/GMOLE SOLUTION)                   C
```

```
C       HEAT=OVERALL HEAT OF SOLUTION (CAL/KG H2O)                      C
C       HTJUN=HEAT CONTRIBUTION FROM SINGLE REACTION (DELTA N * K)      C
C       H2OMW=MOLECULAR WEIGHT OF PURE WATER                            C
C       IGUESS=FLAG TO INDICATE IF USER SUPPLIED INITIAL GUESS          C
C              FOR THE ACTIVITY COEFFICIENT RATIOS AND COMPONENT        C
C              MOLALITIES (IGUESS=1) ARE TO BE USED IN PLACE            C
C              OF THE BUILT IN DEFAULTS (IGUESS=Ø)                      C
C       IMIN=THE ITERATION NUMBER THAT PRODUCES THE MINIMUM             C
C              VALUE OF THE NORMALIZED ERROR SQUARE SUM                 C
C       INPRT=FLAG TO INDICATE IF ALL OF COMPUTER PRINTOUT              C
C              IS ALSO TO BE PRINTED TO THE COMPUTER                    C
C              SCREEN (INPRT NOT EQUAL Ø)                               C
C       IREP=FLAG INDICATING IF THE ENTIRE ITERATIVE PROCEDURE          C
C              IS BEING PERFORMED FOR THE FIRST TIME WITH               C
C              A SET OF INPUT DATA (IREP=Ø) OR IF IT HAS BEEN           C
C              PERFORMED AT LEAST ONCE PREVIOUSLY (IREP>Ø)              C
C       ITCNT=FLAG TO COUNT NUMBER OF ITERATIONS REQUIRED TO SOLVE      C
C              SYSTEM OF EQUATIONS AS GIVEN IN FIGURE 13                C
C       ITOLF=FLAG TO INDICATE IF THE USER SUPPLIED TOLERANCE           C
C              FOR SOLVING THE SYSTEM OF EQUATIONS AS GIVEN             C
C              IN FIGURE 13 HAS BEEN MET (ITOLF=1,OTHERWISE             C
C              ITOLF=Ø).  THIS FLAG IS DETERMINED IN SUBROUTINE         C
C              TOLER                                                    C
C       ITPRT=FLAG CONTROLLING AMOUNT OF OUTPUT DESIRED.                C
C              ITPRT=Ø GIVES THE LEAST AMOUNT OF OUTPUT, WHILE          C
C              ITPRT=2 GIVES THE GREATEST AMOUNT OF OUTPUT              C
C       JJJ=COUNTER FOR DATA POINT IN A PARTICULAR DATA SET (JJJ        C
C              RANGES FROM 1 TO THE NUMBER OF POINTS IN THE DATA        C
C              SET)                                                     C
C       JJJJ=FLAG TO INDICATE IF USER WANTS TO SUPPLY A NEW VALUE       C
C              OF DELINC AND/OR ln K2 FOR THE NEXT SET OF 11            C
C              ITERATIONS                                               C
C       JSAVE=FLAG TO INDICATE IF THE SOLUTION COMPOSITION IS FOR       C
C              THE INITIAL COMPOSITION (JSAVE=Ø) OR THE FINAL           C
C              COMPOSITION (JSAVE=1)                                    C
C       KIT=COUNTER FOR THE NUMBER OF ITERATIONS ON ln K FOR A          C
C              SINGLE VALUE OF KITCNT (KIT RANGES FROM 1 TO 11).        C
C              USED AS DO LOOP COUNTER                                  C
C       KITCNT=COUNTER FOR THE NUMBER OF TIMES THAT THE SET OF          C
C              11 ITERATIONS ON ln K2 IS REPEATED                       C
C       KKFLAG=FLAG TO INDICATE IF THE USER HAS CHANGED THE             C
C              VLAUES OF ln K2 AND DELINC WHICH THE PROGRAM             C
C              CALCULATED FOR THE NEXT SET OF 11 ITERATIONS             C
C              ON ln K2 (KKFLAG=1; IF NO CHANGE MODE, KKFLAG=Ø)         C
C       KKK=KIT MINUS ALTERNATE COUNTS USED WITHIN DO LOOP              C
C       KMIN=ITERATION NUMBER THAT PRODUCES THE MINIMUM DIFFERENCE      C
C              BETWEEN A USER SUPPLIED VALUE OF ln K2 AND THE 11        C
C              VALUES OF ln K2                                          C
C       KOPT=OPTION NUMBER DESCRIBED IN BODY OF THIS THESIS             C
C       KOPTFL=FLAG TO INDICATE IF THE LOADING POINT HAS BEEN           C
C              EXCEEDED (KOPTFL=1) FOR A PROGRAM OPTION (KOPT)          C
C              OF 1                                                     C
C       LLL=COUNTER FOR THE DATA SET NUMBER BEING EXAMINED              C
C              (LLL RANGES FROM 1 TO THE TOTAL NUMBER OF DATA           C
C              SETS INCLUDED)                                           C
C       MINFLG=IMIN                                                     C
C       NCHNGS=FLAG TO INDICATE IF THE USER HAS SUPPLIED A NEW          C
C              VALUE OF ln K2 FOR THE NEXT SET OF 11 ITERATIONS         C
C              (NCHNGS=1; NCHNGS=Ø IF THE USER HAS NOT SUPPLIED         C
C              A NEW VALUE OF ln K2)                                    C
C       NCNT=TOTAL NUMBER OF VALUES OF ln K2 TRIED FROM START OF        C
C              COMPUTER PROGRAM                                         C
C       NCOMP=TOTAL NUMBER OF CHEMICAL COMPONENTS (7 FOR THE            C
C              MDEA SYSTEM)                                             C
```

```
C       NGUESS=FLAG TO INDICATE IF A SET OF GUESSES FOR THE              C
C              MOLALITIES AND THE ACTIVITY COEFFICIENT RATIOS            C
C              HAS BEEN MADE (NGUESS=1; NGUESS=Ø INDICATES               C
C              THAT NO SET OF GUESSES HAS BEEN MADE)                     C
C       NKEY=KEY REACTION MINUS REACTION NUMBER FOR WHICH ln K2          C
C              IS UNKNOWN                                                C
C       NNCNT=FLAG TO INDICATE IF A PREVIOUS PASS THROUGH THE            C
C              SUBROUTINE GAMMAK HAS BEEN MADE (NNCNT=1;                 C
C              NNCNT=Ø INDICATES NO PASS HAS BEEN MADE PREVIOUSLY        C
C       NNN1=NUMBER OF COMPONENTS IN THE INITIAL SOLUTION BEFORE         C
C              ADDITION OF CO2 (NNN1=4)                                  C
C       NNN2=NUMBER OF COMPONENTS IN FINAL SOLUTION (NNN2=7)             C
C       NNN3=NUMBER OF COMPONENTS IN FINAL SOLUTION FOR KOPT=1           C
C              (NNN3=8)                                                  C
C       NRXNS=NUMBER OF REACTIONS (NRXNS=5)                              C
C       NSETS=NUMBER OF DATA SETS                                        C
C       NTOTAL=TOTAL NUMBER OF DATA POINTS FROM ALL DATA SETS            C
C       ORCO2=STOICIOMETRIC MOLAL CONCENTRATION OF CO2 MIXED             C
C              WITH THE MDEA SOLUTION                                    C
C       ORMDEA=STOICHIOMETRIC MOLAL CONCENTRATION OF MDEA IN             C
C              THE SOLUTION                                              C
C       PCO2=PARTIAL PRESSURE OF CO2                                     C
C       PH2O=PARTIAL PRESSURE OF H2O                                     C
C       PMDEA=PARTIAL PRESSURE OF MDEA                                   C
C       PTOT=THEORETICAL TOTAL PRESSURE ASSUMING ALL CO2 IS ABSORBED     C
C       PUREMW=MOLECULAR WEIGHT OF PURE MDEA                             C
C       R=UNIVERSAL GAS CONSTANT                                         C
C       SAVEK=TEMPORARY STORAGE FOR VALUE OF ln K2 WHICH PRODUCES        C
C              MINIMUM VALUE OF ERROR SUM SQUARE                         C
C       SERNRM=NORMALIZED ERROR SQUARE SUM                               C
C       SUMDEN=DENOMINATOR GIVEN BY EQUATION 4Ø                          C
C       SUMHT=SUMMATION OF DELTA N MULTIPLIED BY DELTA H FOR             C
C              EACH REACTION EXCEPT REACTION NKEY FOR USE                C
C              IN EQUATION 31                                            C
C       SUMNUM=NUMERATOR GIVEN BY EQUATION 39                            C
C       T=TEMPERATURE IN KELVIN                                          C
C       TEMP=TEMPERATURE IN FARENHEIT                                    C
C       TEMP1=TEMPERATURE IN CELSIUS                                     C
C       THEAT=CALCULATED TOTAL HEAT OF SOLUTION (CAL/KG H2O)             C
C       TOL=TOLERANCE USED IN SUBROUTINE TOLER TO TEST                   C
C              CONVERGENCE OF SOLUTION PROCEDURE                         C
C       TOL1=TOLERANCE USED IN SUBROUTINE SOLVE TO TEST                  C
C              CONVERGENCE FOR SOLVING SET OF 7 EQUATIONS IN             C
C              7 UNKNOWNS                                                C
C       TOTMOL=TOTAL MOLALITY (TOTAL MOLES/KG H2O) OF ALL                C
C              SPECIES IN SOLUTION                                       C
C       VAPH2O=MOLES OF H2O VAPORIZED FOR LOADINGS GREATER               C
C              THAN THE LOADING POINT (MOLE/KG H2O)                      C
C       VAPMDE=MOLES OF MOLECULAR MDEA VAPORIZED FOR LOADINGS            C
C              GREATER THAN THE LOADING POINT (MOLE/KG MDEA)             C
C       VPH2O=VAPOR PRESSURE OF H2O                                      C
C       VPMDEA=VAPOR PRESSURE OF PURE MDEA                               C
C       WTMOL=MOLECULAR WEIGHT OF AQUEOUS MDEA SOLUTION                  C
C       XH2O=STOICHIOMETRIC MOLE FRACTION OF H2O IN AQUEOUS PHASE        C
C       XMDEA=STOICHIOMETRIC MOLE FRATION OF MDEA IN AQUEOUS PHASE       C
C       XXH2O=CALCULATED MOLE FRACTION OF MOLECULAR H2O                  C
C       XXMDEA=CALCULATED MOLE FRACTION OF MOLECULAR MDEA                C
C       YCO2=CALCULATED MOLE FRACTION OF CO2 IN VAPOR PHASE              C
C       YH2O=CALCULATED MOLE FRACTION OF H2O IN VAPOR PHASE              C
C       YMDEA=CALCULATED MOLE FRACTION OF MDEA IN VAPOR PHASE            C
C       YTOT=TOTAL MOLAL CONCENTRATION OF VAPOR PHASE (MOLE/KG H2O)      C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                        C
```

```
C       SUBROUTINE AND SUBPROGRAM IDENTIFICATION AND DESCRIPTION        C
C                                                                       C
C       DATA=SUBROUTINE TO MODIFY SET OF DATA INPUT BY THE INPUT        C
C               DATA SET.  OPTIONS INCLUDE ADDING AND/OR DELETING       C
C               DATA SETS, ADDING AND/OR DELETING DATA POINTS,          C
C               AND/OR CORRECTING EXISTING DATA POINTS                  C
C       F=SUBPROGRAM CALLED IN SOLVE WHICH CALCULATES THE VALUES        C
C               OF THE FUNCTIONS F(I) WHOSE SOLUTIONS GIVES THE         C
C               COMPOSITION OF THE SOLUTION.  THE FUNCTIONS ARE         C
C               DEFINED IN FIGURE 13                                    C
C       FP=SUBPROGRAM CALLED IN SOLVE WHICH CALCULATES EACH             C
C               NUMERICAL VALUE OF THE JACOBIAN MATRIX                  C
C       GAMMAK=SUBROUTINE TO CALCULATE EACH OF THE ACTIVITIY            C
C               COEFFICIENT RATIOS DEFINED IN FIGURE 13                 C
C       GUESS=SUBROUTINE ESTABLISHING INITIAL GUESSES FOR USE           C
C               IN THE SOLUTION PROCEDURE                               C
C       INVER=SUBROUTINE CALLED BY SOLVE TO INVERT THE MATRIX           C
C               USED IN THE SOLUTION PROCEDURE                          C
C       MULT=SUBROUTINE CALLED BY SOLVE TO MULTIPLY MATRICES            C
C       OUT1=SUBROUTINE USED ONLY BY PROGRAM OPTION 1 FOR               C
C               CREATING AN OUTPUT FILE                                 C
C       OUTPUT=SUBROUTINE FOR CREATING AN OUTPUT FILE FOR ALL           C
C               PROGRAM OPTIONS                                         C
C       SOLVE=SUBROUTINE TO SOLVE SYSTEM OF EQUATIONS                   C
C       TOLER=SUBROUTINE TO CHECK IF THE CURRENT SET OF SOLUTIONS       C
C               IS WITHIN A SPECIFIED TOLERANCE OF THE FORMER           C
C               SET OF SOLUTIONS                                        C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /GAM/ P10(10),P11(10),P12(10),P13(10),T,PHI(10),
     1         DEBYE(10),NRXNS,ITCNT,KIT,KITCNT,QB(3),QC(3),QD(3)
      COMMON /SOL/ X(10),CONST(10),ORCO2,ORMDEA
      COMMON /GS/ NGUESS,CONCO2(10,60),CONMDE(10),NPTS(10)
      COMMON /TOL/ GAM(1,10,10,60),GAM0(1,10,10,1),XSAV(1,10,10,60),
     1         XSAV0(1,10,10,1)
      DIMENSION XCO2(10,60),BTU2(10,60),
     2         CHEAT(10,60),A(10),B(10),C(10),D(10),E(10),DIFF(11),
     3         EQKLN(10),DELH(10),DELN(10),CNAME(10),
     4         CC(10),CC0(10),CHARGE(10),XOLD0(11,10,10,1),
     5         XOLD(11,10,10,60),GSAVE0(11,10,10,1),
     6         GSAVE(11,10,10,60),DELNS(10,60),QCORR(10,60),
     7         DELHS(11),ERR(11),EQKLNS(11),PERCEN(10),CO2(10,60),
     8         BTU(10,60),SOLNMW(10),SYSID(10),GAMMA(10),
     9         PRESS(10),EQPCO2(10,60),BTU1(10,60)
      OPEN(UNIT=7,STATUS='OLD',FILE='INPUT.DAT')
      OPEN(UNIT=8,STATUS='OLD',FILE='INPUT.PAR')
      OPEN(UNIT=9,STATUS='OLD',FILE='PLOTEXP.DAT')
      OPEN(UNIT=10,STATUS='OLD',FILE='PLOTLOAD.DAT')
      OPEN(UNIT=11,STATUS='OLD',FILE='PLOTLOD2.DAT')
      OPEN(UNIT=13,STATUS='OLD',FILE='OUTPUT.DAT')
      OPEN(UNIT=1 ,STATUS='OLD',FILE='PLOTCOMP.DAT')
      REWIND 1
      REWIND 9
      REWIND 13
      WRITE(6,250)
  250 FORMAT(' ENTER THE NUMBER CORRESPONDING TO THE OPTION DESIRED:',
     1 //9X,'-1:  FIT THE DATA TO BEST VALUES OF LN K, DELTA H'/,
     2   10X,'0:  FIX LN K AND FIND BEST VALUE OF DELTA H AND ERROR'/,
     3   10X,'1:  FIX LN K AND DELTA H AND GENERATE LOADING CURVES'/,
     4   10X,'    (LOADING VS. BTU/LB MDEA [EXP. AND CALCULATED])')
```

```
      READ(5,*) KOPT
      READ(7,*) NSETS
      NTOTAL=0
      IREP=0
      DO 20 L=1,NSETS
              READ(7,3) SYSID(L)
    3         FORMAT(A4)
              READ(7,*) PERCEN(L),TEMP,PRESS(L)
              READ(7,*) NPTS(L),PUREMW,WTMOL
              READ(7,*) (CO2(L,I),BTU(L,I), I=1,NPTS(L))
              NTOTAL=NTOTAL+NPTS(L)
   20 CONTINUE
      READ(8,*) NRXNS,NCOMP,TOL,TOL1
      READ(8,*) (I,CHARGE(I),I=1,NCOMP+1)
      READ(8,*) (I,A(I),B(I),C(I),D(I),E(I), I=1,NRXNS)
      READ(8,*)(P10(I),P11(I),P12(I),P13(I),PHI(I),DEBYE(I),I=1,NRXNS)
      READ(8,*) (QB(I),QC(I),QD(I),I=1,3)
      READ(8,21) (I,CNAME(I),I=1,NCOMP)
      READ(8,*) NKEY
   21 FORMAT(2X,I3,2X,A10)
    1 CALL DATA(PERCEN,PRESS,NPTS,NSETS,NTOTAL,CO2,BTU,IREP,
     1          MINFLG,NNN1,NNN2,XOLD,XOLD0,GSAVE,GSAVE0,NRXNS,SYSID)
      IF(KOPT.EQ.1)THEN
              DELHMD=13505.14
              IF(TEMP.EQ.60.0) THEN
                      VPMDEA=0.00
                      VPH2O=0.25611
                      DELH2O=10604.95
              ELSEIF(TEMP.EQ.140.0) THEN
                      VPMDEA=0.00423
                      VPH2O=2.8892
                      DELH2O=10149.56
              ELSEIF(TEMP.EQ.240.0) THEN
                      VPMDEA=0.11080
                      VPH2O=24.968
                      DELH2O=9530.04
              ELSEIF(TEMP.EQ.300.0) THEN
                      VPMDEA=0.54143
                      VPH2O=67.005
                      DELH2O=9107.68
              ENDIF
      ENDIF
      IREP=IREP+1
      WRITE(6,2)
    2 FORMAT(' ENTER EITHER 0, 1, OR 2 TO CONTROL AMOUNT OF PRINTED ',
     1          'OUTPUT:'/10X,'0:  SUMMARY OF INPUT DATA;'/14X,'LN K ',
     2          'AND DELTA H VS. ERROR'/14X,'FINAL VALUE OF LN K AND',
     3          ' DELTA H WITH'/19X,'COMPARISON OF QEXP AND QCALC'//,
     4          10X,'1:  SAME AS "0" PLUS;'/14X,'DETAILS ON EACH ',
     5          'ITERATION ON LN K'//10X,'2:  SAME AS "1" PLUS;'/,
     6          14X,'DETAILS ON EACH DATA POINT FOR EACH ITERATION')
      READ(5,*) ITPRT
      WRITE(6,*) ' ENTER 0 TO TURN OFF THE PRINTING OF ALL BUT THE ',
     1          'ITERATION RECORD AND FINAL ANSWER TO THE SCREEN'
      READ(5,*) INPRT
      IF(INPRT.NE.0) WRITE(6,5) TEMP
      WRITE(13,5) TEMP
    5 FORMAT(////9X,'ANALYSIS OF EQUILIBRIUM CONSTANT AND HEAT OF ',
     1          'REACTION'/16X,'FOR THE PROTONATION OF MDEA AT ',F5.1,
     2          ' F')
      DO 30 L=1,NSETS
              IF(INPRT.NE.0) WRITE(6,6) L,SYSID(L),PRESS(L),PERCEN(L)
              WRITE(13,6) L,SYSID(L),PRESS(L),PERCEN(L)
    6         FORMAT(//27X,'DATA SET NUMBER ',I2//,
```

```
     1                    19X,'SYSTEM          (RUN#.TRIAL):  ',A4/,
     3                    19X,'PRESSURE        (PSIA)       : ',F5.1/,
     4                    19X,'CONCENTRATION (WT. % MDEA):  ',F4.1//,
     5                  /30X,'INPUT DATA'//25X,'MOLE CO2        BTU'/,
     6                  25X,'---------    -------'/,
     7                  25X,'MOLE MDEA    LB MDEA'/)
               DO 29 I=1,NPTS(L)
                     IF(INPRT.NE.0) WRITE(6,8) CO2(L,I),BTU(L,I)
                     WRITE(13,8) CO2(L,I),BTU(L,I)
  8                  FORMAT(26X,F7.5,5X,F7.2)
 29            CONTINUE
 30    CONTINUE
       IF(INPRT.NE.0) WRITE(6,10) NRXNS,NCOMP,CHARGE(1)
       WRITE(13,10) NRXNS,NCOMP,CHARGE(1)
 10    FORMAT('1',26X,'INPUT PARAMETERS'////,
     1         20X,'NUMBER OF REACTIONS   :  ',I2//,
     2         20X,'NUMBER OF COMPONENTS :  ',I2//,
     3         20X,'CHARGES ON COMPONENTS:   1, ',F3.0)
       IF(INPRT.NE.0) WRITE(6,11) (I,CHARGE(I),I=2,NCOMP)
       WRITE(13,11) (I,CHARGE(I),I=2,NCOMP)
 11    FORMAT(44X,I2,', 'F3.0)
       PUREMW=119.163
       H2OMW=18.0152
       CO2MW=44.0099
       DO 35 L=1,NSETS
               SOLNMW(L)=100./((PERCEN(L)/PUREMW)+
     1                       ((100.-PERCEN(L))/H2OMW))
 35    CONTINUE
       TEMP1=(TEMP-32.0)/1.8
       T=TEMP1+273.15
       R=1.98717
       DO 40 J=1,NRXNS
               EQKLN(J)=-1.0*(A(J) + B(J)*T + C(J)/T + D(J)*DLOG(T)
     2                  + E(J)/(T*T))
               DELH(J)= R * ( C(J) - D(J)*T - B(J)*T*T + 2*E(J)/T )
 40    CONTINUE
       DELH(1)=239.00574*(61.49 - 0.2415*TEMP1 + 8.090D-04*TEMP1*TEMP1
     1         -3.316D-06*TEMP1*TEMP1*TEMP1)
       IF(INPRT.NE.0) WRITE(6,45) TOL,TOL1,(EQKLN(I),I=1,NRXNS),
     1         (DELH(I),I=1,NRXNS)
       WRITE(13,45) TOL,TOL1,(EQKLN(I),I=1,NRXNS),(DELH(I),
     1         I=1,NRXNS)
 45    FORMAT(///7X,'TOLERANCE FOR ACTIVITY COEFFICIENT CONVERGENCE: ',
     1      D7.1//7X,'TOLERANCE FOR SIMULTANEOUS EQUATION SOLUTIONS : ',
     2      D7.1////14X,'VALUES FOR LN K, DELTA H FOR EACH REACTION'///,
     3      24X,'LN K      [=]  UNITLESS'//24X,'DELTA H  [=]  CAL/GMOLE',
     4      ///17X,'1',11X,'2',11X,'3',11X,'4',11X,'5'//,
     5       3X,'LN K',7X,F7.3,5X,F7.3,5X,F7.3,5X,F7.3,5X,F7.3//,
     6       3X,'DELTA H',3X,F9.2,3X,F9.2,3X,F9.2,3X,F9.2,3X,F9.2/)
       IF(INPRT.NE.0) WRITE(6,50)
       WRITE(13,50)
 50    FORMAT('1',27X,'CONVERTED DATA'////4X,'(NOTE:  "CORRECTED ',
     1         'HEAT OF SOLUTION" IS TOTAL HEAT OF SOLUTION'/15X,
     2         ' LESS HEAT OF ABSORPTION OF GASEOUS CO2.)'///58X,
     3         'CORRECTED'/10X,'MOLE      HEAT OF   MOLALITY      ',
     4         'MOLALITY      HEAT OF'/,
     5                    8X,'FRACTION   SOLUTION      CO2        ',
     6         '  MDEA         SOLUTION'/,
     7            2X,'POINT    CO2      (J/MOLE) (MOLE/KG H2O) (M',
     8         'OLE/KG H2O) (CAL/KG H2O)')
       DO 100 L=1,NSETS
               IF(INPRT.NE.0) WRITE(6,60) L
               WRITE(13,60) L
 60            FORMAT(/27X,'DATA SET NUMBER ',I2/)
```

```
              DO 90 J=1,NPTS(L)
                      XCO2(L,J)=1./(1.+100.*PUREMW/
     1                        (CO2(L,J)*SOLNMW(L)*PERCEN(L)))
                      XH2O=(1.0-XCO2(L,J))/((H2OMW*PERCEN(L)/
     1                        ((100.0-PERCEN(L))*PUREMW))+1.0)
                      XMDEA=1.0-XCO2(L,J)-XH2O
                      CONCO2(L,J)=1000.0*XCO2(L,J)/(H2OMW*
     1                        (1.0-XCO2(L,J)-XMDEA))
                      CONMDE(L)=1000.0*XMDEA/(H2OMW*
     1                        (1.0-XCO2(L,J)-XMDEA))
                      HEAT=BTU(L,J)*555.555556*PERCEN(L)/
     1                        (100.0-PERCEN(L))
                      HE=BTU(L,J)*PUREMW*XMDEA*
     1                        1054.35/453.592375
                      CHEAT(L,J)=HEAT-CONCO2(L,J)*DELH(NRXNS)
                      IF(INPRT.NE.0) WRITE(6,85) J,XCO2(L,J),HE,
     1                        CONCO2(L,J),CONMDE(L),CHEAT(L,J)
                      WRITE(13,85)J,XCO2(L,J),HE,CONCO2(L,J),
     1                        CONMDE(L),CHEAT(L,J)
  85                  FORMAT(3X,I3,3X,F7.5,3X,F8.2,4X,F7.4,7X,F7.4,
     1                        6X,F9.1)
  90              CONTINUE
 100      CONTINUE
          WRITE(6,101) ITPRT
          WRITE(13,101) ITPRT
 101      FORMAT('1',9X,'ITPRT = ',I1///27X,'ITERATION RECORD'////)
          IF(KOPT.EQ.1) THEN
                  WRITE(6,*) 'ENTER VALUE OF DELTA H FOR RXN NUMBER ',NKEY
                  READ(5,*) DELH(NKEY)
          ENDIF
          IF(KOPT.EQ.0.OR.KOPT.EQ.1) THEN
                  WRITE(6,*) 'ENTER VALUE OF LN K TO BE HELD FIXED'
                  READ(5,*) EQKLN(NKEY)
                  GOTO 109
          ENDIF
          IF(IREP.GT.1) THEN
                  EQKLN(NKEY)=EQKLNS(MINFLG)
                  WRITE(6,200) EQKLN(NKEY)
 200              FORMAT(/' BEST VALUE OF LN K FROM LAST RUN WAS ',F10.5)
                  GOTO 210
          ENDIF
          WRITE(6,102)
 102      FORMAT(' IF YOU WISH TO USE THE VALUE OF LN K CALCULATED',
     1           'BY '/5X,'THE CORRELATION, ENTER "0";'/,
     3           5X,' OTHERWISE, ENTER THE NUMERICAL VALUE OF LN K')
          READ(5,*) FLAGK
          IF(FLAGK.NE.0.0) THEN
                  EQKLN(NKEY)=FLAGK
          ENDIF
 210      DELINC=0.20
          WRITE(6,103) DELINC
 103      FORMAT(' CURRENT VALUE OF DELINC IS ',F7.5//,
     1           ' IF YOU WISH TO USE A DIFFERENT VALUE, ENTER THAT ',
     2           'VALUE;'/5X,'OTHERWISE, ENTER "0.0"')
          READ(5,*) FLAGD
          IF(FLAGD.NE.0.0) THEN
                  DELINC=FLAGD
          ENDIF
          IF(ITPRT.EQ.0) THEN
                  WRITE(6,104)
                  WRITE(13,104)
 104              FORMAT(15X,'NUMBER    LN K       DELTA H    N. ERROR ',
     1                   'SQUARED')
          ENDIF
```

```
109   NNCNT=0
      KITCNT=0
      KKFLAG=0
105   KITCNT=KITCNT+1
      DO 700 KIT=1,11
              SUMNUM=0
              SUMDEN=0
              IF(ITPRT.GT.0) THEN
                      NCNT=11*(KITCNT-1)+KIT
                      WRITE(6,106) NCNT
                      WRITE(13,106) NCNT
106                   FORMAT('1',9X,'ITERATION NUMBER = ',I3)
              ENDIF
              IF(KITCNT.NE.1.AND.KIT.EQ.1.AND.KKFLAG.EQ.0) GOTO 530
              DO 500 L=1,NSETS
                      KOPTFL=0
                      DO 400 J=1,NPTS(L)
                              IF(J.EQ.1) THEN
                                      JSAVE=0
                                      ORMDEA=CONMDE(L)
                                      IF(ITPRT.GT.0) THEN
                                              WRITE(6,107) J
                                              WRITE(13,107) J
107                                           FORMAT(15X,'J = ',I3)
                                      ENDIF
                                      LLL=L
                                      NNN1=4
                                      KKK=KIT
                                      JJJ=J
                                      CALL GUESS(X,GAMMA,NRXNS,KITCNT,
     1                                        KIT,J,KKK,JJJ,MINFLG,
     2                                        GSAVE0,XOLD0,NNN1,LLL,L,
     3                                        JSAVE,IREP,0)
                                      IF(NGUESS.EQ.1)THEN
                                              WRITE(6,108) L,SYSID(L),
     1                                             PERCEN(L),PRESS(L)
108                                           FORMAT(' DATA SET ',
     1                                        I2,'  SYSTEM ',A4,
     2                                        '  WEIGHT PERCENT:  ',
     3                                        F5.1,'  PRESSURE ',
     4                                        '(PSIA):  ',F5.1)
                                              WRITE(6,110)
110                                           FORMAT(/' INITIAL ',
     1                                                'COMPOSITION')
                                              WRITE(6,111)
111                                           FORMAT(/' IF YOU WISH ',
     1                                        'TO ENTER YOUR OWN ',
     2                                        'GUESSES FOR X AND ',
     3                                        'GAMMA, ENTER 1'/,
     4                                        ' OTHERWISE, ENTER 0')
                                              READ(5,*) IGUESS
                                              IF(IGUESS.EQ.0) THEN
                                                   DO 120 I=1,NRXNS
                                                          GAMMA(I)=1.0
120                                                CONTINUE
                                                   X(1)=DLOG(0.4D-10)
                                                   X(2)=DLOG(2.5D-03)
                                                   X(3)=DLOG(ORMDEA)
                                                   X(4)=X(2)
                                              ELSE
                                                      WRITE(6,*)' EN',
     1                                                'TER GUESS FOR',
     2                                                'GAMMA FOR REA',
     3                                                'CTION 1'
```

```
                                        READ(5,*)
     1                                         GAMMA(1)
                                        DO 125 I=1,NNN1
                                           WRITE(6,124)
     1                                        I,CNAME(I)
   124                                     FORMAT(/' E',
     1                                     'NTER GUESS',
     2                                     ' FOR MOLAL',
     3                                     'ITY OF COM',
     4                                     'PONENT ',I2,
     5                                     ' (',A10,')')
                                           READ(5,*)
     1                                        GUES
                                           X(I)=
     1                                        DLOG(GUES)
   125                                     CONTINUE
                              ENDIF
                        ENDIF
                        ITCNT=1
   130                  DO 140 I=1,NRXNS
                              IF(GAMMA(I).LE.0.0)
     1                              GAMMA(I)=1.0
                              CONST(I) = EQKLN(I)-
     1                              DLOG(GAMMA(I))
   140                  CONTINUE
                        CALL SOLVE(NNN1,TOL1,JSAVE,
     1                        ITPRT,0)
                        CALL TOLER(NNN1,X,ITCNT,CC0,
     1                        GAMMA,TOL,J,ITOLF,KIT,
     2                        XOLD0,GSAVE0,ITPRT,
     3                        NRXNS,JSAVE,L,KOPT,0)
                        IF(ITOLF.EQ.1) GOTO 150
                        CALL GAMMAK(JSAVE,GAMMA,CHARGE,
     1                        X,CC0,NNN1,NNCNT)
                        ITCNT=ITCNT+1
                        GOTO 130
                  ENDIF
   150            JSAVE=1
                  IF(ITPRT.GT.0) THEN
                        WRITE(6,107) J
                        WRITE(13,107) J
                  ENDIF
                  ORCO2=CONCO2(L,J)
                  NNN2=NCOMP
                  KKK=KIT
                  JJJ=J
                  LLL=L
                  CALL GUESS(X,GAMMA,NRXNS,KITCNT,KIT,J,
     1                  KKK,JJJ,MINFLG,GSAVE,XOLD,NNN2,
     2                  LLL,L,JSAVE,IREP,0)
                  IF(NGUESS.EQ.1)THEN
                        WRITE(6,108) L,SYSID(L),
     1                        PERCEN(L),PRESS(L)
                        WRITE(6,151) J
   151                  FORMAT(/' FINAL COMPOSITION ',
     1                        'FOR POINT ',I3)
                        WRITE(6,111)
                        READ(5,*) IGUESS
                        IF(IGUESS.EQ.0) THEN
                              DO 160 I=1,NRXNS
                                 GAMMA(I)=
     1                                 GSAVE0(KKK,L,I,1)
   160                        CONTINUE
                              X(1)=DLOG(3.0D-09)
```

```
                                X(2)=DLOG(6.ØD-Ø4)
                                X(3)=DLOG(ORMDEA*Ø.95)
                                X(4)=DLOG(ORMDEA*Ø.Ø5)
                                X(5)=DLOG(ORCO2*Ø.Ø1)
                                X(6)=DLOG(ORCO2*Ø.82)
                                X(7)=DLOG(ORCO2*Ø.17)
                        ELSE
                                DO 165 I=1,NRXNS
                                        WRITE(6,164) I
164                                     FORMAT(' ENTER',
     1                                  ' GAMMA FOR RE',
     2                                  'ACTION ',I2)
                                        READ(5,*)
     1                                          GAMMA(I)
165                                 CONTINUE
                                DO 169 I=1,NNN2
                                        WRITE(6,124)
     1                                          I,CNAME(I)
                                        READ(5,*) GUES
                                        X(I)=DLOG(GUES)
169                                 CONTINUE
                        ENDIF
                ENDIF
                ITCNT=1
170             DO 180 I=1,NRXNS
                        IF(GAMMA(I).LE.Ø.Ø)
     1                          GAMMA(I)=1.Ø
                        CONST(I) = EQKLN(I)-
     1                          DLOG(GAMMA(I))
180             CONTINUE
                CALL SOLVE(NNN2,TOL1,JSAVE,ITPRT,Ø)
                CALL TOLER(NNN2,X,ITCNT,CC,GAMMA,TOL,J,
     1                  ITOLF,KIT,XOLD,GSAVE,ITPRT,
     2                  NRXNS,JSAVE,L,KOPT,Ø)
                IF(ITOLF.EQ.1) GOTO 300
                CALL GAMMAK(JSAVE,GAMMA,CHARGE,X,CC,
     1                  NNN2,NNCNT)
                ITCNT=ITCNT+1
                GOTO 170
300             IF(KOPT.EQ.1) THEN
                        EQPCO2(L,J)=14.696*CC(5)*GAMMA(
     1                      NRXNS)/DEXP(EQKLN(NRXNS))
                        IF(KOPTFL.EQ.1) GOTO 320
                        TOTML=CC(1)+CC(2)+CC(3)+CC(4)+
     1                          CC(5)+CC(6)+CC(7)+
     2                          1ØØØ.Ø/18.Ø152
                        XXMDEA=CC(3)/TOTML
                        XXH2O=(1ØØØ.Ø/18.Ø152)/TOTML
                        PMDEA=XXMDEA*VPMDEA
                        PH2O=XXH2O*VPH2O
                        PTOT=PMDEA+PH2O+EQPCO2(L,J)
                        IF(PTOT.GT.PRESS(L)) THEN
                                CC(5)=DEXP(EQKLN(NRXNS))
     1                                  *(PRESS(L)-PMDEA
     2                                  -PH2O)/
     3                                  GAMMA(NRXNS)
                                CC(8)=ORCO2-CC(5)-CC(6)
     1                                  -CC(7)
                                GOTO 320
                        ENDIF
                        CC(8)=Ø.Ø
                        GOTO 335
                ELSE
                        GOTO 350Ø
```

```
                      ENDIF
320                   NNN3=NCOMP+1
                      KKK=KIT
                      JJJ=J
                      LLL=L
                      CALL GUESS(X,GAMMA,NRXNS,KITCNT,KIT,J,
     1                        KKK,JJJ,MINFLG,GSAVE,XOLD,NNN3,
     2                        LLL,L,JSAVE,IREP,KOPTFL)
                      IF(KOPTFL.EQ.0) THEN
                              X(5)=DLOG(CC(5))
                              X(NRXNS+1)=DLOG(CC(NRXNS+1))
                              KOPTFL=1
                      ENDIF
                      ITCNT=1
325                   TOTML=0.0
                      DO 326 II=1,NRXNS
                              TOTML=TOTML+DEXP(X(II))
326                   CONTINUE
                      TOTML=TOTML+1000.0/18.0152
                      XXMDEA=DEXP(X(3))/TOTML
                      XXH2O=(1000.0/18.0152)/TOTML
                      PMDEA=XXMDEA*VPMDEA
                      PH2O=XXH2O*VPH2O
                      PCO2=PRESS(L)-PH2O-PMDEA
                      DO 330 I=1,NRXNS
                              IF(GAMMA(I).LE.0.0)
     1                                GAMMA(I)=1.0
                              CONST(I) = EQKLN(I)-
     1                                DLOG(GAMMA(I))
                              CONST(NRXNS)=EQKLN(NRXNS)-DLOG(
     1                                GAMMA(NRXNS))+DLOG(PCO2
     2                                /14.696)
330                   CONTINUE
                      CALL SOLVE(NNN3,TOL1,JSAVE,ITPRT,KOPTFL)
                      CALL TOLER(NNN3,X,ITCNT,CC,GAMMA,TOL,J,
     1                        ITOLF,KIT,XOLD,GSAVE,ITPRT,
     2                        NRXNS,JSAVE,L,KOPT,KOPTFL)
                      IF(ITOLF.EQ.1) GOTO 335
                      CALL GAMMAK(JSAVE,GAMMA,CHARGE,X,CC,
     1                        NNN3,NNCNT)
                      ITCNT=ITCNT+1
                      GOTO 325
335                   IF(CC(8).LE.0.0) THEN
                              CC(8)=0.0
                              VAPH2O=0.0
                              VAPMDE=0.0
                              GOTO 340
                      ENDIF
                      YH2O=PH2O/PRESS(L)
                      YMDEA=PMDEA/PRESS(L)
                      YCO2=PCO2/PRESS(L)
                      YTOT=CC(8)/YCO2
                      VAPH2O=YTOT*YH2O
                      VAPMDE=YTOT*YMDEA
340                   DELN(1)=CC(2)-CC0(2)
                      DELN(2)=CC(3)-CC0(3)
                      DELN(3)=CC(6)+CC(7)
                      DELN(4)=CC(7)
                      DELN(5)=ORCO2-CC(8)
                      THEAT=0.0
                      DO 345 JJ=1,NRXNS
                              HTJUN=DELN(JJ)*DELH(JJ)
                              THEAT=THEAT+DELN(JJ)*DELH(JJ)
345                   CONTINUE
```

```
                        THEAT=THEAT+VAPH2O*DELH2O+VAPMDE*DELHMD
                        BTU1(L,J)=THEAT*(100.0-PERCEN(L))/
     1                                  (PERCEN(L)*555.555556)
                        BTU2(L,J)=BTU1(L,J)*PUREMW/CO2MW/
     1                                  CO2(L,J)
                        GOTO 400
350                     DELN(1)=CC(2)-CC0(2)
                        DELN(2)=CC(3)-CC0(3)
                        DELN(3)=CC(6)+CC(7)
                        DELN(4)=CC(7)
                        DELNS(L,J)=DELN(NKEY)
                        SUMHT=0.0
                        DO 360 MM=1,NRXNS-1
                                IF(MM.NE.NKEY) THEN
                                        SUMHT=SUMHT
     1                                        +DELN(MM)*DELH(MM)
                                ENDIF
360                     CONTINUE
                        QCORR(L,J)=CHEAT(L,J)-SUMHT
                        SUMNUM=SUMNUM+(QCORR(L,J)*DELNS(L,J)
     1                          /NPTS(L))
                        SUMDEN=SUMDEN+(DELNS(L,J)*DELNS(L,J)
     1                          /NPTS(L))
400                     CONTINUE
500             CONTINUE
                IF(KOPT.EQ.1) THEN
                        CALL OUT1(NPTS,EQKLN,BTU,BTU1,EQPCO2,SYSID,
     1                          NNN1,NNN3,XSAV0,XSAV,CO2,DELH,NSETS,
     2                          NTOTAL,NRXNS,NKEY,INPRT,BTU2)
                        STOP
                ENDIF
                DELHC=SUMNUM/SUMDEN
510             SERNRM=0.0
                DO 525 L=1,NSETS
                        DO 520 J=1,NPTS(L)
                                ERRO=(QCORR(L,J)-DELNS(L,J)*DELHC)**2.
                                ERNORM=ERRO/NPTS(L)
                                SERNRM=SERNRM+ERNORM
520                     CONTINUE
525             CONTINUE
530             DELHS(KIT)=DELHC
                ERR(KIT)=SERNRM
                EQKLNS(KIT)=EQKLN(NKEY)
                IF(KOPT.EQ.0) THEN
                        MINFLG=1
                        CALL OUTPUT(NPTS,MINFLG,XCO2,DELHS,
     1                          EQKLNS,CHEAT,SYSID,ERR,NNN1,NNN2,
     2                          XOLD0,XOLD,CO2,DELH,CONCO2,
     3                          NSETS,NTOTAL,NRXNS,NKEY,INPRT)
                        WRITE(6,*) ' DO YOU WANT TO DO ANOTHER RUN ',
     1                          'WITH THIS DATA?'
                        READ(5,721) ANS
721                     FORMAT(A1)
                        IF (ANS.EQ.'Y'.OR.ANS.EQ.'y') THEN
                                GOTO 1
                        ELSE
                                STOP
                        ENDIF
                ENDIF
                NCNT=11*(KITCNT-1)+KIT
                IF(ITPRT.EQ.0) THEN
                        WRITE(6,540) NCNT,EQKLN(NKEY),DELHC,SERNRM
                        WRITE(13,540) NCNT,EQKLN(NKEY),DELHC,SERNRM
540                     FORMAT(16X,I3,3X,F8.4,3X,F9.2,3X,D11.5)
```

```
                ELSE
                        WRITE(6,545) NCNT,EQKLN(NKEY),DELHC,SERNRM
                        WRITE(13,545) NCNT,EQKLN(NKEY),DELHC,SERNRM
545             FORMAT(//10X,'SOLUTION REACHED FOR ITERATION ',
     1                  'NUMBER ',I3,' ON LN K'//20X,'RESULTS:'/,
     2                  20X,'LN K = ',F7.3,/20X,'DELTA H = ',F9.2/,
     3                  20X,'NORMALIZED SQUARE ERROR = ',D11.5)
                ENDIF
                IF(KIT.LE.5) THEN
                        EQKLN(NKEY)=EQKLN(NKEY)+DELINC
                ELSEIF(KIT.EQ.6) THEN
                        EQKLN(NKEY)=EQKLN(NKEY)-(DELINC*KIT)
                ELSE
                        EQKLN(NKEY)=EQKLN(NKEY)-DELINC
                ENDIF
700     CONTINUE
        IMIN=1
        ERRMIN=ERR(1)
        DO 720 I=1,11
                IF(ERR(I).LT.ERRMIN) THEN
                        IMIN=I
                        ERRMIN=ERR(I)
                ENDIF
720     CONTINUE
        MINFLG=IMIN
        IF(MINFLG.NE.6.AND.MINFLG.NE.11) THEN
                IF(DELINC.LT.0.0005) THEN
                        CALL OUTPUT(NPTS,MINFLG,XCO2,
     1                          DELHS,EQKLNS,CHEAT,SYSID,ERR,NNN1,NNN2,
     2                          XOLD0,XOLD,CO2,DELH,CONCO2,
     3                          NSETS,NTOTAL,NRXNS,NKEY,INPRT)
                        WRITE(6,*) ' DO YOU WANT TO DO ANOTHER RUN ',
     1                          'WITH THIS DATA?'
                        READ(5,721) ANS
                        IF (ANS.EQ.'Y'.OR.ANS.EQ.'y') THEN
                                GOTO 1
                        ELSE
                                STOP
                        ENDIF
                ENDIF
                DELINC=DELINC/5.0
        ENDIF
        EQKLN(NKEY)=EQKLNS(MINFLG)
        KKFLAG=0
        NCHNGS=0
        WRITE(6,722) EQKLN(NKEY),DELINC
722     FORMAT(//' FOR THE NEXT SET OF 11 ITERATIONS, THE STARTING VALUE',
     1          /5X,' FOR LN K WILL BE ',F8.4/5X,' INCREMENT WILL BE ',
     2          F6.4//10X,' IF THIS IS OK, ',
     3          'ENTER "0"'/10X,' OTHERWISE, ENTER "1"'/)
        READ(5,*) JJJJ
        IF(JJJJ.EQ.0) GOTO 729
723     WRITE(6,724) EQKLN(NKEY),DELINC
724     FORMAT(///' THE CURRENT VALUES OF LN K AND INCREMENT ARE:'//,
     1          5X,'LN K = ',F8.4/5X,'INCREMENT = ',F6.4//'IF YOU WISH',
     2          ' TO CHANGE THE STARTING VALUE FOR LN K, ENTER "-1"'/,
     3          'ENTER "1" TO CHANGE THE INCREMENT VALUE, "0" TO EXIT'/)
        READ(5,*) JJJJ
        IF(JJJJ.EQ.0) THEN
                IF(NCHNGS.EQ.0) GOTO 729
                KKFLAG=1
        ELSEIF(JJJJ.GT.0) THEN
                WRITE(6,*) 'ENTER NEW VALUE FOR INCREMENT'
                READ(5,*) DELINC
```

```
                GOTO 723
        ELSE
                SAVEK=EQKLN(NKEY)
                WRITE(6,*) ' ENTER VALUE FOR LN K'
                READ(5,*) EQKLN(NKEY)
                IF(SAVEK.NE.EQKLN(NKEY)) NCHNGS=1
                GOTO 723
        ENDIF
        DO 725 I=1,11
                DIFF(I)=DABS( EQKLN(NKEY)-EQKLNS(I) )
  725   CONTINUE
        KMIN=1
        DIFMIN=DIFF(1)
        DO 726 I=1,11
                IF(DIFF(I).LT.DIFMIN) THEN
                        KMIN=I
                        DIFMIN=DIFF(I)
                ENDIF
  726   CONTINUE
        MINFLG=KMIN
        GOTO 105
  729   DO 760 L=1,NSETS
                DO 730 I=1,NNN1
                        XOLD0(1,L,I,1)=XOLD0(MINFLG,L,I,1)
  730           CONTINUE
                GSAVE0(1,L,1,1)=GSAVE0(MINFLG,L,1,1)
                DO 745 I=1,NNN2
                        DO 740 J=1,NPTS(L)
                                XOLD(1,L,I,J)=XOLD(MINFLG,L,I,J)
  740                   CONTINUE
  745           CONTINUE
                DO 755 I=1,NRXNS
                        DO 750 J=1,NPTS(L)
                                GSAVE(1,L,I,J)=GSAVE(MINFLG,L,I,J)
  750                   CONTINUE
  755           CONTINUE
  760   CONTINUE
        DELHS(1)=DELHS(MINFLG)
        ERR(1)=ERR(MINFLG)
        SERNRM=ERR(MINFLG)
        EQKLNS(1)=EQKLNS(MINFLG)
        DELHC=DELHS(1)
        GOTO 105
  800   STOP
        END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                          C
C                          SUBROUTINE TOLER                                C
C                                                                          C
C       SUBROUTINE TOLER CHECKS FOR CONVERGENCE IN THE MOLAL               C
C       CONCENTRATIONS FOR EACH OF THE SPECIES IN SOLUTION.  THE           C
C       SUBROUTINE IS CALLED AFTER EACH TIME THE SOLVE SUBROUTINE          C
C       IS COMPLETED.  THE SOLVE SUBROUTINE RETURNS VALUES OF THE          C
C       MOLAL CONCENTRATIONS WHICH SATISFY THE SYSTEM OF EQUATIONS         C
C       DEFINED IN FIGURE 13.  THESE MOLAL CONCENTRATIONS ARE              C
C       CHECKED AGAINST THE CONCENTRATIONS CALCULATED IN THE PRE-          C
C       VIOUS PASS THROUGH THE SOLVE SUBROUTINE.  IF THE SPECIFIED         C
C       TOLERANCE IS MET, THEN THE MOLALITIES ARE STORED AND EXE-          C
C       CUTION OF THE PROGRAM CONTINUES.  IF THE TOLERANCE IS NOT          C
C       MET, THEN NEW VALUES OF THE ACTIVITY COEFFICIENT RATIOS            C
C       ARE CALCULATED AND SUBROUTINE SOLVE IS CALLED AGAIN.               C
C                                                                          C
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C               IDENTIFICATION AND DESCRIPTION OF ARRAYS NOT                   C
C                       INCLUDED IN MAIN PROGRAM                               C
C                                                                              C
C       CCC=MOLALITY (GMOLE/KG H2O) FOR EACH COMPONENT                         C
C       GGG=STORAGE FOR VALUES OF GAMMA                                        C
C       XXX=STORAGE FOR VALUES OF COMPONENT MOLALITIES                         C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C               IDENTIFICATION AND DESCRIPTION OF VARIBLES NOT                 C
C                       INCLUDED IN MAIN PROGRAM                               C
C                                                                              C
C       CNEW=THE CURRENT VALUES OF THE MOLAL CONCENTRATIONS OF                 C
C               EACH COMPONENT.                                                C
C       JJJ=FLAG STORING THE NUMERICAL VALUE OF THE DATA POINT                 C
C               BEING ANALYZED                                                 C
C       NNN=NUMBER OF SPECIES IN AQUEOUS SOLUTION FOR WHICH                    C
C               COMPOSITION IS DETERMINED                                      C
C       NTOL=NUMBER OF SPECIES FOR WHICH TOLERANCE IS MET                      C
C       TEST=PERCENT DIFFERNCE BETWEEN CURRENT MOLAL CONCENTRATION             C
C               AND THE CONCENTRATION FROM THE PREVIOUS PASS                   C
C               THROUGH THE PROGRAM                                            C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
      SUBROUTINE TOLER(NNN,X,ITCNT,CCC,GAMMA,TOL,J,ITOLF,KIT,XXX,GGG,
     1                 ITPRT,NRXNS,JSAVE,L,KOPT,KOPTFL)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TOL/ GAM(1,10,10,60),GAM0(1,10,10,1),XSAV(1,10,10,60),
     1          XSAV0(1,10,10,1)
      DIMENSION X(10),GAMMA(10),CCC(10),XXX(11,10,10,60),
     1          GGG(11,10,10,60)
      ITOLF=0
      IF(ITCNT.EQ.1) THEN
              IF(ITPRT.GT.0) THEN
                      WRITE(6,10) ITCNT
   10                 FORMAT(20X,'ITCNT = ',I2)
              ENDIF
              RETURN
      ENDIF
      NTOL=0
      DO 20 I=1,NNN
              CNEW=DEXP(X(I))
              TEST=DABS( (CNEW-CCC(I))/CCC(I) )
              IF(TEST.LE.TOL) NTOL=NTOL+1
   20 CONTINUE
      IF(ITPRT.GT.0) THEN
             WRITE(6,30) ITCNT,NTOL
   30         FORMAT(20X,'ITCNT = ',I2,'     NTOL = ',I1)
      ENDIF
      IF(JSAVE.EQ.0) THEN
              JJJ=1
      ELSE
              JJJ=J
      ENDIF
      IF(NTOL.EQ.NNN) THEN
              DO 35 I=1,NNN
                      IF(KOPTFL.NE.1) THEN
```

```
                        XXX(KIT,L,I,JJJ)=X(I)
                ENDIF
                CCC(I)=DEXP(X(I))
                IF(KOPT.EQ.1) THEN
                        IF(JSAVE.EQ.Ø) THEN
                                XSAVØ(1,L,I,JJJ)=X(I)
                        ELSE
                                XSAV(1,L,I,JJJ)=X(I)
                        ENDIF
                ENDIF
 35         CONTINUE
            DO 4Ø I=1,NRXNS
                IF(KOPTFL.NE.1) THEN
                        GGG(KIT,L,I,JJJ)=GAMMA(I)
                ENDIF
                IF(KOPT.EQ.1) THEN
                        IF(JSAVE.EQ.Ø) THEN
                                GAMØ(1,L,I,JJJ)=GAMMA(I)
                        ELSE
                                GAM(1,L,I,JJJ)=GAMMA(I)
                        ENDIF
                ENDIF
 4Ø         CONTINUE
            IF(ITPRT.GT.Ø) THEN
                WRITE(6,45) ITCNT
                WRITE(13,45) ITCNT
 45             FORMAT(2ØX,'SOLUTION REACHED AFTER ',I2,
     1                  ' ITERATIONS'/)
                IF(ITPRT.EQ.2) THEN
                        WRITE(6,5Ø)
                        WRITE(13,5Ø)
 5Ø                     FORMAT(2ØX,'GAMMA(I)',5X,'CCC(I)',7X,
     1                          'X(I)'//)
                        WRITE(6,55) (GAMMA(I),CCC(I),X(I),
     1                                  I=1,NNN)
                        WRITE(13,55) (GAMMA(I),CCC(I),X(I),
     1                                  I=1,NNN)
 55                     FORMAT((2ØX,F8.6,3X,D12.6,2X,F9.5))
                ENDIF
            ENDIF
            ITOLF=1
        ENDIF
        RETURN
        END

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                      C
C                       SUBROUTINE GUESS                               C
C                                                                      C
C       SUBROUTINE GUESS ESTABLISHES GUESSES FOR THE VALUES OF THE     C
C       ACTIVITY COEFFICIENT RATIONS AND THE MOLALITIES OF EACH        C
C       COMPONENT FOR EACH DATA POINT IN THE INPUT DATA FILE.          C
C       THE GUESSES ARE ALL FROM PREVIOUS SOLUTIONS: EITHER SOLU-      C
C       TIONS FOR THE IDENTICAL DATA POINT WITH A DIFFERENT VALUE      C
C       OF ln K OR SOLUTIONS FOR DIFFERENT DATA POINTS WITH IDEN-      C
C       TICAL VALUES OF ln K.                                          C
C                                                                      C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                      C
C               IDENTIFICATION AND DESCRIPTION OF ARRAYS               C
C                       NOT INCLUDED IN MAIN PROGRAM                   C
C                                                                      C
C       DIFF=DIFFERENCE BETWEEN THE STOICHIOMETRIC MOLALITY OF         C
```

```
C               MDEA FOR THE CURRENT DATA SET AND THE STOICHIO-          C
C               METRIC MOLALITY OF MDEA FOR THE PREVIOUS DATA SETS       C
C       GGG=STORAGE FOR VALUES OF GAMMA                                  C
C       XXX=STORAGE FOR VALUES OF COMPONENT MOLALITIES                   C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                        C
C               IDENTIFICATION AND DESCRIPTION OF VARIABLES              C
C                       NOT INCLUDED IN MAIN PROGRAM                     C
C                                                                        C
C       DIF=DIFFERENCE BETWEEN THE STOICHIOMETRIC MOLALITY OF            C
C               CO2 FOR THE CURRENT DATA SET AND THE STOICHIO-           C
C               METRIC MOLALITY OF CO2 FOR EACH OF THE PREVIOUS          C
C               DATA POINTS AND DATA SETS                                C
C       DIFMIN=MINIMUM VALUE OF ARRAY DIFF OR OF THE VARIOUS             C
C               VALUES OF DIF                                            C
C       JMIN=DATA POINT NUMBER WHICH PRODUCES DIFMIN THE MINIMUM         C
C               VALUE OF DIF                                             C
C       KFLAG=KOPTFL IN MAIN PROGRAM                                     C
C       LMIN=DATA SET NUMBER WHICH PRODUCES DIFMIN, THE MINIMUM          C
C               OF DIF                                                   C
C       NNN=NUMBER OF COMPONENTS FOR WHICH A MOLALITY GUESS IS           C
C               TO BE MADE                                               C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      SUBROUTINE GUESS(X,GAMMA,NRXNS,KITCNT,KIT,J,KKK,JJJ,MINFLG,GGG,
     1                 XXX,NNN,LLL,L,JSAVE,IREP,KFLAG)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TOL/ GAM(1,10,10,60),GAM0(1,10,10,1),XSAV(1,10,10,60),
     1       XSAV0(1,10,10,1)
      COMMON /GS/ NGUESS,CONCO2(10,60),CONMDE(10),NPTS(10)
      DIMENSION GGG(11,10,10,60),XXX(11,10,10,60),DIFF(10),X(10),
     1                 GAMMA(10)
      NGUESS=0
      IF(KITCNT.EQ.1) THEN
              IF(KIT.EQ.1) THEN
                      IF(IREP.GT.1) THEN
                              KKK=MINFLG
                              GOTO 29
                      ENDIF
                      IF(L.EQ.1) THEN
                              IF(J.EQ.1) THEN
                                      NGUESS=1
                                      RETURN
                              ELSE
                                      JJJ=J-1
                              ENDIF
                      ELSE
                              IF(J.EQ.1) THEN
                                      IF(JSAVE.EQ.0) THEN
                                              DO 5 I=1,L-1
                                                      DIFF(I)=DABS(
     1                                                  CONMDE(I)-
     2                                                  CONMDE(L))
     5                                        CONTINUE
                                              LMIN=1
                                              DIFMIN=DIFF(1)
                                              DO 10 I=1,L-1
                                                      IF(DIFF(I).LT.
     1                                                  DIFMIN) THEN
                                                              LMIN=I
                                                              DIFMIN=
```

```
     1                                                        DIFF(I)
                                                    ENDIF
    10                                          CONTINUE
                                                IF(DIFMIN.LE.0.01)THEN
                                                    LLL=LMIN
                                                ELSE
                                                    NGUESS=1
                                                    RETURN
                                                ENDIF
                                            ELSE
                                               LMIN=0
                                               JMIN=0
                                               DIFMIN=1000.0
                                               DO 25 I=1,L-1
                                                  IF(DIFF(I).LE.0.01) THEN
                                                     DO 15 JCNT=1,NPTS(I)
                                                       DIF=DABS(CONC02(I,JCNT)-
     2                                                      CONC02(L,J))
                                                       IF(DIF.LT.DIFMIN)
     1                                                                THEN
                                                          LMIN=I
                                                          JMIN=JCNT
                                                          DIFMIN=DIF
                                                       ENDIF
    15                                                CONTINUE
                                                  ENDIF
    25                                            CONTINUE
                                                  IF(JMIN.EQ.0.AND.LMIN.EQ.0)
     1                                                      THEN
                                                     NGUESS=1
                                                     RETURN
                                                  ELSE
                                                     LLL=LMIN
                                                     JJJ=JMIN
                                                  ENDIF
                                            ENDIF
                                 ELSE
                                            JJJ=J-1
                                 ENDIF
                        ENDIF
                ELSEIF(KIT.EQ.7) THEN
                        KKK=1
                ELSE
                        KKK=KIT-1
                ENDIF
        ELSE
                IF(KIT.EQ.1) THEN
                        KKK=MINFLG
                ELSEIF(KIT.EQ.7) THEN
                        KKK=1
                ELSE
                        KKK=KIT-1
                ENDIF
        ENDIF
    29  DO 30 I=1,NRXNS
                GAMMA(I)=GGG(KKK,LLL,I,JJJ)
                IF(KFLAG.EQ.1) THEN
                        GAMMA(I)=GAM(KKK,LLL,I,JJJ)
                ENDIF
    30  CONTINUE
        DO 40 I=1,NNN
                X(I)=XXX(KKK,LLL,I,JJJ)
                IF(KFLAG.EQ.1) THEN
                        X(I)=XSAV(KKK,LLL,I,JJJ)
```

```
            ENDIF
 40   CONTINUE
      RETURN
      END


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                        SUBROUTINE OUTPUT                                     C
C                                                                              C
C       SUBROUTINE OUTPUT IS CALLED AFTER THE FINAL SOLUTION IS                C
C       CALCULATED.  IT SIMPLY CREATES THE FINAL OUTPUT FOR                    C
C       OPTIONS -1 AND Ø (KOPT=-1, KOPT=Ø)                                     C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                DESCRIPTION AND IDENTIFICATION OF ARRAYS                      C
C                        NOT INCLUDED IN MAIN PROGRAM                          C
C                                                                              C
C       CM=VALUES OF MOLALITIES FOR EACH COMPONENT FOR EACH DATA               C
C                POINT FOR EACH DATA SET.  CALCULATED FROM VALUES              C
C                OF ln K AND DELTA H WHICH GIVE MIMIMUM ERROR                  C
C                SQUARE SUM                                                    C
C       CONTR=PERCENTAGE OF TOTAL HEAT ATTRIBUTABLE TO EACH OF                 C
C                THE REACTIONS FOR EACH DATA POINT IN EACH DATA                C
C                SET                                                           C
C       DELN=DELTA N FOR EACH COMPONENT FOR A SPECIFIC DATA POINT              C
C       DLOAD=VALUES OF CO2 LOADING (GMOLE CO2/GMOLE MDEA)                     C
C       FRAC=PERCENTAGE OF ORIGINAL CO2 EXISTING AS AQUEOUS CO2,               C
C                BICARBONATE ION, AND CARBONATE ION; PERCENTAGE                C
C                OF ORIGINAL MDEA EXISTING AS AQUEOUS MDEA AND                 C
C                PROTONATED MDEA                                               C
C       HTCALC=CORRECTED HEAT OF SOLUTION CALCULATED BY EQUATION 8             C
C                EXCLUDING THE CO2 ABSORPTION REACTION                         C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                DESCRIPTION AND IDENTIFICATION OF VARIABLES                   C
C                        NOT INCLUDED IN MAIN PROGRAM                          C
C                                                                              C
C       AVGRD=AVERAGE RELATIVE DEVIATION OF THE CALCULATED HEATS               C
C                OF SOLUTION FROM THE EXPERIMENTALLY MEASURED                  C
C                HEATS OF SOLUTION FOR A SINGLE DATA SET                       C
C       DENOM1=SUM OF MOLALITIES OF MDEA AND PROTONATED MDEA;                  C
C                ORIGINAL MDEA MOLALITY                                        C
C       DENOM2=SUM OF MOLALITIES OF AQUEOUS CO2, AQUEOUS BICAR-                C
C                BONATE ION, AND AQUEOUS CARBONATE ION; ORIGINAL               C
C                CO2 MOLALITY                                                  C
C       E=RELATIVE DEVIATION OF THE CALCULATED HEAT OF SOLUTION                C
C                FROM THE EXPERIMENTALLY DETERMINED HEAT OF SOLUTION           C
C                FOR A SINGLE DATA POINT                                       C
C       ORIG1=ORIGINAL CONCENTRATION OF OH- IN SOLUTION                        C
C       ORIG2=ORIGINAL CONCENTRATION OF MDEA IN SOLUTION                       C
C       ORIG3=ORIGINAL CONCENTRATION OF BICARBONATE IN SOLUTION                C
C       ORIG4=ORIGINAL CONCENTRATION OF CARBONATE IN SOLUTION                  C
C       SSUME=TOTAL SUM OF THE RELATIVE DEVIATIONS FOR EACH DATA               C
C                POINT AND EACH DATA SET                                       C
C       TMRD=TOTAL MEAN RELATIVE DEVIATION; THE AVERAGE OF THE                 C
C                RELATIVE DEVIATIONS OVER ALL DATA POINTS AND                  C
C                ALL DATA SETS (SSUME/TOTAL # DATA POINTS)                     C
C       TOTHTC=OVERALL HEAT OF SOLUTION GIVEN BY EQUATION 8                    C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
      SUBROUTINE OUTPUT(NPTS,MINFLG,XCO2,DELHS,EQKLNS,
     1          CHEAT,SYSID,ERR,NNN1,NNN2,XOLDØ,XOLD,CO2,DELH,
     2          CONCO2,NSETS,NTOTAL,NRXNS,NKEY,INPRT)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION XCO2(1Ø,6Ø),DELHS(11),DLOAD(1Ø,61),
     1          CM(1Ø,1Ø,61),DELH(1Ø),EQKLNS(11),CHEAT(1Ø,6Ø),
     2          ERR(11),XOLDØ(11,1Ø,1Ø,1),DELN(1Ø),XOLD(11,1Ø,1Ø,6Ø),
     3          CO2(1Ø,6Ø),CONCO2(1Ø,6Ø),FRAC(1Ø,1Ø,61),SYSID(1Ø),
     4          NPTS(1Ø),CONTR(1Ø,1Ø,6Ø),HTCALC(6Ø)
      WRITE(6,1) EQKLNS(MINFLG),DELHS(MINFLG),ERR(MINFLG)
      WRITE(13,1) EQKLNS(MINFLG),DELHS(MINFLG),ERR(MINFLG)
    1 FORMAT('1',41X,'SOLUTION REACHED'///37X,'LN K         :  ',
     1          F8.4/37X,'DELTA H      :  ',F9.2/37X,'NORM. SQ. ERR.:  ',
     2          D11.5////41X,'SUMMARY OF DATA FIT'///,
     3          4X,'       EXPERIMENTAL   CALCULATED                ',
     3             'PERCENT CONTRIBUTION TO TOTAL HEAT OF SOLUTION'/,
     4          4X,'           HEAT OF        HEAT OF                 '/,
     5          4X,'         SOLUTION       SOLUTION       PERCENT    '/,
     6          4X,'POINT  (CAL/KG H2O)   (CAL/KG H2O)      ERROR    ',
     7                '   RXN1      RXN2      RXN3      RXN4      RXN5')
      DO 21Ø L=1,NSETS
              DO 2ØØ J=1,NPTS(L)
                      IF(J.EQ.1) THEN
                              DLOAD(L,J)=Ø.Ø
                              DO 15Ø KK=1,NNN2
                                      IF(KK.LE.NNN1) THEN
                                              CM(L,KK,J)=DEXP(XOLDØ
     1                                                (MINFLG,L,KK,J))
                                      ELSE
                                              CM(L,KK,J)=Ø.Ø
                                      ENDIF
15Ø                                   CONTINUE
                      ENDIF
                      DLOAD(L,J+1)=CO2(L,J)
                      DO 175 KK=1,NNN2
                              CM(L,KK,J+1)=DEXP(XOLD(MINFLG,L,KK,J))
175                   CONTINUE
2ØØ           CONTINUE
21Ø   CONTINUE
      SSUME=Ø.Ø
      DO 3ØØ L=1,NSETS
              SUME=Ø.Ø
              DO 26Ø J=1,NPTS(L)
                      IF(J.EQ.1) THEN
                              ORIG1=CM(L,2,J)
                              ORIG2=CM(L,3,J)
                              ORIG3=Ø.Ø
                              ORIG4=Ø.Ø
                              WRITE(6,215) L
                              WRITE(13,215) L
215                           FORMAT(/42X,'DATA SET NUMBER ',I2/)
                      ENDIF
                      DELN(1)=CM(L,2,J+1)-ORIG1
                      DELN(2)=CM(L,3,J+1)-ORIG2
                      DELN(3)=CM(L,6,J+1)+CM(L,7,J+1)-ORIG3
                      DELN(4)=CM(L,7,J+1)-ORIG4
                      HTCALC(J)=Ø.Ø
                      DO 22Ø MM=1,NRXNS-1
                              IF(MM.NE.NKEY) THEN
                                      HTCALC(J)=HTCALC(J)+
     1                                        DELN(MM)*DELH(MM)
                              ELSE
```

```
                                        HTCALC(J)=HTCALC(J)+
     1                                          DELHS(MINFLG)*
     2                                          DELN(NKEY)
                             ENDIF
  220                    CONTINUE
                         E=((HTCALC(J)-CHEAT(L,J))/CHEAT(L,J))*100.0
                         SUME=SUME+DABS(E)
                         TOTHTC=HTCALC(J)+CONCO2(L,J)*DELH(NRXNS)
                         CONTR(L,NRXNS,J)=100.0
                         DO 230 MM=1,NRXNS-1
                                 IF(MM.NE.NKEY) THEN
                                         CONTR(L,MM,J)=100.0*DELN(MM)*
     1                                          DELH(MM)/TOTHTC
                                 ELSE
                                         CONTR(L,MM,J)=100.0*DELN(NKEY)*
     1                                          DELHS(MINFLG)/TOTHTC
                                 ENDIF
                                 CONTR(L,NRXNS,J)=CONTR(L,NRXNS,J)-
     1                                  CONTR(L,MM,J)
  230                    CONTINUE
                         WRITE(6,250) J,CHEAT(L,J),HTCALC(J),E,
     1                           (CONTR(L,I,J),I=1,NRXNS)
                         WRITE(13,250) J,CHEAT(L,J),HTCALC(J),E,
     1                           (CONTR(L,I,J),I=1,NRXNS)
  250                    FORMAT(5X,I3,4X,F10.2,4X,F10.2,4X,F8.3,2X,
     1                           5(3X,F6.2))
  260            CONTINUE
                 AVGRD=SUME/NPTS(L)
                 WRITE(6,265) AVGRD
                 WRITE(13,265) AVGRD
  265            FORMAT(//,28X,'MEAN OF THE ABSOLUTE PERCENT ERROR IS ',
     1                   F9.4//)
                 SSUME=SSUME+SUME
                 WRITE(9,270) SYSID(L),NPTS(L),2
  270            FORMAT(1X,'MOLE FRACTION CO2 VS. ',
     1                   'Q FOR RUN ',A4/1X,I3,', ',I1)
                 WRITE(9,275)(XCO2(L,II),CHEAT(L,II),II=1,NPTS(L))
  275            FORMAT (2X,F7.5,',  ',F9.1)
                 WRITE(9,280)
  280            FORMAT()
                 WRITE(9,275)(XCO2(L,II),HTCALC(II),II=1,NPTS(L))
                 WRITE(9,280)
  300    CONTINUE
         TMRD=SSUME/NTOTAL
         WRITE(6,310) TMRD
         WRITE(13,310) TMRD
  310    FORMAT(///,28X,'TOTAL MEAN OF THE PERCENT ERROR IS ',F9.4)
         IF(INPRT.NE.0) WRITE(6,340)
         WRITE(13,340)
  340    FORMAT(//'1',33X,'COMPOSITIONS FOR EACH DATA POINT'///,
     1          39X,'COMPONENT 1:  [H+]'/39X,'COMPONENT 2:  [OH-]'/,
     2          39X,'COMPONENT 3:  [MDEA]'/39X,'COMPONENT 4:  [MDEAH+]',
     3          /39X,'COMPONENT 5:  [CO2]'/39X,'COMPONENT 6:  [HCO3-]'/,
     4          39X,'COMPONENT 7:  [CO3-2]'//,
     5          2X,'LOADING',31X,'MOLALITY (GMOLE/KG H2O)'//,
     6          1X,'MOLE CO2'/1X,'---------'/1X,'MOLE MDEA',6X,'1',12X,
     7          '2',12X,'3',12X,'4',12X,'5',12X,'6',12X,'7')
        DO 401 L=1,NSETS
                 DO 400 J=1,NPTS(L)
                         IF(J.EQ.1) THEN
                                 IF(INPRT.NE.0) WRITE(6,215) L
                                 WRITE(13,215) L
                                 IF(INPRT.NE.0) WRITE(6,380) DLOAD(L,J),
     1                                  (CM(L,I,J),I=1,NNN2)
```

```
                        WRITE(13,380) DLOAD(L,J),
     1                            (CM(L,I,J),I=1,NNN2)
                    ENDIF
                    IF(INPRT.NE.0) WRITE(6,380) DLOAD(L,J+1),
     1                        (CM(L,I,J+1),I=1,NNN2)
                    WRITE(13,380) DLOAD(L,J+1),(CM(L,I,J+1),
     1                        I=1,NNN2)
 380                FORMAT(2X,F7.5,10(2X,D11.5))
 400            CONTINUE
 401    CONTINUE
        WRITE(13,405)
 405    FORMAT('1')
        DO 605 L=1,NSETS
            DO 580 J=1,NPTS(L)
                IF(J.EQ.1) THEN
                    DO 570 I=1,NNN2-2
                        IF(I.LE.2) THEN
                            DENOM1=CM(L,3,J)+
     1                              CM(L,4,J)
                            FRAC(L,1,J)=100.0*
     1                              CM(L,3,J)/DENOM1
                            FRAC(L,2,J)=100.0-
     1                              FRAC(L,1,J)
                        ELSE
                            FRAC(L,I,J)=0.00
                        ENDIF
 570                CONTINUE
                ENDIF
                DENOM1=CM(L,3,J+1)+CM(L,4,J+1)
                DENOM2=CM(L,5,J+1)+CM(L,6,J+1)+CM(L,7,J+1)
                FRAC(L,1,J+1)=100.0*CM(L,3,J+1)/DENOM1
                FRAC(L,2,J+1)=100.0-FRAC(L,1,J+1)
                FRAC(L,3,J+1)=100.0*CM(L,5,J+1)/DENOM2
                FRAC(L,4,J+1)=100.0*CM(L,6,J+1)/DENOM2
                FRAC(L,5,J+1)=100.0-FRAC(L,3,J+1)-FRAC(L,4,J+1)
 580        CONTINUE
            WRITE(1,585) SYSID(L),NPTS(L)+1,NNN2-2
 585        FORMAT(' LOADING VS. COMPOSITION FOR ',
     1             'SYSTEM ',A4/1X,I3,', ',I3)
            DO 595 I=1,NNN2-2
                WRITE(1,590) (DLOAD(L,N),FRAC(L,I,N),
     1                    N=1,NPTS(L)+1)
 590            FORMAT(3X,F9.6,',   ',F10.6)
                WRITE(1,280)
 595        CONTINUE
 605    CONTINUE
 610    RETURN
        END


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                     C
C                        SUBROUTINE OUT1                              C
C                                                                     C
C       SUBROUTINE OUT1 IS CALLED FOR PROGRAM OPTION 1 TO CREATE      C
C       THE FINAL OUTPUT                                              C
C                                                                     C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                     C
C               DESCRIPTION AND IDENTIFICATION OF ARRAYS              C
C                     NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                     C
```

```
C       BTUCO2=EXPERIMENTAL HEAT OF SOLUTION IN UNITS OF BTU/LB CO2      C
C       CM=VALUES OF MOLALITIES FOR EACH COMPONENT FOR EACH DATA         C
C               POINT FOR EACH DATA SET                                  C
C       DLOAD=VALUES OF CO2 LOADING (GMOLE CO2/GMOLE MDEA)               C
C       PTLOAD=LOADING POINT FOR EACH DATA SET                           C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                        C
C                DESCRIPTION AND IDENTIFICATION OF VARIABLES             C
C                        NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                        C
C       AVGRD=AVERAGE RELATIVE DEVIATION OF THE CALCULATED HEATS         C
C               OF SOLUTION FROM THE EXPERIMENTALLY MEASURED HEATS       C
C               OF SOLUTION FOR A SINGLE DATA SET                        C
C       E=RELATIVE DEVIATION OF THE CALCULATED HEAT OF SOLUTION          C
C               FROM THE EXPERIMENTALLY DETERMINED HEAT OF SOLUTION      C
C               FOR A SINGLE DATA POINT                                  C
C       SSUME=TOTAL SUM OF THE RELATIVE DEVIATIONS FOR EACH DATA         C
C               POINT AND EACH DATA SET                                  C
C       SUME=SUM OF THE RELATIVE DEVIATIONS (E) FOR EACH DATA            C
C               POINT FOR A SINGLE DATA SET                              C
C       TMRD=TOTAL MEAN RELATIVE DEVIATION; THE AVERAGE OF THE REL-      C
C               ATIVE DEVIATIONS OVER ALL DATA POINTS AND ALL            C
C               DATA SETS                                                C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
      SUBROUTINE OUT1(NPTS,EQKLN,BTU,BTU1,EQPCO2,SYSID,NNN1,NNN3,
     1          XSAVØ,XSAV,CO2,DELH,NSETS,NTOTAL,NRXNS,NKEY,INPRT,BTU2)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION DELH(1Ø),DLOAD(1Ø,61),BTU2(1Ø,6Ø),PTLOAD(1Ø),
     1          CM(1Ø,1Ø,61),EQKLN(1Ø),CO2(1Ø,6Ø),SYSID(1Ø),
     2          XSAVØ(1,1Ø,1Ø,1),XSAV(1,1Ø,1Ø,6Ø),BTUCO2(6Ø),
     4          NPTS(1Ø),BTU(1Ø,6Ø),BTU1(1Ø,6Ø),EQPCO2(1Ø,6Ø)
      WRITE(6,1) EQKLN(NKEY),DELH(NKEY)
      WRITE(13,1) EQKLN(NKEY),DELH(NKEY)
    1 FORMAT('1',56X,'MDEA PROTONATION'///52X,'LN K        :  ',
     1          F8.4/52X,'DELTA H     :  ',F9.2,
     2          ////49X,'SUMMARY OF FIT FOR LOADING CURVE'///,
     3          17X,'LOADING'/1Ø1X,'EQUILIBRIUM'/,
     4          8X,'         MOLE CO2    EXPERIMENTAL     CALCULATED  ',
     5                '   EXPERIMENTAL    CALCULATED',
     6                '                 PRESSURE'/,
     6          8X,'         ---------   HEAT OF SOLN    HEAT OF SOLN ',
     7                '   HEAT OF SOLN   HEAT OF SOL',
     7                   'N   RELATIVE     OF CO2'/,
     8          8X,'POINT    MOLE MDEA   (BTU/LB MDEA)   (BTU/LB MDEA)',
     9                '   (BTU/LB CO2)   (BTU/LB CO2',
     9                   ')     ERROR       (PSIA)')
      DO 21Ø L=1,NSETS
              PTLOAD(L)=Ø.Ø
              DO 2ØØ J=1,NPTS(L)
                      IF(J.EQ.1) THEN
                              DLOAD(L,J)=Ø.Ø
                              DO 15Ø KK=1,NNN3
                                      IF(KK.LE.NNN1) THEN
                                              CM(L,KK,J)=DEXP(XSAVØ
     1                                                 (1,L,KK,J))
                                      ELSE
                                              CM(L,KK,J)=Ø.Ø
                                      ENDIF
```

```
150                         CONTINUE
                        ENDIF
                        DLOAD(L,J+1)=CO2(L,J)
                        DO 175 KK=1,NNN3
                                IF(XSAV(1,L,KK,J).EQ.0.0) THEN
                                        CM(L,KK,J+1)=0.0
                                ELSE
                                        CM(L,KK,J+1)=DEXP(XSAV
   1                                            (1,L,KK,J))
                                ENDIF
175                     CONTINUE
                        IF(PTLOAD(L).EQ.0.0) THEN
                                IF(CM(L,NNN3,J+1).GT.0.0.AND.CM(L,NNN3,
   1                                 J).GT.0.0) THEN
                                        PTLOAD(L)=DLOAD(L,J)+(DLOAD(L,
   1                                            J)-DLOAD(L,J+1))*(-1.0*
   2                                            CM(L,NNN3,J)/(CM(L,NNN3,
   3                                            J)-CM(L,NNN3,J+1)))
                                ENDIF
                        ENDIF
200             CONTINUE
210     CONTINUE
        SSUME=0.0
        DO 300 L=1,NSETS
                SUME=0.0
                WRITE(6,215) L
                WRITE(13,215) L
215             FORMAT(/51X,'DATA SET NUMBER ',I2/)
                DO 260 J=1,NPTS(L)
                        BTUCO2(J)=BTU(L,J)*119.163/44.0099/CO2(L,J)
                        E=((BTU1(L,J)-BTU(L,J))/BTU(L,J))*100.0
                        SUME=SUME+DABS(E)
                        WRITE(6,250) J,CO2(L,J),BTU(L,J),BTU1(L,J),
   1                            BTUCO2(J),BTU2(L,J),E,EQPCO2(L,J)
                        WRITE(13,250) J,CO2(L,J),BTU(L,J),BTU1(L,J),
   1                            BTUCO2(J),BTU2(L,J),E,EQPCO2(L,J)
250                     FORMAT(9X,I3,4X,F9.6,7X,F7.2,9X,F7.2,9X,F7.2,
   1                            8X,F7.2,6X,F7.2,4X,F8.2)
260             CONTINUE
                WRITE(6,263) PTLOAD(L)
                WRITE(13,263) PTLOAD(L)
263             FORMAT(//43X,'THE LOADING POINT IS ',F8.5)
                AVGRD=SUME/NPTS(L)
                WRITE(6,265) AVGRD
                WRITE(13,265) AVGRD
265             FORMAT(//,38X,'MEAN OF THE ABSOLUTE PERCENT ERROR IS ',
   1                    F9.4//)
                SSUME=SSUME+SUME
                WRITE(10,270) SYSID(L),NPTS(L)+1,2
270             FORMAT(1X,'LOADING VS. ',
   1                    'Q FOR RUN ',A4/1X,I3,', ',I1)
                WRITE(10,274)
274             FORMAT(2x,'0.00000,  0.0000')
                WRITE(10,275)(CO2(L,II),BTU(L,II),II=1,NPTS(L))
275             FORMAT (2X,F7.5,',  ',F9.1)
                WRITE(10,280)
280             FORMAT()
                WRITE(10,274)
                WRITE(10,275)(CO2(L,II),BTU1(L,II),II=1,NPTS(L))
                WRITE(10,280)
                WRITE(11,285) SYSID(L),NPTS(L),2
285             FORMAT(1X,'LOADING VS. ',
   1                    'Q FOR RUN ',A4/1X,I3,', ',I1)
                WRITE(11,275)(CO2(L,II),BTUCO2(II),II=1,NPTS(L))
```

```
                WRITE(11,280)
                WRITE(11,275)(CO2(L,II),BTU2(L,II),II=1,NPTS(L))
                WRITE(11,280)
  300   CONTINUE
        TMRD=SSUME/NTOTAL
        WRITE(6,310) TMRD
        WRITE(13,310) TMRD
  310   FORMAT(///,28X,'TOTAL MEAN OF THE PERCENT ERROR IS ',F9.4)
        IF(INPRT.NE.0) WRITE(6,340)
        WRITE(13,340)
  340   FORMAT(//'1',33X,'COMPOSITIONS FOR EACH DATA POINT'///,
     1          39X,'COMPONENT 1:  [H+]'/39X,'COMPONENT 2:  [OH-]'/,
     2          39X,'COMPONENT 3:  [MDEA]'/39X,'COMPONENT 4:  [MDEAH+]',
     3          /39X,'COMPONENT 5:  [CO2]'/39X,'COMPONENT 6:  [HCO3-]'/,
     4          39X,'COMPONENT 7:  [CO3-2]'/39X,'COMPONENT 8:  CO2(G)'/,
     5          2X,'LOADING',31X,'MOLALITY (GMOLE/KG H2O)'//,
     6          1X,'MOLE CO2'/1X,'---------'/1X,'MOLE MDEA',6X,'1',12X,
     7          '2',12X,'3',12X,'4',12X,'5',12X,'6',12X,'7',12X,'8')
        DO 401 L=1,NSETS
                DO 400 J=1,NPTS(L)
                        IF(J.EQ.1) THEN
                                IF(INPRT.NE.0) WRITE(6,215) L
                                WRITE(13,215) L
                                IF(INPRT.NE.0) WRITE(6,380) DLOAD(L,J),
     1                                  (CM(L,I,J),I=1,NNN3)
                                WRITE(13,380) DLOAD(L,J),
     1                                  (CM(L,I,J),I=1,NNN3)
                        ENDIF
                        IF(INPRT.NE.0) WRITE(6,380) DLOAD(L,J+1),
     1                          (CM(L,I,J+1),I=1,NNN3)
                        WRITE(13,380) DLOAD(L,J+1),(CM(L,I,J+1),
     1                          I=1,NNN3)
  380                   FORMAT(2X,F7.5,10(2X,D11.5))
  400           CONTINUE
  401   CONTINUE
  610   RETURN
        END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                         SUBROUTINE GAMMAK                                    C
C                                                                              C
C       SUBROUTINE GAMMAK CALCULATES THE ACTIVITY COEFFICIENT RATIOS           C
C       FOR EACH OF THE REACTIONS FROM VALUES OF TEMPERATURE AND               C
C       COMPONENT MOLALITIES                                                   C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C               DESCRIPTION AND IDENTIFICATION OF ARRAYS                       C
C                       NOT INCLUDED IN MAIN PROGRAM                           C
C                                                                              C
C       CCC=COMPONENT MOLALITIES                                               C
C       Q=CONSTANTS USED TO CALCULATED THE ACTIVITIY COEFFICIENT               C
C               RATIOS FOR THE CO2 ABSORPTION REACTION                         C
C       RATIO=ACTIVITY COEFFICIENT RATIO                                       C
C       SUMP=TEMPERATURE DEPENDENT CONSTANT USED IN CALCULATING THE            C
C               ACTIVITY COEFFICIENT RATIOS FOR REACTIONS 1, 3, AND 4          C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
C                                                                       C
C               DESCRIPTION AND IDENTIFICATION OF VARIABLES             C
C                       NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                       C
C       ALPHA=CONSTANT USED TO CALCULATE DEBYE-HUCKEL TERM USED         C
C               TO CALCULATE GAMMAK FOR REACTIONS 1, 3, AND 4           C
C       BEE=CONSTANT USED IN CALCULATION OF THE OSMOTIC COEFFICIENT     C
C       BETA=CONSTANT USED IN CALCULATING THE DEBYE-HUCKEL TERM         C
C               OF THE ACTIVITY COEFFICIENT RATIOS                      C
C       CEE=CONSTANT USED IN CALCULATION OF THE OSMOTIC COEFFICIENT     C
C       DH=DEBYE-HUCKEL TERM                                            C
C       DIELEC=DIELECTRIC CONSTANT                                      C
C       FEE=CONSTANT USED IN CALCULATION OF ACTIVITY COEFFICIENT        C
C               RATIOS FOR REACTIONS 1, 3, AND 4                        C
C       GAMMAR= -LOG OF THE ACTIVITY COEFFICIENT                        C
C       GCO2=ACTIVITY COEFFICIENT FOR AQUEOUS CO2                       C
C       GH=ACTIVITY COEFFICIENT FOR HYDROGEN ION                        C
C       GMDEA=ACTIVITY COEFFICIENT OF PROTONATED MDEA                   C
C       J=FLAG INDICATING IF THE SOLUTION COMPOSITION CALCULATED        C
C               IS THE INITIAL COMPOSITION (J=0) OR THE FINAL           C
C               COMPOSITION (J NOT EQUAL TO 0)                          C
C       JJ=NUMBER OF ACTIVITY COEFFICIENTS TO BE CALCULATED             C
C       NNN=NUMBER OF CHEMICAL SPECIES FOR WHICH THE MOLALITY           C
C               WAS DETERMINED                                          C
C       OSMOT=OSMOTIC COEFFICIENT                                       C
C       ROW=DENSITY OF WATER                                            C
C       SEE=CONSTANT USED IN CALCULATION OF ACTIVITY COEFFICIENT        C
C               RATIOS FOR REACTIONS 1, 3, AND 4                        C
C       STRION=MOLAL IONIC STRENGTH                                     C
C       SUMBET=CONSTANT USED IN CALCULATION OF THE DEBYE-HUCKEL TERM    C
C       SUMZM=SUMMATION OF CHARGE SQUARED (Z**2) TIMES COMPONENT        C
C               MOLALITY (M)                                            C
C       TEMPC=TEMPERATURE IN CENTIGRADE                                 C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      SUBROUTINE GAMMAK(J,RATIO,CHARGE,X,CCC,NNN,NNCNT)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /GAM/ P10(10),P11(10),P12(10),P13(10),T,PHI(10),
     1        DEBYE(10),NRXNS,ITCNT,KIT,KITCNT,QB(3),QC(3),QD(3)
      DIMENSION SUMP(10),RATIO(10),X(10),CCC(10),CHARGE(10),Q(3)
      NNCNT=NNCNT+1
      SUMZM=0.0
      DO 5 I=1,NNN
              CCC(I)=DEXP(X(I))
              SUMZM=SUMZM+CCC(I)*(CHARGE(I)**2.0)
    5 CONTINUE
      STRION=SUMZM/2.0
      IF(NNCNT.EQ.1) THEN
              TEMPC=T-273.15
              ROW=1.00157-1.56096D-04*TEMPC-2.69491D-06*TEMPC*TEMPC
              DIELEC=5321./T+233.76-0.9297*T+1.417D-03*T*T-8.292D-07
     1                *T*T*T
              ALPHA=1.17202*DSQRT(ROW)*((2.33752D+04/(DIELEC*T))**1.5)
              IF(TEMPC.LT.107.70) THEN
                      BETA=0.980075+0.707654D-02*TEMPC-2.97433D-05
     1                        *TEMPC*TEMPC
              ELSE
                      BETA=1.64801-2.83246D-03*TEMPC+4.67896D-06
     1                        *TEMPC*TEMPC
              ENDIF
              BEE=4.4357D-02+2.1424D-04*TEMPC-1.21582D-06*TEMPC*TEMPC
```

```
                CEE=4.86989D-03-6.65184D-05*TEMPC+1.69534D-07*TEMPC
     1                  *TEMPC
                SEE=-2.97627+4.80688D-02*T-2.69280D-04*T*T+7.49524D-07
     1                  *T*T*T-1.02352D-09*T*T*T*T+5.58004D-13*T*T*T*T*T
                DO 10 K=1,NRXNS
                        SUMP(K)=P10(K)+P11(K)/T+P12(K)*T*T
   10           CONTINUE
        ENDIF
        IF(J.EQ.0) THEN
                JJ=1
        ELSE
                JJ=NRXNS
        ENDIF
        FEE=(1.0-(1.0+2.0*DSQRT(STRION)-2.0*STRION)
     1          *DEXP(-2.0*DSQRT(STRION)))/(4.0*STRION)
        SUMBET=1.0+BETA*DSQRT(STRION)
        DH=(ALPHA/(BETA*BETA*BETA*STRION))*
     1          (SUMBET-2.0*DLOG(SUMBET)-(1.0/SUMBET))
        OSMOT=1.0-DH+BEE*STRION+CEE*STRION**2.0
        DO 100 I=1,JJ
                RATIO(I)=0.0
                IF(I.NE.2.AND.I.NE.NRXNS) THEN
                        GAMMAR=(DEBYE(I)*SEE*DSQRT(STRION)/(1.0+
     1                          DSQRT(STRION)))+((SUMP(I)+P13(I)*FEE)
     2                          *STRION)+(PHI(I)*OSMOT*STRION)
                        RATIO(I)=10.0**(GAMMAR*(-1.0))
                ELSEIF(I.EQ.NRXNS) THEN
                        DO 70 K=1,3
                                Q(K)=(1.0-DEXP((STRION**1.3)*QD(K)))*
     1                                  QC(K)-QB(K)*STRION
   70                   CONTINUE
                        GCO2=Q(1)/T + Q(2) + Q(3)*T
                        RATIO(I)=DEXP(GCO2)
                ELSEIF(I.EQ.2) THEN
                        GMDEA=DEXP((-1.0*ALPHA*DSQRT(STRION)/(1.0+
     1                          226.350*DSQRT(STRION/(DIELEC*T))))
     2                          +2.0*(-0.0375)*CCC(6))
                        GH=DEXP((-1.0*ALPHA*DSQRT(STRION)/(1.0+1.2*DSQRT
     1                          (STRION)))+STRION*(0.18352-0.25503*DEXP
     2                          (-2.0*DSQRT(STRION)))+STRION*STRION*
     3                          (-0.00059))
                        RATIO(I)=GH/GMDEA
                ENDIF
  100   CONTINUE
        RETURN
        END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                            C
C                        SUBROUTINE SOLVE                                    C
C                                                                            C
C       SUBROUTINE SOLVE TAKES THE VALUES OF THE ACTIVITY COEFFICIENT        C
C       RATIOS, INITIAL STOICHIOMETRIC MOLALITIES OF CO2 AND MDEA,           C
C       AND GUESSES FOR THE COMPONENT MOLALITIES AND FINDS VALUES            C
C       OF THE COMPONENT MOLALITIES USING BROYDEN'S METHOD WHICH             C
C       REPRESENT A SOLUTION TO THE SYSTEM OF EQUATIONS                      C
C                                                                            C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
C                                                                       C
C               DESCRIPTION AND IDENTIFICATION OF ARRAYS                C
C                       NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                       C
C       A=TWO-DIMENSIONAL ARRAY USED IN SOLUTION PROCEDURE              C
C       C=INVERTED A MATRIX                                             C
C       S=ONE-DIMENSIONAL ARRAY USED IN BROYDEN'S METHOD SOLUTION        C
C               PROCEDURE                                               C
C       V=ONE-DIMENSIONAL ARRAY HOLDING VALUES OF THE EQUATIONS         C
C               DEFINED IN FIGURE 13                                    C
C       Y=ONE-DIMENSIONAL ARRAY USED IN BROYDEN'S METHOD SOLUTION        C
C               PROCEDURE                                               C
C       Z=ONE-DIMENSIONAL ARRAY USED IN BROYDEN'S METHOD SOLUTION        C
C               PROCEDURE                                               C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C               IDENTIFICATION AND DESCRIPTION OF VARIABLES             C
C                       NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                       C
C       ACC=ACCUMULATION                                                C
C       ICASE=FLAG INDICATING IF THE SOLUTION COMPOSITION CALCULATED    C
C               IS FOR THE INITIAL COMPOSITION (ICASE=0) OR THE         C
C               FINAL COMPOSITION (ICASE NOT EQUAL TO 0)                C
C       K=COUNTER FOR THE NUMBER OF PASSES THROUGH BROYDEN'S            C
C               METHOD BEFORE A SOLUTION IS CONVERGED UPON              C
C       N=NUMBER OF EQUATIONS WHOSE SOLUTION IS TO BE FOUND             C
C       NN=MAXIMUM NUMBER OF PASSES THROUGH BROYDEN'S METHOD            C
C       P=CONSTANT USED IN BROYDEN'S SOLUTION PROCEDURE                 C
C       SN=SUM OF THE RELATIVE ERROR BETWEEN CURRENT PASS THROUGH       C
C               BROYDEN'S PROCEDURE AND THE PREVIOUS PASS THROUGH       C
C               BROYDEN'S PROCEDURE                                     C
C       TOL=TOLERANCE USED TO ESTABLISH CONVERGENCE                     C
C       VV=CONSTANT USED IN BROYDEN'S SOLUTION PROCEDURE                C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C               SUBROUTINES AND SUBPROGRAMS CALLED                      C
C                       BY SUBROUTINE SOLVE                             C
C                                                                       C
C       F, FP, INVER, MULT                                              C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC



      SUBROUTINE SOLVE(N,TOL,ICASE,ITPRT,KOPTFL)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /SOL/ X(10),CONST(10),ORCO2,ORMDEA
      DIMENSION A(10,10),C(10,10),Y(10),S(10),Z(10),V(10)
      NN=80
      SN=0.0
      K=0
      IF(ITPRT.EQ.2) WRITE(6,3) K,(X(I),I=1,N),SN
      DO 15 I=1,N
              DO 14 J=1,N
                      A(I,J) = FP(I,J,X)
14            CONTINUE
15    CONTINUE
      DO 20 I=1,N
              V(I)=F(I,ICASE,KOPTFL)
20    CONTINUE
      CALL INVER(N,A,C)
```

```
      K=1
      CALL MULT(N,A,V,S,SN)
      DO 30 I=1,N
              X(I)=X(I)+S(I)
   30 CONTINUE
      IF(ITPRT.EQ.2) WRITE(6,3) K,(X(I),I=1,N),SN
   35 DO 40 I=1,N
              VV=F(I,ICASE,KOPTFL)
              Y(I)=VV-V(I)
              V(I)=VV
   40 CONTINUE
      CALL MULT(N,A,Y,Z,ZN)
      P=0.0
      DO 60 I=1,N
              P=P-S(I)*Z(I)
              DO 55 J=1,N
                      C(I,J)=(S(I)+Z(I))*S(J)
   55         CONTINUE
   60 CONTINUE
      IF(P.LE.1.0D-16) GOTO 155
      DO 100 I=1,N
              C(I,I)=C(I,I) + P
  100 CONTINUE
      DO 150 I=1,N
              DO 140 J=1,N
                      ACC=0.0
                      DO 130 LLL=1,N
                              ACC=ACC+C(I,LLL)*A(LLL,J)/P
  130                 CONTINUE
                      Z(J)=ACC
  140         CONTINUE
              DO 145 J=1,N
                      A(I,J)=Z(J)
  145         CONTINUE
  150 CONTINUE
  155 CALL MULT(N,A,V,S,SN)
      DO 160 I=1,N
              X(I) = X(I) + S(I)
  160 CONTINUE
      IF(ITPRT.EQ.2) WRITE(6,3) K+1,(X(I),I=1,N),SN
      IF(SN.LE.TOL) THEN
C             WRITE(6,6)
              RETURN
      ELSE
      ENDIF
      IF(K.LT.NN) THEN
              K=K+1
              GOTO 35
      ELSE
              WRITE(6,4)
      ENDIF
      RETURN
    3 FORMAT(1X,I2,5(1X,E15.8,1X),/10X,6(1X,E15.8,1X)///)
    4 FORMAT(1X,'MAXIMUM NUMBER OF ITERATIONS REACHED')
    6 FORMAT(1X,'PROCEDURE COMPLETED SUCCESSFULLY')
      END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
C                                                                       C
C                              FUNCTION FP                              C
C                                                                       C
C       FUNCTION FP IS A SUBPROGRAM WHICH CALCULATES A SINGLE           C
C       ELEMENT OF THE JACOBIAN MATRIX FOR EACH PASS THROUGH THE        C
C       SUBPROGRAM.  THE ELEMENT CALCULATED IS THE (I,J) ELEMENT,       C
C       GIVEN BY d[F(I)]/d[X(J)], WHERE F AND X ARE DEFINED AS IN       C
C       FIGURE 13.                                                      C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C               IDENTIFICATION AND DESCRIPTION OF VARIABLES             C
C                     NOT INCLUDED IN MAIN PROGRAM                      C
C                                                                       C
C       FP=NUMERICAL VALUE OF THE (I,J) ELEMENT OF THE JACOBIAN         C
C               MATRIX USED IN BROYDEN'S SOLUTION METHOD                C
C       I=ROW NUMBER (OR EQUATION NUMBER) FOR WHICH JACOBIAN            C
C               MATRIX ELEMENT IS FOUND                                 C
C       H=COLUMN NUMBER (OR VARIABLE NUMBER) FOR WHICH JACOBIAN         C
C               MATRIX ELEMENT IS FOUND                                 C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      FUNCTION FP(I,J,X)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(10)
      FP=0.0
      IF (I.EQ.1) THEN
              IF(J.EQ.1) FP=DEXP(X(1))
              IF(J.EQ.2) FP=-1.0*DEXP(X(2))
              IF(J.EQ.4) FP=DEXP(X(4))
              IF(J.EQ.6) FP=-1.0*DEXP(X(6))
              IF(J.EQ.7) FP=-2.0*DEXP(X(7))
      ELSEIF (I.EQ.2) THEN
              IF(J.EQ.3) FP=-1.0*DEXP(X(3))
              IF(J.EQ.4) FP=-1.0*DEXP(X(4))
      ELSEIF (I.EQ.3) THEN
              IF(J.EQ.1) FP=-1.0
              IF(J.EQ.2) FP=-1.0
      ELSEIF (I.EQ.4) THEN
              IF(J.EQ.1) FP=-1.0
              IF(J.EQ.3) FP=-1.0
              IF(J.EQ.4) FP=1.0
      ELSEIF (I.EQ.5) THEN
              IF(J.GE.5) FP=-1.0*DEXP(X(J))
      ELSEIF (I.EQ.6) THEN
              IF(J.EQ.1) FP=-1.0
              IF(J.EQ.5) FP=1.0
              IF(J.EQ.6) FP=-1.0
      ELSEIF(I.EQ.7) THEN
              IF(J.EQ.1) FP=-1.0
              IF(J.EQ.6) FP=1.0
              IF(J.EQ.7) FP=-1.0
      ELSEIF(I.EQ.8) THEN
              IF(J.EQ.5) FP=-1.0
      ENDIF
      RETURN
      END


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
C                                                                       C
C                              FUNCTION F                               C
C                                                                       C
C       FUNCTION F IS A SUBPROGRAM WHICH CALCULATES A SINGLE            C
C       ELEMENT OF THE ONE-DIMENSIONAL VECTOR WHICH CONTAINS            C
C       NUMERICAL VALUES OF THE SYSTEM OF EQUATIONS WHOSE SOLUTION      C
C       IS FOUND IN SUBROUTINE SOLVE.  THE EQUATIONS ARE DEFINED        C
C       FIGURE 13.                                                      C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C               IDENTIFICATION AND DESCRIPTION OF VARIABLES             C
C                       NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                       C
C       F=NUMERICAL VALUE OF THE (I) ELEMENT OF THE VECTOR              C
C       I=EQUATION NUMBER FOR WHICH THE VALUE OF F IS FOUND             C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      FUNCTION F(I,ICASE,KOPTFL)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /SOL/ X(10),CONST(10),ORCO2,ORMDEA
      IF(I.EQ.1) THEN
              IF(ICASE.EQ.0) THEN
                      F=DEXP(X(1)) + DEXP(X(4)) - DEXP(X(2))
              ELSE
                      F=DEXP(X(1))+DEXP(X(4))-DEXP(X(2))-DEXP(X(6))
     1                        -2.0*DEXP(X(7))
              ENDIF
      ELSE
      ENDIF
      IF(I.EQ.2) F=ORMDEA-DEXP(X(3))-DEXP(X(4))
      IF(I.EQ.3) F=CONST(1)-X(1)-X(2)
      IF(I.EQ.4) F=CONST(2)-X(1)-X(3)+X(4)
      IF(I.EQ.5) THEN
              IF(KOPTFL.EQ.0) THEN
                      F=ORCO2-DEXP(X(5))-DEXP(X(6))-DEXP(X(7))
              ELSE
                      F=ORCO2-DEXP(X(5))-DEXP(X(6))-DEXP(X(7))
     1                        -DEXP(X(8))
              ENDIF
      ENDIF
      IF(I.EQ.6) F=CONST(3)-X(1)-X(6)+X(5)
      IF(I.EQ.7) F=CONST(4)-X(1)-X(7)+X(6)
      IF(I.EQ.8) F=CONST(5)-X(5)
      RETURN
      END


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C                       SUBROUTINE MULT                                 C
C                                                                       C
C       SUBROUTINE MULT MULTIPLIES THE MATRIX A BY THE VECTOR Y         C
C       RESULTING IN THE VECTOR Z FOR USED IN BROYDEN'S SOLUTION        C
C       METHOD.                                                         C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C               IDENTIFICATION AND DESCRIPTION OF ARRAYS                C
C                       NOT INCLUDED IN MAIN PROGRAM                    C
```

```
C                                                                       C
C       A=SAME AS ARRAY A IN SUBROUTINE SOLVE                           C
C       Y=SAME AS ARRAY V IN SUBROUTINE SOLVE                           C
C       Z=SAME AS ARRAY S IN SUBROUTINE SOLVE                           C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C               IDENTIFICATION AND DESCRIPTION OF VARIABLES             C
C                       NOT INCLUDED IN MAIN PROGRAM                    C
C                                                                       C
C       ZN=SAME AS VARIABLE SN IN SUBROUTINE SOLVE                      C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      SUBROUTINE MULT(N,A,Y,Z,ZN)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(10,10),Y(10),Z(10)
      ZN=0.0
      DO 15 I=1,N
              Z(I)=0.0
              DO 10 J=1,N
                      Z(I)=Z(I)-A(I,J)*Y(J)
10            CONTINUE
              ZN=ZN+Z(I)*Z(I)
15    CONTINUE
      ZN=DSQRT(ZN)
      RETURN
      END



CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                       C
C                       SUBROUTINE INVER                                C
C                                                                       C
C       SUBROUTINE INVER FINDS THE INVERSE OF THE MATRIX A AND          C
C       STORES IT IN THE MATRIX A AND RETURNS TO THE SOLVE SUB-         C
C       ROUTINE.  NO ARRAY OR VARIABLE IDENTIFICATION IS GIVEN          C
C       HERE.                                                           C
C                                                                       C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC


      SUBROUTINE INVER(N,A,B)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(10,10),B(10,10)
      DO 20 I=1,N
              DO 10 J=1,N
                      B(I,J)=0.0
                      IF(J.EQ.I) B(I,J)=1.0
10            CONTINUE
20    CONTINUE
      DO 100 I=1,N
              I1=I+1
              I2=I
              IF(I.NE.N) THEN
                      DO 30 J=I1,N
                              IF(DABS(A(J,I)).GT.DABS(A(I2,I))) I2=J
30                    CONTINUE
```

```
                        IF (I2.NE.I) THEN
                                DO 40 J=1,N
                                        C=A(I,J)
                                        A(I,J)=A(I2,J)
                                        A(I2,J)=C
                                        C=B(I,J)
                                        B(I,J)=B(I2,J)
                                        B(I2,J)=C
   40                           CONTINUE
                        ELSE
                        ENDIF
                ELSE
                ENDIF
                DO 50 J=1,N
                        IF(J.NE.I) THEN
                                C=A(J,I)/A(I,I)
                                DO 45 K=1,N
                                        A(J,K)=A(J,K)-C*A(I,K)
                                        B(J,K)=B(J,K)-C*B(I,K)
   45                           CONTINUE
                        ELSE
                        ENDIF
   50           CONTINUE
  100   CONTINUE
        DO 120 I=1,N
                C=A(I,I)
                DO 110 J=1,N
                        A(I,J)=B(I,J)/C
  110           CONTINUE
  120   CONTINUE
        RETURN
        END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                          SUBROUTINE DATA                                     C
C                                                                              C
C       SUBROUTINE DATA MODIFIES THE SET OF DATA USED IN THE MAIN              C
C       PROGRAM.  OPTIONS INCLUDE ADDING AND/OR DELETING ENTIRE                C
C       DATA SETS, ADDING AND/OR DELETING DATA POINTS FROM DATA                C
C       SETS READ INTO THE MAIN PROGRAM OR ADDED TO THE SET OF DATA            C
C       THROUGH THIS SUBROUTINE, AND/OR CORRECTING EXISTING DATA               C
C       POINTS.                                                                C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                IDENTIFICATION AND DESCRIPTION OF ARRAYS                      C
C                        NOT INCLUDED IN MAIN PROGRAM                          C
C                                                                              C
C       DIFF=DIFFERENCE BETWEEN THE WEIGHT PERCENT MDEA FOR THE                C
C               DATA SET TO BE ADDED AND THE WEIGHT PERCENT                    C
C               MDEA FOR ALL OF THE OTHER EXISTING DATA SETS                   C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C                IDENTIFICATION AND DESCRIPTION OF VARIABLES                   C
C                        NOT INCLUDED IN MAIN PROGRAM                          C
C                                                                              C
C       DIF=DIFFERENCE BETWEEN THE VALUE OF ACID GAS LOADIG FOR                C
C               A SPECIFIC DATA POINT IN A NEW DATA SET AND THE                C
C               VALUES OF ACID GAS LOADINGS FOR EACH OF THE OTHER              C
C               DATA POINTS                                                    C
```

```
C       DIFMIN=MINIMUM VALUE OF DIF OVER ALL OF THE DATA POINTS          C
C       IADD=FLAG USED IN DATA SET ADD/DELETE OPTION.  IADD=Ø            C
C               TO EXIT THIS OPTION; IADD=1 TO ADD ONE DATA SET;         C
C               IADD=-1 TO DELETE ONE OR MORE DATA SETS                  C
C       ICHECK=FLAG USED TO SELECT EDITING OPTION:  ICHECK=-1            C
C               TO SEE CURRENT LISTING OF DATA; ICHECK=Ø TO              C
C               RETURN TO MAIN PROGRAM; ICHECK=1 TO CORRECT AN           C
C               EXISTING DATA POINT; ICHECK=2 TO ADD OR DELETE           C
C               DATA POINT(S) FROM AN EXISTING DATA SET; ICHECK=3        C
C               ADD OR DELETE ENTIRE DATA SETS                           C
C       IDEL=FLAG USED TO ADD OR DELETE DATA POINTS FROM AN EXIST-       C
C               ING DATA SET:  IDEL=-1Ø TO SEE DATA POINTS FROM A        C
C               SPECIFIC DATA SET; IDEL=-1 TO DELETE POINTS FROM         C
C               THE DATA SET; IDEL=Ø TO EXIT THIS OPTION; IDEL>Ø         C
C               TO ADD N DATA POINTS TO DATA SET                         C
C       JJJJ=DATA POINT NUMBER WHICH IS TO BE CORRECTED                  C
C       JMIN=DATA POINT NUMBER IN DATA SET LMIN WHICH PROVIDES           C
C               DIFMIN                                                   C
C       JSTART=DATA POINT NUMBER WHERE CORRECTED DATA POINT IS TO        C
C               BE CHANGED TO                                            C
C       JUNKK=JUNK VARIABLE USED AS A NUMBERED LINE FOR A "GOTO"         C
C               STATEMENT                                                C
C       KCOL=COLUMN NUMBER CONTAINING DATA TO BE CORRECTED:  KCOL=1      C
C               TO CHANGE VALUE OF LOADING; KCOL=2 TO CHANGE             C
C               VALUE OF BTU/LB MDEA                                     C
C       LDEL=FLAG USED IN MENU FOR DELETING DATA SETS:  LDEL=Ø           C
C               TO EXIT THIS PROGRAM OPTION; LDEL>Ø TO INDICATE          C
C               WHICH DATA SET IS TO BE DELETED                          C
C       LEND=NEW MAXIMUM DATA POINT NUMBER FOR A PARTICULAR DATA         C
C               SET TO WHICH DATA POINTS ARE BEING ADDED                 C
C       LLLL=DATA SET NUMBER CONTAINING DATA POINT TO BE CORRECTED       C
C       LMIN=DATA SET NUMBER CONTAINING JMIN WHICH GIVES DIFMIN          C
C       LSET=LLLL                                                        C
C       LSTART=DATA POINT NUMBER TO BE ADDED TO A PARTICULAR DATA        C
C               SET                                                      C
C       MIN=FLAG INDICATING IF THE DATA SET TO BE ADDED HAS A WEIGHT     C
C               PERCENT MDEA EQUAL TO A WEIGHT PERCENT FOR AN            C
C               EXISTING DATA SET (MIN=1; OTHERWISE MIN=Ø)               C
C       SAVEB=TEMPORARY STORAGE FOR VALUES OF BTU/LB MDEA IN SORT-       C
C               ING ROUTINE                                              C
C       SAVEC=TEMPORARY STORAGE FOR VALUES OF ACID GAS LOADING IN        C
C               SORTING ROUTINE                                          C
C       STUFF=NEW VALUE OF ACID GAS LOADING OR TOTAL HEAT OF ABSORP-     C
C               TION (BTU/LB MDEA) FOR EXISTING DATA POINT CORRECTION    C
C       SVEG=TEMPORARY STORAGE FOR VALUES OF ACTIVITY COEFFICIENT        C
C               RATIOS IN SORTING ROUTINE                                C
C       SVEX=TEMPORARY STORAGE FOR VALUES OF LOG MOLALITY IN SORTING     C
C               ROUTINE                                                  C
C                                                                        C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC



      SUBROUTINE DATA(PERCEN,PRESS,NPTS,NSETS,NTOTAL,CO2,BTU,IREP,
     1          MINFLG,NNN1,NNN2,XOLD,XOLDØ,GSAVE,GSAVEØ,NRXNS,SYSID)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION PERCEN(1Ø),PRESS(1Ø),NPTS(1Ø),CO2(1Ø,6Ø),BTU(1Ø,6Ø),
     1          SAVEX(1Ø),SAVEG(1Ø),DIFF(1Ø),XOLD(11,1Ø,1Ø,6Ø),
     2          XOLDØ(11,1Ø,1Ø,1),GSAVEØ(11,1Ø,1Ø,1),SYSID(1Ø),
     3          GSAVE(11,1Ø,1Ø,6Ø)
   99 GOTO 145
  1ØØ WRITE(6,125)
  125 FORMAT(5X,'THIS IS A LISTING OF THE DATA YOU HAVE INPUT.')
```

```
      DO 140 L=1,NSETS
             WRITE(6,130) L
130          FORMAT(/20X,' DATA SET NUMBER ',I2/11X,'N',3X,
     1              'MOLE CO2/MOLE MDEA',4X,'BTU/LB MDEA'/)
             DO 137 I=1,NPTS(L)
                    WRITE(6,135) I,CO2(L,I),BTU(L,I)
135                 FORMAT(9X,I3,7X,F8.4,11X,F8.2)
137          CONTINUE
140   CONTINUE
145   TYPE 150
150   FORMAT(/20X,'MAIN EDITING MENU'//,
     1 7X,'  ENTER:'/,
     1 9X,'-1:  SEE LISTING OF DATA AGAIN'/,
     1 10X,'0:  EXIT TO MAIN PROGRAM'/,
     1 10X,'1:  CORRECT AN EXISTING DATA POINT'/,
     1 10X,'2:  ADD OR DELETE DATA POINTS FROM'/,
     2 10X,'    AN EXISTING DATA SET'/,
     3 10X,'3:  ADD OR DELETE DATA SETS')
      ACCEPT*,ICHECK
      IF(ICHECK.EQ.0) GOTO 500
      IF(ICHECK.LT.0) GOTO 100
      IF(ICHECK.EQ.1) GOTO 300
      IF(ICHECK.EQ.2) GOTO 400
200   WRITE(6,205)
205   FORMAT(15X,'DATA SET ADD/DELETE MENU'//,
     1 5X,'THIS OPTION IS TO ADD OR DELETE ENTIRE DATA SETS'/,
     1 7X,'ENTER:'/,
     2 9X,'-1:  DELETE ONE OR MORE DATA SETS'/,
     3 10X,'0:  EXIT TO MAIN EDITING MENU'/,
     2 10X,'1:  ADD ONE DATA SET')
      ACCEPT*,IADD
      IF(IADD.EQ.0)GOTO 145
      IF(IADD.GT.0)THEN
             NSETS=NSETS+1
             WRITE(6,210) NSETS
210          FORMAT(10X,'DATA SET NUMBER ',I2,' ADDED TO DATA'/,
     1       10X,'INPUT NUMBER OF DATA POINTS IN THIS DATA SET')
             ACCEPT*,NPTS(NSETS)
             WRITE(6,215)
215          FORMAT(10X,'ENTER PRESSURE (PSIA), AND CONCENTRATION',
     1       ' (WT. % MDEA)'/15X,'FOR THIS DATA SET')
             ACCEPT*,PRESS(NSETS)
             ACCEPT*,PERCEN(NSETS)
             MIN=0
             IF(IREP.GT.0) THEN
                    DO 220 L=1,NSETS-1
                           DIFF(L)=DABS( PERCEN(L)-PERCEN(NSETS) )
                           IF(DIFF(L).LE.0.001) THEN
                                  MIN=1
                           ENDIF
220                 CONTINUE
                    IF(MIN.EQ.0) THEN
                           WRITE(6,*) ' CAN"T ADD THIS DATA SET ',
     1                            'FOR REPETITION>1.'
                           WRITE(6,*) ' IF YOU WISH TO ADD THIS ',
     1                     'SET, PLEASE DO SO ON INITIAL RUN.'
                           NSETS=NSETS-1
                           GOTO 200
                    ENDIF
             ENDIF
             DO 230 J=1,NPTS(NSETS)
                    WRITE(6,225) NSETS,J
225                 FORMAT(10X,'ENTER CO2(I), BTU(I) FOR DATA SET ',
     1              I2,', POINT #',I3)
```

```
                ACCEPT*,CO2(NSETS,J)
                ACCEPT*,BTU(NSETS,J)
230         CONTINUE
            WRITE(6,235)
235         FORMAT(//25X,'NEW DATA SET')
            WRITE(6,130) NSETS
            WRITE(6,135) (I,CO2(NSETS,I),BTU(NSETS,I),
     1                          I=1,NPTS(NSETS))
            IF(IREP.GT.0) THEN
                DO 260 J=1,NPTS(NSETS)
                    JMIN=0
                    LMIN=0
                    DIFMIN=1000.0
                    DO 245 L=1,NSETS-1
                        IF(DIFF(L).LT.0.001) THEN
                            DO 240 JJ=1,NPTS(L)
                                DIF=DABS(CO2(L,JJ)-CO2(NSETS,J))
                                IF(DIF.LT.DIFMIN) THEN
                                    LMIN=L
                                    JMIN=JJ
                                    DIFMIN=DIF
                                ENDIF
240                         CONTINUE
                        ENDIF
245                 CONTINUE
                    DO 250 I=1,NNN2
                        XOLD(MINFLG,NSETS,I,J)=XOLD(MINFLG,LMIN,
     1                          I,JMIN)
250                 CONTINUE
                    DO 255 I=1,NRXNS
                        GSAVE(MINFLG,NSETS,I,J)=GSAVE(MINFLG,
     1                          LMIN,I,JMIN)
255                 CONTINUE
260             CONTINUE
                DO 261 I=1,NNN1
                    XOLD0(MINFLG,NSETS,I,1)=XOLD0(MINFLG,LMIN,I,1)
261             CONTINUE
                GSAVE0(MINFLG,NSETS,1,1)=GSAVE0(MINFLG,LMIN,1,1)
            ENDIF
            GOTO 200
        ELSE
265         WRITE(6,270)
270         FORMAT(20X,'DATA SET DELETE MENU'//,
     1          7X,'ENTER:'/,
     1          10X,'0:  EXIT TO DATA SET ADD/DELETE MENU'/,
     2          10X,'L:  DATA SET NUMBER THAT YOU WISH TO DELETE')
            ACCEPT*,LDEL
            IF(LDEL.EQ.0) GOTO 200
            NSETS=NSETS-1
            DO 295 L=LDEL,NSETS
                PERCEN(L)=PERCEN(L+1)
                PRESS(L)=PRESS(L+1)
                NPTS(L)=NPTS(L+1)
                SYSID(L)=SYSID(L+1)
                DO 275 J=1,NPTS(L)
                    CO2(L,J)=CO2(L+1,J)
                    BTU(L,J)=BTU(L+1,J)
275             CONTINUE
                IF(IREP.GT.0) THEN
                    DO 280 I=1,NNN1
                        XOLD0(MINFLG,L,I,1)=XOLD0(MINFLG,
     1                      L+1,I,1)
280                 CONTINUE
                    GSAVE0(MINFLG,L,1,1)=GSAVE0(MINFLG,L+1,1,1)
```

```
                        DO 288 I=1,NNN2
                            DO 284,J=1,NPTS(L)
                                XOLD(MINFLG,L,I,J)=XOLD(MINFLG,L+1,
     1                                          I,J)
284                         CONTINUE
288                     CONTINUE
                        DO 294 I=1,NRXNS
                            DO 290 J=1,NPTS(L)
                               GSAVE(MINFLG,L,I,J)=GSAVE(MINFLG,
     1                                          L+1,I,J)
290                         CONTINUE
294                     CONTINUE
                    ENDIF
295             CONTINUE
        ENDIF
        GOTO 265
300     WRITE(6,305)
305     FORMAT(5X,'EXISTING POINT CORRECTION MENU'//,
     1  5X,'  ENTER:'/,
     1  5X,'     0:  EXIT TO MAIN EDITING MENU'/,
     1  4X,'L,J,COL:  DATA SET NUMBER, POINT NUMBER, COLUMN'/,
     1  4X,'          NUMBER IN WHICH ERROR OCCURS')
        ACCEPT*,LLLL
        IF(LLLL.EQ.0) GOTO 145
        LSET=LLLL
        ACCEPT*,JJJJ
        ACCEPT*,KCOL
        WRITE(6,310) LLLL,JJJJ,KCOL
310     FORMAT(10X,'DATA SET NUMBER ',I2,5X,'POINT NUMBER ',I3,
     1  5X,'COLUMN NUMBER ',I1)
        IF(KCOL.EQ.1) THEN
                WRITE(6,320) CO2(LLLL,JJJJ)
320             FORMAT(10X,'OLD VALUE OF LOADING: ',F9.6/,
     1          10X,'ENTER NEW VALUE; NEGATIVE VALUE TERMINATES',
     2          ' CORRECTION PROCEDURE')
                ACCEPT*,STUFF
                IF(STUFF.LE.0.0) GOTO 300
                CO2(LLLL,JJJJ)=STUFF
                JMIN=0
                DIFMIN=1000.0
                DO 325 J=1,NPTS(LSET)
                        IF(J.NE.JJJJ) THEN
                                DIF=DABS(CO2(LSET,J)-STUFF)
                                IF(DIF.LT.DIFMIN) THEN
                                        JMIN=J
                                        DIFMIN=DIF
                                ENDIF
                        ENDIF
325             CONTINUE
                IF(STUFF.LT.CO2(LSET,JMIN)) THEN
                        JSTART=JMIN
                ELSE
                        JSTART=JMIN+1
                ENDIF
                IF(JSTART.EQ.JJJJ) GOTO 300
                IF(IREP.GT.0) THEN
                        DO 330 I=1,NNN2
                                XOLD(MINFLG,LSET,I,JJJJ)=XOLD(MINFLG,
     1                                  LSET,I,JSTART-1)
330                     CONTINUE
                        DO 335 I=1,NRXNS
                                GSAVE(MINFLG,LSET,I,JMIN)=GSAVE(MINFLG,
     1                                  LSET,I,JSTART-1)
335                     CONTINUE
```

```
                ENDIF
                DO 360 NN=2,NPTS(LSET)
                        DO 350 KK=NN-1,1,-1
                                IF(CO2(LSET,KK+1).LT.CO2(LSET,KK)) THEN
                                        SAVEC=CO2(LSET,KK+1)
                                        SAVEB=BTU(LSET,KK+1)
                                        CO2(LSET,KK+1)=CO2(LSET,KK)
                                        BTU(LSET,KK+1)=BTU(LSET,KK)
                                        CO2(LSET,KK)=SAVEC
                                        BTU(LSET,KK)=SAVEB
                                        IF(IREP.GT.0) THEN
                                            DO 340 I=1,NNN2
                                                SVEX=XOLD(MINFLG,
     1                                                    LSET,I,KK+1)
                                                XOLD(MINFLG,LSET,I,KK+1)
     1                                               =XOLD(MINFLG,LSET,I,KK)
                                                XOLD(MINFLG,LSET,I,KK)
     1                                                    =SVEX
340                                         CONTINUE
                                            DO 345 I=1,NRXNS
                                                SVEG=GSAVE(MINFLG,LSET,
     1                                                    I,KK+1)
                                                GSAVE(MINFLG,LSET,I,
     1                                                KK+1)=GSAVE(MINFLG,
     2                                                LSET,I,KK)
                                                GSAVE(MINFLG,LSET,I,KK)=
     1                                                    SVEG
345                                         CONTINUE
                                        ENDIF
                                ELSE
                                        GOTO 355
                                ENDIF
350                     CONTINUE
355                     JUNKK=JJ
360             CONTINUE
        ELSE
                WRITE(6,380) BTU(LLLL,JJJJ)
380             FORMAT(10X,'OLD VALUE OF HEAT (BTU/LB MDEA): ',F7.2/,
     1          10X,'ENTER NEW VALUE; A VALUE OF 0 TERMINATES',
     2          ' CORRECTION PROCEDURE')
                ACCEPT*,STUFF
                IF(STUFF.EQ.0.0) GOTO 300
                BTU(LLLL,JJJJ)=STUFF
        ENDIF
        GOTO 300
400     WRITE(6,405)
405     FORMAT(15X,'ADD/DELETE MENU FOR DATA POINTS'/,
     1  15X,'     IN EXISTING DATA SETS'//,
     1  7X,'ENTER:'/,
     1  10X,'0:  EXIT TO MAIN EDITING MENU'/,
     1  10X,'L:  NUMBER OF THE DATA SET FOR WHICH YOU WISH'/,
     2  10X,'    TO ADD OR DELETE POINTS')
        ACCEPT*,LSET
        IF(LSET.EQ.0) GOTO 145
409     WRITE(6,410) LSET
410     FORMAT(15X,'ADD/DELETE MENU FOR DATA SET ',I2//,
     1  7X,'ENTER:'/,
     2  8X,'-10:  SEE DATA POINTS FOR THIS DATA SET'/,
     3  8X,' -1:  ENTER DELETE MENU FOR DELETING POINTS'/,
     4  8X,'      FROM THIS DATA SET'/,
     1  10X,'0:  EXIT TO MAIN ADD/DELETE MENU FOR EXISTING'/,
     1  10X,'    DATA SETS'/,
     1  8X,'N>0:  ADD N POINTS TO THE DATA SET')
        ACCEPT*,IDEL
```

```
      IF(IDEL.EQ.-10) THEN
              WRITE(6,130) LSET
              DO 411 I=1,NPTS(LSET)
                      WRITE(6,135) I,CO2(LSET,I),BTU(LSET,I)
411           CONTINUE
              GOTO 409
      ENDIF
      IF(IDEL.EQ.0)GOTO 400
      IF(IDEL.GT.0)THEN
              LSTART=NPTS(LSET)+1
              LEND=NPTS(LSET)+IDEL
              NPTS(LSET)=NPTS(LSET)+IDEL
              DO 420 L=LSTART,LEND
                      WRITE(6,225) LSET,L
                      ACCEPT*,CO2(LSET,L)
                      ACCEPT*,BTU(LSET,L)
                      IF(IREP.GT.0) THEN
                              DO 412 I=1,NNN2
                                      XOLD(MINFLG,LSET,I,L)=XOLD(
     1                                        MINFLG,LSET,I,LSTART-1)
412                           CONTINUE
                              DO 418 I=1,NRXNS
                                      GSAVE(MINFLG,LSET,I,L)=GSAVE(
     1                                        MINFLG,LSET,I,LSTART-1)
418                           CONTINUE
                      ENDIF
420           CONTINUE
              DO 445 NN=2,NPTS(LSET)
                      DO 440 KK=NN-1,1,-1
                              IF(CO2(LSET,KK+1).LT.CO2(LSET,KK)) THEN
                                      SAVEC=CO2(LSET,KK+1)
                                      SAVEB=BTU(LSET,KK+1)
                                      CO2(LSET,KK+1)=CO2(LSET,KK)
                                      BTU(LSET,KK+1)=BTU(LSET,KK)
                                      CO2(LSET,KK)=SAVEC
                                      BTU(LSET,KK)=SAVEB
                                      IF(IREP.GT.0) THEN
                                          DO 425 I=1,NNN2
                                              XOLD(MINFLG,LSET,I,KK+1)
     1                                        =XOLD(MINFLG,LSET,I,KK)
425                                       CONTINUE
                                          DO 430 I=1,NRXNS
                                              GSAVE(MINFLG,LSET,I,
     1                                        KK+1)=GSAVE(MINFLG,
     2                                        LSET,I,KK)
430                                       CONTINUE
                                      ENDIF
                              ELSE
                                      GOTO 441
                              ENDIF
440                   CONTINUE
441                   JUNKK=JJ
445           CONTINUE
              GOTO 409
      ELSE
450           WRITE(6,455) LSET
455           FORMAT(15X,'DELETE MENU FOR DELETING POINTS'/,
     1        15X,'       FROM DATA SET ',I2//,
     1        7X,'ENTER:'/,
     1        9X,'-1:  REVIEW DATA FROM DATA SET'/,
     1        10X,'0:  EXIT TO ADD/DELETE MENU FOR THIS DATA SET'/,
     1        10X,'N:  NUMBER OF THE DATA POINT YOU WISH TO DELETE')
              ACCEPT*,IDEL
              IF(IDEL.EQ.-1) THEN
```

```
                        WRITE(6,130) LSET
                        DO 459 I=1,NPTS(LSET)
                                WRITE(6,135) I,CO2(LSET,I),BTU(LSET,I)
459                     CONTINUE
                        GOTO 450
                ENDIF
                IF(IDEL.EQ.0) GOTO 409
                NPTS(LSET)=NPTS(LSET)-1
                DO 475 J=IDEL,NPTS(LSET)
                        CO2(LSET,J)=CO2(LSET,J+1)
                        BTU(LSET,J)=BTU(LSET,J+1)
                        IF(IREP.GT.0) THEN
                                DO 460 I=1,NNN2
                                        XOLD(MINFLG,LSET,I,J)=XOLD(
     1                                          MINFLG,LSET,I,J+1)
460                             CONTINUE
                                DO 465 I=1,NRXNS
                                        GSAVE(MINFLG,LSET,I,J)=GSAVE(
     1                                          MINFLG,LSET,I,J+1)
465                             CONTINUE
                        ENDIF
475             CONTINUE
        ENDIF
        GOTO 450
500     NTOTAL=0
        DO 520 L=1,NSETS
                NTOTAL=NTOTAL+NPTS(L)
520     CONTINUE
        RETURN
        END
```

Data File INPUT.DAT

This data file contains the individual experimental data points and data sets. The first line of the input file contains the value of NSETS, the number of data sets contained in the input file. Then, for each data set, the first line contains an identification number and the second line contains values of wt. % MDEA (PERCEN(L)), temperature (TEMP), and pressure (PRESS(L)). The third line contains the number of data points in this data set (NPTS(L)), the molecular weight of MDEA (PUREMW), and the molecular weight of the aqueous MDEA solution (WTMOL). The following lines contain the experimental data. Each of these lines describes a single data point; the first of the pair of numbers is the loading value, and the second is the overall heat of solution (Btu/lb MDEA).

```
    2
16.1
  20.000     300.00     212.6000
  19       119.1699982         21.6990471
         0.0519972        -12.8162069
         0.0823508        -19.3131409
         0.0964466        -21.1985188
         0.1152635        -26.7721614
         0.1266214        -29.4640007
         0.1393755        -31.6818924
         0.1435370        -34.6696625
         0.1499204        -33.6409149
         0.1622793        -37.4009571
         0.1793778        -42.1643753
         0.1905102        -45.8882332
         0.2066680        -46.9649315
         0.2169855        -51.1045876
         0.2295441        -53.4322281
         0.2421141        -54.4586945
         0.2457476        -55.2070961
         0.2608507        -57.8685417
         0.2625298        -56.4326668
         0.2642092        -61.9326515
18.1
  40.000     300.00     212.6000
  16       119.1699982         27.2765160
         0.0282527         -7.3898196
         0.0345143         -8.2980270
         0.0444156        -11.7722645
         0.0486015        -11.6856489
         0.0555484        -13.1005754
         0.0638300        -15.3457127
         0.0714601        -16.7695103
         0.0803199        -19.2727213
         0.0898600        -21.2189052
         0.0985271        -24.8393555
         0.1082103        -25.6007786
         0.1191382        -27.3232841
         0.1205894        -27.3651524
         0.1284104        -31.0019188
         0.1309826        -30.5781040
         0.1321013        -30.3393250
```

Input Data File INPUT.PAR

This file contains the parameters used in program execution. These values are independent of the experimental data points. The first line of this data file contains the values of the variables NRXNS, NCOMP, TOL, and TOL1 (See documented computer program for identification and description of these variables). The second through the ninth lines contain values of the component number (I) and the ionic charge on that component (CHARGE(I)). The tenth through the fourteenth lines contain values of the reaction number (I), along with the corresponding values of A(I), B(I), C(I), D(I), and E(I) for each reaction. The fifteenth through nineteenth lines contain values of P10, P11, P12, P13, PHI, and DEBYE for each of the reactions. The twentieth through twenty-second lines contain values of QB(I), QC(I), and QD(I) for I=1, 3. Finally, the twenty-third through thirtieth lines contain values of the component number (I) and component name (CNAME(I)).

```
 5,7,5.ØD-Ø4,1.ØD-Ø5
1, 1.Ø
2, -1.Ø
3, Ø.Ø
4, 1.Ø
5, Ø.Ø
6, -1.Ø
7, -2.Ø
8, Ø.Ø
1,-3361.1189, -Ø.51917065, 179690.18, 534.51952,-8891663.9
2, 3.0154811,Ø.ØØ37761995, 4610.5676,       Ø.Ø,       Ø.Ø
3, 3653.1643,  Ø.59521486,-196965.31,-577.Ø3321,11762966.Ø
4,-213.40693,-Ø.Ø23309934, 8Ø25.Ø613, 37.3ØØ95Ø, 418333.61
5, 2Ø8.Ø2333, Ø.Ø3Ø346227,-7279.7238,-32.595Ø93,-316Ø4.Ø5
  -Ø.611Ø9Ø,  87.6450,  1.8698D-Ø6,  -Ø.244560,  -Ø.Ø157,  2.Ø
        Ø.Ø,       Ø.Ø,          Ø.Ø,         Ø.Ø,       Ø.Ø,  Ø.Ø
  -Ø.688379,  136.722, 1.93521D-Ø6,  -Ø.124789,  -Ø.Ø157,  2.Ø
9.56741D-Ø3, -47.4Ø28, 2.3Ø264D-Ø7,  -Ø.159489,       Ø.Ø,  4.Ø
        Ø.Ø,       Ø.Ø,          Ø.Ø,         Ø.Ø,       Ø.Ø,  Ø.Ø
    -653.3,    -155.3,      -2.5Ø4
    3.9398,    1.1695,      -2.276
 -Ø.ØØ6491,-Ø.ØØ1981,      -2.163
    1           H+
    2          OH-
    3         MDEA
    4      MDEAH+
    5         CO2
    6        HCO3-
    7       CO3-2
    2
```

APPENDIX H

OUTPUT DATA FROM COMPUTER MODEL FOR 288.7 K, 333.2 K, 388.7 K, AND 422.0 K

ANALYSIS OF EQUILIBRIUM CONSTANT AND HEAT OF REACTION
FOR THE PROTONATION OF MDEA AT 60.0 F

DATA SET NUMBER 1

SYSTEM	(RUN#.TRIAL):	1.2
PRESSURE	(PSIA) :	162.6
CONCENTRATION	(WT. % MDEA):	20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.19580	-31.94
0.25386	-43.22
0.25386	-44.46
0.31693	-55.60
0.39357	-69.99
0.59160	-98.19
0.88551	-150.07
1.09834	-183.73
1.14803	-188.20
1.20088	-189.51
1.25693	-190.15
1.38240	-191.52
2.36187	-191.44
3.34579	-194.80
6.79001	-197.24
7.33907	-121.81

DATA SET NUMBER 2

SYSTEM	(RUN#.TRIAL):	1.3
PRESSURE	(PSIA) :	162.6
CONCENTRATION	(WT. % MDEA):	20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.17242	-28.81
0.42468	-70.26
0.52129	-91.93
0.63983	-111.16
0.68533	-117.68
0.78201	-136.34
0.88053	-150.13
0.96031	-160.34
0.96826	-166.46
1.05001	-174.22
1.12540	-182.33
1.23352	-189.64

1.51693	-191.69
2.11456	-191.71
2.93020	-185.16
2.93020	-185.16
4.65391	-182.77

DATA SET NUMBER 3

SYSTEM (RUN#.TRIAL): 2.1
PRESSURE (PSIA) : 22.6
CONCENTRATION (WT. % MDEA): 20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.05751	-12.44
0.12995	-15.67
0.22368	-39.42
0.34787	-61.62
0.52385	-89.28
0.64299	-103.99
0.78521	-111.30
0.85832	-114.74
0.97297	-119.39
1.11796	-121.77
1.22243	-124.12
1.34307	-130.00
1.35275	-128.40
1.49737	-129.64
1.57821	-128.82
1.63914	-131.70
1.76114	-133.65
1.85754	-132.00
1.86506	-135.11
1.97886	-136.41
2.09578	-141.67
2.24252	-140.34
2.39656	-142.63
2.56830	-142.50
2.76163	-147.81
2.96892	-148.52
3.52061	-148.95
3.85768	-155.06
4.71562	-156.29
5.31900	-156.85
6.04818	-160.55

DATA SET NUMBER 4

SYSTEM (RUN#.TRIAL): 3.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 40.0

INPUT DATA

MOLE CO2	BTU

MOLE MDEA	LB MDEA
0.11389	-21.44
0.17715	-29.01
0.26572	-45.85
0.39861	-70.25
0.56700	-96.68
0.59159	-108.05
0.62018	-117.98
0.62250	-112.86
0.62250	-119.94
0.72133	-128.31
0.80358	-137.28
0.84489	-141.59
0.88981	-159.87
0.89326	-163.07
0.89326	-154.53
0.94603	-158.86
1.07141	-178.75
1.13749	-189.99
1.13749	-189.17
1.21549	-191.99
1.30271	-192.48
1.39536	-192.27
1.51769	-195.34
1.78560	-194.40
2.15033	-194.46
2.41061	-193.19

DATA SET NUMBER 5

SYSTEM	(RUN#.TRIAL):	3.3
PRESSURE	(PSIA) :	162.6
CONCENTRATION	(WT. % MDEA):	40.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.10587	-19.25
0.13132	-24.09
0.13691	-23.27
0.16476	-30.20
0.20610	-39.54
0.20667	-36.34
0.24707	-44.24
0.27788	-47.63
0.29571	-53.32
0.33641	-58.69
0.33827	-57.67
0.35199	-59.91
0.35816	-61.28
0.35862	-61.89
0.38958	-67.59
0.40178	-70.84
0.45534	-80.51
0.46352	-82.44
0.47326	-87.10
0.47528	-81.54
0.49327	-92.81

0.51898	-89.55
0.54601	-99.62
0.55722	-97.59
0.57365	-102.68
0.58467	-103.32
0.62983	-112.20
0.63019	-116.95
0.64071	-111.52
0.65002	-113.03
0.66525	-117.83
0.67275	-122.28
0.67374	-119.68
0.72332	-127.48
0.72704	-129.27
0.76531	-138.82
0.79503	-144.67
0.80119	-139.85
0.84667	-145.46
0.85923	-150.98
0.89825	-160.11
0.94977	-166.65
0.95520	-169.27
1.00084	-172.80
1.04054	-177.19
1.07404	-184.27
1.10667	-196.54
1.11012	-188.18
1.16578	-196.07
1.20134	-196.74
1.24551	-198.44
1.39424	-195.62
2.21448	-194.75

DATA SET NUMBER 6

SYSTEM	(RUN#.TRIAL):	4.1
PRESSURE	(PSIA) :	22.6
CONCENTRATION	(WT. % MDEA):	40.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.18020	-30.34
0.40848	-70.07
0.51335	-91.02
0.53663	-95.60
0.58746	-103.29
0.61531	-107.44
0.63533	-109.17
0.66918	-111.47
0.69755	-112.19
0.71091	-122.92
0.77495	-123.21
0.81694	-125.34
0.82628	-128.60
0.86559	-130.03
0.90811	-133.80
0.96541	-129.12
0.96541	-133.10

0.98018	-136.48
0.98018	-136.75
1.02431	-136.24
1.02431	-131.13
1.02431	-136.25
1.04001	-139.77
1.08921	-139.65
1.08921	-136.37
1.10575	-142.93
1.16525	-142.82
1.17851	-145.16
1.23575	-148.46
1.32945	-150.46
1.34472	-149.84
1.42404	-154.14
1.54296	-151.07
1.56662	-158.32
1.67262	-155.94
1.82223	-158.39
1.98915	-163.47
2.23680	-171.14
2.45961	-170.50
2.79524	-177.23

DATA SET NUMBER 7

SYSTEM (RUN#.TRIAL): 5.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 60.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.07915	-11.67
0.18468	-31.51
0.27911	-48.68
0.34550	-59.47
0.43410	-77.89
0.55814	-98.80
0.59137	-106.07
0.64260	-115.66
0.74122	-130.76
0.76671	-140.96
0.79626	-143.93
0.85084	-154.55
0.85679	-153.22
0.91156	-163.61
0.92489	-169.12
0.98026	-174.95
0.98207	-174.53
1.04576	-185.81
1.05278	-189.01
1.05432	-187.27
1.13899	-199.09
1.14677	-201.27
1.22160	-201.10
1.24354	-197.22
1.25009	-208.17
1.31583	-201.64

1.34573	-200.62
1.36180	-200.59
1.36944	-205.32
1.43350	-199.82
1.45190	-200.55
1.53479	-199.55
1.57081	-199.77
1.58507	-200.23
1.60776	-199.72
1.66836	-203.77
1.92777	-199.86
2.17445	-204.28
2.36856	-200.53
2.49483	-201.52
3.35579	-198.92
5.12427	-196.17

DATA SET NUMBER 8

SYSTEM (RUN#.TRIAL): 5.3
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 60.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.06820	-11.73
0.10635	-18.32
0.15917	-28.68
0.18607	-33.81
0.21979	-38.65
0.24025	-46.41
0.27098	-47.70
0.29308	-51.96
0.29741	-56.36
0.33682	-59.49
0.37139	-66.35
0.41096	-76.37
0.45297	-86.41
0.45392	-80.84
0.48048	-92.75
0.50192	-91.37
0.50399	-93.25
0.52950	-96.63
0.53061	-95.86
0.53505	-101.90
0.56664	-101.64
0.59754	-107.53
0.59997	-108.88
0.63394	-113.95
0.63928	-120.08
0.67713	-127.11
0.67994	-118.64
0.72239	-131.51
0.73109	-138.14
0.77568	-141.48
0.78035	-140.52
0.83559	-149.39
0.84086	-153.76

0.89815	-165.25
0.90190	-159.50
0.90566	-169.10
0.97769	-175.24
0.98585	-185.14
1.07183	-193.20
1.17695	-198.81

DATA SET NUMBER 9

SYSTEM	(RUN#.TRIAL):	6.1
PRESSURE	(PSIA) :	22.6
CONCENTRATION	(WT. % MDEA):	60.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.07893	-12.35
0.12328	-21.12
0.18485	-31.72
0.27731	-48.71
0.43296	-78.11
0.45430	-82.67
0.53009	-96.26
0.58977	-107.67
0.62356	-113.22
0.65570	-118.79
0.70092	-126.81
0.74227	-131.78
0.74262	-134.70
0.74262	-135.34
0.79405	-138.97
0.84534	-140.60
0.84867	-141.83
0.89903	-143.04
0.90935	-144.17
0.97423	-147.31
1.04376	-147.65
1.13994	-154.80
1.14415	-152.79
1.23292	-152.78
1.36587	-159.95
1.67624	-164.61

INPUT PARAMETERS

NUMBER OF REACTIONS : 5

NUMBER OF COMPONENTS : 7

CHARGES ON COMPONENTS:
1, 1.
2, -1.
3, Ø.
4, 1.
5, Ø.
6, -1.
7, -2.

TOLERANCE FOR ACTIVITY COEFFICIENT CONVERGENCE: Ø.5D-Ø3

TOLERANCE FOR SIMULTANEOUS EQUATION SOLUTIONS : Ø.1D-Ø4

VALUES FOR LN K, DELTA H FOR EACH REACTION

LN K [=] UNITLESS

DELTA H [=] CAL/GMOLE

	1	2	3	4	5
LN K	-32.986	-2Ø.Ø75	-14.768	-24.ØØ4	-3.11Ø
DELTA H	13842.4Ø	8536.52	2987.36	4167.Ø3	-5146.6Ø

CONVERTED DATA

(NOTE: "CORRECTED HEAT OF SOLUTION" IS TOTAL HEAT OF SOLUTION LESS HEAT OF ABSORPTION OF GASEOUS CO2.)

POINT	MOLE FRACTION CO2	HEAT OF SOLUTION (J/MOLE)	MOLALITY CO2 (MOLE/KG H2O)	MOLALITY MDEA (MOLE/KG H2O)	CORRECTED HEAT OF SOLUTION (CAL/KG H2O)
			DATA SET NUMBER 1		
1	0.00708	-319.92	0.4108	2.0980	-2322.0
2	0.00916	-432.04	0.5326	2.0980	-3262.4
3	0.00916	-444.41	0.5326	2.0980	-3434.3
4	0.01141	-554.48	0.6649	2.0980	-4300.3
5	0.01413	-696.09	0.8257	2.0980	-5471.8
6	0.02109	-969.65	1.2412	2.0980	-7250.3
7	0.03124	-1466.54	1.8578	2.0980	-11281.9
8	0.03846	-1782.07	2.3043	2.0980	-13658.4
9	0.04013	-1822.30	2.4085	2.0980	-13743.3
10	0.04190	-1831.57	2.5194	2.0980	-13354.2
11	0.04377	-1834.18	2.6370	2.0980	-12838.0
12	0.04793	-1839.37	2.9002	2.0980	-11673.7
13	0.07920	-1778.23	4.9551	2.0980	-1087.1
14	0.10861	-1751.58	7.0194	2.0980	9070.9
15	0.19826	-1595.20	14.2452	2.0980	45920.0
16	0.21091	-969.64	15.3971	2.0980	62324.2
			DATA SET NUMBER 2		
1	0.00624	-288.78	0.3617	2.0980	-2139.3
2	0.01523	-697.97	0.8910	2.0980	-5173.1
3	0.01863	-910.10	1.0936	2.0980	-7139.9
4	0.02277	-1095.82	1.3423	2.0980	-8530.7
5	0.02435	-1158.21	1.4378	2.0980	-8944.8
6	0.02769	-1337.28	1.6406	2.0980	-10492.7
7	0.03107	-1467.43	1.8473	2.0980	-11344.4
8	0.03379	-1562.78	2.0147	2.0980	-11900.5
9	0.03406	-1621.95	2.0314	2.0980	-12664.3
10	0.03683	-1692.74	2.2029	2.0980	-12860.0
11	0.03937	-1766.88	2.3610	2.0980	-13172.7
12	0.04299	-1830.75	2.5879	2.0980	-13019.9
13	0.05235	-1832.49	3.1825	2.0980	-10245.3
14	0.07150	-1795.62	4.4363	2.0980	-3794.8
15	0.09642	-1687.69	6.1475	2.0980	5922.1
16	0.09642	-1687.69	6.1475	2.0980	5922.1
17	0.14493	-1576.52	9.7637	2.0980	24865.0
			DATA SET NUMBER 3		
1	0.00209	-125.21	0.1207	2.0980	-1106.6
2	0.00471	-157.37	0.2726	2.0980	-773.9
3	0.00808	-394.45	0.4693	2.0980	-3060.0
4	0.01251	-613.83	0.7298	2.0980	-4802.4
5	0.01872	-883.77	1.0990	2.0980	-6743.9
6	0.02288	-1025.00	1.3490	2.0980	-7500.4
7	0.02780	-1091.53	1.6473	2.0980	-6980.1
8	0.03031	-1122.37	1.8007	2.0980	-6668.6
9	0.03422	-1163.19	2.0413	2.0980	-6077.1
10	0.03912	-1180.35	2.3454	2.0980	-4842.1

11	0.04262	-1198.69	2.5646	2.0980	-4039.7
12	0.04663	-1250.23	2.8177	2.0980	-3553.9
13	0.04695	-1234.45	2.8380	2.0980	-3227.5
14	0.05171	-1240.15	3.1414	2.0980	-1838.2
15	0.05435	-1228.89	3.3110	2.0980	-851.6
16	0.05633	-1253.68	3.4389	2.0980	-593.1
17	0.06027	-1266.94	3.6948	2.0980	453.2
18	0.06336	-1247.16	3.8971	2.0980	1723.7
19	0.06360	-1276.27	3.9128	2.0980	1372.0
20	0.06722	-1283.53	4.1516	2.0980	2420.8
21	0.07091	-1327.79	4.3969	2.0980	2952.2
22	0.07550	-1308.76	4.7047	2.0980	4722.3
23	0.08027	-1323.27	5.0279	2.0980	6067.3
24	0.08553	-1314.51	5.3882	2.0980	7939.5
25	0.09138	-1354.78	5.7938	2.0980	9289.2
26	0.09757	-1351.99	6.2287	2.0980	11429.2
27	0.11365	-1331.83	7.3861	2.0980	17325.2
28	0.12319	-1371.50	8.0933	2.0980	20116.6
29	0.14657	-1345.52	9.8932	2.0980	29209.3
30	0.16228	-1325.48	11.1591	2.0980	35646.5
31	0.18051	-1327.19	12.6889	2.0980	43006.3

DATA SET NUMBER 4

1	0.01032	-538.03	0.6372	5.5946	-4660.0
2	0.01596	-723.98	0.9911	5.5946	-5643.9
3	0.02375	-1135.07	1.4866	5.5946	-9329.1
4	0.03521	-1718.98	2.2301	5.5946	-14543.0
5	0.04935	-2330.88	3.1721	5.5946	-19481.7
6	0.05138	-2599.37	3.3097	5.5946	-22983.8
7	0.05373	-2831.27	3.4697	5.5946	-25838.9
8	0.05392	-2707.84	3.4826	5.5946	-23875.7
9	0.05392	-2877.80	3.4826	5.5946	-26499.2
10	0.06195	-3052.53	4.0355	5.5946	-26754.1
11	0.06853	-3242.92	4.4957	5.5946	-27706.7
12	0.07180	-3333.09	4.7268	5.5946	-28115.0
13	0.07533	-3749.01	4.9781	5.5946	-33590.7
14	0.07560	-3822.88	4.9974	5.5946	-34675.7
15	0.07560	-3622.78	4.9974	5.5946	-31514.5
16	0.07971	-3707.73	5.2927	5.5946	-31598.8
17	0.08933	-4128.39	5.9941	5.5946	-35356.5
18	0.09432	-4363.78	6.3638	5.5946	-37614.3
19	0.09432	-4344.96	6.3638	5.5946	-37310.8
20	0.10014	-4381.38	6.8001	5.5946	-36109.1
21	0.10656	-4361.23	7.2881	5.5946	-33779.5
22	0.11328	-4323.78	7.8064	5.5946	-31035.4
23	0.12201	-4349.51	8.4908	5.5946	-28648.1
24	0.14052	-4237.47	9.9897	5.5946	-20588.6
25	0.16450	-4120.36	12.0302	5.5946	-10106.5
26	0.18081	-4013.58	13.4863	5.5946	-2142.7

DATA SET NUMBER 5

1	0.00960	-483.61	0.5923	5.5946	-4082.8
2	0.01188	-603.72	0.7347	5.5946	-5141.7
3	0.01238	-582.75	0.7660	5.5946	-4675.0
4	0.01486	-754.47	0.9217	5.5946	-6440.8
5	0.01852	-984.11	1.1530	5.5946	-8708.9
6	0.01857	-904.55	1.1562	5.5946	-7509.4
7	0.02212	-1097.21	1.3822	5.5946	-9272.3
8	0.02481	-1177.94	1.5546	5.5946	-9639.3
9	0.02636	-1316.67	1.6544	5.5946	-11234.9
10	0.02988	-1444.05	1.8821	5.5946	-12052.1
11	0.03004	-1418.57	1.8925	5.5946	-11618.7

12	0.03122	-1471.90	1.9692	5.5946	-12053.7
13	0.03175	-1504.87	2.0037	5.5946	-12385.4
14	0.03179	-1519.79	2.0063	5.5946	-12598.0
15	0.03444	-1655.06	2.1796	5.5946	-13815.4
16	0.03548	-1732.79	2.2478	5.5946	-14668.1
17	0.04002	-1960.09	2.5474	5.5946	-16708.1
18	0.04071	-2005.64	2.5932	5.5946	-17187.4
19	0.04153	-2117.19	2.6477	5.5946	-18632.6
20	0.04170	-1981.76	2.6590	5.5946	-16516.2
21	0.04321	-2251.95	2.7596	5.5946	-20170.1
22	0.04536	-2168.06	2.9035	5.5946	-18224.0
23	0.04761	-2406.12	3.0547	5.5946	-21174.4
24	0.04854	-2354.73	3.1174	5.5946	-20099.0
25	0.04990	-2474.19	3.2093	5.5946	-21513.8
26	0.05081	-2487.15	3.2710	5.5946	-21432.3
27	0.05452	-2690.29	3.5236	5.5946	-23420.1
28	0.05455	-2804.05	3.5257	5.5946	-25168.1
29	0.05541	-2671.57	3.5845	5.5946	-22856.4
30	0.05617	-2705.54	3.6366	5.5946	-23147.3
31	0.05741	-2816.64	3.7218	5.5946	-24485.3
32	0.05802	-2921.08	3.7638	5.5946	-25916.6
33	0.05810	-2858.76	3.7693	5.5946	-24925.9
34	0.06211	-3032.12	4.0466	5.5946	-26387.4
35	0.06241	-3073.74	4.0675	5.5946	-26943.4
36	0.06548	-3289.99	4.2816	5.5946	-29378.2
37	0.06785	-3420.02	4.4478	5.5946	-30690.5
38	0.06834	-3304.31	4.4823	5.5946	-28727.5
39	0.07194	-3423.51	4.7367	5.5946	-29494.7
40	0.07293	-3549.66	4.8071	5.5946	-31177.6
41	0.07599	-3751.85	5.0253	5.5946	-33435.0
42	0.08000	-3888.23	5.3136	5.5946	-34374.9
43	0.08042	-3947.60	5.3439	5.5946	-35189.8
44	0.08394	-4014.46	5.5993	5.5946	-35182.6
45	0.08698	-4102.71	5.8214	5.5946	-35664.1
46	0.08953	-4254.74	6.0088	5.5946	-37321.8
47	0.09200	-4525.81	6.1914	5.5946	-40927.7
48	0.09226	-4332.18	6.2107	5.5946	-37734.2
49	0.09644	-4493.02	6.5221	5.5946	-39053.6
50	0.09909	-4495.07	6.7210	5.5946	-38276.6
51	0.10236	-4517.48	6.9681	5.5946	-37635.1
52	0.11320	-4399.46	7.8002	5.5946	-32307.2
53	0.16858	-4106.41	12.3891	5.5946	-8367.8

DATA SET NUMBER 6

1	0.01623	-757.04	1.0081	5.5946	-6049.9
2	0.03605	-1712.95	2.2853	5.5946	-14190.2
3	0.04489	-2204.70	2.8720	5.5946	-18929.9
4	0.04683	-2311.05	3.0022	5.5946	-19957.8
5	0.05104	-2485.81	3.2866	5.5946	-21340.7
6	0.05333	-2579.51	3.4424	5.5946	-22076.9
7	0.05497	-2616.49	3.5544	5.5946	-22141.1
8	0.05773	-2663.77	3.7438	5.5946	-22017.5
9	0.06003	-2674.39	3.9025	5.5946	-21466.9
10	0.06111	-2926.87	3.9773	5.5946	-25057.0
11	0.06625	-2917.74	4.3355	5.5946	-23321.1
12	0.06959	-2957.41	4.5704	5.5946	-22898.5
13	0.07033	-3032.11	4.6227	5.5946	-23839.8
14	0.07343	-3055.62	4.8426	5.5946	-23238.0
15	0.07676	-3132.81	5.0805	5.5946	-23408.4
16	0.08121	-3008.66	5.4011	5.5946	-20025.3
17	0.08121	-3101.43	5.4011	5.5946	-21499.9
18	0.08235	-3176.16	5.4837	5.5946	-22325.3
19	0.08235	-3182.38	5.4837	5.5946	-22424.3

20	0.08574	-3158.95	5.7306	5.5946	-20967.0
21	0.08574	-3040.49	5.7306	5.5946	-19074.8
22	0.08574	-3159.15	5.7306	5.5946	-20970.2
23	0.08694	-3236.41	5.8184	5.5946	-21820.2
24	0.09068	-3220.55	6.0937	5.5946	-20361.7
25	0.09068	-3144.75	6.0937	5.5946	-19144.5
26	0.09193	-3291.50	6.1862	5.5946	-21097.9
27	0.09640	-3272.88	6.5191	5.5946	-19345.7
28	0.09739	-3322.89	6.5933	5.5946	-19831.1
29	0.10164	-3382.37	6.9135	5.5946	-19404.0
30	0.10851	-3401.69	7.4377	5.5946	-17446.6
31	0.10962	-3383.41	7.5232	5.5946	-16776.4
32	0.11534	-3458.21	7.9669	5.5946	-16086.3
33	0.12379	-3356.96	8.6322	5.5946	-11524.5
34	0.12545	-3511.35	8.7646	5.5946	-13527.6
35	0.13281	-3429.61	9.3576	5.5946	-9596.8
36	0.14299	-3442.46	10.1946	5.5946	-6194.1
37	0.15407	-3506.93	11.1285	5.5946	-3269.1
38	0.16999	-3602.40	12.5140	5.5946	1020.3
39	0.18381	-3529.29	13.7605	5.5946	7670.7
40	0.20378	-3578.81	15.6382	5.5946	14842.3

DATA SET NUMBER 7

1	0.01442	-588.97	0.9964	12.5878	-4598.1
2	0.03301	-1560.02	2.3247	12.5878	-14292.5
3	0.04906	-2370.29	3.5133	12.5878	-22486.3
4	0.06003	-2861.98	4.3491	12.5878	-27172.0
5	0.07428	-3691.65	5.4643	12.5878	-36782.0
6	0.09352	-4585.66	7.0257	12.5878	-46175.3
7	0.09854	-4895.70	7.4441	12.5878	-50078.5
8	0.10617	-5293.11	8.0889	12.5878	-54750.6
9	0.12050	-5888.38	9.3303	12.5878	-60948.0
10	0.12413	-6321.38	9.6512	12.5878	-67794.0
11	0.12830	-6424.14	10.0231	12.5878	-68360.4
12	0.13591	-6837.64	10.7102	12.5878	-73667.4
13	0.13673	-6772.64	10.7851	12.5878	-72179.0
14	0.14421	-7169.30	11.4746	12.5878	-77290.3
15	0.14601	-7395.03	11.6423	12.5878	-81016.5
16	0.15341	-7583.81	12.3393	12.5878	-82290.4
17	0.15365	-7563.32	12.3621	12.5878	-81820.4
18	0.16200	-7972.67	13.1638	12.5878	-87093.7
19	0.16291	-8101.09	13.2522	12.5878	-89304.4
20	0.16311	-8024.78	13.2716	12.5878	-87757.9
21	0.17393	-8420.95	14.3374	12.5878	-92122.3
22	0.17491	-8502.78	14.4353	12.5878	-93429.4
23	0.18422	-8399.93	15.3772	12.5878	-88444.0
24	0.18691	-8210.61	15.6534	12.5878	-83787.7
25	0.18771	-8657.98	15.7359	12.5878	-92488.7
26	0.19565	-8304.56	16.5634	12.5878	-82790.9
27	0.19921	-8225.94	16.9398	12.5878	-80003.0
28	0.20111	-8205.08	17.1421	12.5878	-78934.7
29	0.20201	-8389.04	17.2382	12.5878	-82380.5
30	0.20948	-8087.96	18.0446	12.5878	-73648.4
31	0.21160	-8095.57	18.2762	12.5878	-73061.1
32	0.22101	-7959.04	19.3196	12.5878	-66857.5
33	0.22503	-7926.97	19.7731	12.5878	-64712.9
34	0.22661	-7928.83	19.9526	12.5878	-64168.2
35	0.22911	-7883.30	20.2381	12.5878	-62278.6
36	0.23571	-7974.08	21.0010	12.5878	-61723.1
37	0.26273	-7544.74	24.2663	12.5878	-41663.1
38	0.28671	-7460.81	27.3715	12.5878	-29366.3
39	0.30451	-7141.00	29.8149	12.5878	-13663.9
40	0.31562	-7061.64	31.4044	12.5878	-6309.2

41	0.38284	-6285.83	42.2420	12.5878	51635.6
42	0.48645	-5158.22	64.5032	12.5878	168497.3

DATA SET NUMBER 8

1	0.01245	-593.29	0.8585	12.5878	-5359.3
2	0.01928	-920.08	1.3388	12.5878	-8379.1
3	0.02858	-1426.43	2.0035	12.5878	-13587.4
4	0.03325	-1673.62	2.3422	12.5878	-16121.6
5	0.03904	-1901.58	2.7666	12.5878	-17967.8
6	0.04252	-2275.27	3.0242	12.5878	-23111.4
7	0.04770	-2325.97	3.4110	12.5878	-22197.1
8	0.05139	-2523.73	3.6892	12.5878	-24313.1
9	0.05211	-2735.52	3.7437	12.5878	-27701.9
10	0.05861	-2867.53	4.2398	12.5878	-27755.6
11	0.06424	-3179.13	4.6750	12.5878	-31233.5
12	0.07060	-3634.32	5.1730	12.5878	-37020.2
13	0.07726	-4082.59	5.7019	12.5878	-42664.3
14	0.07741	-3818.73	5.7139	12.5878	-37959.5
15	0.08157	-4361.61	6.0482	12.5878	-46164.3
16	0.08490	-4281.06	6.3180	12.5878	-43624.5
17	0.08522	-4367.57	6.3441	12.5878	-45056.1
18	0.08915	-4506.66	6.6653	12.5878	-46223.7
19	0.08932	-4470.02	6.6792	12.5878	-45512.1
20	0.09000	-4747.91	6.7351	12.5878	-50254.3
21	0.09481	-4710.89	7.1328	12.5878	-47993.5
22	0.09947	-4958.02	7.5217	12.5878	-50895.9
23	0.09983	-5018.28	7.5523	12.5878	-51864.2
24	0.10489	-5222.49	7.9800	12.5878	-53889.4
25	0.10568	-5498.67	8.0472	12.5878	-58653.6
26	0.11124	-5784.20	8.5235	12.5878	-62056.7
27	0.11165	-5396.43	8.5589	12.5878	-54819.2
28	0.11780	-5940.30	9.0933	12.5878	-62791.9
29	0.11905	-6230.89	9.2028	12.5878	-67752.4
30	0.12540	-6335.47	9.7641	12.5878	-67645.7
31	0.12606	-6287.92	9.8229	12.5878	-66546.6
32	0.13380	-6625.75	10.5183	12.5878	-70360.4
33	0.13453	-6813.52	10.5846	12.5878	-73655.3
34	0.14239	-7256.48	11.3057	12.5878	-79524.6
35	0.14290	-6999.76	11.3530	12.5878	-74488.4
36	0.14341	-7416.71	11.4003	12.5878	-82246.4
37	0.15307	-7599.41	12.3070	12.5878	-82697.8
38	0.15415	-8018.33	12.4097	12.5878	-90416.7
39	0.16537	-8256.23	13.4920	12.5878	-91559.8
40	0.17869	-8360.68	14.8152	12.5878	-89430.6

DATA SET NUMBER 9

1	0.01438	-623.49	0.9936	12.5878	-5182.2
2	0.02228	-1057.10	1.5518	12.5878	-9610.3
3	0.03304	-1570.53	2.3269	12.5878	-14459.0
4	0.04876	-2372.46	3.4907	12.5878	-22626.9
5	0.07410	-3702.88	5.4500	12.5878	-37040.4
6	0.07747	-3904.96	5.7187	12.5878	-39460.5
7	0.08924	-4488.88	6.6727	12.5878	-45876.0
8	0.09830	-4971.08	7.4239	12.5878	-51519.0
9	0.10335	-5197.97	7.8493	12.5878	-53953.7
10	0.10810	-5424.93	8.2538	12.5878	-56516.1
11	0.11470	-5748.01	8.8230	12.5878	-60264.1
12	0.12065	-5933.48	9.3435	12.5878	-61733.3
13	0.12070	-6064.23	9.3479	12.5878	-64137.0
14	0.12070	-6093.34	9.3479	12.5878	-64675.9
15	0.12799	-6204.99	9.9954	12.5878	-64370.4
16	0.13515	-6226.24	10.6410	12.5878	-62405.0

17	0.13561	-6277.26	10.6829	12.5878	-63212.2
18	0.14251	-6280.44	11.3168	12.5878	-60961.1
19	0.14391	-6319.71	11.4467	12.5878	-61234.3
20	0.15261	-6391.57	12.2634	12.5878	-59644.9
21	0.16174	-6337.05	13.1386	12.5878	-55418.7
22	0.17405	-6546.73	14.3494	12.5878	-55153.1
23	0.17458	-6457.41	14.4023	12.5878	-53202.3
24	0.18561	-6370.83	15.5197	12.5878	-47445.7
25	0.20159	-6538.80	17.1933	12.5878	-44804.9
26	0.23656	-6434.45	21.1002	12.5878	-28578.9

MDEA PROTONATION

LN K : -20.0000
DELTA H : 9497.60

SUMMARY OF FIT FOR LOADING CURVE

POINT	LOADING MOLE CO2 / MOLE MDEA	EXPERIMENTAL HEAT OF SOLN (BTU/LB MDEA)	CALCULATED HEAT OF SOLN (BTU/LB MDEA)	EXPERIMENTAL HEAT OF SOLN (BTU/LB CO2)	CALCULATED HEAT OF SOLN (BTU/LB CO2)	RELATIVE ERROR	EQUILIBRIUM PRESSURE OF CO2 (PSIA)
			DATA SET NUMBER 1				
1	0.195801	-31.94	-38.62	-441.69	-534.07	20.91	0.08
2	0.253856	-43.22	-49.23	-461.03	-525.13	13.90	0.15
3	0.253856	-44.46	-49.23	-474.24	-525.13	10.73	0.15
4	0.316932	-55.60	-60.57	-475.01	-517.46	8.94	0.25
5	0.393567	-69.99	-74.12	-481.54	-509.90	5.89	0.44
6	0.591603	-98.19	-108.22	-449.41	-495.32	10.21	1.49
7	0.885505	-150.07	-156.58	-458.87	-478.77	4.34	10.87
8	1.098344	-183.73	-182.62	-452.92	-450.20	-0.60	124.02
9	1.148029	-188.20	-185.83	-443.87	-438.28	-1.26	174.74
10	1.200880	-189.51	-185.81	-427.29	-418.96	-1.95	230.73
11	1.256928	-190.15	-185.80	-409.61	-400.25	-2.29	291.18
12	1.382404	-191.52	-185.77	-375.12	-363.86	-3.00	428.24
13	2.361871	-191.44	-185.53	-219.47	-212.69	-3.09	1511.42
14	3.345787	-194.80	-185.29	-157.64	-149.95	-4.88	2602.26
15	6.790010	-197.24	-184.46	-78.65	-73.56	-6.48	6422.21
16	7.339066	-121.81	-184.33	-44.94	-68.01	51.32	7031.20

THE LOADING POINT IS 1.13612

MEAN OF THE ABSOLUTE PERCENT ERROR IS 9.3617

DATA SET NUMBER 2

1	0.172425	-28.81	-34.29	-452.37	-538.44	19.03	0.06
2	0.424680	-70.26	-79.56	-447.97	-507.22	13.23	0.54
3	0.521286	-91.93	-96.25	-477.51	-499.92	4.69	0.99
4	0.639827	-111.16	-116.36	-470.42	-492.42	4.68	1.97
5	0.685332	-117.68	-123.98	-464.94	-489.82	5.35	2.58
6	0.782014	-136.34	-139.95	-472.07	-484.57	2.65	4.79
7	0.880532	-150.13	-155.80	-461.66	-479.07	3.77	10.38
8	0.960313	-160.34	-167.74	-452.08	-472.96	4.62	24.88
9	0.968257	-166.46	-168.83	-465.48	-472.12	1.43	27.60
10	1.050014	-174.22	-178.22	-449.26	-459.56	2.29	78.86
11	1.125396	-182.33	-184.93	-438.68	-444.94	1.43	151.31
12	1.233523	-189.64	-185.81	-416.27	-407.85	-2.02	265.84
13	1.516928	-191.69	-185.74	-342.16	-331.53	-3.11	576.29
14	2.114562	-191.71	-185.59	-245.48	-237.65	-3.19	1237.39
15	2.930197	-185.16	-185.40	-171.09	-171.31	0.13	2141.44
16	2.930197	-185.16	-185.40	-171.09	-171.31	0.13	2141.44
17	4.653909	-182.77	-184.98	-106.34	-107.62	1.21	4052.98

THE LOADING POINT IS 1.13612

MEAN OF THE ABSOLUTE PERCENT ERROR IS 4.2906

DATA SET NUMBER 3

1	0.057511	-12.44	-12.26	-585.60	-577.00	-1.47	0.01
2	0.129947	-15.67	-26.31	-326.60	-548.19	67.85	0.03
3	0.223682	-39.42	-43.74	-477.19	-529.49	10.96	0.11
4	0.347873	-61.62	-66.07	-479.63	-514.22	7.21	0.32
5	0.523853	-89.28	-96.69	-461.47	-499.74	8.29	1.00
6	0.642990	-103.99	-116.89	-437.90	-492.23	12.41	2.01
7	0.785209	-111.30	-140.48	-383.79	-484.40	26.21	4.89
8	0.858320	-114.74	-152.28	-361.96	-480.39	32.72	8.53
9	0.972967	-119.39	-166.52	-332.26	-463.41	39.47	29.38
10	1.117959	-121.77	-166.27	-294.93	-402.69	36.54	143.71
11	1.222434	-124.12	-166.08	-274.92	-367.87	33.81	253.88
12	1.343075	-130.00	-165.87	-262.08	-334.39	27.59	385.12
13	1.352746	-128.40	-165.85	-257.01	-331.97	29.17	395.71
14	1.497372	-129.64	-165.60	-234.43	-299.44	27.73	554.73
15	1.578212	-128.82	-165.45	-221.02	-283.86	28.43	643.91
16	1.639139	-131.70	-165.35	-217.55	-273.13	25.55	711.21
17	1.761142	-133.65	-165.13	-205.48	-253.88	23.55	846.10
18	1.857542	-132.00	-164.96	-192.41	-240.45	24.97	952.77
19	1.865057	-135.11	-164.95	-196.15	-239.47	22.08	961.09
20	1.978862	-136.41	-164.75	-186.65	-225.42	20.77	1087.09
21	2.095781	-141.67	-164.54	-183.03	-212.58	16.14	1216.59

22	2.242520	-140.34	-164.28	-169.44	-198.35	17.06	1379.16
23	2.396565	-142.63	-164.01	-161.14	-185.30	14.99	1549.87
24	2.568297	-142.50	-163.70	-150.23	-172.59	14.88	1740.22
25	2.761627	-147.81	-163.36	-144.92	-160.17	10.52	1954.55
26	2.968924	-148.52	-163.00	-135.45	-148.65	9.75	2184.38
27	3.520606	-148.95	-162.02	-114.56	-124.61	8.77	2796.12
28	3.857678	-155.06	-161.43	-108.83	-113.30	4.10	3169.92
29	4.715620	-156.29	-159.91	-89.74	-91.82	2.32	4121.42
30	5.319005	-156.85	-158.84	-79.85	-80.86	1.27	4790.64
31	6.048177	-160.55	-157.55	-71.87	-70.53	-1.86	5599.39

THE LOADING POINT IS 0.95187

MEAN OF THE ABSOLUTE PERCENT ERROR IS 19.6281

DATA SET NUMBER 4

1	0.113895	-21.44	-24.08	-509.61	-572.36	12.31	0.05
2	0.177149	-29.01	-36.28	-443.41	-554.48	25.05	0.15
3	0.265718	-45.85	-52.70	-467.16	-537.02	14.95	0.42
4	0.398613	-70.25	-76.38	-477.22	-518.80	8.71	1.27
5	0.567002	-96.68	-105.25	-461.68	-502.61	8.87	3.85
6	0.591589	-108.05	-109.39	-494.52	-500.64	1.24	4.48
7	0.620183	-117.98	-114.17	-515.08	-498.45	-3.23	5.35
8	0.622501	-112.86	-114.56	-490.89	-498.27	1.50	5.43
9	0.622501	-119.94	-114.56	-521.70	-498.27	-4.49	5.43
10	0.721329	-128.31	-130.89	-481.65	-491.33	2.01	10.15
11	0.803581	-137.28	-144.25	-462.56	-486.06	5.08	18.08
12	0.844892	-141.59	-150.86	-453.77	-483.47	6.55	25.20
13	0.889814	-159.87	-157.93	-486.47	-480.57	-1.21	38.35
14	0.893264	-163.07	-158.47	-494.29	-480.34	-2.82	39.75
15	0.893264	-154.53	-158.47	-468.42	-480.34	2.55	39.75
16	0.946033	-158.86	-166.44	-454.68	-476.36	4.77	75.39
17	1.071407	-178.75	-172.93	-451.75	-437.01	-3.26	486.90
18	1.137489	-189.99	-172.91	-452.24	-411.59	-8.99	847.08
19	1.137489	-189.17	-172.91	-450.29	-411.59	-8.59	847.08
20	1.215488	-191.99	-172.89	-427.68	-385.14	-9.95	1292.87
21	1.302707	-192.48	-172.87	-400.06	-359.31	-10.19	1799.38
22	1.395355	-192.27	-172.85	-373.10	-335.41	-10.10	2340.92
23	1.517691	-195.34	-172.82	-348.49	-308.33	-11.53	3058.37
24	1.785601	-194.40	-172.76	-294.79	-261.97	-11.13	4633.29
25	2.150334	-194.46	-172.68	-244.86	-217.43	-11.20	6780.25
26	2.410608	-193.19	-172.62	-216.99	-193.89	-10.65	8313.07

THE LOADING POINT IS 0.99437

MEAN OF THE ABSOLUTE PERCENT ERROR IS 7.7280

DATA SET NUMBER 5

1	0.105871	-19.25	-22.49	-492.42	-575.19	16.81	0.05
2	0.131318	-24.09	-27.49	-496.74	-566.74	14.09	0.08
3	0.136914	-23.27	-28.57	-460.12	-565.07	22.81	0.08
4	0.164755	-30.20	-33.92	-496.29	-557.51	12.34	0.13
5	0.206100	-39.54	-41.72	-519.41	-548.07	5.52	0.22
6	0.206667	-36.34	-41.82	-476.13	-547.96	15.08	0.23
7	0.247069	-44.24	-49.29	-484.86	-540.22	11.42	0.35
8	0.277879	-47.63	-54.91	-464.09	-535.04	15.29	0.47
9	0.295709	-53.32	-58.13	-488.25	-532.27	9.02	0.56
10	0.336413	-58.69	-65.41	-472.40	-526.49	11.45	0.79
11	0.338271	-57.67	-65.74	-461.60	-526.24	14.00	0.80
12	0.351986	-59.91	-68.18	-460.85	-524.44	13.80	0.89
13	0.358158	-61.28	-69.27	-463.30	-523.66	13.03	0.94
14	0.358624	-61.89	-69.35	-467.31	-523.60	12.05	0.94
15	0.389585	-67.59	-74.80	-469.74	-519.84	10.66	1.19
16	0.401782	-70.84	-76.93	-477.39	-518.44	8.60	1.30
17	0.455337	-80.51	-86.22	-478.75	-512.72	7.09	1.88
18	0.463521	-82.44	-87.63	-481.57	-511.90	6.30	1.99
19	0.473262	-87.10	-89.31	-498.32	-510.94	2.53	2.12
20	0.475283	-81.54	-89.65	-464.54	-510.75	9.95	2.15
21	0.493271	-92.81	-92.74	-509.43	-509.04	-0.08	2.41
22	0.518981	-89.55	-97.12	-467.21	-506.70	8.45	2.85
23	0.546011	-99.62	-101.71	-494.00	-504.36	2.10	3.38
24	0.557221	-97.59	-103.60	-474.19	-503.42	6.16	3.62
25	0.573653	-102.68	-106.37	-484.67	-502.07	3.59	4.01
26	0.584674	-103.32	-108.22	-478.48	-501.19	4.75	4.29
27	0.629827	-112.20	-115.78	-482.34	-497.73	3.19	5.68
28	0.630194	-116.95	-115.84	-502.46	-497.70	-0.95	5.69
29	0.640712	-111.52	-117.59	-471.29	-496.93	5.44	6.08
30	0.650023	-113.03	-119.14	-470.83	-496.25	5.40	6.44
31	0.665247	-117.83	-121.66	-479.57	-495.17	3.25	7.09
32	0.672751	-122.28	-122.90	-492.13	-494.64	0.51	7.43
33	0.673735	-119.68	-123.06	-480.96	-494.57	2.83	7.47
34	0.723315	-127.48	-131.22	-477.20	-491.20	2.93	10.29
35	0.727042	-129.27	-131.83	-481.42	-490.95	1.98	10.54
36	0.765311	-138.82	-138.07	-491.13	-488.47	-0.54	13.68
37	0.795027	-144.67	-142.88	-492.71	-486.59	-1.24	16.95
38	0.801190	-139.85	-143.87	-472.63	-486.21	2.87	17.75
39	0.846667	-145.46	-151.14	-465.17	-483.36	3.91	25.59
40	0.859235	-150.98	-153.14	-475.76	-482.56	1.43	28.58

41	0.898251	-160.11	-159.24	-482.61	-480.00	-0.54	41.91
42	0.949774	-166.65	-166.98	-475.09	-476.02	0.20	79.52
43	0.955196	-169.27	-167.75	-479.82	-475.52	-0.90	86.09
44	1.000836	-172.80	-172.94	-467.49	-467.87	0.08	181.16
45	1.040536	-177.19	-172.93	-461.07	-450.00	-2.40	335.37
46	1.074041	-184.27	-172.92	-464.53	-435.94	-6.15	500.57
47	1.106675	-196.54	-172.92	-480.86	-423.07	-12.02	675.60
48	1.110120	-188.18	-172.92	-458.99	-421.75	-8.11	694.55
49	1.165784	-196.07	-172.90	-455.40	-401.58	-11.82	1007.45
50	1.201342	-196.74	-172.90	-443.42	-389.68	-12.12	1211.29
51	1.245507	-198.44	-172.89	-431.40	-375.84	-12.88	1466.63
52	1.394244	-195.62	-172.85	-379.90	-335.68	-11.64	2334.41
53	2.214485	-194.75	-172.66	-238.12	-211.11	-11.34	7158.01

THE LOADING POINT IS 0.99437

MEAN OF THE ABSOLUTE PERCENT ERROR IS 7.2384

DATA SET NUMBER 6

1	0.180195	-30.34	-36.85	-455.95	-553.77	21.46	0.16
2	0.408478	-70.07	-78.10	-464.46	-517.68	11.46	1.36
3	0.513351	-91.02	-96.16	-480.08	-507.20	5.65	2.75
4	0.536626	-95.60	-100.12	-482.39	-505.16	4.72	3.18
5	0.587463	-103.29	-108.69	-476.07	-500.97	5.23	4.37
6	0.615306	-107.44	-113.36	-472.80	-498.82	5.50	5.19
7	0.635328	-109.17	-116.69	-465.27	-497.32	6.89	5.88
8	0.669182	-111.47	-122.31	-451.03	-494.89	9.72	7.26
9	0.697545	-112.19	-126.99	-435.48	-492.93	13.19	8.70
10	0.710912	-122.92	-129.19	-468.17	-492.03	5.10	9.48
11	0.774949	-123.21	-139.63	-430.50	-487.86	13.32	14.64
12	0.816941	-125.34	-146.40	-415.41	-485.22	16.81	20.04
13	0.826285	-128.60	-147.90	-421.42	-484.64	15.00	21.59
14	0.865592	-130.03	-148.53	-406.76	-464.62	14.23	30.29
15	0.908110	-133.80	-148.46	-398.94	-442.66	10.96	46.71
16	0.965409	-129.12	-148.37	-362.14	-416.12	14.91	100.63
17	0.965409	-133.10	-148.37	-373.30	-416.12	11.47	100.63
18	0.980177	-136.48	-148.34	-377.01	-409.78	8.69	127.83
19	0.980177	-136.75	-148.34	-377.75	-409.78	8.48	127.83
20	1.024311	-136.24	-148.27	-360.14	-391.93	8.83	265.10
21	1.024311	-131.13	-148.27	-346.63	-391.93	13.07	265.10
22	1.024311	-136.25	-148.27	-360.16	-391.93	8.82	265.10
23	1.040012	-139.77	-148.24	-363.88	-385.95	6.06	332.97
24	1.089213	-139.65	-148.16	-347.16	-368.31	6.09	580.79
25	1.089213	-136.37	-148.16	-338.99	-368.31	8.65	580.79
26	1.105747	-142.93	-148.13	-349.98	-362.73	3.64	670.51

27	1.165249	-142.82	-148.03	-331.87	-343.98	3.65	1004.40
28	1.178507	-145.16	-148.01	-333.51	-340.06	1.96	1080.15
29	1.235755	-148.46	-147.92	-325.29	-324.10	-0.37	1410.10
30	1.329448	-150.46	-147.76	-306.43	-300.94	-1.79	1955.44
31	1.344722	-149.84	-147.74	-301.70	-297.47	-1.40	2044.67
32	1.424038	-154.14	-147.60	-293.08	-280.65	-4.24	2508.95
33	1.542962	-151.07	-147.41	-265.10	-258.67	-2.42	3206.77
34	1.566623	-158.32	-147.37	-273.62	-254.70	-6.92	3345.75
35	1.672618	-155.94	-147.19	-252.44	-238.27	-5.61	3968.74
36	1.822226	-158.39	-146.94	-235.35	-218.34	-7.23	4848.78
37	1.989154	-163.47	-146.66	-222.51	-199.64	-10.28	5831.27
38	2.236801	-171.14	-146.25	-207.16	-177.03	-14.54	7289.43
39	2.459614	-170.50	-145.88	-187.70	-160.59	-14.44	8601.72
40	2.795244	-177.23	-145.32	-171.68	-140.77	-18.01	10578.81

THE LOADING POINT IS 0.83064

MEAN OF THE ABSOLUTE PERCENT ERROR IS 8.7704

DATA SET NUMBER 7

1	0.079153	-11.67	-17.55	-399.24	-600.38	50.38	0.05
2	0.184679	-31.51	-38.23	-461.95	-560.55	21.34	0.44
3	0.279105	-48.68	-55.53	-472.27	-538.74	14.08	1.44
4	0.345500	-59.47	-67.30	-466.03	-527.44	13.18	2.77
5	0.434096	-77.89	-82.66	-485.80	-515.60	6.13	5.86
6	0.558136	-98.80	-103.70	-479.30	-503.07	4.96	14.89
7	0.591371	-106.07	-109.26	-485.64	-500.27	3.01	18.91
8	0.642600	-115.66	-117.78	-487.33	-496.29	1.84	27.30
9	0.741216	-130.76	-134.02	-477.66	-489.57	2.49	56.62
10	0.766709	-140.96	-138.18	-497.79	-487.98	-1.97	69.19
11	0.796257	-143.93	-142.98	-489.44	-486.20	-0.66	88.23
12	0.850842	-154.55	-151.77	-491.81	-482.99	-1.79	144.79
13	0.856789	-153.22	-152.72	-484.22	-482.64	-0.33	153.60
14	0.911563	-163.61	-153.59	-485.99	-456.22	-6.13	285.36
15	0.924887	-169.12	-153.59	-495.11	-449.64	-9.18	341.46
16	0.980259	-174.95	-153.58	-483.26	-424.21	-12.22	874.71
17	0.982071	-174.53	-153.58	-481.20	-423.42	-12.01	907.09
18	1.045762	-185.81	-153.56	-481.09	-397.60	-17.35	2978.86
19	1.052779	-189.01	-153.56	-486.11	-394.95	-18.75	3290.59
20	1.054324	-187.27	-153.56	-480.94	-394.37	-18.00	3360.38
21	1.138993	-199.09	-153.54	-473.29	-365.01	-22.88	7510.23
22	1.146771	-201.27	-153.54	-475.21	-362.53	-23.71	7906.78
23	1.221598	-201.10	-153.53	-445.74	-340.29	-23.66	11764.09
24	1.243538	-197.22	-153.52	-429.42	-334.28	-22.16	12903.78
25	1.250090	-208.17	-153.52	-450.89	-332.52	-26.25	13244.64
26	1.315833	-201.64	-153.51	-414.93	-315.88	-23.87	16672.94

27	1.345733	-200.62	-153.50	-403.66	-308.85	-23.49	18235.77
28	1.361800	-200.59	-153.50	-398.83	-305.20	-23.48	19076.24
29	1.369437	-205.32	-153.50	-405.95	-303.49	-25.24	19475.88
30	1.433498	-199.82	-153.48	-377.43	-289.91	-23.19	22830.88
31	1.451900	-200.55	-153.48	-374.00	-286.22	-23.47	23795.36
32	1.534788	-199.55	-153.46	-352.03	-270.74	-23.09	28142.62
33	1.570812	-199.77	-153.46	-344.35	-264.51	-23.18	30033.11
34	1.585073	-200.23	-153.45	-342.03	-262.13	-23.36	30781.67
35	1.607758	-199.72	-153.45	-336.36	-258.42	-23.17	31972.49
36	1.668358	-203.77	-153.44	-330.70	-249.02	-24.70	35154.48
37	1.927766	-199.86	-153.38	-280.72	-215.43	-23.26	48783.41
38	2.174449	-204.28	-153.33	-254.38	-190.93	-24.94	61750.05
39	2.368557	-200.53	-153.29	-229.24	-175.24	-23.56	71955.27
40	2.494829	-201.52	-153.27	-218.71	-166.34	-23.95	78594.60
41	3.355790	-198.92	-153.09	-160.50	-123.52	-23.04	********
42	5.124267	-196.17	-152.72	-103.66	-80.70	-22.15	********

THE LOADING POINT IS 0.86228

MEAN OF THE ABSOLUTE PERCENT ERROR IS 17.5142

DATA SET NUMBER 8

1	0.068203	-11.73	-15.27	-465.81	-606.36	30.17	0.03
2	0.106354	-18.32	-23.08	-466.48	-587.57	25.96	0.10
3	0.159166	-28.68	-33.40	-487.87	-568.16	16.46	0.30
4	0.186068	-33.81	-38.49	-492.02	-560.16	13.85	0.45
5	0.219785	-38.65	-44.76	-476.12	-551.44	15.82	0.72
6	0.240247	-46.41	-48.51	-523.06	-546.72	4.52	0.93
7	0.270981	-47.70	-54.07	-476.65	-540.32	13.36	1.32
8	0.293079	-51.96	-58.03	-480.04	-536.15	11.69	1.67
9	0.297411	-56.36	-58.81	-513.13	-535.37	4.33	1.74
10	0.336818	-59.49	-65.78	-478.24	-528.78	10.57	2.56
11	0.371394	-66.35	-71.83	-483.74	-523.66	8.25	3.49
12	0.410956	-76.37	-78.68	-503.19	-518.41	3.02	4.87
13	0.452970	-86.41	-85.90	-516.53	-513.44	-0.60	6.80
14	0.453923	-80.84	-86.06	-482.21	-513.33	6.45	6.85
15	0.480483	-92.75	-90.59	-522.67	-510.47	-2.33	8.40
16	0.501918	-91.37	-94.22	-492.90	-508.29	3.12	9.87
17	0.503986	-93.25	-94.57	-500.97	-508.09	1.42	10.02
18	0.529503	-96.63	-98.88	-494.14	-505.65	2.33	12.09
19	0.530611	-95.86	-99.07	-489.19	-505.54	3.34	12.19
20	0.535050	-101.90	-99.82	-515.67	-505.13	-2.04	12.59
21	0.566641	-101.64	-105.13	-485.69	-502.33	3.43	15.83
22	0.597542	-107.53	-110.29	-487.24	-499.77	2.57	19.76
23	0.599971	-108.88	-110.70	-491.37	-499.57	1.67	20.11
24	0.633945	-113.95	-116.35	-486.70	-496.94	2.10	25.65

25	0.639283	-120.08	-117.23	-508.60	-496.54	-2.37	26.65
26	0.677127	-127.11	-123.49	-508.27	-493.82	-2.84	35.05
27	0.679936	-118.64	-123.96	-472.46	-493.62	4.48	35.78
28	0.722390	-131.51	-130.94	-492.92	-490.78	-0.43	49.03
29	0.731092	-138.14	-132.36	-511.61	-490.21	-4.18	52.38
30	0.775679	-141.48	-139.64	-493.85	-487.43	-1.30	74.38
31	0.780350	-140.52	-140.40	-487.58	-487.15	-0.09	77.28
32	0.835592	-149.39	-149.33	-484.09	-483.88	-0.04	125.11
33	0.840859	-153.76	-150.17	-495.11	-483.57	-2.33	131.48
34	0.898148	-165.25	-153.59	-498.19	-463.04	-7.05	241.43
35	0.901901	-159.50	-153.59	-478.85	-461.11	-3.70	252.68
36	0.905659	-169.10	-153.59	-505.56	-459.19	-9.17	264.72
37	0.977693	-175.24	-153.58	-485.32	-425.32	-12.36	831.22
38	0.985849	-185.14	-153.58	-508.49	-421.80	-17.05	979.20
39	1.071828	-193.20	-153.56	-488.05	-387.92	-20.52	4175.08
40	1.176948	-198.81	-153.54	-457.38	-353.22	-22.77	9454.92

THE LOADING POINT IS 0.86228

MEAN OF THE ABSOLUTE PERCENT ERROR IS 7.5032

DATA SET NUMBER 9

1	0.078930	-12.35	-17.51	-423.82	-600.50	41.69	0.05
2	0.123280	-21.12	-26.44	-463.78	-580.70	25.21	0.15
3	0.184852	-31.72	-38.27	-464.64	-560.50	20.63	0.45
4	0.277311	-48.71	-55.21	-475.61	-539.09	13.35	1.41
5	0.432960	-78.11	-82.47	-488.47	-515.74	5.58	5.81
6	0.454304	-82.67	-86.12	-492.72	-513.29	4.18	6.87
7	0.530090	-96.26	-98.98	-491.69	-505.59	2.83	12.14
8	0.589773	-107.67	-109.00	-494.32	-500.40	1.23	18.69
9	0.623564	-113.22	-113.19	-491.63	-491.48	-0.03	23.81
10	0.655697	-118.79	-113.14	-490.55	-467.20	-4.76	30.00
11	0.700917	-126.81	-113.07	-489.86	-436.79	-10.83	41.75
12	0.742265	-131.78	-113.01	-480.72	-412.24	-14.25	57.08
13	0.742615	-134.70	-113.01	-491.11	-412.04	-16.10	57.23
14	0.742615	-135.34	-113.01	-493.47	-412.04	-16.50	57.23
15	0.794051	-138.97	-112.93	-473.89	-385.09	-18.74	86.60
16	0.845341	-140.60	-112.86	-450.36	-361.48	-19.74	137.24
17	0.848669	-141.83	-112.85	-452.51	-360.04	-20.43	141.75
18	0.899030	-143.04	-112.78	-430.81	-339.65	-21.16	244.01
19	0.909348	-144.17	-112.76	-429.29	-335.75	-21.79	277.36
20	0.974226	-147.31	-112.66	-409.42	-313.12	-23.52	776.57
21	1.043759	-147.65	-112.56	-383.01	-291.99	-23.76	2891.72
22	1.139945	-154.80	-112.42	-367.70	-267.01	-27.38	7558.67
23	1.144150	-152.79	-112.41	-361.58	-266.02	-26.43	7773.00

24	1.232917	-152.78	-112.28	-335.53	-246.57	-26.51	12351.74
25	1.365871	-159.95	-112.08	-317.08	-222.18	-29.93	19289.26
26	1.676239	-164.61	-111.61	-265.89	-180.29	-32.19	35568.37

THE LOADING POINT IS 0.61499

MEAN OF THE ABSOLUTE PERCENT ERROR IS 18.0289

TOTAL MEAN OF THE PERCENT ERROR IS 11.2407

COMPOSITIONS FOR EACH DATA POINT

COMPONENT 1: [H+]
COMPONENT 2: [OH-]
COMPONENT 3: [MDEA]
COMPONENT 4: [MDEAH+]
COMPONENT 5: [CO2]
COMPONENT 6: [HCO3-]
COMPONENT 7: [CO3-2]
COMPONENT 8: CO2(G)

LOADING MOLALITY (GMOLE/KG H2O)

MOLE CO2

MOLE MDEA

DATA SET NUMBER 1

1	2	3	4	5	6	7	8
0.00000	0.22699D-11	0.23079D-02	0.20957D+01	0.23079D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.19580	0.63600D-09	0.14286D-04	0.15810D+01	0.51695D+00	0.21017D-03	0.30422D+00	0.10636D+00	0.00000D+00
0.25386	0.84673D-09	0.10623D-04	0.14490D+01	0.64896D+00	0.37010D-03	0.41548D+00	0.11673D+00	0.00000D+00
0.25386	0.84673D-09	0.10623D-04	0.14490D+01	0.64896D+00	0.37010D-03	0.41548D+00	0.11674D+00	0.00000D+00
0.31693	0.11008D-08	0.80226D-05	0.13107D+01	0.78729D+00	0.61237D-03	0.54132D+00	0.12298D+00	0.00000D+00
0.39357	0.14592D-08	0.58851D-05	0.11484D+01	0.94955D+00	0.10300D-02	0.69978D+00	0.12488D+00	0.00000D+00
0.59160	0.28710D-08	0.27501D-05	0.75232D+00	0.13456D+01	0.32042D-02	0.11303D+01	0.10768D+00	0.00000D+00
0.88551	0.12016D-07	0.57888D-06	0.22030D+00	0.18777D+01	0.21298D-01	0.17953D+01	0.41199D-01	0.00000D+00
1.09834	0.11503D-06	0.57655D-07	0.24223D-01	0.20737D+01	0.23546D+00	0.20639D+01	0.49177D-02	0.00000D+00
1.14803	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.24987D-01

1.20088	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.13586D+00
1.25693	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.25345D+00
1.38240	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.51670D+00
2.36187	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.25716D+01
3.34579	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.46358D+01
6.79001	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.11862D+02
7.33907	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.13014D+02

DATA SET NUMBER 2

0.00000	0.22699D-11	0.23079D-02	0.20957D+01	0.23079D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.17242	0.55593D-09	0.16361D-04	0.16357D+01	0.46226D+00	0.16028D-03	0.26092D+00	0.10066D+00	0.00000D+00
0.42468	0.16255D-08	0.52176D-05	0.10841D+01	0.10138D+01	0.12485D-02	0.76559D+00	0.12413D+00	0.00000D+00
0.52129	0.22540D-08	0.36124D-05	0.88955D+00	0.12084D+01	0.21787D-02	0.97451D+00	0.11695D+00	0.00000D+00
0.63983	0.34183D-08	0.22611D-05	0.66021D+00	0.14378D+01	0.41732D-02	0.12386D+01	0.99593D-01	0.00000D+00
0.68533	0.40742D-08	0.18593D-05	0.57476D+00	0.15232D+01	0.53833D-02	0.13416D+01	0.90783D-01	0.00000D+00
0.78201	0.62837D-08	0.11557D-05	0.39830D+00	0.16997D+01	0.96699D-02	0.15623D+01	0.68695D-01	0.00000D+00
0.88053	0.11561D-07	0.60285D-06	0.22844D+00	0.18695D+01	0.20365D-01	0.17844D+01	0.42568D-01	0.00000D+00
0.96031	0.24879D-07	0.27217D-06	0.10966D+00	0.19883D+01	0.47895D-01	0.19453D+01	0.21497D-01	0.00000D+00
0.96826	0.27360D-07	0.24691D-06	0.99963D-01	0.19980D+01	0.53044D-01	0.19587D+01	0.19675D-01	0.00000D+00
1.05001	0.73998D-07	0.89918D-07	0.37537D-01	0.20604D+01	0.15004D+00	0.20453D+01	0.75797D-02	0.00000D+00
1.12540	0.13983D-06	0.47382D-07	0.19948D-01	0.20780D+01	0.28708D+00	0.20699D+01	0.40567D-02	0.00000D+00
1.23352	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.20435D+00
1.51693	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.79892D+00
2.11456	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.20527D+01
2.93020	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.37639D+01
2.93020	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.37639D+01
4.65391	0.14987D-06	0.44194D-07	0.18618D-01	0.20793D+01	0.30798D+00	0.20718D+01	0.37882D-02	0.73802D+01

DATA SET NUMBER 3

0.00000	0.22699D-11	0.23079D-02	0.20957D+01	0.23079D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.05751	0.18720D-09	0.45551D-04	0.19236D+01	0.17433D+00	0.16458D-04	0.66991D-01	0.53649D-01	0.00000D+00
0.12995	0.41580D-09	0.21755D-04	0.17378D+01	0.36012D+00	0.88548D-04	0.18498D+00	0.87560D-01	0.00000D+00
0.22368	0.73488D-09	0.12318D-04	0.15170D+01	0.58097D+00	0.28021D-03	0.35704D+00	0.11196D+00	0.00000D+00
0.34787	0.12378D-08	0.70582D-05	0.12445D+01	0.85350D+00	0.76259D-03	0.60463D+00	0.12443D+00	0.00000D+00
0.52385	0.22736D-08	0.35772D-05	0.88448D+00	0.12135D+01	0.22099D-02	0.98015D+00	0.11667D+00	0.00000D+00
0.64299	0.34589D-08	0.22314D-05	0.65422D+00	0.14437D+01	0.42467D-02	0.12457D+01	0.99017D-01	0.00000D+00
0.78521	0.63873D-08	0.11354D-05	0.39260D+00	0.17054D+01	0.98758D-02	0.15696D+01	0.67896D-01	0.00000D+00
0.85832	0.98414D-08	0.71456D-06	0.26543D+00	0.18325D+01	0.16848D-01	0.17352D+01	0.48660D-01	0.00000D+00
0.97297	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.44257D-01
1.11796	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.34845D+00
1.22243	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.56763D+00
1.34307	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.82073D+00
1.35275	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.84102D+00
1.49737	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.11444D+01
1.57821	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.13140D+01
1.63914	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.14419D+01
1.76114	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.16978D+01
1.85754	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.19001D+01

1.86506	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.19158D+01
1.97886	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.21546D+01
2.09578	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.23999D+01
2.24252	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.27077D+01
2.39656	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.30309D+01
2.56830	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.33912D+01
2.76163	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.37968D+01
2.96892	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.42317D+01
3.52061	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.53891D+01
3.85768	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.60963D+01
4.71562	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.78962D+01
5.31900	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.91621D+01
6.04818	0.22568D-07	0.30084D-06	0.12055D+00	0.19774D+01	0.43101D-01	0.19304D+01	0.23524D-01	0.10692D+02

DATA SET NUMBER 4

0.00000	0.14088D-11	0.38212D-02	0.55908D+01	0.38212D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.11389	0.34673D-09	0.24199D-04	0.46810D+01	0.91354D+00	0.12497D-03	0.36062D+00	0.27645D+00	0.00000D+00
0.17715	0.50425D-09	0.14710D-04	0.42532D+01	0.13414D+01	0.31785D-03	0.64016D+00	0.35059D+00	0.00000D+00
0.26572	0.71226D-09	0.86855D-05	0.37001D+01	0.18945D+01	0.76795D-03	0.10771D+01	0.40869D+00	0.00000D+00
0.39861	0.10381D-08	0.45850D-05	0.29372D+01	0.26574D+01	0.19709D-02	0.17989D+01	0.42925D+00	0.00000D+00
0.56700	0.15897D-08	0.22079D-05	0.20483D+01	0.35463D+01	0.50767D-02	0.27879D+01	0.37920D+00	0.00000D+00
0.59159	0.16981D-08	0.19821D-05	0.19242D+01	0.36704D+01	0.57849D-02	0.29374D+01	0.36649D+00	0.00000D+00
0.62018	0.18390D-08	0.17446D-05	0.17814D+01	0.38132D+01	0.67351D-02	0.31127D+01	0.35022D+00	0.00000D+00
0.62250	0.18512D-08	0.17264D-05	0.17699D+01	0.38246D+01	0.68189D-02	0.31270D+01	0.34884D+00	0.00000D+00
0.62250	0.18512D-08	0.17264D-05	0.17699D+01	0.38246D+01	0.68189D-02	0.31270D+01	0.34884D+00	0.00000D+00
0.72133	0.25381D-08	0.10743D-05	0.12899D+01	0.43047D+01	0.11759D-01	0.37429D+01	0.28091D+00	0.00000D+00
0.80358	0.35800D-08	0.67282D-06	0.90600D+00	0.46886D+01	0.19674D-01	0.42635D+01	0.21255D+00	0.00000D+00
0.84489	0.44767D-08	0.50718D-06	0.71958D+00	0.48750D+01	0.26634D-01	0.45254D+01	0.17482D+00	0.00000D+00
0.88981	0.60964D-08	0.35031D-06	0.52384D+00	0.50707D+01	0.39334D-01	0.48069D+01	0.13194D+00	0.00000D+00
0.89326	0.62671D-08	0.33924D-06	0.50922D+00	0.50854D+01	0.40677D-01	0.48282D+01	0.12860D+00	0.00000D+00
0.89326	0.62671D-08	0.33924D-06	0.50922D+00	0.50854D+01	0.40677D-01	0.48282D+01	0.12860D+00	0.00000D+00
0.94603	0.10579D-07	0.18836D-06	0.29837D+00	0.52962D+01	0.74742D-01	0.51396D+01	0.78293D-01	0.00000D+00
1.07141	0.21019D-07	0.90611D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.43101D+00
1.13749	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.80071D+00
1.13749	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.80071D+00
1.21549	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.12371D+01
1.30271	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.17250D+01
1.39536	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.22434D+01
1.51769	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.29278D+01
1.78560	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.44266D+01
2.15033	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.64672D+01
2.41061	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.79233D+01

DATA SET NUMBER 5

0.00000	0.14088D-11	0.38212D-02	0.55908D+01	0.38212D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.10587	0.32566D-09	0.26131D-04	0.47379D+01	0.85667D+00	0.10723D-03	0.32775D+00	0.26444D+00	0.00000D+00
0.13132	0.39150D-09	0.20751D-04	0.45598D+01	0.10348D+01	0.16853D-03	0.43420D+00	0.30030D+00	0.00000D+00

0.13691	0.40561D-09	0.19815D-04	0.45214D+01	0.10732D+01	0.18402D-03	0.45843D+00	0.30737D+00	0.00000D+00
0.16476	0.47433D-09	0.16036D-04	0.43345D+01	0.12601D+01	0.27231D-03	0.58287D+00	0.33860D+00	0.00000D+00
0.20610	0.57300D-09	0.12200D-04	0.40674D+01	0.15272D+01	0.44000D-03	0.77803D+00	0.37457D+00	0.00000D+00
0.20667	0.57433D-09	0.12157D-04	0.40638D+01	0.15308D+01	0.44262D-03	0.78078D+00	0.37499D+00	0.00000D+00
0.24707	0.66877D-09	0.96092D-05	0.38130D+01	0.17816D+01	0.65356D-03	0.98159D+00	0.40000D+00	0.00000D+00
0.27788	0.74070D-09	0.81482D-05	0.36273D+01	0.19672D+01	0.84876D-03	0.11403D+01	0.41347D+00	0.00000D+00
0.29571	0.78264D-09	0.74390D-05	0.35219D+01	0.20727D+01	0.97662D-03	0.12341D+01	0.41930D+00	0.00000D+00
0.33641	0.88022D-09	0.60995D-05	0.32860D+01	0.23085D+01	0.13138D-02	0.14530D+01	0.42775D+00	0.00000D+00
0.33827	0.88476D-09	0.60461D-05	0.32754D+01	0.23191D+01	0.13308D-02	0.14632D+01	0.42799D+00	0.00000D+00
0.35199	0.91855D-09	0.56691D-05	0.31975D+01	0.23971D+01	0.14610D-02	0.15384D+01	0.42934D+00	0.00000D+00
0.35816	0.93393D-09	0.55091D-05	0.31626D+01	0.24320D+01	0.15224D-02	0.15725D+01	0.42974D+00	0.00000D+00
0.35862	0.93509D-09	0.54972D-05	0.31600D+01	0.24346D+01	0.15271D-02	0.15751D+01	0.42977D+00	0.00000D+00
0.38958	0.10143D-08	0.47741D-05	0.29871D+01	0.26075D+01	0.18635D-02	0.17479D+01	0.42981D+00	0.00000D+00
0.40178	0.10465D-08	0.45207D-05	0.29198D+01	0.26748D+01	0.20097D-02	0.18168D+01	0.42899D+00	0.00000D+00
0.45534	0.11975D-08	0.35746D-05	0.26296D+01	0.29650D+01	0.27575D-02	0.21243D+01	0.42034D+00	0.00000D+00
0.46352	0.12222D-08	0.34503D-05	0.25859D+01	0.30087D+01	0.28888D-02	0.21720D+01	0.41833D+00	0.00000D+00
0.47326	0.12522D-08	0.33082D-05	0.25342D+01	0.30604D+01	0.30518D-02	0.22289D+01	0.41572D+00	0.00000D+00
0.47528	0.12585D-08	0.32795D-05	0.25235D+01	0.30711D+01	0.30866D-02	0.22408D+01	0.41515D+00	0.00000D+00
0.49327	0.13163D-08	0.30352D-05	0.24287D+01	0.31659D+01	0.34108D-02	0.23466D+01	0.40962D+00	0.00000D+00
0.51898	0.14043D-08	0.27176D-05	0.22946D+01	0.32999D+01	0.39249D-02	0.24992D+01	0.40039D+00	0.00000D+00
0.54601	0.15048D-08	0.24185D-05	0.21553D+01	0.34392D+01	0.45391D-02	0.26611D+01	0.38907D+00	0.00000D+00
0.55722	0.15493D-08	0.23038D-05	0.20981D+01	0.34965D+01	0.48191D-02	0.27287D+01	0.38391D+00	0.00000D+00
0.57365	0.16180D-08	0.21446D-05	0.20146D+01	0.35800D+01	0.52594D-02	0.28282D+01	0.37588D+00	0.00000D+00
0.58467	0.16665D-08	0.20434D-05	0.19590D+01	0.36356D+01	0.55764D-02	0.28952D+01	0.37019D+00	0.00000D+00
0.62983	0.18908D-08	0.16699D-05	0.17337D+01	0.38609D+01	0.70912D-02	0.31721D+01	0.34439D+00	0.00000D+00
0.63019	0.18928D-08	0.16672D-05	0.17318D+01	0.38627D+01	0.71051D-02	0.31744D+01	0.34416D+00	0.00000D+00
0.64071	0.19521D-08	0.15887D-05	0.16800D+01	0.39146D+01	0.75175D-02	0.32394D+01	0.33760D+00	0.00000D+00
0.65002	0.20072D-08	0.15218D-05	0.16343D+01	0.39603D+01	0.79045D-02	0.32971D+01	0.33162D+00	0.00000D+00
0.66525	0.21032D-08	0.14169D-05	0.15599D+01	0.40347D+01	0.85858D-02	0.33917D+01	0.32152D+00	0.00000D+00
0.67275	0.21535D-08	0.13672D-05	0.15234D+01	0.40712D+01	0.89459D-02	0.34384D+01	0.31639D+00	0.00000D+00
0.67374	0.21603D-08	0.13608D-05	0.15186D+01	0.40760D+01	0.89944D-02	0.34446D+01	0.31571D+00	0.00000D+00
0.72332	0.25564D-08	0.10633D-05	0.12805D+01	0.43141D+01	0.11896D-01	0.37554D+01	0.27937D+00	0.00000D+00
0.72704	0.25915D-08	0.10429D-05	0.12628D+01	0.43318D+01	0.12157D-01	0.37788D+01	0.27648D+00	0.00000D+00
0.76531	0.30111D-08	0.84663D-06	0.10827D+01	0.45118D+01	0.15317D-01	0.40207D+01	0.24557D+00	0.00000D+00
0.79503	0.34359D-08	0.70988D-06	0.94520D+00	0.46494D+01	0.18565D-01	0.42092D+01	0.22010D+00	0.00000D+00
0.80119	0.35386D-08	0.68308D-06	0.91694D+00	0.46776D+01	0.19355D-01	0.42483D+01	0.21467D+00	0.00000D+00
0.84667	0.45249D-08	0.50053D-06	0.71169D+00	0.48829D+01	0.27010D-01	0.45366D+01	0.17315D+00	0.00000D+00
0.85923	0.48965D-08	0.45454D-06	0.65615D+00	0.49384D+01	0.29915D-01	0.46159D+01	0.16129D+00	0.00000D+00
0.89825	0.65299D-08	0.32347D-06	0.48822D+00	0.51064D+01	0.42748D-01	0.48588D+01	0.12377D+00	0.00000D+00
0.94977	0.11076D-07	0.17916D-06	0.28477D+00	0.53098D+01	0.78677D-01	0.51600D+01	0.74906D-01	0.00000D+00
0.95520	0.11867D-07	0.16625D-06	0.26551D+00	0.53291D+01	0.84936D-01	0.51889D+01	0.70084D-01	0.00000D+00
1.00084	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.36199D-01
1.04054	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.25830D+00
1.07404	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.44575D+00
1.10667	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.62832D+00
1.11012	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.64760D+00
1.16578	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.95901D+00
1.20134	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.11579D+01
1.24551	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.14050D+01
1.39424	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.22371D+01
2.21448	0.21019D-07	0.90612D-07	0.14887D+00	0.54457D+01	0.15749D+00	0.53654D+01	0.40132D-01	0.68260D+01

DATA SET NUMBER 6

0.00000	0.14088D-11	0.38212D-02	0.55908D+01	0.38212D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.18020	0.51155D-09	0.14410D-04	0.42334D+01	0.13612D+01	0.32964D-03	0.65441D+00	0.35338D+00	0.00000D+00
0.40848	0.10646D-08	0.43882D-05	0.28830D+01	0.27115D+01	0.20935D-02	0.18548D+01	0.42836D+00	0.00000D+00
0.51335	0.13845D-08	0.27842D-05	0.23239D+01	0.32707D+01	0.38068D-02	0.24656D+01	0.40254D+00	0.00000D+00
0.53663	0.14689D-08	0.25186D-05	0.22035D+01	0.33911D+01	0.43165D-02	0.26047D+01	0.39318D+00	0.00000D+00
0.58746	0.16792D-08	0.20185D-05	0.19449D+01	0.36497D+01	0.56596D-02	0.29122D+01	0.36871D+00	0.00000D+00
0.61531	0.18137D-08	0.17833D-05	0.18057D+01	0.37889D+01	0.65622D-02	0.30827D+01	0.35311D+00	0.00000D+00
0.63533	0.19213D-08	0.16285D-05	0.17065D+01	0.38881D+01	0.73033D-02	0.32061D+01	0.34098D+00	0.00000D+00
0.66918	0.21293D-08	0.13907D-05	0.15407D+01	0.40539D+01	0.87725D-02	0.34162D+01	0.31884D+00	0.00000D+00
0.69755	0.23357D-08	0.12118D-05	0.14036D+01	0.41910D+01	0.10267D-01	0.35934D+01	0.29876D+00	0.00000D+00
0.71091	0.24456D-08	0.11332D-05	0.13396D+01	0.42550D+01	0.11075D-01	0.36773D+01	0.28884D+00	0.00000D+00
0.77495	0.31375D-08	0.80087D-06	0.10379D+01	0.45567D+01	0.16279D-01	0.40818D+01	0.23745D+00	0.00000D+00
0.81694	0.38297D-08	0.61689D-06	0.84518D+00	0.47494D+01	0.21604D-01	0.43483D+01	0.20057D+00	0.00000D+00
0.82628	0.40251D-08	0.57913D-06	0.80292D+00	0.47917D+01	0.23118D-01	0.44075D+01	0.19206D+00	0.00000D+00
0.86559	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.19553D+00
0.90811	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.43340D+00
0.96541	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.75396D+00
0.96541	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.75396D+00
0.98018	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.83658D+00
0.98018	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.83658D+00
1.02431	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.10835D+01
1.02431	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.10835D+01
1.02431	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.10835D+01
1.04001	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.11713D+01
1.08921	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.14466D+01
1.08921	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.14466D+01
1.10575	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.15391D+01
1.16525	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.18720D+01
1.17851	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.19462D+01
1.23575	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.22664D+01
1.32945	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.27906D+01
1.34472	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.28761D+01
1.42404	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.33198D+01
1.54296	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.39851D+01
1.56662	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.41175D+01
1.67262	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.47105D+01
1.82223	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.55475D+01
1.98915	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.64814D+01
2.23680	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.78669D+01
2.45961	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.91134D+01
2.79524	0.41228D-08	0.56190D-06	0.78331D+00	0.48113D+01	0.23878D-01	0.44352D+01	0.18805D+00	0.10991D+02

DATA SET NUMBER 7

0.00000	0.95200D-12	0.58113D-02	0.12582D+02	0.58113D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.07915	0.21281D-09	0.30804D-04	0.11031D+02	0.15566D+01	0.92128D-04	0.43592D+00	0.56035D+00	0.00000D+00
0.18468	0.33761D-09	0.97235D-05	0.93743D+01	0.32135D+01	0.56598D-03	0.14347D+01	0.88939D+00	0.00000D+00
0.27911	0.39571D-09	0.47786D-05	0.80801D+01	0.45077D+01	0.13939D-02	0.25162D+01	0.99576D+00	0.00000D+00

0.34550	0.42472D-09	0.31153D-05	0.72320D+01	0.53558D+01	0.22583D-02	0.33379D+01	0.10089D+01	0.00000D+00
0.43410	0.45877D-09	0.18424D-05	0.61539D+01	0.64339D+01	0.38954D-02	0.44869D+01	0.97349D+00	0.00000D+00
0.55814	0.51429D-09	0.91244D-06	0.47175D+01	0.78703D+01	0.76312D-02	0.61658D+01	0.85222D+00	0.00000D+00
0.59137	0.53402D-09	0.75512D-06	0.43440D+01	0.82438D+01	0.90806D-02	0.66261D+01	0.80884D+00	0.00000D+00
0.64260	0.57183D-09	0.56055D-06	0.37764D+01	0.88114D+01	0.11896D-01	0.73426D+01	0.73442D+00	0.00000D+00
0.74122	0.68992D-09	0.30265D-06	0.27096D+01	0.98782D+01	0.20662D-01	0.87411D+01	0.56855D+00	0.00000D+00
0.76671	0.73760D-09	0.25413D-06	0.24394D+01	0.10148D+02	0.24163D-01	0.91057D+01	0.52137D+00	0.00000D+00
0.79626	0.80813D-09	0.20499D-06	0.21293D+01	0.10458D+02	0.29313D-01	0.95291D+01	0.46468D+00	0.00000D+00
0.85084	0.10110D-08	0.13108D-06	0.15667D+01	0.11021D+02	0.43998D-01	0.10311D+02	0.35490D+00	0.00000D+00
0.85679	0.10420D-08	0.12418D-06	0.15064D+01	0.11081D+02	0.46234D-01	0.10396D+02	0.34259D+00	0.00000D+00
0.91156	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.62033D+00
0.92489	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.78805D+00
0.98026	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.14851D+01
0.98207	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.15079D+01
1.04576	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.23096D+01
1.05278	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.23979D+01
1.05432	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.24174D+01
1.13899	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.34832D+01
1.14677	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.35811D+01
1.22160	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.45230D+01
1.24354	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.47992D+01
1.25009	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.48816D+01
1.31583	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.57092D+01
1.34573	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.60856D+01
1.36180	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.62878D+01
1.36944	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.63840D+01
1.43350	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.71903D+01
1.45190	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.74220D+01
1.53479	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.84654D+01
1.57081	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.89188D+01
1.58507	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.90983D+01
1.60776	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.93839D+01
1.66836	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.10147D+02
1.92777	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.13412D+02
2.17445	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.16517D+02
2.36856	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.18961D+02
2.49483	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.20550D+02
3.35579	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.31388D+02
5.12427	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.53649D+02

DATA SET NUMBER 8

0.00000	0.95200D-12	0.58114D-02	0.12582D+02	0.58114D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.06820	0.19256D-09	0.36639D-04	0.11224D+02	0.13642D+01	0.67004D-04	0.35277D+00	0.50569D+00	0.00000D+00
0.10635	0.25536D-09	0.21351D-04	0.10573D+02	0.20146D+01	0.17328D-03	0.66266D+00	0.67594D+00	0.00000D+00
0.15917	0.31566D-09	0.12205D-04	0.97489D+01	0.28389D+01	0.41101D-03	0.11674D+01	0.83573D+00	0.00000D+00
0.18607	0.33870D-09	0.96095D-05	0.93542D+01	0.32336D+01	0.57520D-03	0.14497D+01	0.89195D+00	0.00000D+00
0.21979	0.36266D-09	0.73221D-05	0.88781D+01	0.37097D+01	0.82491D-03	0.18219D+01	0.94387D+00	0.00000D+00
0.24025	0.37514D-09	0.62805D-05	0.85977D+01	0.39901D+01	0.10017D-02	0.20563D+01	0.96687D+00	0.00000D+00
0.27098	0.39170D-09	0.50512D-05	0.81869D+01	0.44009D+01	0.13055D-02	0.24186D+01	0.99118D+00	0.00000D+00
0.29308	0.40234D-09	0.43519D-05	0.78981D+01	0.46897D+01	0.15543D-02	0.26857D+01	0.10020D+01	0.00000D+00

0.29741	0.40431D-09	0.42291D-05	0.78421D+01	0.47457D+01	0.16063D-02	0.27386D+01	0.10035D+01	0.00000D+00
0.33682	0.42123D-09	0.32877D-05	0.73407D+01	0.52471D+01	0.21298D-02	0.32282D+01	0.10094D+01	0.00000D+00
0.37139	0.43488D-09	0.26614D-05	0.69114D+01	0.56764D+01	0.26724D-02	0.36683D+01	0.10041D+01	0.00000D+00
0.41096	0.44994D-09	0.21065D-05	0.64306D+01	0.61572D+01	0.34042D-02	0.41820D+01	0.98760D+00	0.00000D+00
0.45297	0.46616D-09	0.16538D-05	0.59305D+01	0.66573D+01	0.43351D-02	0.47378D+01	0.95979D+00	0.00000D+00
0.45392	0.46653D-09	0.16447D-05	0.59192D+01	0.66686D+01	0.43584D-02	0.47505D+01	0.95903D+00	0.00000D+00
0.48048	0.47736D-09	0.14145D-05	0.56081D+01	0.69797D+01	0.50472D-02	0.51067D+01	0.93650D+00	0.00000D+00
0.50192	0.48661D-09	0.12532D-05	0.53596D+01	0.72282D+01	0.56677D-02	0.53965D+01	0.91584D+00	0.00000D+00
0.50399	0.48753D-09	0.12386D-05	0.53357D+01	0.72521D+01	0.57309D-02	0.54246D+01	0.91372D+00	0.00000D+00
0.52950	0.49947D-09	0.10727D-05	0.50428D+01	0.75450D+01	0.65642D-02	0.57725D+01	0.88626D+00	0.00000D+00
0.53061	0.50001D-09	0.10660D-05	0.50302D+01	0.75576D+01	0.66028D-02	0.57876D+01	0.88499D+00	0.00000D+00
0.53505	0.50220D-09	0.10396D-05	0.49795D+01	0.76083D+01	0.67594D-02	0.58484D+01	0.87991D+00	0.00000D+00
0.56664	0.51907D-09	0.86951D-06	0.46215D+01	0.79663D+01	0.79786D-02	0.62833D+01	0.84152D+00	0.00000D+00
0.59754	0.53805D-09	0.72884D-06	0.42751D+01	0.83127D+01	0.93788D-02	0.67120D+01	0.80034D+00	0.00000D+00
0.59997	0.53965D-09	0.71869D-06	0.42480D+01	0.83398D+01	0.94991D-02	0.67459D+01	0.79695D+00	0.00000D+00
0.63394	0.56466D-09	0.58990D-06	0.38716D+01	0.87162D+01	0.11361D-01	0.72210D+01	0.74759D+00	0.00000D+00
0.63928	0.56902D-09	0.57160D-06	0.38128D+01	0.87750D+01	0.11688D-01	0.72960D+01	0.73947D+00	0.00000D+00
0.67713	0.60451D-09	0.45546D-06	0.33991D+01	0.91887D+01	0.14334D-01	0.78297D+01	0.67954D+00	0.00000D+00
0.67994	0.60749D-09	0.44767D-06	0.33686D+01	0.92192D+01	0.14557D-01	0.78694D+01	0.67490D+00	0.00000D+00
0.72239	0.66054D-09	0.34262D-06	0.29107D+01	0.96771D+01	0.18492D-01	0.84725D+01	0.60233D+00	0.00000D+00
0.73109	0.67356D-09	0.32366D-06	0.28176D+01	0.97702D+01	0.19457D-01	0.85966D+01	0.58682D+00	0.00000D+00
0.77568	0.75702D-09	0.23846D-06	0.23449D+01	0.10243D+02	0.25584D-01	0.92341D+01	0.50438D+00	0.00000D+00
0.78035	0.76776D-09	0.23055D-06	0.22958D+01	0.10292D+02	0.26371D-01	0.93011D+01	0.49545D+00	0.00000D+00
0.83559	0.94118D-09	0.14976D-06	0.17223D+01	0.10865D+02	0.38959D-01	0.10093D+02	0.38617D+00	0.00000D+00
0.84086	0.96383D-09	0.14314D-06	0.16684D+01	0.10919D+02	0.40597D-01	0.10169D+02	0.37541D+00	0.00000D+00
0.89815	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.45146D+00
0.90190	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.49871D+00
0.90566	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.54601D+00
0.97769	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.14528D+01
0.98585	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.15554D+01
1.07183	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.26377D+01
1.17695	0.10729D-08	0.11799D-06	0.14508D+01	0.11137D+02	0.48458D-01	0.10475D+02	0.33118D+00	0.39609D+01

DATA SET NUMBER 9

0.00000	0.95200D-12	0.58114D-02	0.12582D+02	0.58114D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.07893	0.21242D-09	0.30907D-04	0.11035D+02	0.15528D+01	0.91574D-04	0.43418D+00	0.55929D+00	0.00000D+00
0.12328	0.27738D-09	0.17548D-04	0.10301D+02	0.22870D+01	0.23768D-03	0.81619D+00	0.73540D+00	0.00000D+00
0.18485	0.33775D-09	0.97092D-05	0.93718D+01	0.32160D+01	0.56712D-03	0.14366D+01	0.88971D+00	0.00000D+00
0.27731	0.39484D-09	0.48371D-05	0.81036D+01	0.44842D+01	0.13741D-02	0.24946D+01	0.99481D+00	0.00000D+00
0.43296	0.45833D-09	0.18544D-05	0.61674D+01	0.64204D+01	0.38701D-02	0.44719D+01	0.97425D+00	0.00000D+00
0.45430	0.46669D-09	0.16412D-05	0.59147D+01	0.66731D+01	0.43677D-02	0.47556D+01	0.95874D+00	0.00000D+00
0.53009	0.49975D-09	0.10691D-05	0.50361D+01	0.75517D+01	0.65846D-02	0.57805D+01	0.88558D+00	0.00000D+00
0.58977	0.53301D-09	0.76208D-06	0.43618D+01	0.82260D+01	0.90050D-02	0.66039D+01	0.81102D+00	0.00000D+00
0.62356	0.55012D-09	0.65893D-06	0.40811D+01	0.85067D+01	0.10278D-01	0.69555D+01	0.77560D+00	0.10794D+00
0.65570	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.51238D+00
0.70092	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.10816D+01
0.74227	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.16021D+01
0.74262	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.16065D+01
0.74262	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.16065D+01

0.79405	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.22540D+01
0.84534	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.28996D+01
0.84867	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.29415D+01
0.89903	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.35754D+01
0.90935	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.37053D+01
0.97423	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.45220D+01
1.04376	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.53972D+01
1.13994	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.66080D+01
1.14415	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.66609D+01
1.23292	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.77783D+01
1.36587	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.94519D+01
1.67624	0.55014D-09	0.65894D-06	0.40811D+01	0.85067D+01	0.10279D-01	0.69555D+01	0.77560D+00	0.13359D+02

ANALYSIS OF EQUILIBRIUM CONSTANT AND HEAT OF REACTION
FOR THE PROTONATION OF MDEA AT 140.0 F

DATA SET NUMBER 1

SYSTEM (RUN#.TRIAL): 7.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.05999	-12.13
0.13494	-27.97
0.23150	-47.93
0.35999	-73.25
0.54212	-105.96
0.67553	-127.68
0.81342	-156.17
0.92682	-171.31
0.94121	-178.55
1.01100	-183.19
1.02635	-186.61
1.07282	-189.84
1.12212	-188.96
1.15668	-186.13
1.23023	-187.79
1.27015	-187.11
1.28970	-189.41
1.42123	-189.82
1.63267	-181.87
1.65796	-190.69
1.85034	-188.02
2.17744	-182.01
2.51781	-183.73
3.13198	-187.84
4.05319	-182.83
4.97443	-173.54

DATA SET NUMBER 2

SYSTEM (RUN#.TRIAL): 7.2
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.21169	-40.97
0.26841	-52.13

0.33071	-61.96
0.36083	-70.04
0.43998	-88.05
0.49736	-92.22
0.53983	-106.42
0.58014	-111.64
0.60909	-117.19
0.65767	-125.57
0.68245	-130.29
0.74112	-138.88
0.74749	-145.00
0.79945	-141.25
0.81313	-157.37
0.91773	-171.70
0.92535	-176.59
1.15310	-194.71
1.16264	-182.59
1.48242	-195.13
1.97665	-195.08
2.79993	-193.86

DATA SET NUMBER 3

SYSTEM (RUN#.TRIAL): 8.1
PRESSURE (PSIA) : 22.6
CONCENTRATION (WT. % MDEA): 20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.22815	-50.49
0.35632	-73.83
0.53241	-108.30
0.58272	-121.70
0.60278	-124.25
0.65076	-129.53
0.68014	-133.08
0.73793	-137.20
0.79858	-138.25
0.80469	-137.80
0.84898	-136.13
0.87205	-141.68
0.92066	-136.99
0.95002	-141.82
0.98858	-143.58
1.08202	-141.61
1.08498	-144.26
1.13105	-142.10
1.24702	-143.01
1.35940	-141.88
1.59696	-139.81
2.12922	-129.32
3.02838	-103.29
4.80977	-78.59

DATA SET NUMBER 4

SYSTEM (RUN#.TRIAL): 9.1

PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 40.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.03322	-6.44
0.04045	-8.08
0.06560	-13.36
0.09108	-18.64
0.10509	-21.25
0.15621	-31.78
0.18324	-37.02
0.36924	-76.27
0.43770	-84.31
0.63447	-120.98
0.73637	-150.07
0.77520	-157.58
0.81417	-162.61
0.85606	-169.97
0.85885	-173.60
0.90119	-180.08
0.90414	-175.93
0.94990	-178.79
0.95300	-180.42
1.00266	-181.31
1.00930	-183.74
1.06351	-186.29
1.11901	-184.18
1.19892	-187.64
1.26642	-184.56
1.45187	-188.52
1.45706	-186.99
1.67262	-187.97
1.91993	-185.42
2.13330	-188.33
2.33616	-190.54
2.57871	-189.88
2.84070	-181.52
5.22783	-109.82

DATA SET NUMBER 5

SYSTEM (RUN#.TRIAL): 10.1
PRESSURE (PSIA) : 22.6
CONCENTRATION (WT. % MDEA): 40.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.18787	-41.47
0.27857	-62.75
0.38759	-84.10
0.42673	-91.58
0.45451	-99.39

0.47505	-105.47
0.48743	-110.62
0.52606	-107.88
0.53867	-108.33
0.58504	-113.84
0.61116	-116.55
0.64083	-117.77
0.67029	-118.79
0.69928	-119.09
0.73251	-119.15
0.82351	-115.07
0.82603	-117.37
0.98978	-112.50
1.09807	-114.67
1.16431	-113.39
1.58464	-110.24
1.69298	-116.05
2.09130	-110.14
2.24410	-112.75
2.45961	-109.08

DATA SET NUMBER 6

SYSTEM (RUN#.TRIAL): 11.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 60.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.02937	-6.64
0.06608	-15.08
0.08853	-18.25
0.11300	-24.57
0.12543	-25.28
0.17365	-34.99
0.17573	-38.80
0.23942	-47.46
0.29350	-60.59
0.33444	-69.19
0.41433	-85.35
0.45653	-94.49
0.48369	-99.09
0.55689	-115.30
0.61718	-126.22
0.65502	-135.10
0.69402	-142.07
0.73074	-151.03
0.73353	-148.26
0.75243	-151.42
0.75945	-157.21
0.76157	-155.58
0.78219	-157.32
0.80553	-159.70
0.83422	-161.03
0.85374	-161.46
0.89168	-161.76
0.92363	-163.05
0.97875	-163.12

1.00146	-162.89
1.04892	-163.87
1.10885	-164.07
1.12460	-164.95
1.21421	-166.27
1.31550	-167.02
1.76125	-160.66

DATA SET NUMBER 7

SYSTEM	(RUN#.TRIAL):	12.1
PRESSURE	(PSIA) :	22.6
CONCENTRATION	(WT. % MDEA):	60.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.01710	-4.45
0.03847	-9.16
0.06599	-14.17
0.10264	-23.40
0.14060	-30.08
0.15395	-33.04
0.23194	-49.66
0.24539	-50.08
0.28845	-61.97
0.32154	-66.41
0.35200	-71.66
0.35925	-72.26
0.36510	-73.99
0.38241	-74.10
0.40089	-74.56
0.42068	-74.57
0.42766	-74.88
0.44181	-73.16
0.49688	-74.26
0.51545	-73.12
0.58971	-71.87
0.61584	-70.94
0.69003	-71.08
0.83891	-68.86
0.88018	-65.67
1.05974	-68.16
1.21470	-63.51

INPUT PARAMETERS

NUMBER OF REACTIONS : 5

NUMBER OF COMPONENTS : 7

CHARGES ON COMPONENTS:
1, 1.
2, -1.
3, Ø.
4, 1.
5, Ø.
6, -1.
7, -2.

TOLERANCE FOR ACTIVITY COEFFICIENT CONVERGENCE: Ø.5D-Ø3

TOLERANCE FOR SIMULTANEOUS EQUATION SOLUTIONS : Ø.1D-Ø4

VALUES FOR LN K, DELTA H FOR EACH REACTION

LN K [=] UNITLESS

DELTA H [=] CAL/GMOLE

	1	2	3	4	5
LN K	-29.98Ø	-18.113	-14.471	-23.351	-4.1ØØ
DELTA H	11758.16	8329.13	-342.42	1384.61	-3353.61

CONVERTED DATA

(NOTE: "CORRECTED HEAT OF SOLUTION" IS TOTAL HEAT OF SOLUTION LESS HEAT OF ABSORPTION OF GASEOUS CO2.)

POINT	MOLE FRACTION CO2	HEAT OF SOLUTION (J/MOLE)	MOLALITY CO2 (MOLE/KG H20)	MOLALITY MDEA (MOLE/KG H20)	CORRECTED HEAT OF SOLUTION (CAL/KG H20)
			DATA SET NUMBER 1		
1	0.00218	-122.10	0.1259	2.0980	-1262.7
2	0.00489	-280.80	0.2831	2.0980	-2935.8
3	0.00836	-479.44	0.4857	2.0980	-5028.0
4	0.01294	-729.33	0.7552	2.0980	-7640.6
5	0.01936	-1048.14	1.1373	2.0980	-10901.9
6	0.02401	-1257.01	1.4172	2.0980	-12979.9
7	0.02877	-1530.03	1.7065	2.0980	-15967.0
8	0.03265	-1671.68	1.9444	2.0980	-17272.2
9	0.03314	-1741.48	1.9746	2.0980	-18177.0
10	0.03551	-1782.32	2.1210	2.0980	-18330.0
11	0.03603	-1814.64	2.1533	2.0980	-18697.2
12	0.03760	-1842.97	2.2507	2.0980	-18817.9
13	0.03926	-1831.32	2.3542	2.0980	-18349.6
14	0.04042	-1801.74	2.4267	2.0980	-17713.8
15	0.04288	-1813.08	2.5810	2.0980	-17425.9
16	0.04421	-1804.05	2.6647	2.0980	-17051.2
17	0.04486	-1825.00	2.7057	2.0980	-17233.4
18	0.04921	-1820.59	2.9817	2.0980	-16364.4
19	0.05612	-1731.66	3.4253	2.0980	-13772.7
20	0.05694	-1814.03	3.4783	2.0980	-14819.2
21	0.06313	-1776.94	3.8820	2.0980	-13095.6
22	0.07347	-1701.10	4.5682	2.0980	-9958.6
23	0.08399	-1697.75	5.2823	2.0980	-7803.8
24	0.10238	-1700.83	6.5708	2.0980	-4052.9
25	0.12863	-1607.10	8.5035	2.0980	3124.0
26	0.15338	-1482.07	10.4362	2.0980	10896.6
			DATA SET NUMBER 2		
1	0.00765	-410.14	0.4441	2.0980	-4201.1
2	0.00968	-520.82	0.5631	2.0980	-5352.5
3	0.01190	-617.64	0.6938	2.0980	-6279.5
4	0.01297	-697.36	0.7570	2.0980	-7188.9
5	0.01577	-874.19	0.9231	2.0980	-9133.5
6	0.01779	-913.71	1.0434	2.0980	-9308.8
7	0.01928	-1052.81	1.1325	2.0980	-10982.3
8	0.02069	-1102.91	1.2171	2.0980	-11424.3
9	0.02170	-1156.51	1.2779	2.0980	-11991.0
10	0.02339	-1237.08	1.3798	2.0980	-12813.3
11	0.02425	-1282.43	1.4318	2.0980	-13294.2
12	0.02628	-1364.11	1.5548	2.0980	-14074.1
13	0.02650	-1423.97	1.5682	2.0980	-14880.2
14	0.02829	-1384.52	1.6772	2.0980	-13992.8
15	0.02876	-1541.80	1.7059	2.0980	-16135.6
16	0.03234	-1676.03	1.9254	2.0980	-17390.4
17	0.03260	-1723.29	1.9414	2.0980	-18015.9
18	0.04030	-1885.02	2.4192	2.0980	-18930.5
19	0.04062	-1767.05	2.4392	2.0980	-17179.4
20	0.05122	-1867.60	3.1101	2.0980	-16672.1

21	0.06715	-1835.76	4.1470	2.0980	-13187.5
22	0.09253	-1774.63	5.8742	2.0980	-7225.5

DATA SET NUMBER 3

1	0.00824	-505.16	0.4786	2.0980	-5407.8
2	0.01281	-735.18	0.7476	2.0980	-7746.6
3	0.01902	-1071.66	1.1170	2.0980	-11295.1
4	0.02078	-1202.12	1.2225	2.0980	-12802.5
5	0.02148	-1226.49	1.2646	2.0980	-13016.4
6	0.02315	-1276.36	1.3653	2.0980	-13411.2
7	0.02417	-1309.98	1.4269	2.0980	-13697.7
8	0.02617	-1347.81	1.5482	2.0980	-13863.8
9	0.02826	-1355.15	1.6754	2.0980	-13582.1
10	0.02847	-1350.54	1.6882	2.0980	-13478.0
11	0.02999	-1331.99	1.7811	2.0980	-12933.1
12	0.03078	-1385.17	1.8295	2.0980	-13541.6
13	0.03244	-1337.08	1.9315	2.0980	-12549.1
14	0.03344	-1382.79	1.9931	2.0980	-13013.3
15	0.03475	-1398.02	2.0740	2.0980	-12986.0
16	0.03791	-1374.38	2.2700	2.0980	-12055.8
17	0.03801	-1399.88	2.2763	2.0980	-12402.0
18	0.03956	-1376.69	2.3729	2.0980	-11777.7
19	0.04344	-1379.91	2.6162	2.0980	-11088.2
20	0.04717	-1363.73	2.8520	2.0980	-10141.4
21	0.05496	-1332.79	3.3504	2.0980	-8181.8
22	0.07196	-1210.64	4.4670	2.0980	-2980.4
23	0.09933	-938.47	6.3534	2.0980	6960.8
24	0.14906	-674.58	10.0907	2.0980	22925.7

DATA SET NUMBER 4

1	0.00303	-162.87	0.1858	5.5946	-1762.6
2	0.00369	-204.13	0.2263	5.5946	-2233.2
3	0.00597	-336.75	0.3670	5.5946	-3716.7
4	0.00827	-468.81	0.5096	5.5946	-5194.8
5	0.00953	-533.76	0.5879	5.5946	-5898.3
6	0.01410	-794.69	0.8739	5.5946	-8840.9
7	0.01650	-923.47	1.0252	5.5946	-10274.6
8	0.03270	-1870.95	2.0657	5.5946	-21319.5
9	0.03853	-2055.80	2.4488	5.5946	-23013.9
10	0.05490	-2899.75	3.5496	5.5946	-32904.2
11	0.06316	-3565.43	4.1197	5.5946	-41764.5
12	0.06627	-3731.50	4.3369	5.5946	-43818.4
13	0.06937	-3837.84	4.5549	5.5946	-44950.6
14	0.07268	-3997.27	4.7893	5.5946	-46890.5
15	0.07290	-4081.57	4.8049	5.5946	-48180.8
16	0.07622	-4218.82	5.0418	5.5946	-49787.2
17	0.07645	-4120.70	5.0583	5.5946	-48197.1
18	0.08001	-4171.53	5.3143	5.5946	-48397.5
19	0.08025	-4208.30	5.3316	5.5946	-48940.6
20	0.08408	-4211.43	5.6095	5.5946	-48338.2
21	0.08459	-4265.70	5.6466	5.5946	-49116.8
22	0.08873	-4305.36	5.9499	5.5946	-49044.4
23	0.09293	-4236.85	6.2604	5.5946	-47219.6
24	0.09891	-4287.91	6.7074	5.5946	-47000.7
25	0.10390	-4194.19	7.0851	5.5946	-44593.8
26	0.11734	-4219.99	8.1226	5.5946	-42581.2
27	0.11771	-4183.96	8.1516	5.5946	-41916.8
28	0.13281	-4134.00	9.3576	5.5946	-38237.1
29	0.14951	-3999.32	10.7412	5.5946	-32651.5
30	0.16341	-3995.69	11.9349	5.5946	-29725.8
31	0.17621	-3980.75	13.0698	5.5946	-26738.9
32	0.19101	-3895.78	14.4268	5.5946	-21945.1

33	0.20641	-3653.27	15.8925	5.5946	-13931.6
34	0.32371	-1883.55	29.2475	5.5946	57410.8

DATA SET NUMBER 5

1	0.01691	-1033.86	1.0511	5.5946	-11833.3
2	0.02487	-1551.84	1.5585	5.5946	-18014.7
3	0.03427	-2059.66	2.1684	5.5946	-23874.7
4	0.03760	-2235.24	2.3874	5.5946	-25912.6
5	0.03995	-2419.96	2.5428	5.5946	-28284.4
6	0.04168	-2563.29	2.6577	5.5946	-30149.8
7	0.04272	-2685.60	2.7270	5.5946	-31825.9
8	0.04595	-2610.20	2.9431	5.5946	-30085.6
9	0.04700	-2618.17	3.0136	5.5946	-30015.1
10	0.05084	-2740.29	3.2730	5.5946	-31186.4
11	0.05299	-2799.28	3.4192	5.5946	-31701.7
12	0.05542	-2821.22	3.5852	5.5946	-31595.3
13	0.05782	-2838.38	3.7500	5.5946	-31419.8
14	0.06017	-2838.39	3.9122	5.5946	-30986.1
15	0.06285	-2831.90	4.0981	5.5946	-30387.5
16	0.07011	-2713.75	4.6072	5.5946	-27169.3
17	0.07031	-2767.27	4.6213	5.5946	-27971.8
18	0.08309	-2615.91	5.5374	5.5946	-23094.5
19	0.09135	-2642.45	6.1432	5.5946	-21868.2
20	0.09633	-2598.71	6.5138	5.5946	-20152.6
21	0.12671	-2441.65	8.8654	5.5946	-11100.3
22	0.13421	-2548.15	9.4715	5.5946	-11217.8
23	0.16071	-2344.34	11.6999	5.5946	-1555.3
24	0.17045	-2372.00	12.5548	5.5946	345.5
25	0.18381	-2257.86	13.7605	5.5946	5747.7

DATA SET NUMBER 6

1	0.00540	-338.33	0.3697	12.5878	-4296.6
2	0.01207	-762.85	0.8318	12.5878	-9777.9
3	0.01610	-919.56	1.1143	12.5878	-11474.2
4	0.02046	-1232.42	1.4224	12.5878	-15706.9
5	0.02266	-1264.83	1.5789	12.5878	-15768.0
6	0.03110	-1736.04	2.1859	12.5878	-21831.3
7	0.03146	-1924.00	2.2120	12.5878	-24913.0
8	0.04238	-2327.26	3.0138	12.5878	-29446.5
9	0.05146	-2942.71	3.6945	12.5878	-38102.3
10	0.05822	-3336.33	4.2098	12.5878	-43539.1
11	0.07114	-4059.00	5.2155	12.5878	-53631.1
12	0.07782	-4461.42	5.7467	12.5878	-59467.2
13	0.08207	-4656.98	6.0886	12.5878	-62152.5
14	0.09333	-5352.63	7.0100	12.5878	-72575.6
15	0.10240	-5800.95	7.7689	12.5878	-79130.4
16	0.10800	-6170.08	8.2452	12.5878	-84928.7
17	0.11370	-6447.26	8.7362	12.5878	-89096.1
18	0.11900	-6812.57	9.1984	12.5878	-95006.9
19	0.11940	-6684.89	9.2336	12.5878	-92586.5
20	0.12210	-6806.36	9.4714	12.5878	-94421.0
21	0.12310	-7058.52	9.5599	12.5878	-98948.3
22	0.12340	-6982.75	9.5864	12.5878	-97497.2
23	0.12632	-7037.40	9.8461	12.5878	-98077.8
24	0.12960	-7117.32	10.1398	12.5878	-99081.2
25	0.13361	-7143.65	10.5010	12.5878	-98978.9
26	0.13631	-7140.26	10.7467	12.5878	-98510.5
27	0.14151	-7110.36	11.2243	12.5878	-97157.2
28	0.14584	-7130.85	11.6264	12.5878	-96882.5
29	0.15321	-7072.52	12.3203	12.5878	-94616.9
30	0.15621	-7037.39	12.6062	12.5878	-93463.7
31	0.16241	-7027.67	13.2036	12.5878	-92276.3

32	0.17011	-6971.65	13.9580	12.5878	-89914.9
33	0.17211	-6992.19	14.1562	12.5878	-89984.1
34	0.18331	-6952.73	15.2842	12.5878	-87299.9
35	0.19561	-6878.76	16.5592	12.5878	-83646.2
36	0.24561	-6205.81	22.1702	12.5878	-59535.4

DATA SET NUMBER 7

1	0.00315	-227.06	0.2152	12.5878	-2985.6
2	0.00706	-465.81	0.4842	12.5878	-6011.3
3	0.01205	-716.70	0.8306	12.5878	-9021.3
4	0.01862	-1175.98	1.2921	12.5878	-15169.7
5	0.02533	-1501.15	1.7698	12.5878	-19131.7
6	0.02767	-1645.02	1.9379	12.5878	-21036.3
7	0.04111	-2438.22	2.9196	12.5878	-31593.4
8	0.04339	-2452.76	3.0889	12.5878	-31371.6
9	0.05062	-3012.13	3.6310	12.5878	-39460.8
10	0.05610	-3209.43	4.0474	12.5878	-41766.1
11	0.06109	-3445.10	4.4309	12.5878	-44859.5
12	0.06227	-3469.41	4.5221	12.5878	-45050.5
13	0.06322	-3548.79	4.5958	12.5878	-46243.8
14	0.06602	-3543.80	4.8137	12.5878	-45610.8
15	0.06899	-3554.41	5.0463	12.5878	-45213.2
16	0.07215	-3542.69	5.2954	12.5878	-44383.8
17	0.07326	-3552.97	5.3833	12.5878	-44344.0
18	0.07550	-3462.95	5.5614	12.5878	-42313.3
19	0.08412	-3482.17	6.2547	12.5878	-40903.7
20	0.08699	-3417.97	6.4884	12.5878	-39169.9
21	0.09829	-3318.24	7.4231	12.5878	-34998.8
22	0.10220	-3260.96	7.7520	12.5878	-33118.1
23	0.11312	-3227.54	8.6860	12.5878	-30100.7
24	0.13426	-3052.57	10.5600	12.5878	-21972.1
25	0.13994	-2891.83	11.0795	12.5878	-17567.2
26	0.16381	-2918.39	13.3397	12.5878	-12066.4
27	0.18337	-2655.62	15.2903	12.5878	-1648.4

MDEA PROTONATION

LN K : -17.8000
DELTA H : 9398.30

SUMMARY OF FIT FOR LOADING CURVE

POINT	LOADING MOLE CO2 / MOLE MDEA	EXPERIMENTAL HEAT OF SOLN (BTU/LB MDEA)	CALCULATED HEAT OF SOLN (BTU/LB MDEA)	EXPERIMENTAL HEAT OF SOLN (BTU/LB CO2)	CALCULATED HEAT OF SOLN (BTU/LB CO2)	RELATIVE ERROR	EQUILIBRIUM PRESSURE OF CO2 (PSIA)
			DATA SET NUMBER 1				
1	0.059993	-12.13	-13.15	-547.47	-593.50	8.41	0.13
2	0.134938	-27.97	-28.52	-561.31	-572.34	1.97	0.65
3	0.231499	-47.93	-47.94	-560.58	-560.71	0.02	2.01
4	0.359987	-73.25	-73.33	-550.93	-551.56	0.11	5.49
5	0.542116	-105.96	-108.54	-529.20	-542.12	2.44	16.34
6	0.675528	-127.68	-133.58	-511.75	-535.41	4.62	33.81
7	0.813418	-156.17	-158.15	-519.84	-526.45	1.27	74.11
8	0.926821	-171.31	-176.07	-500.47	-514.38	2.78	151.45
9	0.941207	-178.55	-177.22	-513.66	-509.81	-0.75	166.37
10	1.010995	-183.19	-177.03	-490.62	-474.12	-3.36	260.32
11	1.026354	-186.61	-176.99	-492.31	-466.92	-5.16	285.91
12	1.072824	-189.84	-176.87	-479.12	-446.38	-6.83	373.15
13	1.122123	-188.96	-176.74	-455.96	-426.46	-6.47	479.07
14	1.156675	-186.13	-176.64	-435.72	-413.50	-5.10	559.44
15	1.230225	-187.79	-176.45	-413.31	-388.35	-6.04	741.81
16	1.270148	-187.11	-176.34	-398.87	-375.92	-5.76	845.17
17	1.289700	-189.41	-176.29	-397.66	-370.11	-6.93	896.58
18	1.421232	-189.82	-175.94	-361.63	-335.19	-7.31	1251.27
19	1.632665	-181.87	-175.37	-301.62	-290.84	-3.57	1837.89
20	1.657961	-190.69	-175.31	-311.41	-286.30	-8.06	1908.76
21	1.850345	-188.02	-174.79	-275.14	-255.78	-7.03	2450.36
22	2.177443	-182.01	-173.92	-226.32	-216.27	-4.44	3377.06
23	2.517814	-183.73	-173.02	-197.59	-186.06	-5.83	4344.90
24	3.131979	-187.84	-171.38	-162.39	-148.16	-8.76	6095.02
25	4.053192	-182.83	-168.92	-122.14	-112.85	-7.61	8723.67
26	4.974426	-173.54	-166.47	-94.46	-90.61	-4.07	11354.02

THE LOADING POINT IS 0.93506

MEAN OF THE ABSOLUTE PERCENT ERROR IS 4.7966

DATA SET NUMBER 2

1	0.211686	-40.97	-43.98	-524.06	-562.57	7.35	1.66
2	0.268408	-52.13	-55.28	-525.92	-557.66	6.03	2.78
3	0.330706	-61.96	-67.58	-507.33	-553.34	9.07	4.48
4	0.360833	-70.04	-73.50	-525.56	-551.51	4.94	5.52
5	0.439978	-88.05	-88.91	-541.86	-547.18	0.98	9.11
6	0.497357	-92.22	-99.98	-502.04	-544.30	8.42	12.72
7	0.539832	-106.42	-108.11	-533.77	-542.23	1.58	16.14
8	0.580145	-111.64	-115.76	-521.06	-540.27	3.69	20.13
9	0.609093	-117.19	-121.21	-520.95	-538.84	3.43	23.56
10	0.657666	-125.57	-130.28	-516.98	-536.36	3.75	30.67
11	0.682448	-130.29	-134.85	-516.93	-535.03	3.50	35.12
12	0.741118	-138.88	-145.51	-507.38	-531.60	4.77	48.66
13	0.747491	-145.00	-146.64	-525.25	-531.19	1.13	50.45
14	0.799452	-141.25	-155.76	-478.38	-527.55	10.28	68.19
15	0.813127	-157.37	-158.11	-524.02	-526.48	0.47	73.98
16	0.917727	-171.70	-174.76	-506.58	-515.61	1.78	142.73
17	0.925354	-176.59	-175.86	-516.71	-514.58	-0.41	150.00
18	1.153097	-194.71	-176.65	-457.21	-414.81	-9.28	550.93
19	1.162641	-182.59	-176.63	-425.22	-411.34	-3.26	573.72
20	1.482417	-195.13	-175.78	-356.41	-321.05	-9.92	1419.64
21	1.976653	-195.08	-174.46	-267.23	-238.97	-10.57	2807.60
22	2.799926	-193.86	-172.26	-187.47	-166.59	-11.14	5148.41

THE LOADING POINT IS 0.93506

MEAN OF THE ABSOLUTE PERCENT ERROR IS 5.2619

DATA SET NUMBER 3

1	0.228148	-50.49	-47.27	-599.25	-561.01	-6.38	1.94
2	0.356324	-73.83	-72.61	-560.99	-551.78	-1.64	5.35
3	0.532410	-108.30	-106.69	-550.75	-542.59	-1.48	15.49
4	0.582722	-121.70	-115.10	-565.47	-534.81	-5.42	20.41
5	0.602783	-124.25	-114.67	-558.13	-515.08	-7.71	22.77
6	0.650758	-129.53	-113.63	-538.93	-472.80	-12.27	29.54
7	0.680141	-133.08	-113.00	-529.78	-449.86	-15.09	34.67

8	0.737933	-137.20	-111.76	-503.42	-410.06	-18.55	47.79
9	0.798580	-138.25	-110.45	-468.73	-374.49	-20.10	67.84
10	0.804688	-137.80	-110.32	-463.69	-371.21	-19.94	70.34
11	0.848978	-136.13	-109.37	-434.15	-348.80	-19.66	92.07
12	0.872052	-141.68	-108.87	-439.89	-338.03	-23.16	106.40
13	0.920660	-136.99	-107.82	-402.89	-317.10	-21.29	145.48
14	0.950022	-141.82	-107.19	-404.20	-305.50	-24.42	176.23
15	0.988579	-143.58	-106.36	-393.25	-291.31	-25.92	226.12
16	1.082018	-141.61	-104.35	-354.37	-261.12	-26.31	391.97
17	1.084985	-144.26	-104.28	-360.00	-260.25	-27.71	398.15
18	1.131051	-142.10	-103.29	-340.16	-247.27	-27.31	499.42
19	1.247021	-143.01	-100.80	-310.51	-218.86	-29.52	785.00
20	1.359398	-141.88	-98.38	-282.60	-195.94	-30.66	1082.97
21	1.596955	-139.81	-93.26	-237.04	-158.12	-33.29	1738.03
22	2.129221	-129.32	-81.80	-164.45	-104.02	-36.75	3240.16
23	3.028384	-103.29	-62.44	-92.35	-55.83	-39.55	5799.62
24	4.809769	-78.59	-24.08	-44.24	-13.56	-69.36	10883.81

THE LOADING POINT IS 0.57728

MEAN OF THE ABSOLUTE PERCENT ERROR IS 22.6458

DATA SET NUMBER 4

1	0.033217	-6.44	-7.85	-525.09	-640.00	21.88	0.09
2	0.040453	-8.08	-9.45	-540.75	-632.45	16.96	0.13
3	0.065598	-13.36	-14.91	-551.37	-615.33	11.60	0.34
4	0.091081	-18.64	-20.34	-554.12	-604.65	9.12	0.66
5	0.105092	-21.25	-23.29	-547.47	-600.18	9.63	0.88
6	0.156208	-31.78	-33.94	-550.92	-588.25	6.78	2.02
7	0.183243	-37.02	-39.49	-547.08	-583.57	6.67	2.85
8	0.369237	-76.27	-76.78	-559.27	-563.04	0.67	14.88
9	0.437705	-84.31	-90.17	-521.55	-557.82	6.96	23.65
10	0.634472	-120.98	-127.74	-516.30	-545.12	5.58	78.44
11	0.736368	-150.07	-146.50	-551.80	-538.69	-2.38	145.54
12	0.775200	-157.58	-149.15	-550.40	-520.96	-5.35	186.36
13	0.814166	-162.61	-149.05	-540.79	-495.70	-8.34	241.40
14	0.856058	-169.97	-148.95	-537.60	-471.11	-12.37	323.66
15	0.858853	-173.60	-148.94	-547.28	-469.55	-14.20	330.25
16	0.901194	-180.08	-148.83	-541.04	-447.17	-17.35	452.69
17	0.904139	-175.93	-148.83	-526.87	-445.69	-15.41	463.03
18	0.949903	-178.79	-148.71	-509.64	-423.89	-16.82	662.91
19	0.953001	-180.42	-148.70	-512.59	-422.49	-17.58	679.45
20	1.002659	-181.31	-148.58	-489.61	-401.23	-18.05	1004.62
21	1.009303	-183.74	-148.56	-492.93	-398.55	-19.15	1056.99
22	1.063510	-186.29	-148.43	-474.30	-377.89	-20.33	1556.99
23	1.119008	-184.18	-148.29	-445.65	-358.81	-19.49	2175.70

24	1.198919	-187.64	-148.09	-423.76	-334.44	-21.08	3177.83
25	1.266418	-184.56	-147.92	-394.59	-316.25	-19.85	4078.13
26	1.451873	-188.52	-147.45	-351.57	-274.98	-21.78	6655.19
27	1.457063	-186.99	-147.44	-347.47	-273.98	-21.15	6728.43
28	1.672618	-187.97	-146.90	-304.29	-237.80	-21.85	9795.46
29	1.919928	-185.42	-146.27	-261.49	-206.29	-21.11	13344.74
30	2.133302	-188.33	-145.74	-239.03	-184.98	-22.61	16418.08
31	2.336158	-190.54	-145.23	-220.84	-168.32	-23.78	19344.85
32	2.578712	-189.88	-144.62	-199.38	-151.85	-23.84	22848.08
33	2.840705	-181.52	-143.96	-173.02	-137.22	-20.69	26634.87
34	5.227828	-109.82	-137.96	-56.88	-71.46	25.63	61181.01

THE LOADING POINT IS 0.75140

MEAN OF THE ABSOLUTE PERCENT ERROR IS 15.4715

DATA SET NUMBER 5

1	0.187875	-41.47	-40.44	-597.62	-582.84	-2.47	3.01
2	0.278568	-62.75	-58.79	-609.93	-571.38	-6.32	7.37
3	0.387593	-84.10	-80.39	-587.48	-561.57	-4.41	16.92
4	0.426727	-91.58	-84.88	-581.09	-538.56	-7.32	22.02
5	0.454507	-99.39	-84.32	-592.11	-502.31	-15.17	26.35
6	0.475046	-105.47	-83.90	-601.15	-478.24	-20.45	30.00
7	0.487428	-110.62	-83.66	-614.50	-464.70	-24.38	32.41
8	0.526056	-107.88	-82.88	-555.26	-426.57	-23.18	41.07
9	0.538670	-108.33	-82.62	-544.52	-415.31	-23.73	44.32
10	0.585038	-113.84	-81.69	-526.87	-378.07	-28.24	58.48
11	0.611163	-116.55	-81.16	-516.37	-359.58	-30.36	68.29
12	0.640834	-117.77	-80.57	-497.60	-340.40	-31.59	81.46
13	0.670289	-118.79	-79.97	-479.85	-323.05	-32.68	97.15
14	0.699276	-119.09	-79.39	-461.11	-307.40	-33.34	115.77
15	0.732511	-119.15	-78.72	-440.44	-290.97	-33.94	142.07
16	0.823505	-115.07	-76.89	-378.36	-252.80	-33.19	257.34
17	0.826032	-117.37	-76.83	-384.72	-251.86	-34.54	261.86
18	0.989783	-112.50	-73.54	-307.74	-201.17	-34.63	909.12
19	1.098070	-114.67	-71.36	-282.75	-175.95	-37.77	1932.34
20	1.164313	-113.39	-70.02	-263.70	-162.84	-38.25	2732.46
21	1.584642	-110.24	-61.56	-188.37	-105.18	-44.17	8539.12
22	1.692985	-116.05	-59.37	-185.60	-94.96	-48.84	10086.91
23	2.091302	-110.14	-51.35	-142.60	-66.48	-53.38	15812.62
24	2.244098	-112.75	-48.27	-136.04	-58.24	-57.19	18016.18
25	2.459614	-109.08	-43.93	-120.08	-48.36	-59.73	21127.54

THE LOADING POINT IS 0.41204

MEAN OF THE ABSOLUTE PERCENT ERROR IS 30.3692

DATA SET NUMBER 6

1	0.029367	-6.64	-7.32	-612.55	-674.71	10.15	0.13
2	0.066079	-15.08	-15.67	-617.95	-642.29	3.94	0.68
3	0.088526	-18.25	-20.63	-558.30	-630.86	13.00	1.27
4	0.113000	-24.57	-25.93	-588.80	-621.36	5.53	2.17
5	0.125432	-25.28	-28.60	-545.61	-617.29	13.14	2.74
6	0.173650	-34.99	-38.77	-545.65	-604.58	10.80	5.87
7	0.175725	-38.80	-39.21	-597.80	-604.11	1.05	6.05
8	0.239421	-47.46	-52.34	-536.78	-591.92	10.27	13.18
9	0.293500	-60.59	-63.28	-558.97	-583.83	4.45	22.92
10	0.334439	-69.19	-71.47	-560.16	-578.59	3.29	33.40
11	0.414328	-85.35	-87.21	-557.74	-569.89	2.18	65.02
12	0.456530	-94.49	-95.41	-560.40	-565.89	0.98	90.15
13	0.483692	-99.09	-100.66	-554.67	-563.47	1.59	110.56
14	0.556885	-115.30	-110.31	-560.61	-536.35	-4.33	188.47
15	0.617178	-126.22	-110.18	-553.75	-483.36	-12.71	289.76
16	0.655017	-135.10	-110.09	-558.45	-455.08	-18.51	379.48
17	0.694022	-142.07	-110.00	-554.28	-429.16	-22.57	502.45
18	0.730743	-151.03	-109.92	-559.60	-407.29	-27.22	657.54
19	0.733532	-148.26	-109.91	-547.27	-405.72	-25.87	671.30
20	0.752427	-151.42	-109.87	-544.90	-395.38	-27.44	773.20
21	0.759454	-157.21	-109.86	-560.49	-391.66	-30.12	815.39
22	0.761566	-155.58	-109.85	-553.13	-390.56	-29.39	828.58
23	0.782192	-157.32	-109.80	-544.57	-380.10	-30.20	970.71
24	0.805526	-159.70	-109.75	-536.82	-368.91	-31.28	1166.08
25	0.834222	-161.03	-109.69	-522.67	-356.01	-31.89	1471.82
26	0.853742	-161.46	-109.64	-512.07	-347.73	-32.09	1733.60
27	0.891682	-161.76	-109.56	-491.19	-332.68	-32.27	2415.81
28	0.923626	-163.05	-109.49	-477.98	-320.96	-32.85	3239.12
29	0.978749	-163.12	-109.36	-451.26	-302.54	-32.96	5463.34
30	1.001464	-162.89	-109.31	-440.40	-295.54	-32.89	6751.46
31	1.048922	-163.87	-109.20	-423.00	-281.89	-33.36	10163.28
32	1.108848	-164.07	-109.07	-400.63	-266.33	-33.52	15558.54
33	1.124596	-164.95	-109.03	-397.14	-262.51	-33.90	17112.56
34	1.214209	-166.27	-108.83	-370.77	-242.69	-34.54	26552.14
35	1.315499	-167.02	-108.60	-343.76	-223.53	-34.97	37845.39
36	1.761247	-160.66	-107.60	-246.99	-165.42	-33.03	89423.99

THE LOADING POINT IS 0.53436

MEAN OF THE ABSOLUTE PERCENT ERROR IS 20.5076

DATA SET NUMBER 7

1	0.017095	-4.45	-4.40	-704.61	-697.51	-1.01	0.04
2	0.038466	-9.16	-9.43	-644.93	-663.74	2.92	0.22
3	0.065985	-14.17	-15.65	-581.38	-642.34	10.49	0.68
4	0.102645	-23.40	-23.70	-617.35	-625.10	1.25	1.75
5	0.140595	-30.08	-31.82	-579.30	-612.84	5.79	3.56
6	0.153953	-33.04	-34.64	-581.13	-609.29	4.85	4.41
7	0.231938	-49.66	-50.81	-579.75	-593.18	2.32	12.13
8	0.245385	-50.08	-53.56	-552.56	-590.95	6.95	14.07
9	0.288454	-61.97	-60.58	-581.65	-568.64	-2.24	21.83
10	0.321537	-66.41	-59.99	-559.21	-505.16	-9.67	29.76
11	0.351998	-71.66	-59.44	-551.24	-457.26	-17.05	38.93
12	0.359248	-72.26	-59.32	-544.62	-447.06	-17.91	41.42
13	0.365099	-73.99	-59.21	-548.71	-439.12	-19.97	43.52
14	0.382412	-74.10	-58.90	-524.69	-417.05	-20.52	50.27
15	0.400890	-74.56	-58.57	-503.61	-395.60	-21.45	58.41
16	0.420680	-74.57	-58.22	-479.97	-374.72	-21.93	68.36
17	0.427664	-74.88	-58.10	-474.06	-367.81	-22.41	72.20
18	0.441808	-73.16	-57.84	-448.34	-354.49	-20.93	80.56
19	0.496883	-74.26	-56.86	-404.64	-309.85	-23.43	121.90
20	0.515451	-73.12	-56.53	-384.07	-296.94	-22.69	139.68
21	0.589707	-71.87	-55.20	-330.00	-253.47	-23.19	238.29
22	0.615836	-70.94	-54.74	-311.89	-240.67	-22.84	287.00
23	0.690030	-71.08	-53.41	-278.90	-209.60	-24.85	488.13
24	0.838910	-68.86	-50.76	-222.26	-163.83	-26.29	1530.20
25	0.880178	-65.67	-50.02	-202.01	-153.88	-23.82	2180.31
26	1.059735	-68.16	-46.82	-174.16	-119.63	-31.31	11061.23
27	1.214696	-63.51	-44.06	-141.57	-98.20	-30.63	26605.28

THE LOADING POINT IS 0.28074

MEAN OF THE ABSOLUTE PERCENT ERROR IS 16.2475

TOTAL MEAN OF THE PERCENT ERROR IS 16.7330

COMPOSITIONS FOR EACH DATA POINT

COMPONENT 1: [H+]
COMPONENT 2: [OH-]
COMPONENT 3: [MDEA]
COMPONENT 4: [MDEAH+]
COMPONENT 5: [CO2]
COMPONENT 6: [HCO3-]
COMPONENT 7: [CO3-2]
COMPONENT 8: CO2(G)
MOLALITY (GMOLE/KG H2O)

LOADING

MOLE CO2

MOLE MDEA

DATA SET NUMBER 1

MOLE MDEA	1	2	3	4	5	6	7	8
0.00000	0.31197D-10	0.35126D-02	0.20945D+01	0.35126D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.05999	0.14158D-08	0.12480D-03	0.19507D+01	0.14727D+00	0.14440D-03	0.10429D+00	0.21427D-01	0.00000D+00
0.13494	0.32357D-08	0.60323D-04	0.17839D+01	0.31406D+00	0.68068D-03	0.25083D+00	0.31582D-01	0.00000D+00
0.23150	0.58741D-08	0.34476D-04	0.15756D+01	0.52238D+00	0.19903D-02	0.44502D+00	0.38662D-01	0.00000D+00
0.35999	0.10164D-07	0.19818D-04	0.13058D+01	0.79222D+00	0.51303D-02	0.70803D+00	0.42085D-01	0.00000D+00
0.54212	0.19130D-07	0.10016D-04	0.93582D+00	0.11621D+01	0.14191D-01	0.10842D+01	0.38984D-01	0.00000D+00
0.67553	0.30451D-07	0.59821D-05	0.67637D+00	0.14216D+01	0.27977D-01	0.13569D+01	0.32331D-01	0.00000D+00
0.81342	0.53358D-07	0.32286D-05	0.42724D+00	0.16707D+01	0.58636D-01	0.16250D+01	0.22839D-01	0.00000D+00
0.92682	0.94507D-07	0.17485D-05	0.25516D+00	0.18428D+01	0.11624D+00	0.18136D+01	0.14610D-01	0.00000D+00
0.94121	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.12894D-01
1.01100	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.15931D+00
1.02635	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.19153D+00
1.07282	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.28902D+00
1.12212	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.39245D+00
1.15668	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.46494D+00
1.23023	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.61924D+00
1.27015	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.70300D+00
1.28970	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.74402D+00
1.42123	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.10200D+01
1.63267	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.14635D+01
1.65796	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.15166D+01
1.85034	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.19202D+01
2.17744	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.26065D+01
2.51781	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.33206D+01
3.13198	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.46091D+01
4.05319	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.65417D+01
4.97443	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.84745D+01

DATA SET NUMBER 2

0.00000	0.31197D-10	0.35126D-02	0.20945D+01	0.35126D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.21169	0.52999D-08	0.38080D-04	0.16179D+01	0.48008D+00	0.16586D-02	0.40486D+00	0.37589D-01	0.00000D+00
0.26841	0.69980D-08	0.29016D-04	0.14973D+01	0.60067D+00	0.27061D-02	0.52017D+00	0.40233D-01	0.00000D+00
0.33071	0.90845D-08	0.22270D-04	0.13666D+01	0.73137D+00	0.42426D-02	0.64779D+00	0.41782D-01	0.00000D+00
0.36083	0.10196D-07	0.19752D-04	0.13040D+01	0.79397D+00	0.51577D-02	0.70977D+00	0.42091D-01	0.00000D+00
0.43998	0.13535D-07	0.14616D-04	0.11414D+01	0.95655D+00	0.82323D-02	0.87312D+00	0.41706D-01	0.00000D+00
0.49736	0.16455D-07	0.11820D-04	0.10253D+01	0.10727D+01	0.11239D-01	0.99174D+00	0.40460D-01	0.00000D+00
0.53983	0.18984D-07	0.10101D-04	0.94036D+00	0.11576D+01	0.14025D-01	0.10795D+01	0.39069D-01	0.00000D+00
0.58014	0.21760D-07	0.86860D-05	0.86066D+00	0.12373D+01	0.17235D-01	0.11625D+01	0.37412D-01	0.00000D+00
0.60909	0.24035D-07	0.77789D-05	0.80403D+00	0.12939D+01	0.19959D-01	0.12219D+01	0.36033D-01	0.00000D+00
0.65767	0.28533D-07	0.64300D-05	0.71034D+00	0.13876D+01	0.25536D-01	0.13208D+01	0.33395D-01	0.00000D+00
0.68245	0.31240D-07	0.58150D-05	0.66329D+00	0.14347D+01	0.28988D-01	0.13709D+01	0.31906D-01	0.00000D+00
0.74112	0.39170D-07	0.45286D-05	0.55446D+00	0.15435D+01	0.39388D-01	0.14874D+01	0.28052D-01	0.00000D+00
0.74749	0.40192D-07	0.44020D-05	0.54289D+00	0.15551D+01	0.40751D-01	0.14999D+01	0.27610D-01	0.00000D+00
0.79945	0.50109D-07	0.34571D-05	0.45105D+00	0.16469D+01	0.54179D-01	0.15992D+01	0.23872D-01	0.00000D+00
0.81313	0.53287D-07	0.32332D-05	0.42773D+00	0.16702D+01	0.58539D-01	0.16245D+01	0.22861D-01	0.00000D+00
0.91773	0.89936D-07	0.18429D-05	0.26716D+00	0.18308D+01	0.10978D+00	0.18004D+01	0.15227D-01	0.00000D+00
0.92535	0.93751D-07	0.17635D-05	0.25707D+00	0.18409D+01	0.11517D+00	0.18115D+01	0.14709D-01	0.00000D+00
1.15310	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.45743D+00
1.16264	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.47745D+00
1.48242	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.11483D+01
1.97665	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.21852D+01
2.79993	0.98888D-07	0.16667D-05	0.24462D+00	0.18533D+01	0.12244D+00	0.18252D+01	0.14063D-01	0.39124D+01

DATA SET NUMBER 3

0.00000	0.31197D-10	0.35126D-02	0.20945D+01	0.35126D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.22815	0.57757D-08	0.35047D-04	0.15827D+01	0.51524D+00	0.19317D-02	0.43822D+00	0.38493D-01	0.00000D+00
0.35632	0.10025D-07	0.20105D-04	0.13133D+01	0.78462D+00	0.50128D-02	0.70048D+00	0.42061D-01	0.00000D+00
0.53241	0.18515D-07	0.10383D-04	0.95514D+00	0.11428D+01	0.13498D-01	0.10641D+01	0.39339D-01	0.00000D+00
0.58272	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.11422D-01
0.60278	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.53509D-01
0.65076	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.15416D+00
0.68014	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.21580D+00
0.73793	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.33705D+00
0.79858	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.46428D+00
0.80469	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.47710D+00
0.84898	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.57002D+00
0.87205	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.61843D+00
0.92066	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.72040D+00
0.95002	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.78201D+00
0.98858	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.86290D+00
1.08202	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.10589D+01
1.08498	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.10652D+01
1.13105	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.11618D+01
1.24702	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.14051D+01
1.35940	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.16409D+01

1.59696	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.21392D+01
2.12922	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.32559D+01
3.02838	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.51423D+01
4.80977	0.21548D-07	0.87806D-05	0.86629D+00	0.12317D+01	0.16985D-01	0.11566D+01	0.37540D-01	0.88796D+01

DATA SET NUMBER 4

0.00000	0.19443D-10	0.58416D-02	0.55887D+01	0.58416D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.03322	0.84747D-09	0.22664D-03	0.53509D+01	0.24365D+00	0.93705D-04	0.12806D+00	0.57680D-01	0.00000D+00
0.04045	0.10172D-08	0.19257D-03	0.53028D+01	0.29178D+00	0.13621D-03	0.16078D+00	0.65405D-01	0.00000D+00
0.06560	0.15910D-08	0.12713D-03	0.51397D+01	0.45483D+00	0.33955D-03	0.27861D+00	0.88048D-01	0.00000D+00
0.09108	0.21525D-08	0.94221D-04	0.49791D+01	0.61552D+00	0.63124D-03	0.40244D+00	0.10649D+00	0.00000D+00
0.10509	0.24543D-08	0.82184D-04	0.48921D+01	0.70243D+00	0.82802D-03	0.47188D+00	0.11523D+00	0.00000D+00
0.15621	0.35241D-08	0.54818D-04	0.45814D+01	0.10131D+01	0.17690D-02	0.73121D+00	0.14094D+00	0.00000D+00
0.18324	0.40758D-08	0.45914D-04	0.44204D+01	0.11742D+01	0.24141D-02	0.87136D+00	0.15139D+00	0.00000D+00
0.36924	0.78898D-08	0.17855D-04	0.33551D+01	0.22395D+01	0.10290D-01	0.18714D+01	0.18403D+00	0.00000D+00
0.43770	0.94550D-08	0.13264D-04	0.29779D+01	0.26167D+01	0.15265D-01	0.22503D+01	0.18318D+00	0.00000D+00
0.63447	0.15695D-07	0.56861D-05	0.19340D+01	0.36606D+01	0.42023D-01	0.33546D+01	0.15297D+00	0.00000D+00
0.73637	0.21420D-07	0.35056D-05	0.14219D+01	0.41727D+01	0.71347D-01	0.39239D+01	0.12438D+00	0.00000D+00
0.77520	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.13316D+00
0.81417	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.35116D+00
0.85606	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.58553D+00
0.85885	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.60117D+00
0.90119	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.83805D+00
0.90414	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.85452D+00
0.94990	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.11106D+01
0.95300	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.11279D+01
1.00266	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.14057D+01
1.00930	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.14429D+01
1.06351	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.17461D+01
1.11901	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.20566D+01
1.19892	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.25037D+01
1.26642	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.28813D+01
1.45187	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.39189D+01
1.45706	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.39479D+01
1.67262	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.51538D+01
1.91993	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.65374D+01
2.13330	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.77312D+01
2.33616	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.88661D+01
2.57871	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.10223D+02
2.84070	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.11689D+02
5.22783	0.22564D-07	0.32462D-05	0.13487D+01	0.42459D+01	0.77448D-01	0.40067D+01	0.11959D+00	0.25044D+02

DATA SET NUMBER 5

0.00000	0.19444D-10	0.58416D-02	0.55887D+01	0.58416D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.18787	0.41696D-08	0.44617D-04	0.43930D+01	0.12016D+01	0.25354D-02	0.89554D+00	0.15300D+00	0.00000D+00
0.27857	0.59968D-08	0.27223D-04	0.38662D+01	0.17283D+01	0.56093D-02	0.13774D+01	0.17546D+00	0.00000D+00
0.38759	0.82940D-08	0.16469D-04	0.32533D+01	0.23413D+01	0.11484D-01	0.19726D+01	0.18437D+00	0.00000D+00
0.42673	0.88484D-08	0.14809D-04	0.31184D+01	0.24761D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.82168D-01
0.45451	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.23758D+00

0.47505	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.35248D+00
0.48743	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.42176D+00
0.52606	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.63787D+00
0.53867	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.70844D+00
0.58504	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.96784D+00
0.61116	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.11140D+01
0.64083	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.12800D+01
0.67029	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.14448D+01
0.69928	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.16070D+01
0.73251	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.17929D+01
0.82351	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.23020D+01
0.82603	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.23161D+01
0.98978	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.32322D+01
1.09807	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.38380D+01
1.16431	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.42086D+01
1.58464	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.65602D+01
1.69298	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.71663D+01
2.09130	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.93948D+01
2.24410	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.10250D+02
2.45961	0.88486D-08	0.14809D-04	0.31184D+01	0.24762D+01	0.13227D-01	0.21078D+01	0.18417D+00	0.11455D+02

DATA SET NUMBER 6

0.00000	0.13195D-10	0.89224D-02	0.12579D+02	0.89224D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.02937	0.77196D-09	0.26300D-03	0.12063D+02	0.52435D+00	0.12218D-03	0.21500D+00	0.15454D+00	0.00000D+00
0.06608	0.14935D-08	0.12419D-03	0.11487D+02	0.11003D+01	0.56989D-03	0.56226D+00	0.26896D+00	0.00000D+00
0.08853	0.18502D-08	0.91611D-04	0.11152D+02	0.14361D+01	0.99012D-03	0.79071D+00	0.32264D+00	0.00000D+00
0.11300	0.21834D-08	0.69599D-04	0.10795D+02	0.17926D+01	0.15722D-02	0.10492D+01	0.37166D+00	0.00000D+00
0.12543	0.23339D-08	0.61443D-04	0.10617D+02	0.19705D+01	0.19176D-02	0.11835D+01	0.39345D+00	0.00000D+00
0.17365	0.28221D-08	0.40242D-04	0.99434D+01	0.26444D+01	0.35833D-02	0.17203D+01	0.46203D+00	0.00000D+00
0.17573	0.28402D-08	0.39579D-04	0.99149D+01	0.26729D+01	0.36670D-02	0.17438D+01	0.46449D+00	0.00000D+00
0.23942	0.33080D-08	0.24768D-04	0.90569D+01	0.35309D+01	0.67560D-02	0.24831D+01	0.52388D+00	0.00000D+00
0.29350	0.36052D-08	0.17360D-04	0.83496D+01	0.42382D+01	0.10259D-01	0.31303D+01	0.55394D+00	0.00000D+00
0.33444	0.37905D-08	0.13478D-04	0.78249D+01	0.47629D+01	0.13545D-01	0.36297D+01	0.56660D+00	0.00000D+00
0.41433	0.40979D-08	0.84229D-05	0.68238D+01	0.57640D+01	0.21925D-01	0.46231D+01	0.57043D+00	0.00000D+00
0.45653	0.42498D-08	0.66191D-05	0.63060D+01	0.62818D+01	0.27682D-01	0.51562D+01	0.56279D+00	0.00000D+00
0.48369	0.43496D-08	0.56754D-05	0.59765D+01	0.66113D+01	0.32002D-01	0.55019D+01	0.55472D+00	0.00000D+00
0.55689	0.45501D-08	0.42622D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53355D+00	0.28356D+00
0.61718	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.10425D+01
0.65502	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53355D+00	0.15188D+01
0.69402	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.20098D+01
0.73074	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.24721D+01
0.73353	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.25072D+01
0.75243	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.27450D+01
0.75945	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.28335D+01
0.76157	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.28600D+01
0.78219	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.31197D+01
0.80553	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.34134D+01
0.83422	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.37746D+01
0.85374	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.40203D+01

0.89168	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.44979D+01
0.92363	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.49000D+01
0.97875	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.55939D+01
1.00146	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.58798D+01
1.04892	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.64772D+01
1.10885	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.72316D+01
1.12460	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.74298D+01
1.21421	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.85578D+01
1.31550	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.98328D+01
1.76125	0.45501D-08	0.42621D-05	0.53695D+01	0.72183D+01	0.41652D-01	0.61512D+01	0.53356D+00	0.15444D+02

DATA SET NUMBER 7

0.00000	0.13195D-10	0.89225D-02	0.12579D+02	0.89225D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.01710	0.48021D-09	0.41458D-03	0.12268D+02	0.31944D+00	0.42973D-04	0.11127D+00	0.10388D+00	0.00000D+00
0.03847	0.96988D-09	0.20725D-03	0.11917D+02	0.67125D+00	0.20450D-03	0.29695D+00	0.18705D+00	0.00000D+00
0.06599	0.14919D-08	0.12437D-03	0.11489D+02	0.10989D+01	0.56835D-03	0.56132D+00	0.26872D+00	0.00000D+00
0.10264	0.20487D-08	0.77756D-04	0.10945D+02	0.16428D+01	0.13101D-02	0.93878D+00	0.35198D+00	0.00000D+00
0.14060	0.25026D-08	0.53306D-04	0.10403D+02	0.21850D+01	0.23849D-02	0.13498D+01	0.41757D+00	0.00000D+00
0.15395	0.26392D-08	0.47387D-04	0.10216D+02	0.23719D+01	0.28391D-02	0.14983D+01	0.43680D+00	0.00000D+00
0.23194	0.32607D-08	0.26082D-04	0.91562D+01	0.34316D+01	0.63384D-02	0.23949D+01	0.51837D+00	0.00000D+00
0.24539	0.33445D-08	0.23780D-04	0.89780D+01	0.36098D+01	0.71001D-02	0.25537D+01	0.52803D+00	0.00000D+00
0.28845	0.35414D-08	0.18833D-04	0.85150D+01	0.40728D+01	0.93516D-02	0.29762D+01	0.54830D+00	0.97137D-01
0.32154	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93513D-02	0.29762D+01	0.54830D+00	0.51363D+00
0.35200	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.89707D+00
0.35925	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.98834D+00
0.36510	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.10620D+01
0.38241	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.12799D+01
0.40089	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.15125D+01
0.42068	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.17616D+01
0.42766	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.18495D+01
0.44181	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.20276D+01
0.49688	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.27209D+01
0.51545	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.29546D+01
0.58971	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.38893D+01
0.61584	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.42182D+01
0.69003	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.51522D+01
0.83891	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.70262D+01
0.88018	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.75457D+01
1.05974	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.98059D+01
1.21470	0.35412D-08	0.18832D-04	0.85150D+01	0.40728D+01	0.93514D-02	0.29762D+01	0.54830D+00	0.11757D+02

ANALYSIS OF EQUILIBRIUM CONSTANT AND HEAT OF REACTION
FOR THE PROTONATION OF MDEA AT 240.0 F

DATA SET NUMBER 1

SYSTEM (RUN#.TRIAL): 13.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.16297	-32.48
0.25665	-58.79
0.25749	-53.15
0.29587	-59.08
0.29587	-65.96
0.36647	-74.62
0.37127	-77.48
0.40855	-82.16
0.49223	-106.61
0.52214	-108.72
0.52385	-122.33
0.54183	-113.15
0.54926	-119.05
0.55240	-122.22
0.58072	-121.68
0.63724	-120.15
0.72231	-120.52
0.80032	-116.53
0.88989	-112.11
0.89809	-119.04
1.01041	-112.90
1.15608	-110.29
1.20088	-105.74
1.24282	-112.47
1.30084	-108.98
1.42883	-101.28
1.59603	-99.27
2.08847	-86.82
2.60940	-74.32
3.12585	-54.73

DATA SET NUMBER 2

SYSTEM (RUN#.TRIAL): 14.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 40.0

INPUT DATA

MOLE CO2	BTU

MOLE MDEA	LB MDEA
0.07844	-16.60
0.13389	-30.77
0.15879	-36.85
0.17343	-40.39
0.18968	-43.17
0.20621	-45.86
0.22325	-52.20
0.22473	-50.93
0.26262	-60.06
0.26354	-61.08
0.30932	-71.03
0.33398	-75.15
0.33514	-74.33
0.36200	-81.59
0.36317	-78.70
0.37683	-79.84
0.39240	-79.31
0.40871	-80.66
0.42578	-80.55
0.46245	-77.58
0.46411	-77.44
0.48230	-78.14
0.50474	-74.25
0.50988	-74.34
0.52498	-77.61
0.54818	-71.95
0.59851	-73.65
0.60058	-69.37
0.71947	-72.42
0.72183	-66.55
0.88050	-65.51
1.09318	-76.31

DATA SET NUMBER 3

SYSTEM (RUN#.TRIAL): 15.1
PRESSURE (PSIA) : 162.6
CONCENTRATION (WT. % MDEA): 60.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.03775	-9.31
0.04919	-12.61
0.06266	-13.93
0.06826	-15.64
0.07687	-17.58
0.08417	-20.21
0.09322	-20.92
0.10135	-24.23
0.10928	-25.49
0.11120	-25.97
0.12079	-27.11
0.12158	-26.79
0.13139	-30.47
0.13457	-32.56
0.14270	-31.54

0.14367	-31.45
0.15481	-34.82
0.16123	-37.24
0.17135	-39.21
0.17475	-38.81
0.18190	-37.60
0.18931	-38.05
0.20151	-38.49
0.23653	-36.51
0.27402	-35.98
0.30223	-35.22
0.34905	-35.80
0.47018	-30.30
0.80603	-22.18

INPUT PARAMETERS

NUMBER OF REACTIONS : 5

NUMBER OF COMPONENTS : 7

CHARGES ON COMPONENTS:
1, 1.
2, -1.
3, Ø.
4, 1.
5, Ø.
6, -1.
7, -2.

TOLERANCE FOR ACTIVITY COEFFICIENT CONVERGENCE: Ø.5D-Ø3

TOLERANCE FOR SIMULTANEOUS EQUATION SOLUTIONS : Ø.1D-Ø4

VALUES FOR LN K, DELTA H FOR EACH REACTION

LN K [=] UNITLESS

DELTA H [=] CAL/GMOLE

	1	2	3	4	5
LN K	-27.75Ø	-16.345	-14.913	-23.366	-4.639
DELTA H	9385.59	8Ø28.19	-4128.78	-1589.Ø1	-1634.2Ø

CONVERTED DATA

(NOTE: "CORRECTED HEAT OF SOLUTION" IS TOTAL HEAT OF SOLUTION LESS HEAT OF ABSORPTION OF GASEOUS CO2.)

POINT	MOLE FRACTION CO2	HEAT OF SOLUTION (J/MOLE)	MOLALITY CO2 (MOLE/KG H20)	MOLALITY MDEA (MOLE/KG H20)	CORRECTED HEAT OF SOLUTION (CAL/KG H20)
			DATA SET NUMBER 1		
1	0.00590	-325.69	0.3419	2.0980	-3952.1
2	0.00926	-587.57	0.5385	2.0980	-7285.5
3	0.00929	-531.15	0.5402	2.0980	-6498.8
4	0.01066	-589.61	0.6207	2.0980	-7191.0
5	0.01066	-658.25	0.6207	2.0980	-8146.3
6	0.01317	-742.85	0.7688	2.0980	-9107.9
7	0.01334	-771.17	0.7789	2.0980	-9488.4
8	0.01466	-816.66	0.8571	2.0980	-10010.6
9	0.01761	-1056.46	1.0327	2.0980	-13118.9
10	0.01866	-1076.29	1.0954	2.0980	-13310.3
11	0.01872	-1210.90	1.0990	2.0980	-15194.1
12	0.01935	-1119.32	1.1367	2.0980	-13857.6
13	0.01961	-1177.35	1.1523	2.0980	-14651.3
14	0.01972	-1208.55	1.1589	2.0980	-15080.5
15	0.02071	-1202.04	1.2183	2.0980	-14909.0
16	0.02268	-1184.52	1.3369	2.0980	-14502.6
17	0.02563	-1184.56	1.5154	2.0980	-14262.0
18	0.02832	-1142.24	1.6791	2.0980	-13441.1
19	0.03139	-1095.45	1.8670	2.0980	-12520.3
20	0.03167	-1162.81	1.8842	2.0980	-13454.5
21	0.03549	-1098.47	2.1198	2.0980	-12216.4
22	0.04040	-1067.57	2.4254	2.0980	-11353.9
23	0.04190	-1021.95	2.5194	2.0980	-10568.6
24	0.04330	-1085.42	2.6074	2.0980	-11359.8
25	0.04523	-1049.59	2.7291	2.0980	-10675.8
26	0.04946	-971.10	2.9976	2.0980	-9167.4
27	0.05493	-946.38	3.3484	2.0980	-8315.5
28	0.07068	-813.86	4.3815	2.0980	-4897.5
29	0.08678	-684.60	5.4744	2.0980	-1375.3
30	0.10220	-495.66	6.5579	2.0980	3115.6
			DATA SET NUMBER 2		
1	0.00713	-418.03	0.4388	5.5946	-5431.7
2	0.01211	-770.99	0.7491	5.5946	-10173.4
3	0.01433	-921.06	0.8884	5.5946	-12195.0
4	0.01563	-1008.39	0.9703	5.5946	-13374.9
5	0.01707	-1076.24	1.0612	5.5946	-14256.2
6	0.01853	-1141.57	1.1537	5.5946	-15101.0
7	0.02003	-1297.26	1.2490	5.5946	-17291.3
8	0.02016	-1265.47	1.2572	5.5946	-16806.7
9	0.02348	-1487.31	1.4693	5.5946	-19842.0
10	0.02356	-1512.63	1.4744	5.5946	-20214.0
11	0.02754	-1751.71	1.7305	5.5946	-23478.6
12	0.02967	-1849.30	1.8685	5.5946	-24779.6
13	0.02977	-1828.97	1.8749	5.5946	-24465.8
14	0.03208	-2002.73	2.0253	5.5946	-26907.7
15	0.03218	-1931.73	2.0318	5.5946	-25828.8
16	0.03335	-1957.16	2.1082	5.5946	-26123.4

17	0.03468	-1941.61	2.1953	5.5946	-25786.8
18	0.03607	-1971.94	2.2866	5.5946	-26139.2
19	0.03752	-1966.21	2.3821	5.5946	-25941.2
20	0.04062	-1887.45	2.5872	5.5946	-24503.5
21	0.04076	-1883.78	2.5965	5.5946	-24436.6
22	0.04229	-1897.97	2.6983	5.5946	-24532.5
23	0.04417	-1799.86	2.8238	5.5946	-22885.3
24	0.04460	-1801.35	2.8526	5.5946	-22873.4
25	0.04586	-1877.94	2.9370	5.5946	-23944.1
26	0.04779	-1737.54	3.0668	5.5946	-21636.9
27	0.05195	-1770.79	3.3484	5.5946	-21805.8
28	0.05212	-1667.59	3.3600	5.5946	-20201.8
29	0.06180	-1723.06	4.0251	5.5946	-20243.4
30	0.06199	-1583.18	4.0383	5.5946	-18049.4
31	0.07460	-1537.48	4.9260	5.5946	-16213.4
32	0.09098	-1759.28	6.1159	5.5946	-18269.6

DATA SET NUMBER 3

1	0.00693	-473.58	0.4752	12.5878	-6984.9
2	0.00901	-639.84	0.6192	12.5878	-9496.6
3	0.01145	-704.89	0.7888	12.5878	-10316.3
4	0.01246	-791.02	0.8592	12.5878	-11632.4
5	0.01401	-887.44	0.9676	12.5878	-13067.4
6	0.01532	-1018.90	1.0595	12.5878	-15109.6
7	0.01694	-1053.14	1.1735	12.5878	-15518.1
8	0.01839	-1217.73	1.2758	12.5878	-18105.5
9	0.01980	-1279.08	1.3756	12.5878	-18990.1
10	0.02014	-1302.70	1.3997	12.5878	-19350.4
11	0.02184	-1357.60	1.5205	12.5878	-20104.1
12	0.02198	-1341.63	1.5305	12.5878	-19825.2
13	0.02371	-1523.16	1.6539	12.5878	-22689.5
14	0.02427	-1626.60	1.6939	12.5878	-24364.0
15	0.02570	-1573.24	1.7963	12.5878	-23345.1
16	0.02587	-1568.52	1.8085	12.5878	-23250.9
17	0.02782	-1733.26	1.9487	12.5878	-25832.3
18	0.02894	-1851.56	2.0295	12.5878	-27716.5
19	0.03070	-1946.06	2.1569	12.5878	-29151.5
20	0.03129	-1924.76	2.1997	12.5878	-28743.6
21	0.03253	-1862.58	2.2898	12.5878	-27591.8
22	0.03381	-1882.32	2.3830	12.5878	-27813.4
23	0.03591	-1899.88	2.5365	12.5878	-27927.9
24	0.04189	-1790.83	2.9774	12.5878	-25555.3
25	0.04821	-1753.38	3.4494	12.5878	-24345.7
26	0.05291	-1707.98	3.8044	12.5878	-23133.9
27	0.06061	-1721.90	4.3938	12.5878	-22652.5
28	0.07996	-1427.41	5.9185	12.5878	-15579.0
29	0.12967	-988.53	10.1461	12.5878	-1905.2

MDEA PROTONATION

LN K : -15.8100
DELTA H : 9047.30

SUMMARY OF FIT FOR LOADING CURVE

POINT	LOADING MOLE CO2 / MOLE MDEA	EXPERIMENTAL HEAT OF SOLN (BTU/LB MDEA)	CALCULATED HEAT OF SOLN (BTU/LB MDEA)	EXPERIMENTAL HEAT OF SOLN (BTU/LB CO2)	CALCULATED HEAT OF SOLN (BTU/LB CO2)	RELATIVE ERROR	EQUILIBRIUM PRESSURE OF CO2 (PSIA)
			DATA SET NUMBER 1				
1	0.162974	-32.48	-36.08	-539.59	-599.40	11.08	15.91
2	0.256654	-58.79	-55.92	-620.24	-589.98	-4.88	39.09
3	0.257493	-53.15	-56.10	-558.87	-589.90	5.55	39.35
4	0.295875	-59.08	-64.06	-540.65	-586.21	8.43	52.47
5	0.295875	-65.96	-64.06	-603.59	-586.21	-2.88	52.47
6	0.366471	-74.62	-78.41	-551.35	-579.33	5.08	83.07
7	0.371265	-77.48	-79.37	-565.07	-578.86	2.44	85.48
8	0.408549	-82.16	-86.77	-544.52	-575.10	5.62	105.88
9	0.492234	-106.61	-95.79	-586.41	-526.91	-10.15	163.47
10	0.522142	-108.72	-95.04	-563.80	-492.85	-12.58	188.59
11	0.523853	-122.33	-95.00	-632.28	-491.02	-22.34	190.11
12	0.541830	-113.15	-94.55	-565.44	-472.49	-16.44	206.61
13	0.549256	-119.05	-94.37	-586.86	-465.19	-20.73	213.72
14	0.552399	-122.22	-94.29	-599.05	-462.16	-22.85	216.79
15	0.580718	-121.68	-93.58	-567.34	-436.32	-23.09	245.91
16	0.637239	-120.15	-92.17	-510.52	-391.63	-23.29	312.71
17	0.722306	-120.52	-90.04	-451.77	-337.54	-25.28	438.09
18	0.800325	-116.53	-88.10	-394.25	-298.05	-24.40	583.23
19	0.889895	-112.11	-85.86	-341.12	-261.24	-23.42	789.46
20	0.898092	-119.04	-85.66	-358.90	-258.24	-28.05	810.54
21	1.010405	-112.90	-82.85	-302.55	-222.02	-26.61	1136.27
22	1.156079	-110.29	-79.22	-258.30	-185.53	-28.17	1653.56
23	1.200880	-105.74	-78.10	-238.41	-176.09	-26.14	1830.98
24	1.242820	-112.47	-77.05	-245.03	-167.86	-31.49	2003.70
25	1.300841	-108.98	-75.60	-226.83	-157.36	-30.63	2251.97
26	1.428828	-101.28	-72.41	-191.92	-137.21	-28.51	2831.12

27	1.596033	-99.27	-68.23	-168.41	-115.75	-31.27	3635.39
28	2.088467	-86.82	-55.94	-112.55	-72.52	-35.57	6167.57
29	2.609399	-74.32	-42.93	-77.11	-44.55	-42.23	8958.58
30	3.125846	-54.73	-30.04	-47.41	-26.02	-45.12	11768.78

THE LOADING POINT IS 0.45912

MEAN OF THE ABSOLUTE PERCENT ERROR IS 20.8105

DATA SET NUMBER 2

1	0.078436	-16.60	-18.03	-573.10	-622.26	8.58	8.66
2	0.133892	-30.77	-30.39	-622.32	-614.55	-1.25	24.06
3	0.158794	-36.85	-35.89	-628.28	-611.92	-2.60	33.74
4	0.173428	-40.39	-39.10	-630.64	-610.50	-3.19	40.31
5	0.189683	-43.17	-42.66	-616.29	-609.00	-1.18	48.43
6	0.206213	-45.86	-46.27	-602.20	-607.55	0.89	57.63
7	0.223247	-52.20	-49.97	-633.07	-606.11	-4.26	68.15
8	0.224726	-50.93	-50.29	-613.58	-605.98	-1.24	69.12
9	0.262624	-60.06	-58.48	-619.18	-602.93	-2.62	96.97
10	0.263541	-61.08	-58.68	-627.58	-602.86	-3.94	97.73
11	0.309322	-71.03	-68.47	-621.74	-599.33	-3.60	140.49
12	0.333977	-75.15	-67.77	-609.26	-549.41	-9.82	168.21
13	0.335137	-74.33	-67.74	-600.53	-547.29	-8.87	169.61
14	0.362004	-81.59	-67.11	-610.24	-501.99	-17.74	204.30
15	0.363170	-78.70	-67.09	-586.77	-500.17	-14.76	205.91
16	0.376829	-79.84	-66.77	-573.64	-479.75	-16.37	225.55
17	0.392397	-79.31	-66.41	-547.26	-458.21	-16.27	249.60
18	0.408713	-80.66	-66.02	-534.39	-437.40	-18.15	276.87
19	0.425784	-80.55	-65.63	-512.24	-417.33	-18.53	307.80
20	0.462453	-77.58	-64.77	-454.20	-379.23	-16.50	383.47
21	0.464114	-77.44	-64.73	-451.76	-377.65	-16.40	387.22
22	0.482305	-78.14	-64.31	-438.70	-361.03	-17.70	430.26
23	0.504737	-74.25	-63.79	-398.31	-342.17	-14.09	488.65
24	0.509880	-74.34	-63.67	-394.80	-338.09	-14.36	502.92
25	0.524977	-77.61	-63.31	-400.28	-326.55	-18.42	546.83
26	0.548179	-71.95	-62.77	-355.39	-310.05	-12.76	620.57
27	0.598511	-73.65	-61.60	-333.19	-278.67	-16.36	810.17
28	0.600578	-69.37	-61.55	-312.75	-277.49	-11.27	818.92
29	0.719467	-72.42	-58.78	-272.53	-221.20	-18.84	1485.27
30	0.721825	-66.55	-58.72	-249.64	-220.27	-11.76	1502.32
31	0.880496	-65.51	-55.02	-201.46	-169.20	-16.01	3119.33
32	1.093177	-76.31	-50.06	-189.02	-124.00	-34.40	7117.26

THE LOADING POINT IS 0.30879

MEAN OF THE ABSOLUTE PERCENT ERROR IS 11.6488

DATA SET NUMBER 3

1	0.037753	-9.31	-9.09	-667.99	-652.02	-2.39	4.20
2	0.049187	-12.61	-11.76	-694.16	-647.27	-6.75	6.90
3	0.062662	-13.93	-14.88	-601.77	-643.18	6.88	10.93
4	0.068258	-15.64	-16.18	-620.55	-641.78	3.42	12.90
5	0.076870	-17.58	-18.17	-619.17	-639.86	3.34	16.26
6	0.084170	-20.21	-19.85	-650.11	-638.41	-1.80	19.45
7	0.093224	-20.92	-21.92	-607.70	-636.79	4.79	23.85
8	0.101353	-24.23	-23.79	-647.26	-635.48	-1.82	28.24
9	0.109281	-25.49	-25.60	-631.46	-634.30	0.45	32.95
10	0.111196	-25.97	-26.04	-632.26	-634.03	0.28	34.16
11	0.120791	-27.11	-28.23	-607.62	-632.72	4.13	40.58
12	0.121583	-26.79	-28.41	-596.65	-632.62	6.03	41.14
13	0.131385	-30.47	-30.64	-627.95	-631.40	0.55	48.47
14	0.134566	-32.56	-31.36	-655.12	-631.02	-3.68	51.02
15	0.142703	-31.54	-33.21	-598.38	-630.09	5.30	57.90
16	0.143672	-31.45	-33.43	-592.66	-629.98	6.30	58.76
17	0.154812	-34.82	-35.95	-609.00	-628.79	3.25	69.21
18	0.161230	-37.24	-37.40	-625.39	-628.13	0.44	75.75
19	0.171346	-39.21	-39.69	-619.63	-627.14	1.21	86.87
20	0.174745	-38.81	-40.45	-601.29	-626.82	4.25	90.85
21	0.181903	-37.60	-42.07	-559.68	-626.16	11.88	99.61
22	0.189311	-38.05	-43.73	-544.20	-625.49	14.94	109.27
23	0.201508	-38.49	-46.47	-517.16	-624.44	20.74	126.58
24	0.236531	-36.51	-48.21	-417.88	-551.88	32.07	187.14
25	0.274025	-35.98	-47.44	-355.51	-468.74	31.85	273.41
26	0.302232	-35.22	-46.86	-315.54	-419.79	33.04	356.39
27	0.349054	-35.80	-45.89	-277.70	-355.99	28.19	537.68
28	0.470175	-30.30	-43.40	-174.50	-249.91	43.22	1396.58
29	0.806026	-22.18	-36.48	-74.52	-122.53	64.43	14079.02

THE LOADING POINT IS 0.21156

MEAN OF THE ABSOLUTE PERCENT ERROR IS 11.9796

TOTAL MEAN OF THE PERCENT ERROR IS 14.7746

COMPOSITIONS FOR EACH DATA POINT

COMPONENT 1: [H+]
COMPONENT 2: [OH-]
COMPONENT 3: [MDEA]
COMPONENT 4: [MDEAH+]
COMPONENT 5: [CO2]
COMPONENT 6: [HCO3-]
COMPONENT 7: [CO3-2]
COMPONENT 8: CO2(G)
MOLALITY (GMOLE/KG H2O)

LOADING

MOLE CO2

MOLE MDEA

DATA SET NUMBER 1

MOLE MDEA	1	2	3	4	5	6	7	8
0.00000	0.26132D-09	0.40210D-02	0.20939D+01	0.40210D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.16297	0.26233D-07	0.81291D-04	0.17588D+01	0.33917D+00	0.95575D-02	0.32563D+00	0.67288D-02	0.00000D+00
0.25665	0.44053D-07	0.51738D-04	0.15738D+01	0.52421D+00	0.22342D-01	0.50806D+00	0.80450D-02	0.00000D+00
0.25749	0.44223D-07	0.51559D-04	0.15721D+01	0.52584D+00	0.22481D-01	0.50968D+00	0.80538D-02	0.00000D+00
0.29587	0.52246D-07	0.44304D-04	0.14982D+01	0.59980D+00	0.29386D-01	0.58294D+00	0.84071D-02	0.00000D+00
0.29587	0.52246D-07	0.44304D-04	0.14982D+01	0.59980D+00	0.29386D-01	0.58294D+00	0.84071D-02	0.00000D+00
0.36647	0.68303D-07	0.34463D-04	0.13652D+01	0.73281D+00	0.44900D-01	0.71512D+00	0.88280D-02	0.00000D+00
0.37127	0.69462D-07	0.33913D-04	0.13563D+01	0.74169D+00	0.46096D-01	0.72396D+00	0.88468D-02	0.00000D+00
0.40855	0.78801D-07	0.30024D-04	0.12879D+01	0.81004D+00	0.56069D-01	0.79210D+00	0.89541D-02	0.00000D+00
0.49223	0.92492D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89968D-02	0.69464D-01
0.52214	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89969D-02	0.13221D+00
0.52385	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.13580D+00
0.54183	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.17351D+00
0.54926	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.18909D+00
0.55240	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.19569D+00
0.58072	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.25510D+00
0.63724	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.37368D+00
0.72231	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.55215D+00
0.80032	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.71583D+00
0.88989	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.90374D+00
0.89809	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.92094D+00
1.01041	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.11566D+01
1.15608	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.14622D+01
1.20088	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.15562D+01
1.24282	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.16442D+01
1.30084	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.17659D+01
1.42883	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.20344D+01

1.59603	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.23852D+01
2.08847	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.34183D+01
2.60940	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.45112D+01
3.12585	0.92491D-07	0.25646D-04	0.11974D+01	0.90061D+00	0.71639D-01	0.88259D+00	0.89970D-02	0.55947D+01

DATA SET NUMBER 2

0.00000	0.16356D-09	0.67161D-02	0.55879D+01	0.67161D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.07844	0.11898D-07	0.18888D-03	0.51379D+01	0.45666D+00	0.50178D-02	0.41112D+00	0.22675D-01	0.00000D+00
0.13389	0.20096D-07	0.11760D-03	0.48274D+01	0.76720D+00	0.12810D-01	0.70543D+00	0.30828D-01	0.00000D+00
0.15879	0.23717D-07	0.10003D-03	0.46896D+01	0.90502D+00	0.17308D-01	0.83723D+00	0.33847D-01	0.00000D+00
0.17343	0.25831D-07	0.91744D-04	0.46090D+01	0.98558D+00	0.20236D-01	0.91455D+00	0.35469D-01	0.00000D+00
0.18968	0.28169D-07	0.83834D-04	0.45199D+01	0.10747D+01	0.23738D-01	0.10003D+01	0.37150D-01	0.00000D+00
0.20621	0.30538D-07	0.76892D-04	0.44297D+01	0.11649D+01	0.27569D-01	0.10874D+01	0.38735D-01	0.00000D+00
0.22325	0.32972D-07	0.70666D-04	0.43371D+01	0.12575D+01	0.31807D-01	0.11769D+01	0.40244D-01	0.00000D+00
0.22473	0.33183D-07	0.70164D-04	0.43291D+01	0.12655D+01	0.32189D-01	0.11847D+01	0.40370D-01	0.00000D+00
0.26262	0.38592D-07	0.58958D-04	0.41247D+01	0.14699D+01	0.42766D-01	0.13832D+01	0.43285D-01	0.00000D+00
0.26354	0.38723D-07	0.58721D-04	0.41198D+01	0.14748D+01	0.43041D-01	0.13880D+01	0.43349D-01	0.00000D+00
0.30932	0.45294D-07	0.48450D-04	0.38759D+01	0.17187D+01	0.57988D-01	0.16264D+01	0.46139D-01	0.00000D+00
0.33398	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.14090D+00
0.33514	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.14739D+00
0.36200	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.29770D+00
0.36317	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.30422D+00
0.37683	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.38064D+00
0.39240	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.46774D+00
0.40871	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.55902D+00
0.42578	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.65452D+00
0.46245	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.85967D+00
0.46411	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.86897D+00
0.48230	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.97074D+00
0.50474	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.10962D+01
0.50988	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.11250D+01
0.52498	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.12095D+01
0.54818	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.13393D+01
0.59851	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.16209D+01
0.60058	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.16324D+01
0.71947	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.22976D+01
0.72183	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.23108D+01
0.88050	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.31984D+01
1.09318	0.45217D-07	0.48554D-04	0.38787D+01	0.17159D+01	0.57801D-01	0.16236D+01	0.46111D-01	0.43883D+01

DATA SET NUMBER 3

0.00000	0.11148D-09	0.10303D-01	0.12577D+02	0.10303D-01	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.03775	0.57833D-08	0.39815D-03	0.12061D+02	0.52643D+00	0.23705D-02	0.41967D+00	0.53181D-01	0.00000D+00
0.04919	0.73453D-08	0.32049D-03	0.11909D+02	0.67916D+00	0.37261D-02	0.55202D+00	0.63413D-01	0.00000D+00
0.06266	0.90839D-08	0.26117D-03	0.11730D+02	0.85794D+00	0.56190D-02	0.70862D+00	0.74527D-01	0.00000D+00
0.06826	0.97744D-08	0.24252D-03	0.11656D+02	0.93187D+00	0.64924D-02	0.77383D+00	0.78900D-01	0.00000D+00
0.07687	0.10801D-07	0.21841D-03	0.11542D+02	0.10453D+01	0.79304D-02	0.87431D+00	0.85391D-01	0.00000D+00
0.08417	0.11639D-07	0.20132D-03	0.11447D+02	0.11412D+01	0.92352D-02	0.95959D+00	0.90691D-01	0.00000D+00

0.09322	0.12638D-07	0.18331D-03	0.11328D+02	0.12597D+01	0.10959D-01	0.10655D+01	0.97026D-01	0.00000D+00
0.10135	0.13498D-07	0.16950D-03	0.11222D+02	0.13659D+01	0.12603D-01	0.11607D+01	0.10251D+00	0.00000D+00
0.10928	0.14305D-07	0.15773D-03	0.11119D+02	0.14692D+01	0.14291D-01	0.12536D+01	0.10769D+00	0.00000D+00
0.11120	0.14495D-07	0.15510D-03	0.11094D+02	0.14941D+01	0.14711D-01	0.12761D+01	0.10891D+00	0.00000D+00
0.12079	0.15422D-07	0.14300D-03	0.10969D+02	0.16187D+01	0.16888D-01	0.13887D+01	0.11492D+00	0.00000D+00
0.12158	0.15496D-07	0.14207D-03	0.10959D+02	0.16289D+01	0.17072D-01	0.13980D+01	0.11540D+00	0.00000D+00
0.13139	0.16395D-07	0.13140D-03	0.10832D+02	0.17559D+01	0.19425D-01	0.15131D+01	0.12130D+00	0.00000D+00
0.13457	0.16678D-07	0.12822D-03	0.10791D+02	0.17970D+01	0.20214D-01	0.15505D+01	0.12317D+00	0.00000D+00
0.14270	0.17381D-07	0.12064D-03	0.10686D+02	0.19020D+01	0.22290D-01	0.16462D+01	0.12784D+00	0.00000D+00
0.14367	0.17463D-07	0.11978D-03	0.10673D+02	0.19145D+01	0.22542D-01	0.16576D+01	0.12839D+00	0.00000D+00
0.15481	0.18378D-07	0.11062D-03	0.10530D+02	0.20579D+01	0.25526D-01	0.17887D+01	0.13455D+00	0.00000D+00
0.16123	0.18883D-07	0.10583D-03	0.10447D+02	0.21403D+01	0.27313D-01	0.18642D+01	0.13799D+00	0.00000D+00
0.17135	0.19647D-07	0.98908D-04	0.10318D+02	0.22700D+01	0.30228D-01	0.19834D+01	0.14324D+00	0.00000D+00
0.17475	0.19895D-07	0.96736D-04	0.10274D+02	0.23135D+01	0.31235D-01	0.20235D+01	0.14497D+00	0.00000D+00
0.18190	0.20406D-07	0.92392D-04	0.10183D+02	0.24050D+01	0.33400D-01	0.21078D+01	0.14853D+00	0.00000D+00
0.18931	0.20916D-07	0.88194D-04	0.10088D+02	0.24995D+01	0.35704D-01	0.21952D+01	0.15212D+00	0.00000D+00
0.20151	0.21717D-07	0.81865D-04	0.99330D+01	0.26548D+01	0.39639D-01	0.23391D+01	0.15782D+00	0.00000D+00
0.23653	0.22343D-07	0.77123D-04	0.98053D+01	0.27825D+01	0.43016D-01	0.24578D+01	0.16233D+00	0.31430D+00
0.27402	0.22343D-07	0.77123D-04	0.98053D+01	0.27825D+01	0.43017D-01	0.24578D+01	0.16233D+00	0.78624D+00
0.30223	0.22343D-07	0.77123D-04	0.98053D+01	0.27825D+01	0.43016D-01	0.24578D+01	0.16233D+00	0.11413D+01
0.34905	0.22343D-07	0.77123D-04	0.98053D+01	0.27825D+01	0.43016D-01	0.24578D+01	0.16233D+00	0.17307D+01
0.47018	0.22343D-07	0.77123D-04	0.98053D+01	0.27825D+01	0.43016D-01	0.24578D+01	0.16233D+00	0.32553D+01
0.80603	0.22343D-07	0.77123D-04	0.98053D+01	0.27825D+01	0.43016D-01	0.24578D+01	0.16233D+00	0.74830D+01

ANALYSIS OF EQUILIBRIUM CONSTANT AND HEAT OF REACTION
FOR THE PROTONATION OF MDEA AT 300.0 F

DATA SET NUMBER 1

SYSTEM	(RUN#.TRIAL):	16.1
PRESSURE	(PSIA) :	212.6
CONCENTRATION	(WT. % MDEA):	20.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.05200	-12.82
0.08235	-19.31
0.09645	-21.20
0.11526	-28.08
0.11526	-25.46
0.12662	-29.46
0.13938	-31.68
0.14354	-34.67
0.14992	-33.64
0.16214	-37.05
0.16242	-37.75
0.17938	-42.16
0.19051	-45.89
0.20639	-59.60
0.20667	-46.96
0.21699	-51.10
0.22954	-53.43
0.24211	-54.46
0.24575	-55.21
0.26085	-57.87
0.26253	-56.43
0.26421	-61.93
0.28914	-58.97
0.30654	-58.94
0.31497	-58.40
0.32087	-55.73
0.33774	-54.60
0.35435	-53.65
0.36675	-54.33
0.40996	-53.00
0.43686	-52.20
0.48143	-47.11
0.50789	-46.47

DATA SET NUMBER 2

SYSTEM	(RUN#.TRIAL):	18.1
PRESSURE	(PSIA) :	212.6
CONCENTRATION	(WT. % MDEA):	40.0

INPUT DATA

MOLE CO2 / MOLE MDEA	BTU / LB MDEA
0.02825	-7.39
0.03451	-8.30
0.04442	-11.77
0.04860	-11.69
0.05555	-13.10
0.06383	-15.35
0.07146	-16.77
0.07999	-18.86
0.08065	-19.68
0.08975	-21.54
0.08975	-20.95
0.09008	-21.17
0.09853	-24.84
0.10821	-25.60
0.11914	-27.32
0.12059	-27.37
0.12841	-31.00
0.13098	-30.58
0.13210	-30.34
0.14240	-31.56
0.14330	-30.61
0.14364	-30.62
0.15520	-30.80
0.16881	-30.73
0.18415	-29.40
0.20066	-29.38
0.21665	-28.43
0.23372	-27.13
0.25427	-26.65
0.27662	-25.07
0.29848	-23.51
0.32169	-22.02
0.35257	-20.97

INPUT PARAMETERS

NUMBER OF REACTIONS : 5

NUMBER OF COMPONENTS : 7

CHARGES ON COMPONENTS:
1, 1.
2, -1.
3, Ø.
4, 1.
5, Ø.
6, -1.
7, -2.

TOLERANCE FOR ACTIVITY COEFFICIENT CONVERGENCE: Ø.5D-Ø3

TOLERANCE FOR SIMULTANEOUS EQUATION SOLUTIONS : Ø.1D-Ø4

VALUES FOR LN K, DELTA H FOR EACH REACTION

LN K [=] UNITLESS

DELTA H [=] CAL/GMOLE

	1	2	3	4	5
LN K	-26.84Ø	-15.534	-15.487	-23.6Ø7	-4.765
DELTA H	7773.Ø7	7825.4Ø	-737Ø.65	-3145.8Ø	-849.38

CONVERTED DATA

(NOTE: "CORRECTED HEAT OF SOLUTION" IS TOTAL HEAT OF SOLUTION LESS HEAT OF ABSORPTION OF GASEOUS CO2.)

POINT	MOLE FRACTION CO2	HEAT OF SOLUTION (J/MOLE)	MOLALITY CO2 (MOLE/KG H2O)	MOLALITY MDEA (MOLE/KG H2O)	CORRECTED HEAT OF SOLUTION (CAL/KG H2O)
			DATA SET NUMBER 1		
1	0.00189	-129.04	0.1091	2.0980	-1687.4
2	0.00299	-194.24	0.1728	2.0980	-2535.6
3	0.00350	-213.09	0.2023	2.0980	-2772.4
4	0.00418	-282.07	0.2418	2.0980	-3694.6
5	0.00418	-255.80	0.2418	2.0980	-3331.3
6	0.00459	-295.86	0.2656	2.0980	-3866.6
7	0.00505	-317.98	0.2924	2.0980	-4151.9
8	0.00520	-347.91	0.3011	2.0980	-4559.5
9	0.00543	-337.51	0.3145	2.0980	-4405.2
10	0.00587	-371.58	0.3402	2.0980	-4857.3
11	0.00588	-378.56	0.3407	2.0980	-4953.5
12	0.00649	-422.58	0.3763	2.0980	-5536.5
13	0.00689	-459.71	0.3997	2.0980	-6033.9
14	0.00746	-596.71	0.4330	2.0980	-7909.7
15	0.00747	-470.22	0.4336	2.0980	-6154.6
16	0.00784	-511.48	0.4552	2.0980	-6711.2
17	0.00829	-534.53	0.4816	2.0980	-7012.1
18	0.00874	-544.55	0.5079	2.0980	-7132.3
19	0.00887	-551.97	0.5156	2.0980	-7229.7
20	0.00941	-578.26	0.5473	2.0980	-7572.5
21	0.00947	-563.88	0.5508	2.0980	-7370.0
22	0.00953	-618.80	0.5543	2.0980	-8130.9
23	0.01042	-588.64	0.6066	2.0980	-7674.7
24	0.01104	-587.97	0.6431	2.0980	-7639.5
25	0.01134	-582.44	0.6608	2.0980	-7549.9
26	0.01155	-555.65	0.6732	2.0980	-7167.9
27	0.01215	-544.11	0.7086	2.0980	-6981.8
28	0.01274	-534.33	0.7434	2.0980	-6820.4
29	0.01318	-540.82	0.7694	2.0980	-6892.1
30	0.01471	-526.82	0.8601	2.0980	-6631.2
31	0.01566	-518.32	0.9165	2.0980	-6471.5
32	0.01723	-467.03	1.0100	2.0980	-5685.1
33	0.01816	-460.24	1.0655	2.0980	-5548.9
			DATA SET NUMBER 2		
1	0.00258	-186.93	0.1581	5.5946	-2602.7
2	0.00315	-209.78	0.1931	5.5946	-2909.3
3	0.00405	-297.35	0.2485	5.5946	-4149.0
4	0.00443	-295.04	0.2719	5.5946	-4097.1
5	0.00506	-330.56	0.3108	5.5946	-4588.1
6	0.00581	-386.92	0.3571	5.5946	-5380.3
7	0.00650	-422.52	0.3998	5.5946	-5871.4
8	0.00727	-474.92	0.4475	5.5946	-6606.5
9	0.00733	-495.49	0.4512	5.5946	-6906.3
10	0.00815	-541.79	0.5021	5.5946	-7550.9
11	0.00815	-526.93	0.5021	5.5946	-7332.1
12	0.00818	-532.49	0.5040	5.5946	-7412.6
13	0.00894	-624.31	0.5512	5.5946	-8731.6

14	0.00981	-642.89	0.6054	5.5946	-8967.6
15	0.01079	-685.46	0.6665	5.5946	-9553.6
16	0.01092	-686.42	0.6746	5.5946	-9562.2
17	0.01162	-777.10	0.7184	5.5946	-10872.0
18	0.01185	-766.30	0.7328	5.5946	-10702.8
19	0.01195	-760.24	0.7391	5.5946	-10609.0
20	0.01287	-789.97	0.7967	5.5946	-11010.5
21	0.01295	-766.13	0.8017	5.5946	-10654.4
22	0.01298	-766.42	0.8036	5.5946	-10657.4
23	0.01401	-770.16	0.8683	5.5946	-10669.7
24	0.01522	-767.49	0.9444	5.5946	-10579.5
25	0.01658	-733.26	1.0302	5.5946	-10014.1
26	0.01804	-731.56	1.1226	5.5946	-9926.5
27	0.01945	-707.02	1.2121	5.5946	-9500.6
28	0.02095	-673.60	1.3076	5.5946	-8937.2
29	0.02275	-660.49	1.4225	5.5946	-8662.1
30	0.02470	-620.15	1.5475	5.5946	-7971.7
31	0.02660	-580.26	1.6698	5.5946	-7287.3
32	0.02861	-542.36	1.7997	5.5946	-6625.3
33	0.03127	-515.26	1.9725	5.5946	-6092.4

MDEA PROTONATION

LN K : -14.9300
DELTA H : 8214.70

SUMMARY OF FIT FOR LOADING CURVE

POINT	LOADING MOLE CO2 / MOLE MDEA	EXPERIMENTAL HEAT OF SOLN (BTU/LB MDEA)	CALCULATED HEAT OF SOLN (BTU/LB MDEA)	EXPERIMENTAL HEAT OF SOLN (BTU/LB CO2)	CALCULATED HEAT OF SOLN (BTU/LB CO2)	RELATIVE ERROR	EQUILIBRIUM PRESSURE OF CO2 (PSIA)
			DATA SET NUMBER 1				
1	0.051997	-12.82	-12.50	-667.38	-651.02	-2.45	8.20
2	0.082351	-19.31	-19.45	-635.00	-639.43	0.70	18.41
3	0.096447	-21.20	-22.61	-595.13	-634.70	6.65	24.30
4	0.115263	-28.08	-26.77	-659.62	-628.80	-4.67	33.26
5	0.115263	-25.46	-26.77	-598.18	-628.80	5.12	33.26
6	0.126621	-29.46	-29.25	-630.05	-625.43	-0.73	39.27
7	0.139375	-31.68	-32.01	-615.48	-621.77	1.02	46.54
8	0.143537	-34.67	-32.90	-654.00	-620.60	-5.11	49.03
9	0.149920	-33.64	-34.26	-607.57	-618.83	1.85	52.97
10	0.162140	-37.05	-36.86	-618.76	-615.52	-0.52	60.90
11	0.162418	-37.75	-36.92	-629.31	-615.45	-2.20	61.09
12	0.179378	-42.16	-40.48	-636.46	-611.00	-4.00	72.96
13	0.190510	-45.89	-42.79	-652.19	-608.15	-6.75	81.28
14	0.206389	-59.60	-46.05	-781.87	-604.18	-22.73	93.89
15	0.206668	-46.96	-46.11	-615.31	-604.11	-1.82	94.12
16	0.216986	-51.10	-48.21	-637.71	-601.59	-5.66	102.79
17	0.229544	-53.43	-50.74	-630.27	-598.56	-5.03	113.85
18	0.242114	-54.46	-53.26	-609.03	-595.58	-2.21	125.47
19	0.245748	-55.21	-53.98	-608.27	-594.72	-2.23	128.93
20	0.260851	-57.87	-56.96	-600.68	-591.21	-1.58	143.82
21	0.262530	-56.43	-57.29	-582.03	-590.83	1.51	145.53
22	0.264209	-61.93	-57.61	-634.69	-590.44	-6.97	147.24
23	0.289143	-58.97	-56.33	-552.19	-527.54	-4.47	173.92
24	0.306540	-58.94	-55.29	-520.59	-488.39	-6.19	193.88
25	0.314965	-58.40	-54.79	-502.05	-470.98	-6.19	203.94
26	0.320866	-55.73	-54.43	-470.25	-459.34	-2.32	211.15

27	0.337739	-54.60	-53.42	-437.75	-428.28	-2.16	232.48
28	0.354351	-53.65	-52.43	-409.97	-400.60	-2.29	254.54
29	0.366753	-54.33	-51.68	-401.10	-381.57	-4.87	271.70
30	0.409963	-53.00	-49.09	-350.07	-324.25	-7.38	336.18
31	0.436861	-52.20	-47.48	-323.53	-294.30	-9.04	380.08
32	0.481426	-47.11	-44.81	-264.95	-252.04	-4.88	459.37
33	0.507892	-46.47	-43.23	-247.73	-230.45	-6.98	510.39

THE LOADING POINT IS 0.26505

MEAN OF THE ABSOLUTE PERCENT ERROR IS 4.4925

DATA SET NUMBER 2

1	0.028253	-7.39	-7.02	-708.21	-672.98	-4.98	5.95
2	0.034514	-8.30	-8.54	-650.98	-669.95	2.91	8.46
3	0.044416	-11.77	-10.92	-717.65	-665.89	-7.21	13.19
4	0.048601	-11.69	-11.93	-651.02	-664.36	2.05	15.46
5	0.055548	-13.10	-13.58	-638.57	-662.00	3.67	19.57
6	0.063830	-15.35	-15.55	-650.96	-659.42	1.30	25.03
7	0.071460	-16.77	-17.35	-635.40	-657.21	3.43	30.59
8	0.079987	-18.86	-19.35	-638.55	-654.90	2.56	37.41
9	0.080652	-19.68	-19.50	-660.75	-654.73	-0.91	37.97
10	0.089749	-21.54	-21.63	-649.81	-652.42	0.40	46.01
11	0.089749	-20.95	-21.63	-631.98	-652.42	3.23	46.01
12	0.090082	-21.17	-21.70	-636.31	-652.34	2.52	46.32
13	0.098527	-24.84	-23.66	-682.61	-650.31	-4.73	54.46
14	0.108210	-25.60	-25.90	-640.58	-648.10	1.17	64.59
15	0.119138	-27.32	-28.41	-620.97	-645.73	3.99	77.06
16	0.120589	-27.37	-28.74	-614.44	-645.42	5.04	78.79
17	0.128410	-31.00	-30.53	-653.70	-643.80	-1.51	88.50
18	0.130983	-30.58	-31.12	-632.10	-643.28	1.77	91.82
19	0.132101	-30.34	-31.37	-621.86	-643.05	3.41	93.29
20	0.142404	-31.56	-33.71	-599.99	-641.02	6.84	107.33
21	0.143301	-30.61	-33.92	-578.28	-640.84	10.82	108.61
22	0.143637	-30.62	-33.99	-577.16	-640.78	11.02	109.09
23	0.155197	-30.80	-36.60	-537.34	-638.58	18.84	126.24
24	0.168808	-30.73	-39.66	-492.91	-636.10	29.05	148.18
25	0.184147	-29.40	-39.40	-432.30	-579.33	34.01	175.25
26	0.200660	-29.38	-38.49	-396.39	-519.35	31.02	207.30
27	0.216655	-28.43	-37.61	-355.32	-469.98	32.27	241.35
28	0.233721	-27.13	-36.66	-314.29	-424.76	35.15	281.11
29	0.254269	-26.65	-35.53	-283.79	-378.36	33.32	333.94
30	0.276616	-25.07	-34.30	-245.42	-335.72	36.79	397.94
31	0.298475	-23.51	-33.09	-213.23	-300.19	40.78	467.60

32	0.321694	-22.02	-31.81	-185.30	-267.74	44.49	549.77
33	0.352568	-20.97	-30.11	-161.07	-231.21	43.55	673.18

THE LOADING POINT IS 0.17092

MEAN OF THE ABSOLUTE PERCENT ERROR IS 14.0836

TOTAL MEAN OF THE PERCENT ERROR IS 9.2881

COMPOSITIONS FOR EACH DATA POINT

COMPONENT 1: [H+]
COMPONENT 2: [OH-]
COMPONENT 3: [MDEA]
COMPONENT 4: [MDEAH+]
COMPONENT 5: [CO2]
COMPONENT 6: [HCO3-]
COMPONENT 7: [CO3-2]
COMPONENT 8: CO2(G)

LOADING — MOLALITY (GMOLE/KG H2O)

MOLE CO2 / MOLE MDEA

DATA SET NUMBER 1

1	2	3	4	5	6	7	8
0.00000	0.64601D-09	0.41229D-02	0.20938D+01	0.41229D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.05200	0.17910D-07	0.25304D-03	0.19917D+01	0.10623D+00	0.45965D-02	0.10300D+00	0.14894D-02	0.00000D+00
0.08235	0.28648D-07	0.17599D-03	0.19333D+01	0.16469D+00	0.10130D-01	0.16076D+00	0.18751D-02	0.00000D+00
0.09645	0.33718D-07	0.15516D-03	0.19067D+01	0.19126D+00	0.13265D-01	0.18705D+00	0.20318D-02	0.00000D+00
0.11526	0.40567D-07	0.13442D-03	0.18718D+01	0.22621D+00	0.17963D-01	0.22163D+00	0.22236D-02	0.00000D+00
0.11526	0.40567D-07	0.13442D-03	0.18718D+01	0.22621D+00	0.17963D-01	0.22163D+00	0.22236D-02	0.00000D+00
0.12662	0.44744D-07	0.12453D-03	0.18509D+01	0.24703D+00	0.21070D-01	0.24225D+00	0.23311D-02	0.00000D+00
0.13938	0.49474D-07	0.11510D-03	0.18278D+01	0.27017D+00	0.24794D-01	0.26517D+00	0.24451D-02	0.00000D+00
0.14354	0.51026D-07	0.11234D-03	0.18203D+01	0.27767D+00	0.26062D-01	0.27259D+00	0.24808D-02	0.00000D+00
0.14992	0.53415D-07	0.10836D-03	0.18089D+01	0.28911D+00	0.28056D-01	0.28394D+00	0.25344D-02	0.00000D+00
0.16214	0.58017D-07	0.10150D-03	0.17871D+01	0.31086D+00	0.32039D-01	0.30549D+00	0.26326D-02	0.00000D+00
0.16242	0.58122D-07	0.10136D-03	0.17866D+01	0.31135D+00	0.32132D-01	0.30598D+00	0.26348D-02	0.00000D+00
0.17938	0.64574D-07	0.93206D-04	0.17568D+01	0.34116D+00	0.38020D-01	0.33555D+00	0.27624D-02	0.00000D+00
0.19051	0.68848D-07	0.88536D-04	0.17375D+01	0.36051D+00	0.42103D-01	0.35474D+00	0.28410D-02	0.00000D+00
0.20639	0.75002D-07	0.82626D-04	0.17102D+01	0.38781D+00	0.48221D-01	0.38183D+00	0.29467D-02	0.00000D+00
0.20667	0.75111D-07	0.82529D-04	0.17097D+01	0.38828D+00	0.48332D-01	0.38230D+00	0.29485D-02	0.00000D+00
0.21699	0.79145D-07	0.79094D-04	0.16921D+01	0.40583D+00	0.52494D-01	0.39972D+00	0.30131D-02	0.00000D+00
0.22954	0.84095D-07	0.75270D-04	0.16710D+01	0.42699D+00	0.57753D-01	0.42073D+00	0.30879D-02	0.00000D+00
0.24211	0.89092D-07	0.71782D-04	0.16500D+01	0.44795D+00	0.63226D-01	0.44156D+00	0.31586D-02	0.00000D+00
0.24575	0.90544D-07	0.70830D-04	0.16440D+01	0.45397D+00	0.64848D-01	0.44754D+00	0.31782D-02	0.00000D+00
0.26085	0.96621D-07	0.67117D-04	0.16192D+01	0.47881D+00	0.71770D-01	0.47223D+00	0.32567D-02	0.00000D+00
0.26253	0.97300D-07	0.66726D-04	0.16164D+01	0.48155D+00	0.72558D-01	0.47496D+00	0.32650D-02	0.00000D+00
0.26421	0.97981D-07	0.66340D-04	0.16137D+01	0.48429D+00	0.73350D-01	0.47768D+00	0.32734D-02	0.00000D+00
0.28914	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47904D+00	0.32776D-02	0.50555D-01
0.30654	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.87053D-01
0.31497	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.10473D+00
0.32087	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.11711D+00

0.33774	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.15251D+00
0.35435	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.18736D+00
0.36675	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.21338D+00
0.40996	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.30403D+00
0.43686	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.36046D+00
0.48143	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.45396D+00
0.50789	0.98320D-07	0.66149D-04	0.16123D+01	0.48566D+00	0.73745D-01	0.47903D+00	0.32775D-02	0.50948D+00

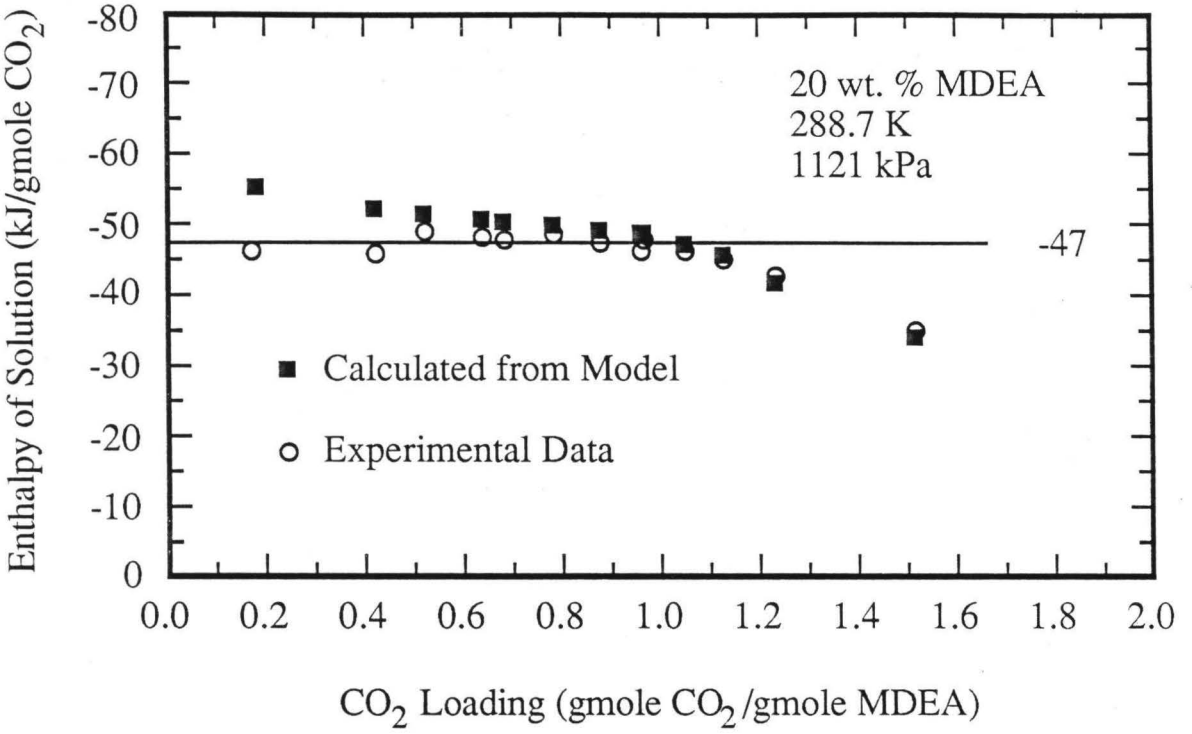
DATA SET NUMBER 2

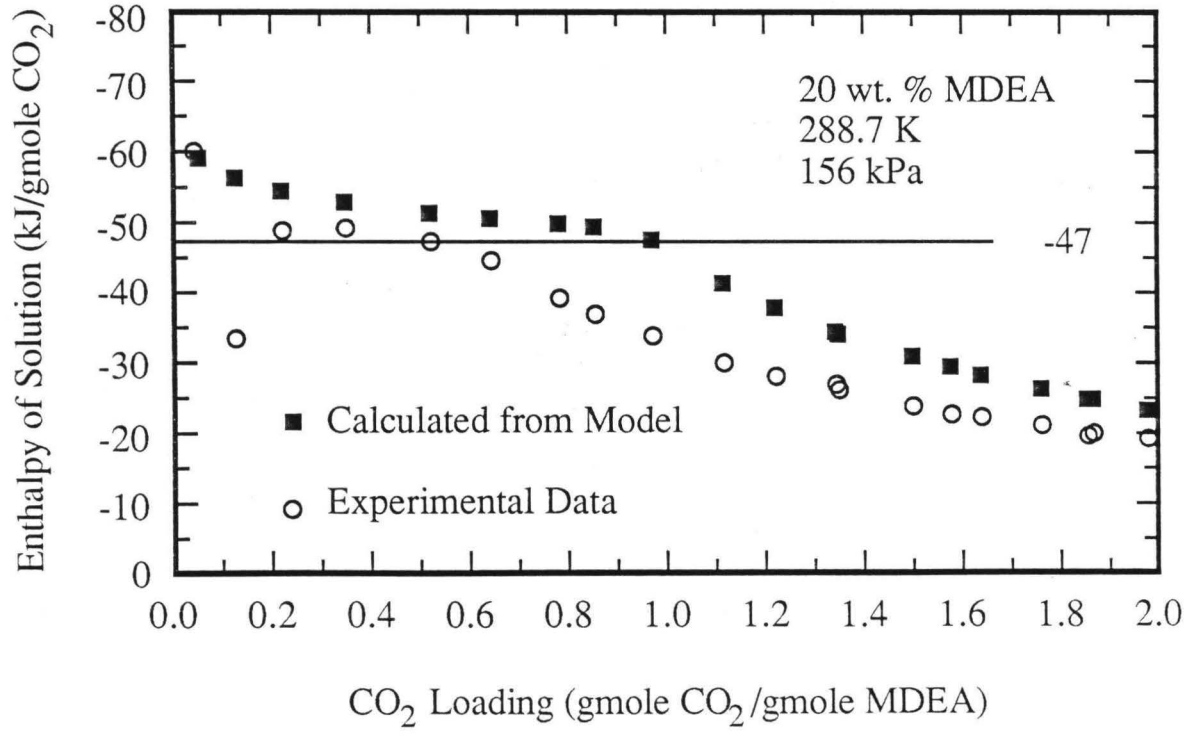
0.00000	0.40546D-09	0.69056D-02	0.55877D+01	0.69056D-02	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00
0.02825	0.99278D-08	0.50691D-03	0.54343D+01	0.16031D+00	0.32777D-02	0.14977D+00	0.50179D-02	0.00000D+00
0.03451	0.12119D-07	0.43549D-03	0.54000D+01	0.19457D+00	0.46105D-02	0.18283D+00	0.56486D-02	0.00000D+00
0.04442	0.15584D-07	0.35948D-03	0.53462D+01	0.24836D+00	0.70648D-02	0.23484D+00	0.65817D-02	0.00000D+00
0.04860	0.17047D-07	0.33561D-03	0.53236D+01	0.27098D+00	0.82210D-02	0.25673D+00	0.69572D-02	0.00000D+00
0.05555	0.19472D-07	0.30297D-03	0.52862D+01	0.30835D+00	0.10286D-01	0.29292D+00	0.75592D-02	0.00000D+00
0.06383	0.22356D-07	0.27223D-03	0.52419D+01	0.35265D+00	0.12973D-01	0.33588D+00	0.82468D-02	0.00000D+00
0.07146	0.25004D-07	0.24943D-03	0.52013D+01	0.39324D+00	0.15654D-01	0.37528D+00	0.88551D-02	0.00000D+00
0.07999	0.27952D-07	0.22844D-03	0.51562D+01	0.43836D+00	0.18873D-01	0.41911D+00	0.95095D-02	0.00000D+00
0.08065	0.28182D-07	0.22696D-03	0.51527D+01	0.44187D+00	0.19133D-01	0.42252D+00	0.95594D-02	0.00000D+00
0.08975	0.31311D-07	0.20866D-03	0.51049D+01	0.48972D+00	0.22830D-01	0.46905D+00	0.10229D-01	0.00000D+00
0.08975	0.31311D-07	0.20866D-03	0.51049D+01	0.48972D+00	0.22830D-01	0.46905D+00	0.10229D-01	0.00000D+00
0.09008	0.31426D-07	0.20805D-03	0.51031D+01	0.49146D+00	0.22970D-01	0.47075D+00	0.10253D-01	0.00000D+00
0.09853	0.34317D-07	0.19377D-03	0.50589D+01	0.53564D+00	0.26627D-01	0.51374D+00	0.10851D-01	0.00000D+00
0.10821	0.37615D-07	0.17975D-03	0.50086D+01	0.58602D+00	0.31067D-01	0.56281D+00	0.11513D-01	0.00000D+00
0.11914	0.41316D-07	0.16628D-03	0.49520D+01	0.64254D+00	0.36381D-01	0.61791D+00	0.12232D-01	0.00000D+00
0.12059	0.41805D-07	0.16465D-03	0.49446D+01	0.65003D+00	0.37111D-01	0.62521D+00	0.12325D-01	0.00000D+00
0.12841	0.44438D-07	0.15639D-03	0.49043D+01	0.69024D+00	0.41135D-01	0.66445D+00	0.12819D-01	0.00000D+00
0.13098	0.45301D-07	0.15386D-03	0.48911D+01	0.70343D+00	0.42493D-01	0.67732D+00	0.12979D-01	0.00000D+00
0.13210	0.45676D-07	0.15278D-03	0.48854D+01	0.70916D+00	0.43089D-01	0.68291D+00	0.13048D-01	0.00000D+00
0.14240	0.49119D-07	0.14354D-03	0.48328D+01	0.76178D+00	0.48720D-01	0.73430D+00	0.13670D-01	0.00000D+00
0.14330	0.49418D-07	0.14279D-03	0.48282D+01	0.76635D+00	0.49223D-01	0.73876D+00	0.13723D-01	0.00000D+00
0.14364	0.49530D-07	0.14251D-03	0.48265D+01	0.76806D+00	0.49412D-01	0.74043D+00	0.13743D-01	0.00000D+00
0.15520	0.53367D-07	0.13352D-03	0.47678D+01	0.82673D+00	0.56073D-01	0.79778D+00	0.14412D-01	0.00000D+00
0.16881	0.57856D-07	0.12426D-03	0.46992D+01	0.89538D+00	0.64322D-01	0.86492D+00	0.15166D-01	0.00000D+00
0.18415	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87531D+00	0.15281D-01	0.73997D-01
0.20066	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.16638D+00
0.21665	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.25587D+00
0.23372	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.35134D+00
0.25427	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.46630D+00
0.27662	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.59132D+00
0.29848	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.71362D+00
0.32169	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.84351D+00
0.35257	0.58550D-07	0.12294D-03	0.46886D+01	0.90599D+00	0.65640D-01	0.87530D+00	0.15280D-01	0.10162D+01

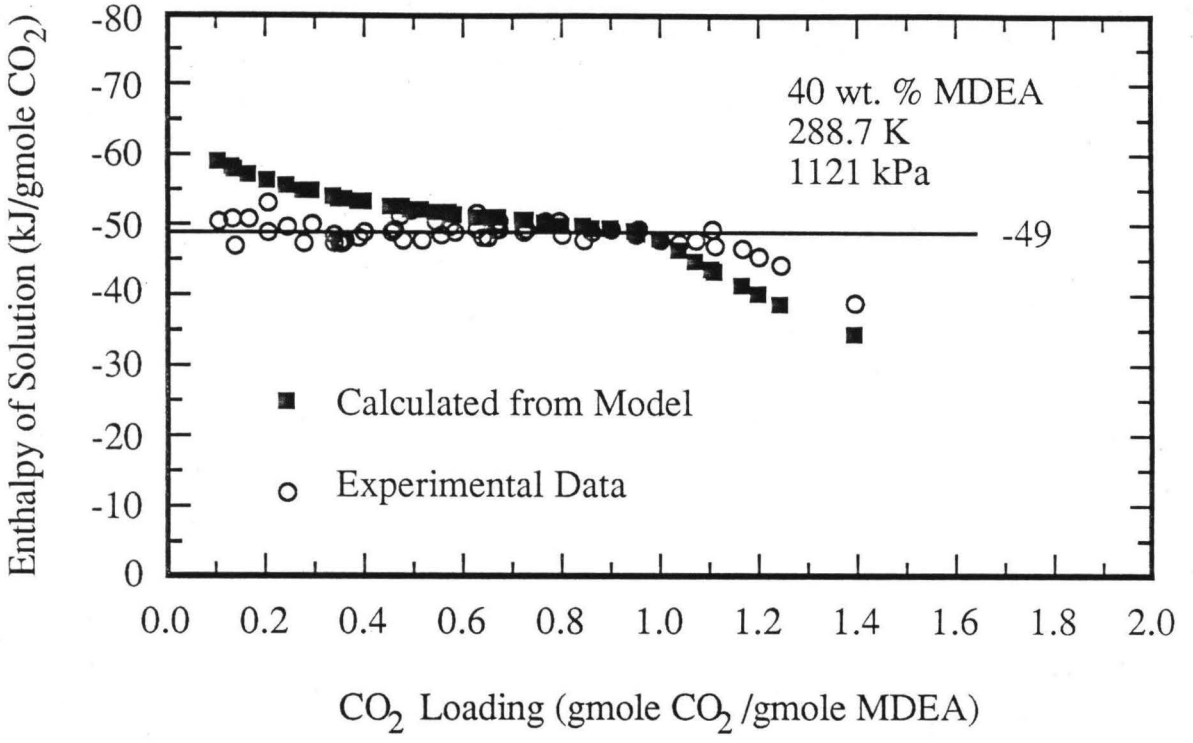
APPENDIX I

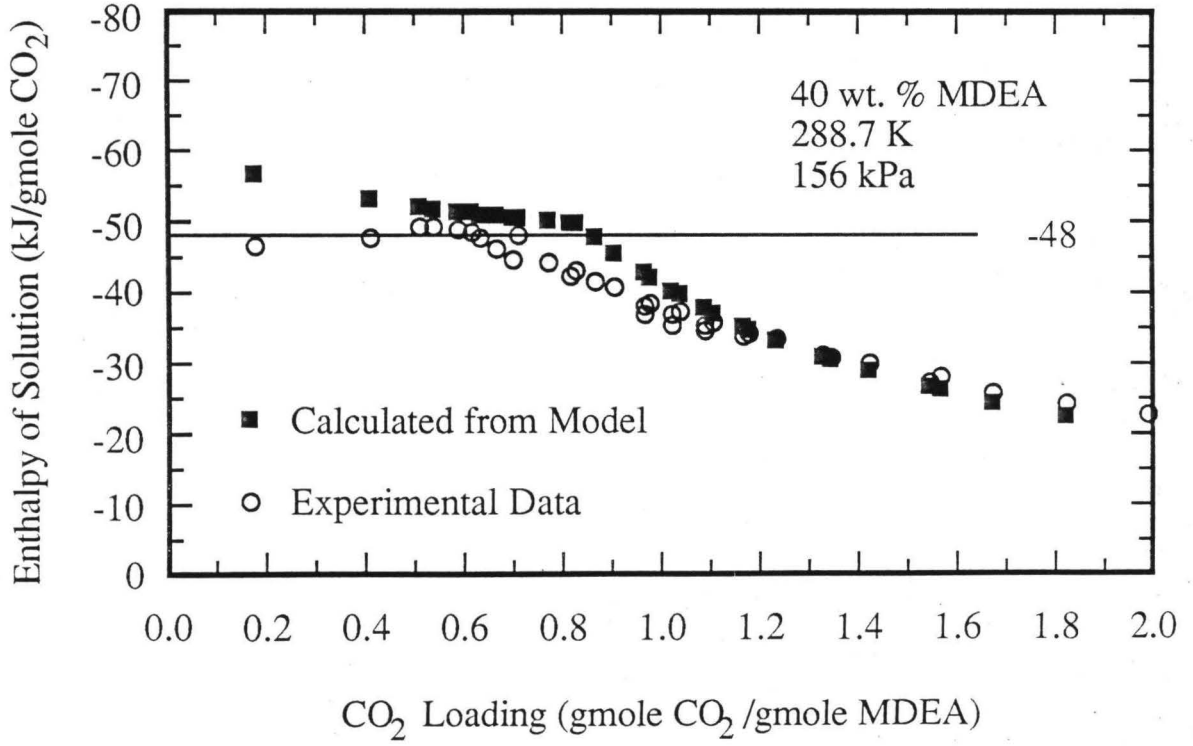
PLOTS OF EXPERIMENTAL DATA AND THE COMPUTER MODEL'S PREDICTIONS

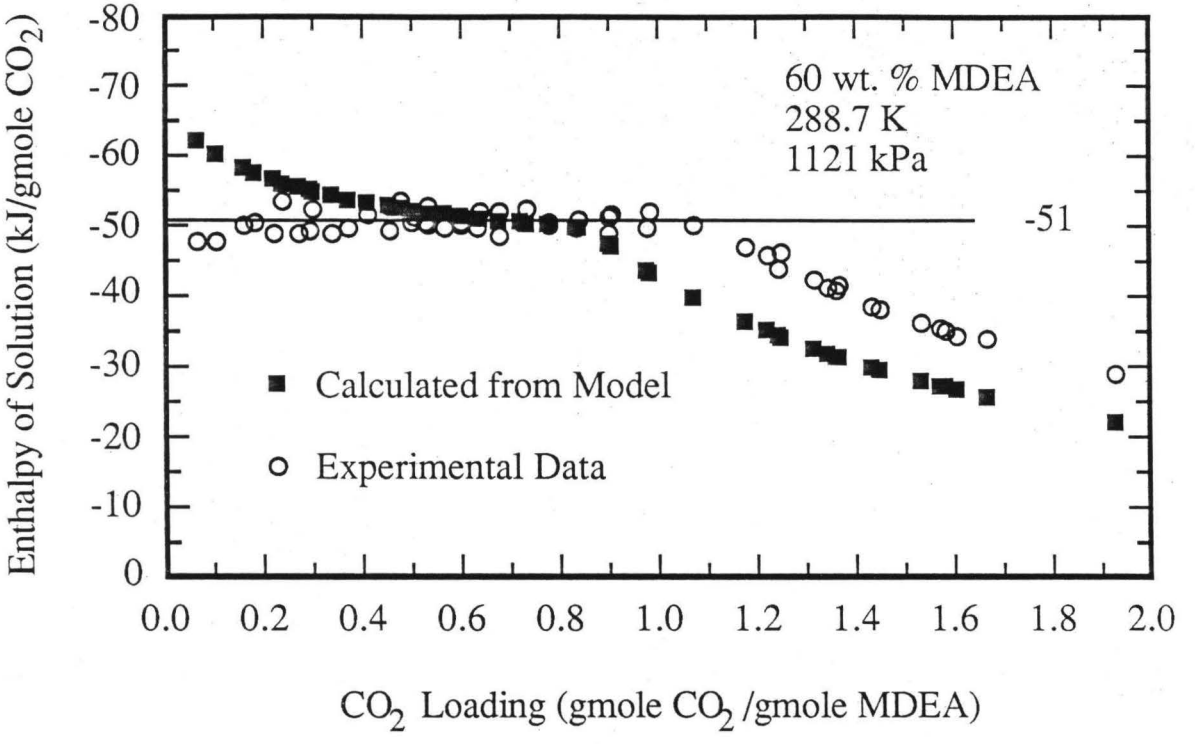
The first 15 plots are of the enthalpy of solution (kJ/gmole CO_2) as a function of acid gas loading for all systems other than those shown in the body of the thesis in figures 22 and 23. The remainder of the plots contain the same data as are in the first set of 15 plots but show the data as the enthalpy of solution (kJ/gmole MDEA) as a function of loading.

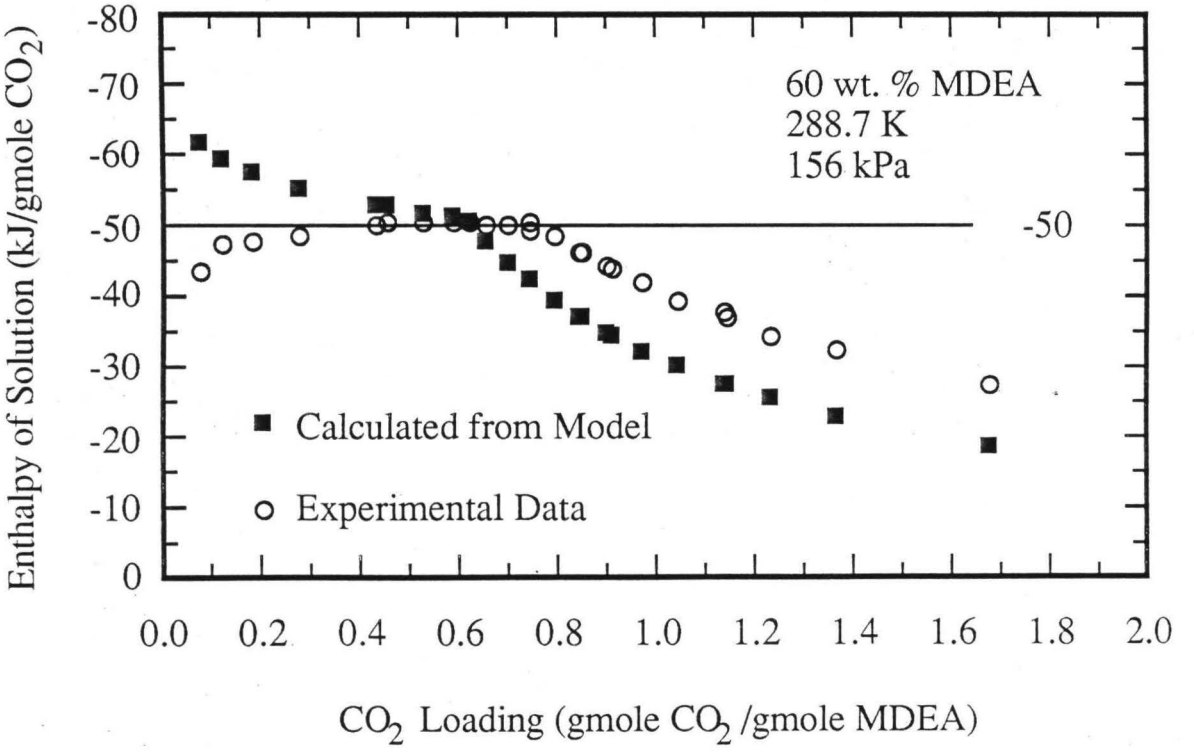

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
20 wt. % MDEA
288.7 K
1121 kPa
-47
Calculated from Model
Experimental Data
CO_2 Loading (gmole CO_2/gmole MDEA)

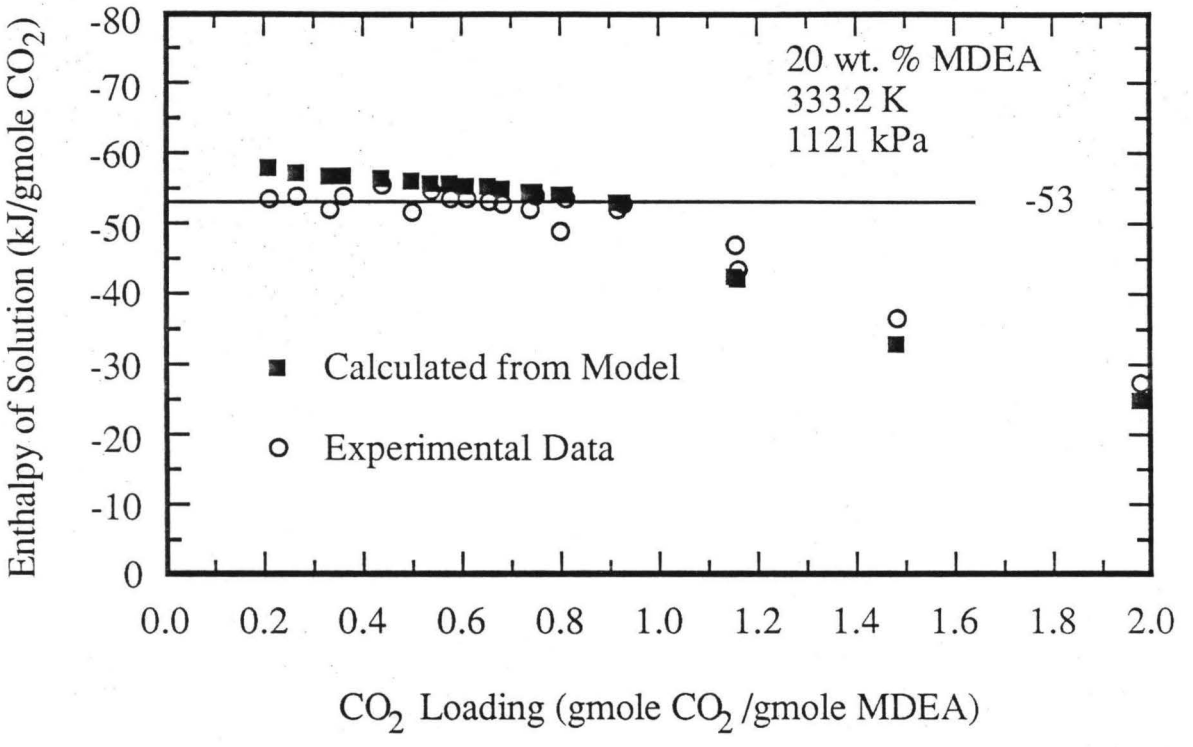

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
20 wt. % MDEA
288.7 K
156 kPa
-47
Calculated from Model
Experimental Data
CO_2 Loading (gmole CO_2/gmole MDEA)

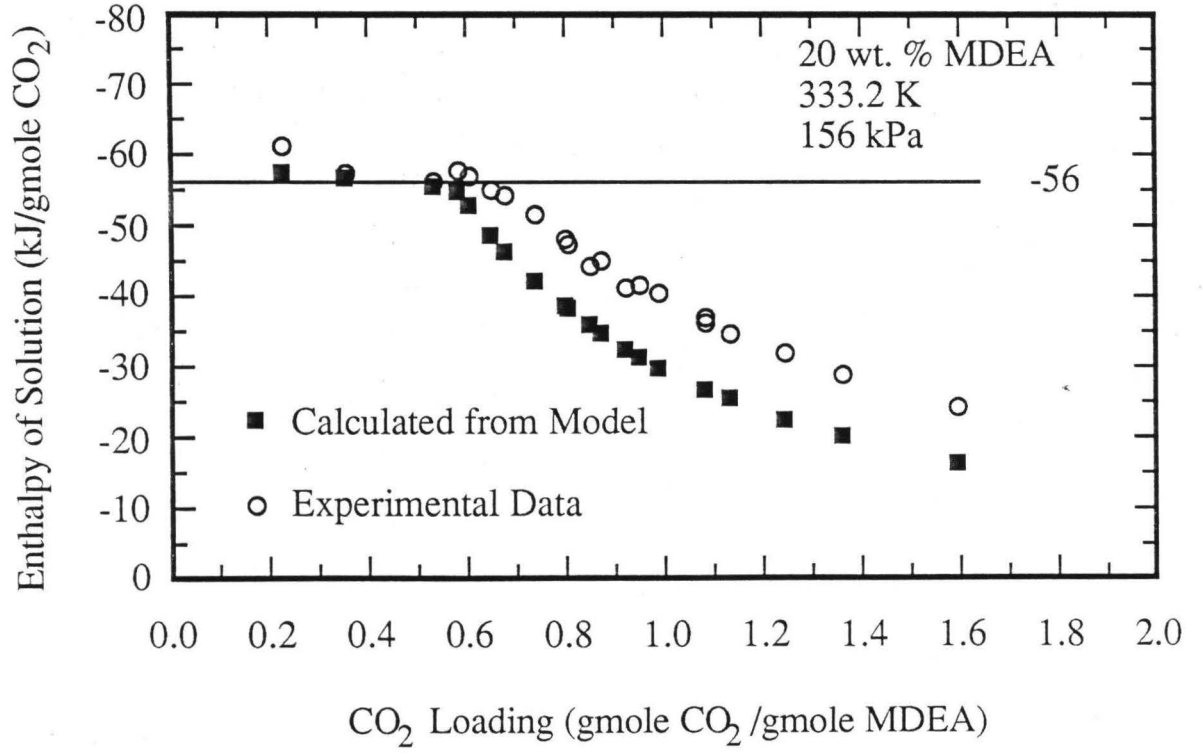

40 wt. % MDEA
288.7 K
1121 kPa
-49
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

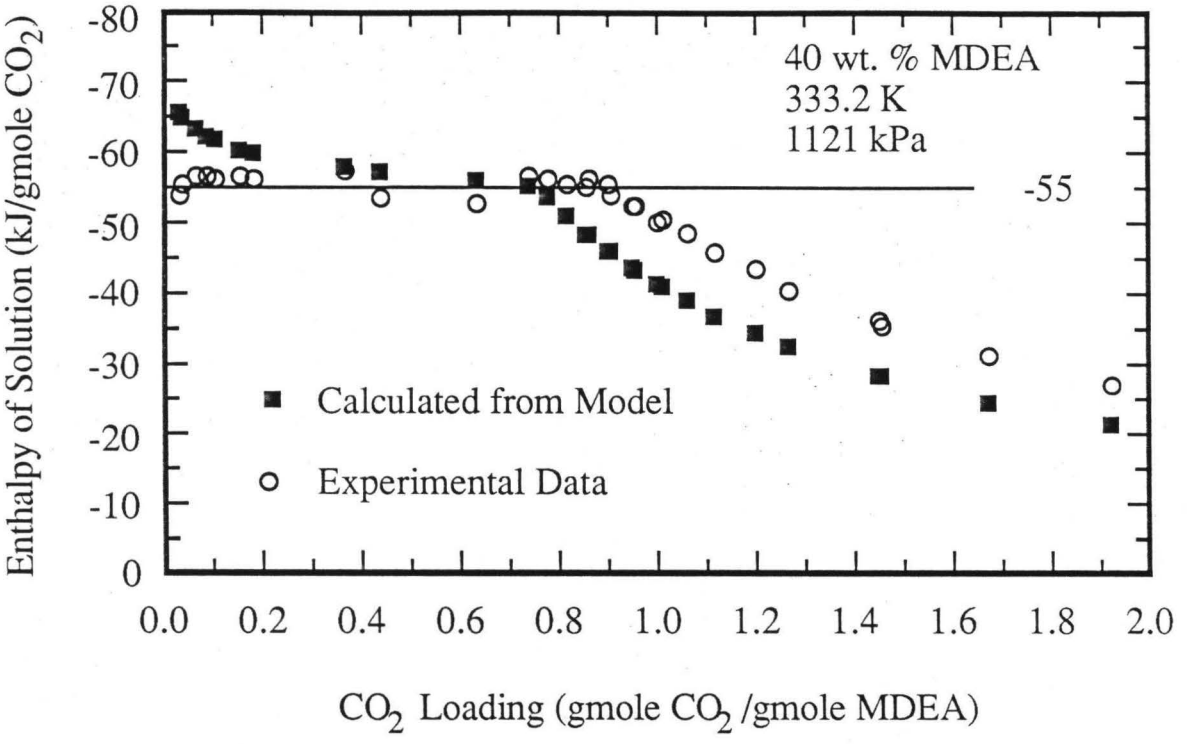

40 wt. % MDEA
288.7 K
156 kPa
-48
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

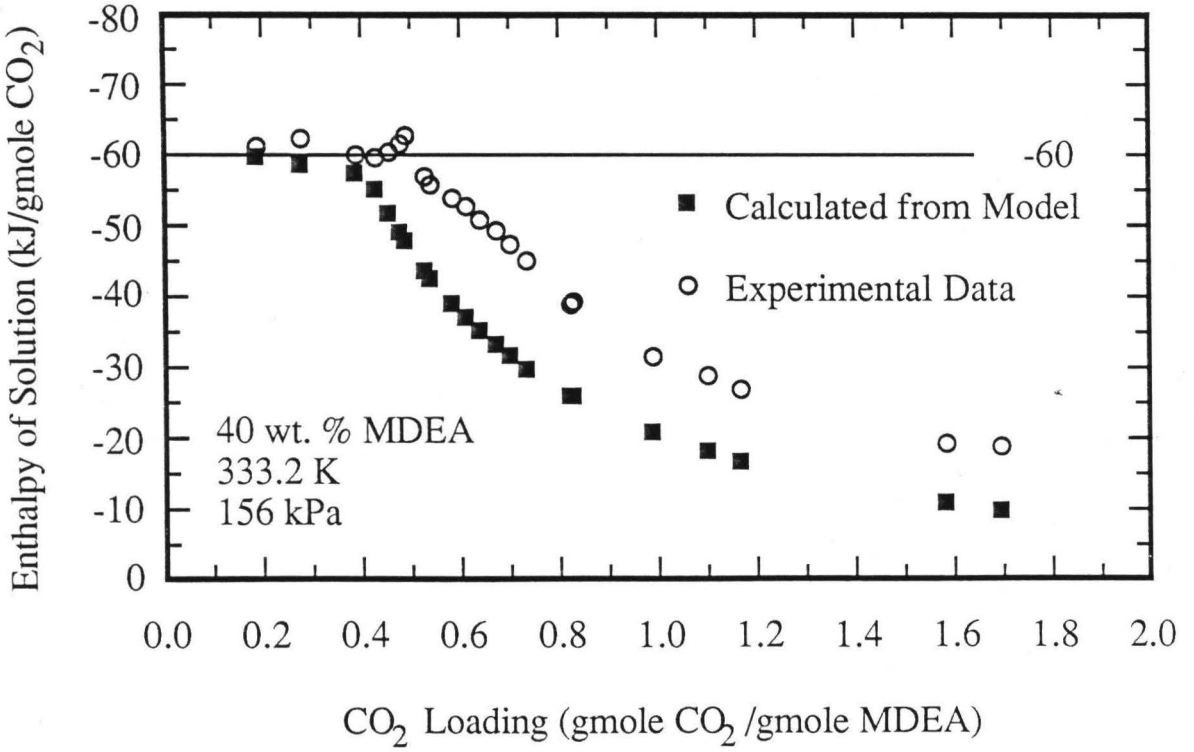

60 wt. % MDEA
288.7 K
1121 kPa
-51
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

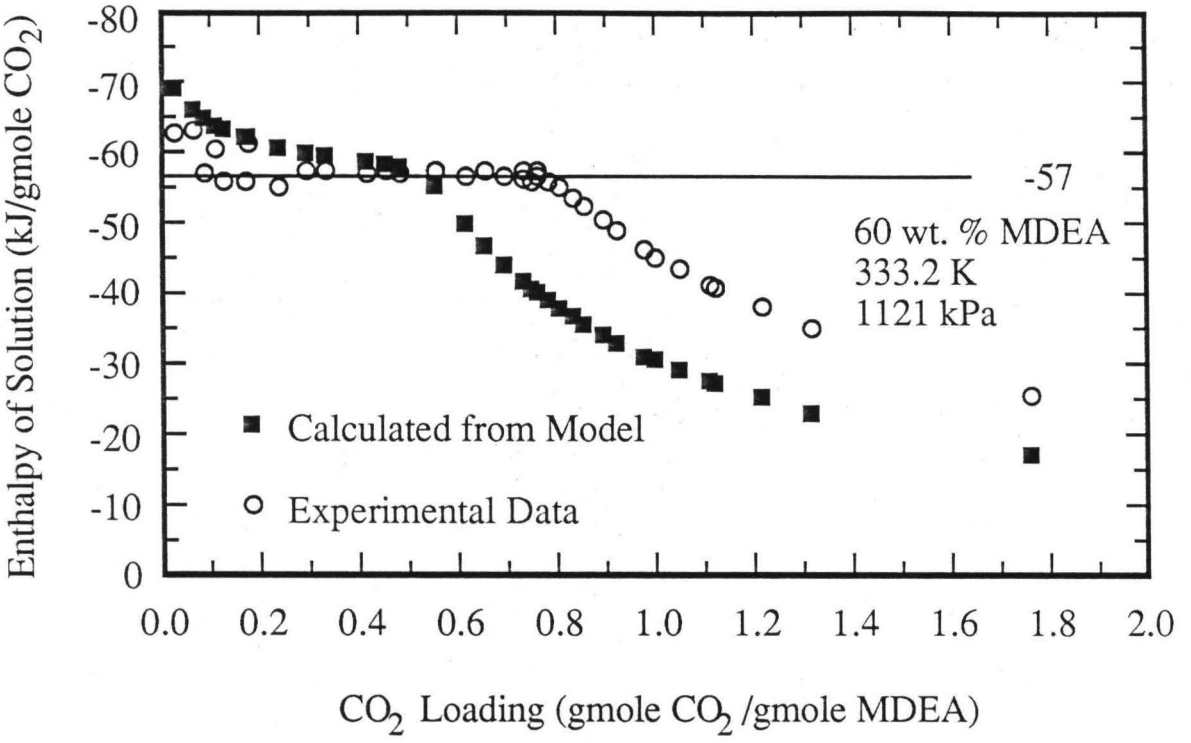

60 wt. % MDEA
288.7 K
156 kPa
-50
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0

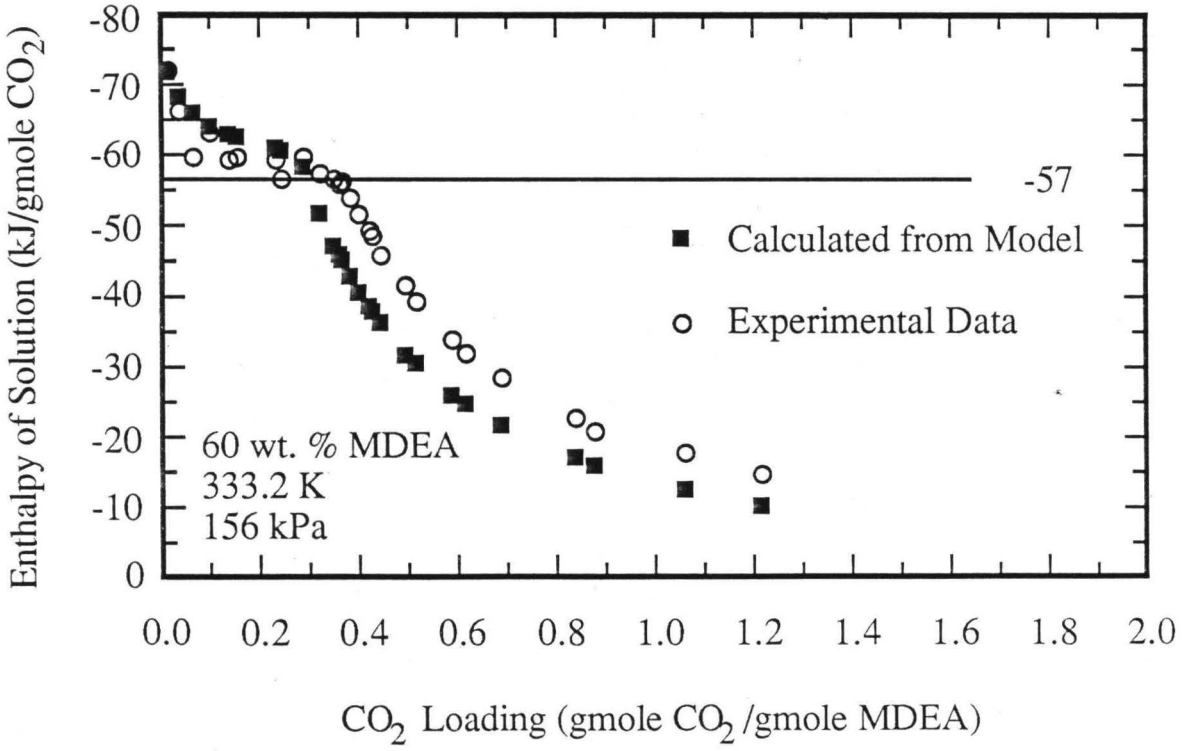

20 wt. % MDEA
333.2 K
1121 kPa
-53
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)

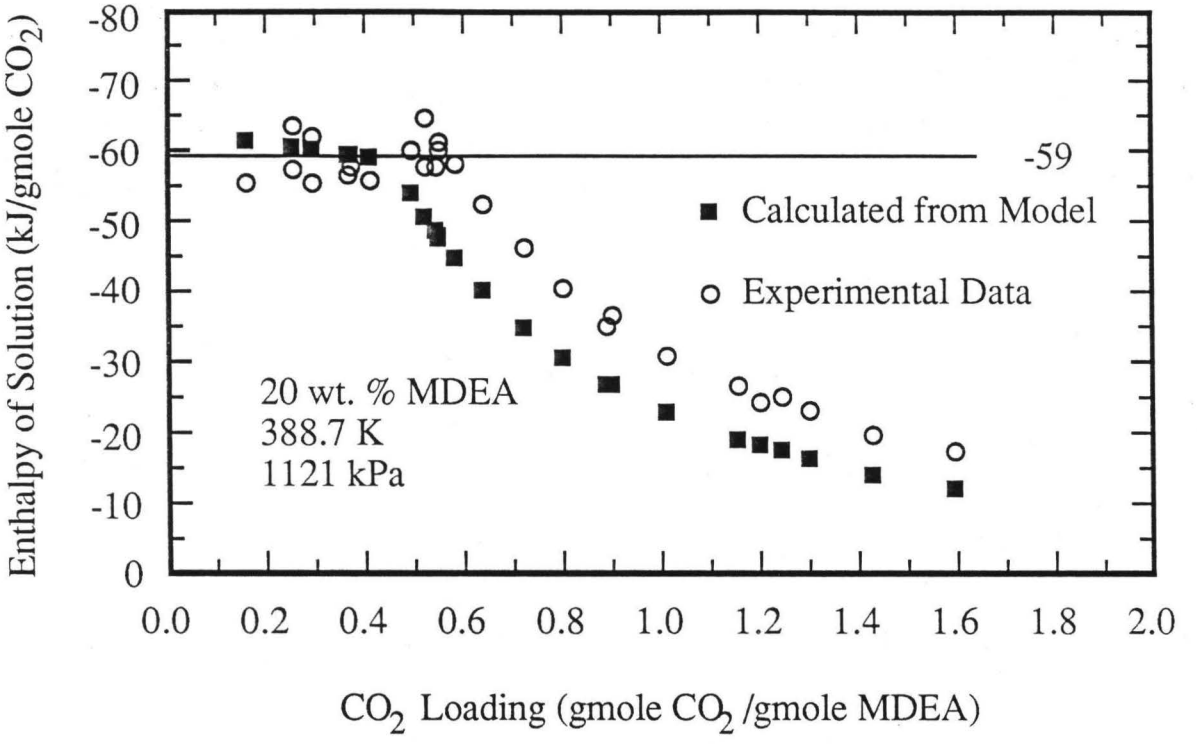

20 wt. % MDEA
333.2 K
156 kPa
-56
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO2)
CO2 Loading (gmole CO2 /gmole MDEA)

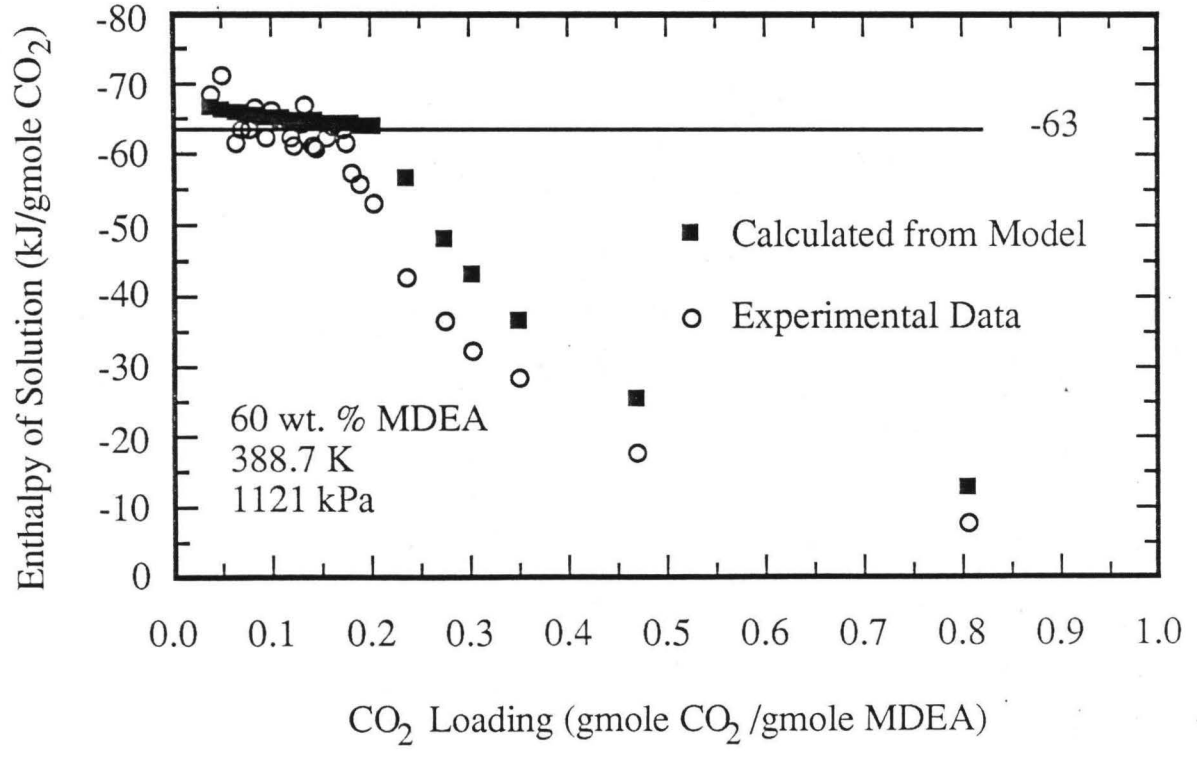

40 wt. % MDEA
333.2 K
1121 kPa
-55
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole CO_2)
CO_2 Loading (gmole CO_2 /gmole MDEA)

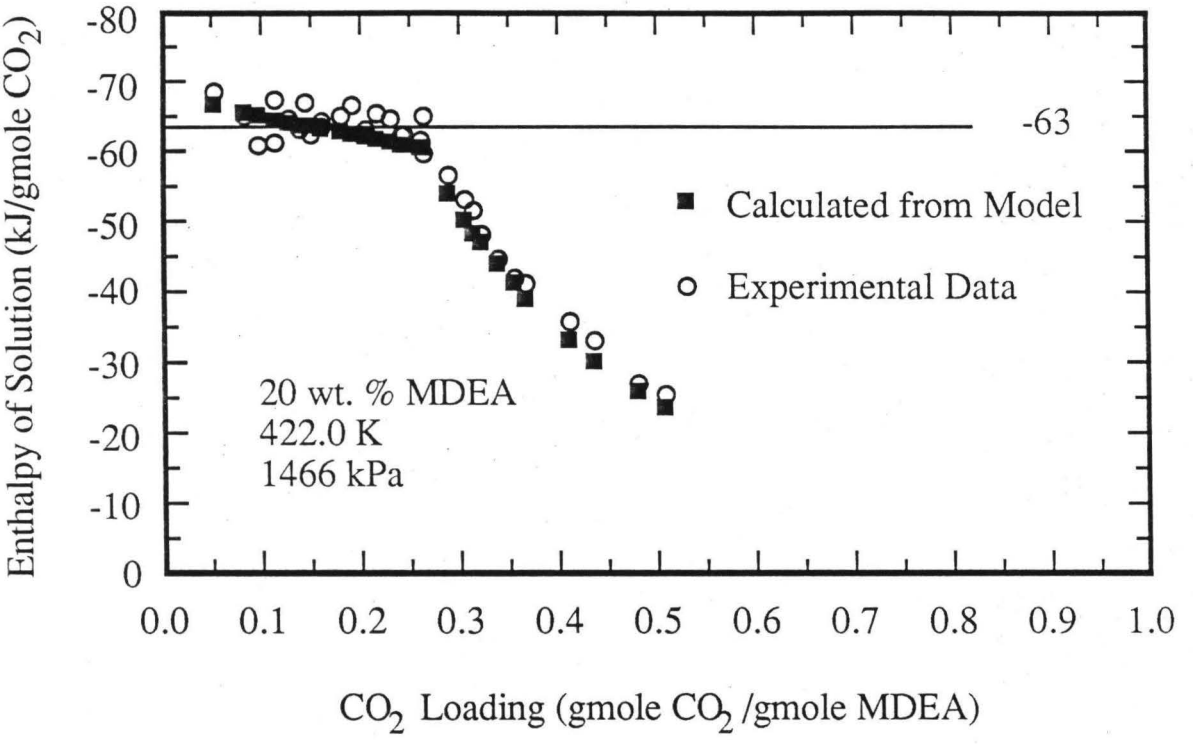

-60
Calculated from Model
Experimental Data
40 wt. % MDEA
333.2 K
156 kPa
Enthalpy of Solution (kJ/gmole CO_2)
CO_2 Loading (gmole CO_2 /gmole MDEA)

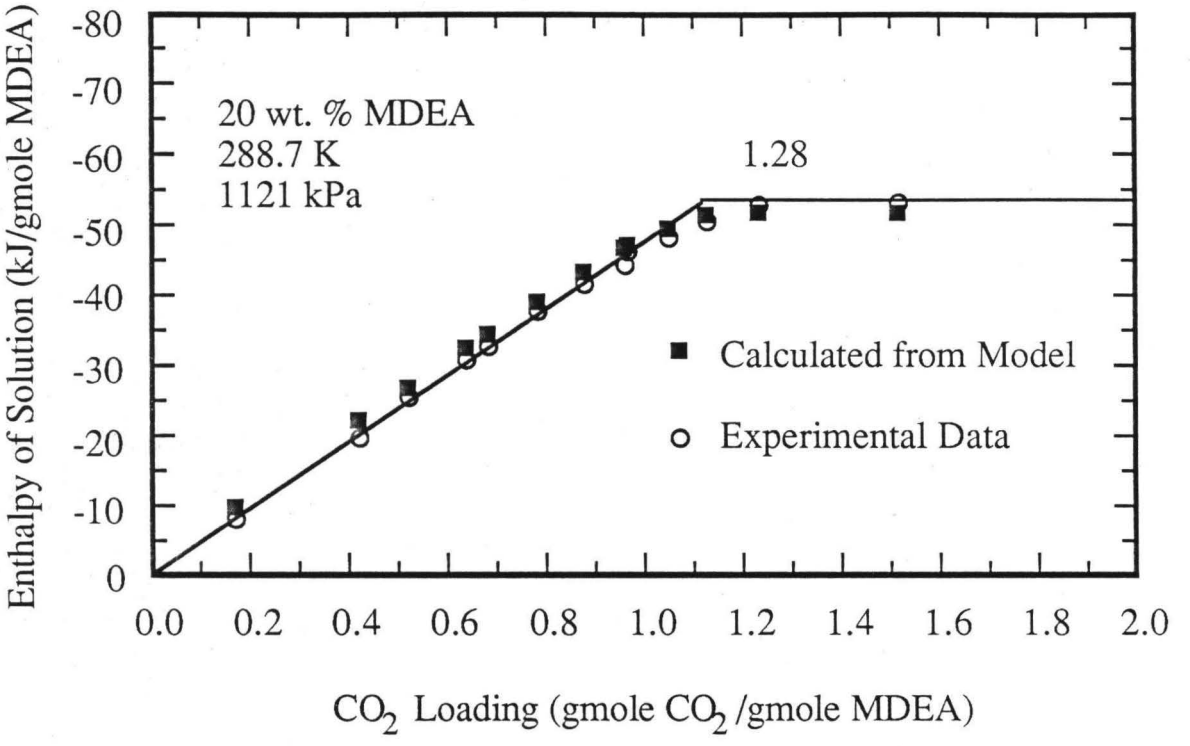

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-57
60 wt. % MDEA
333.2 K
1121 kPa
Calculated from Model
Experimental Data
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

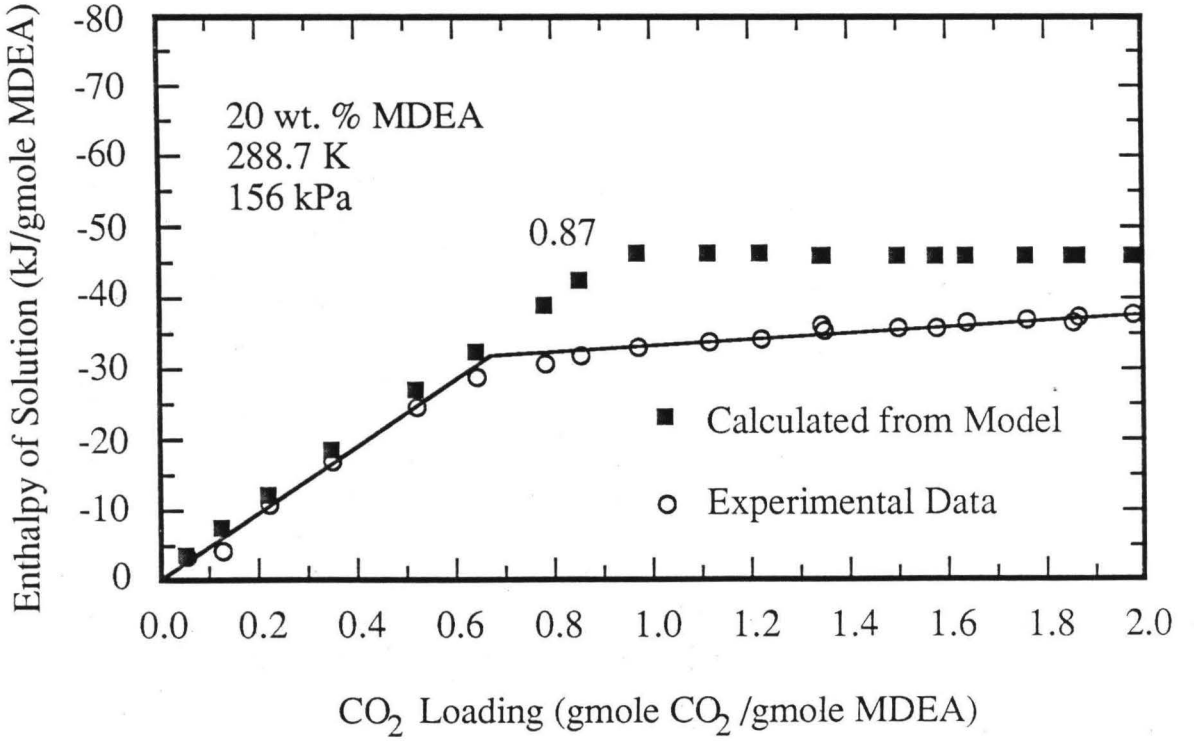

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
-57
Calculated from Model
Experimental Data
60 wt. % MDEA
333.2 K
156 kPa
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO_2 Loading (gmole CO_2 /gmole MDEA)

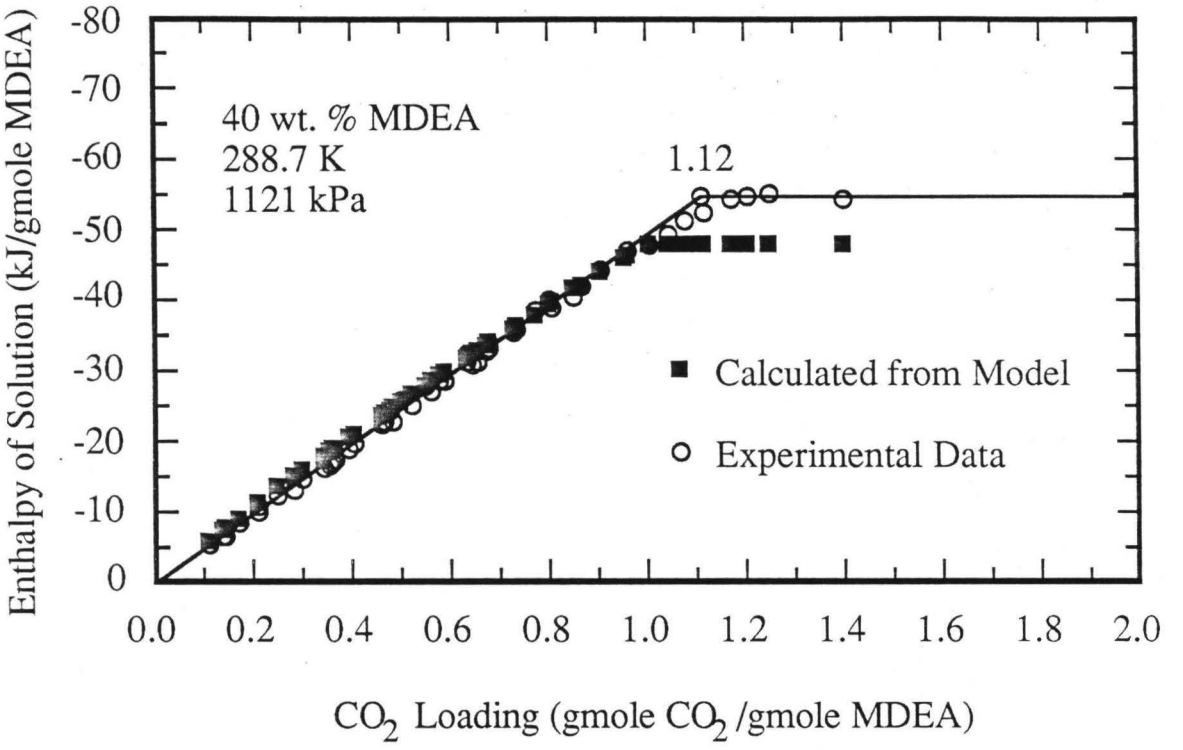

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
-59
Calculated from Model
Experimental Data
20 wt. % MDEA
388.7 K
1121 kPa
CO_2 Loading (gmole CO_2 /gmole MDEA)

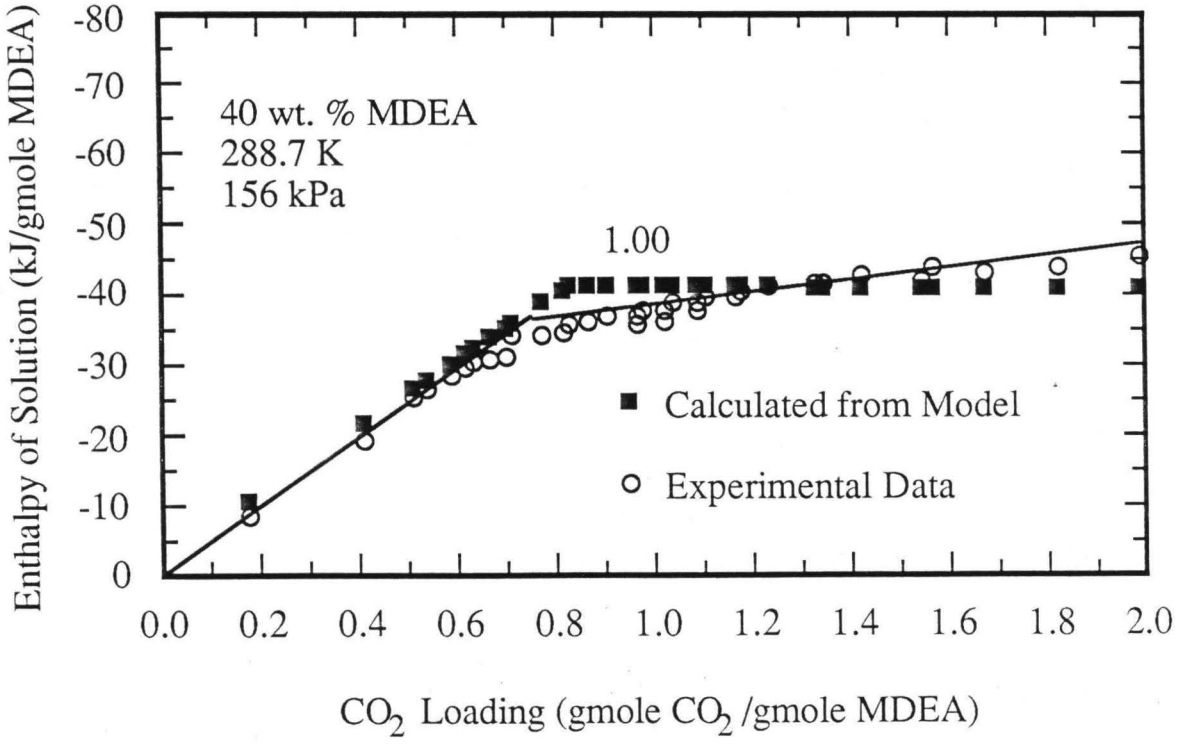

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
-63
Calculated from Model
Experimental Data
60 wt. % MDEA
388.7 K
1121 kPa
CO_2 Loading (gmole CO_2 /gmole MDEA)

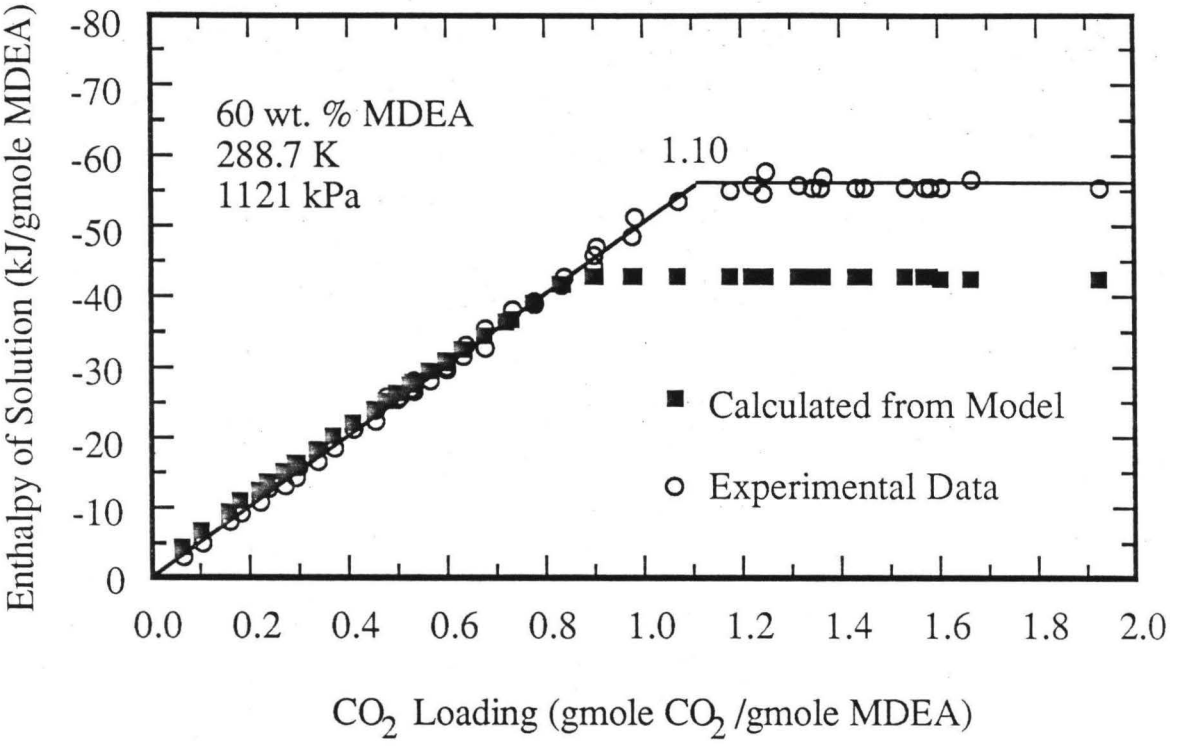

Enthalpy of Solution (kJ/gmole CO_2)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
CO_2 Loading (gmole CO_2 /gmole MDEA)
-63
Calculated from Model
Experimental Data
20 wt. % MDEA
422.0 K
1466 kPa

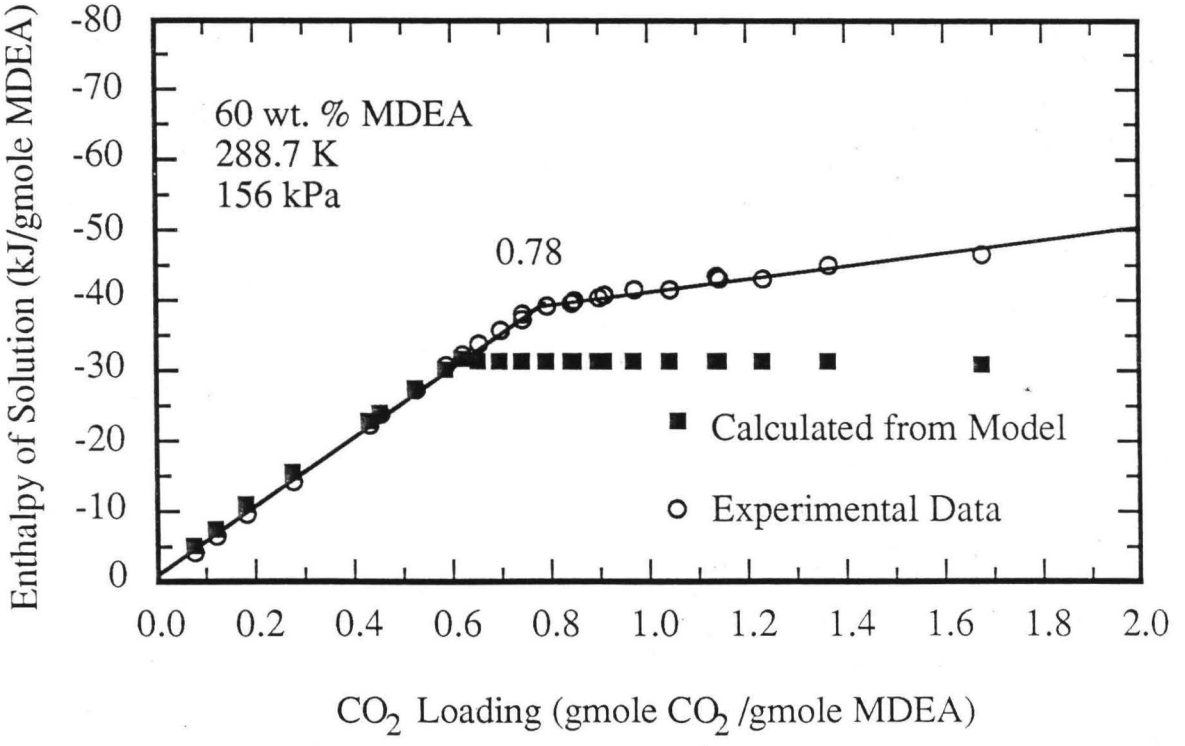

20 wt. % MDEA
288.7 K
1121 kPa
1.28
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

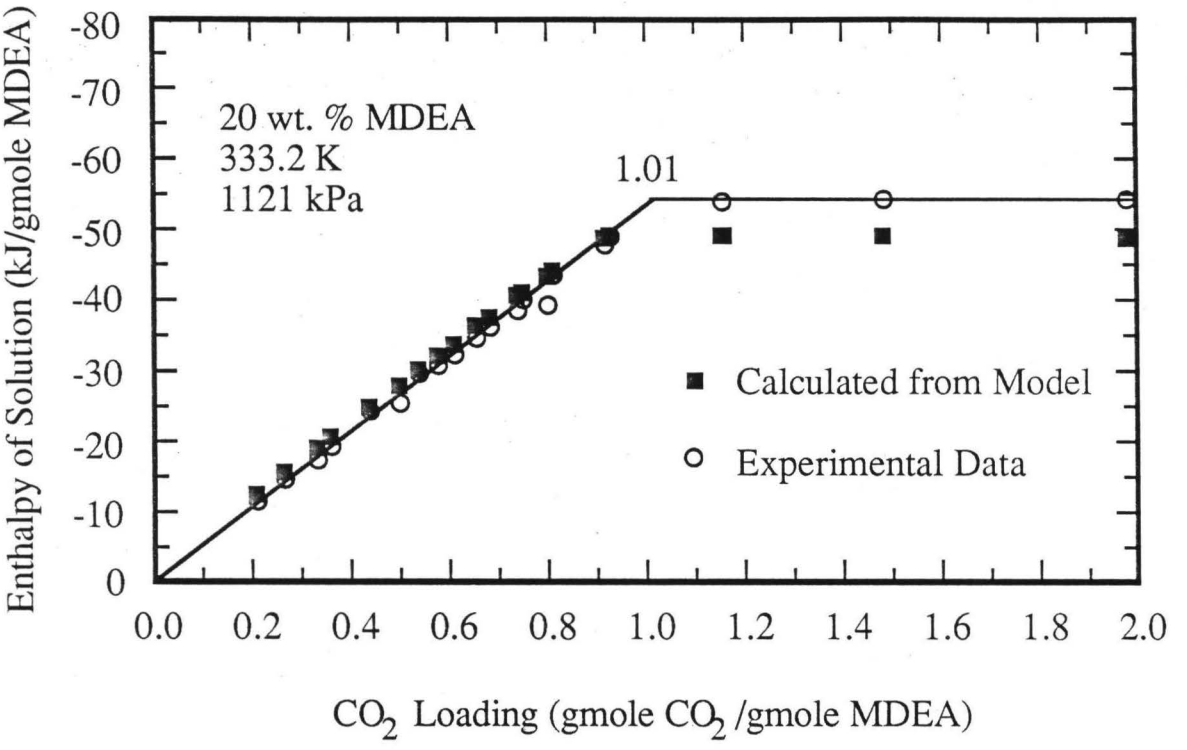

20 wt. % MDEA
288.7 K
156 kPa
0.87
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

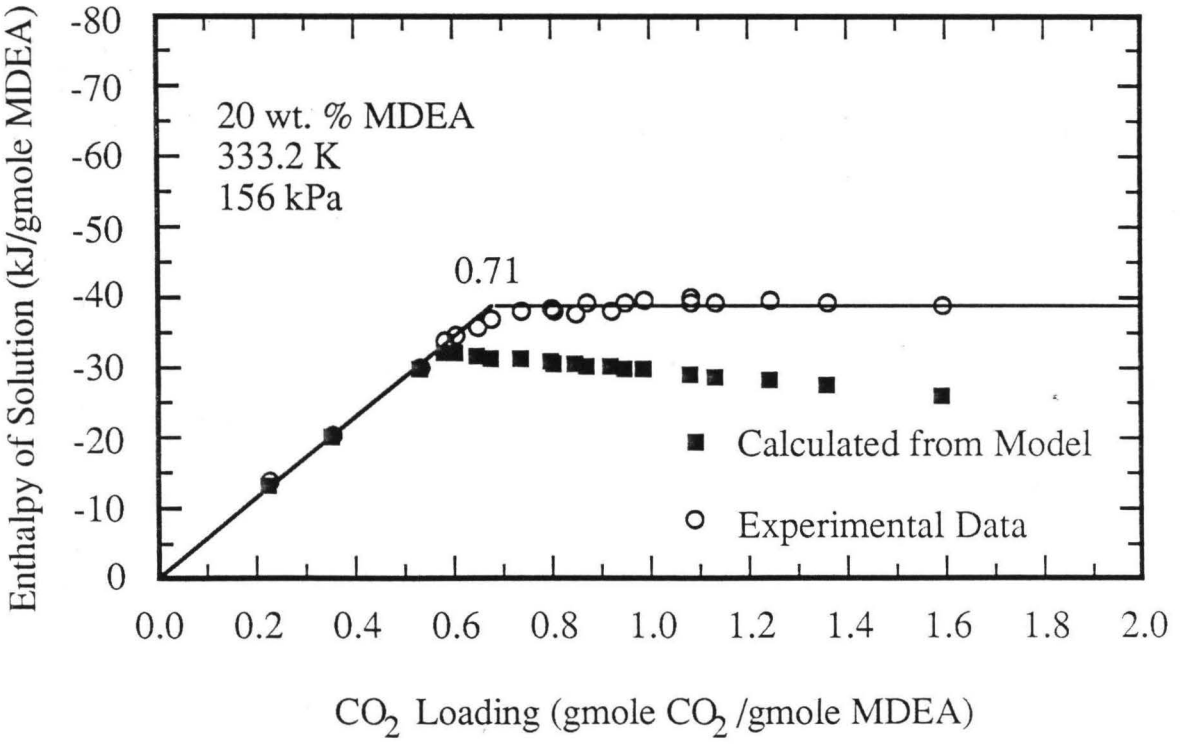

40 wt. % MDEA
288.7 K
1121 kPa
1.12
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

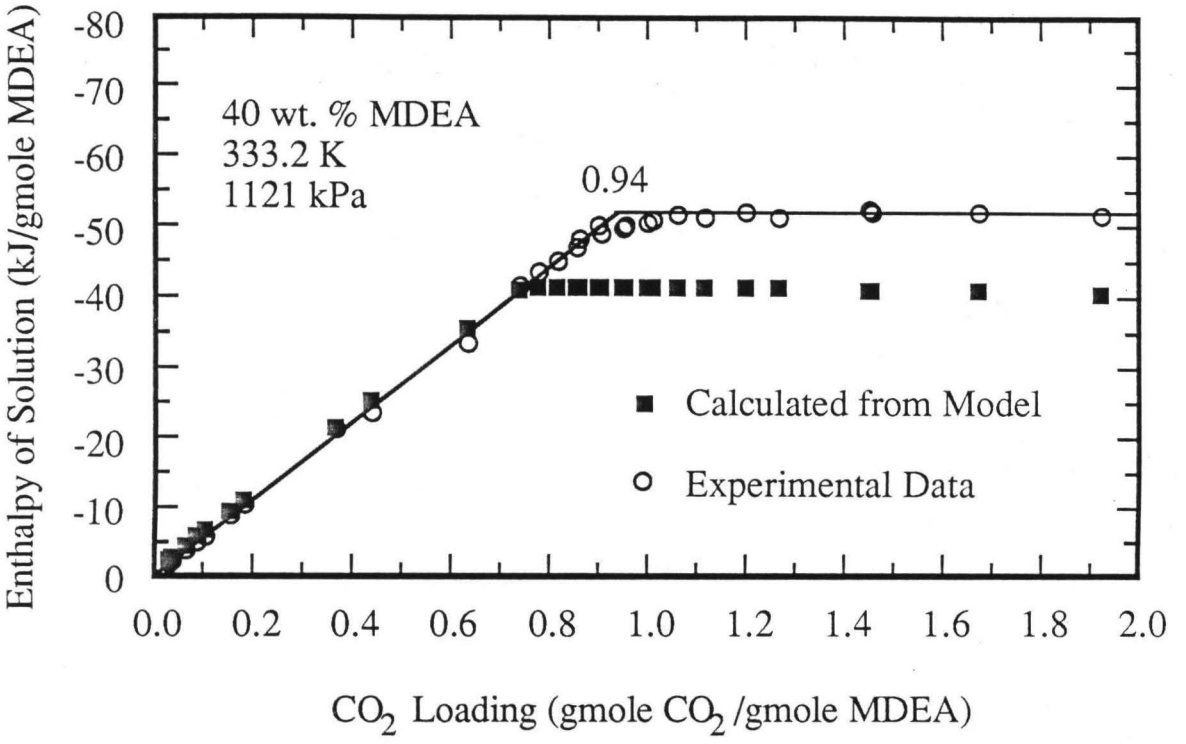

40 wt. % MDEA
288.7 K
156 kPa
1.00
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

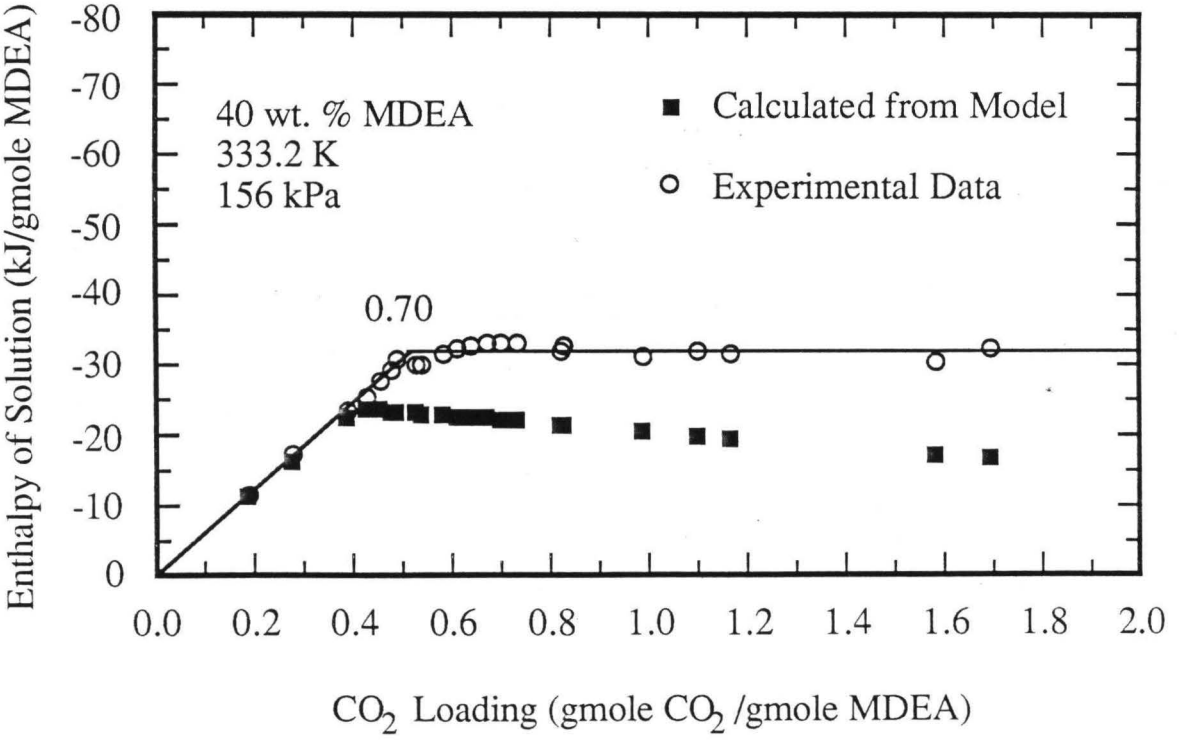

60 wt. % MDEA
288.7 K
1121 kPa
1.10
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

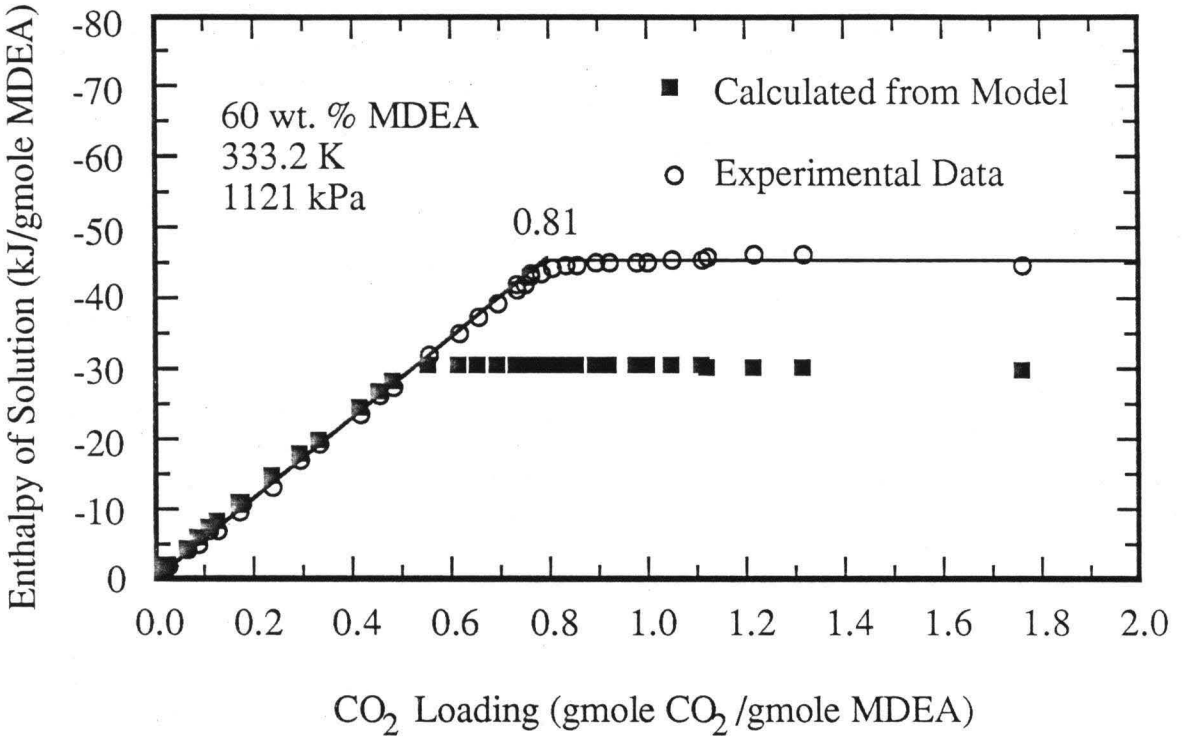

60 wt. % MDEA
288.7 K
156 kPa
0.78
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

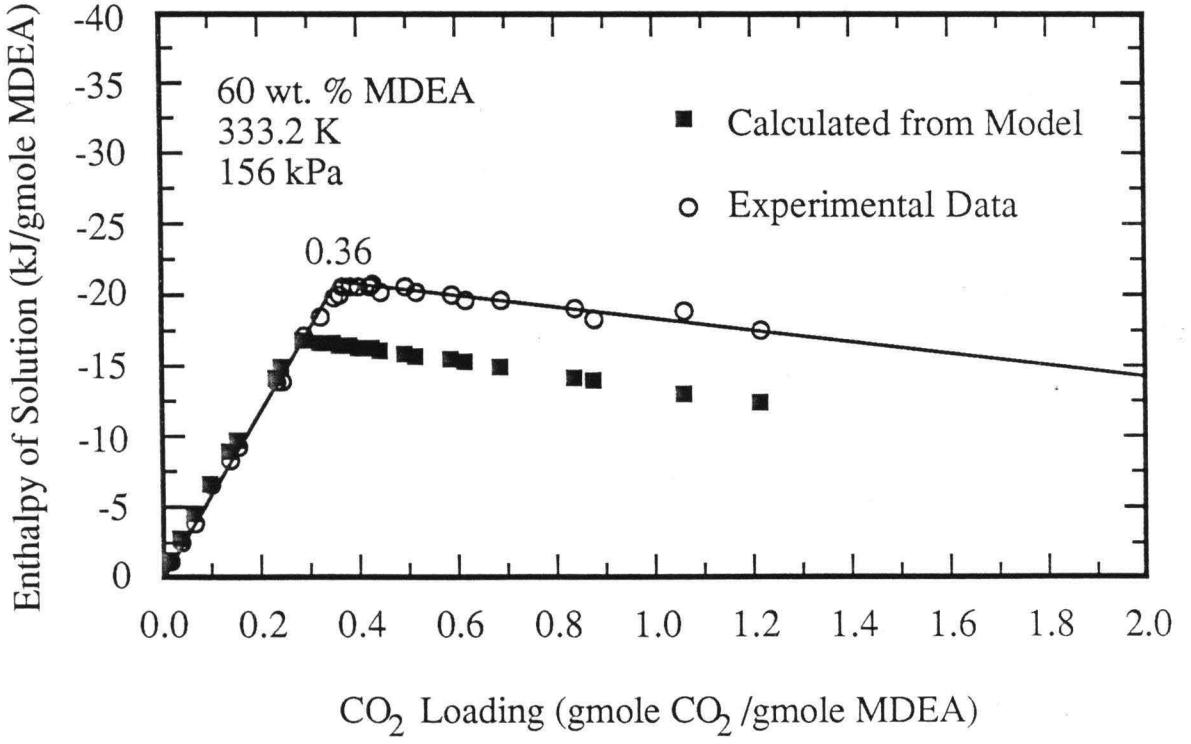

20 wt. % MDEA
333.2 K
1121 kPa
1.01
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

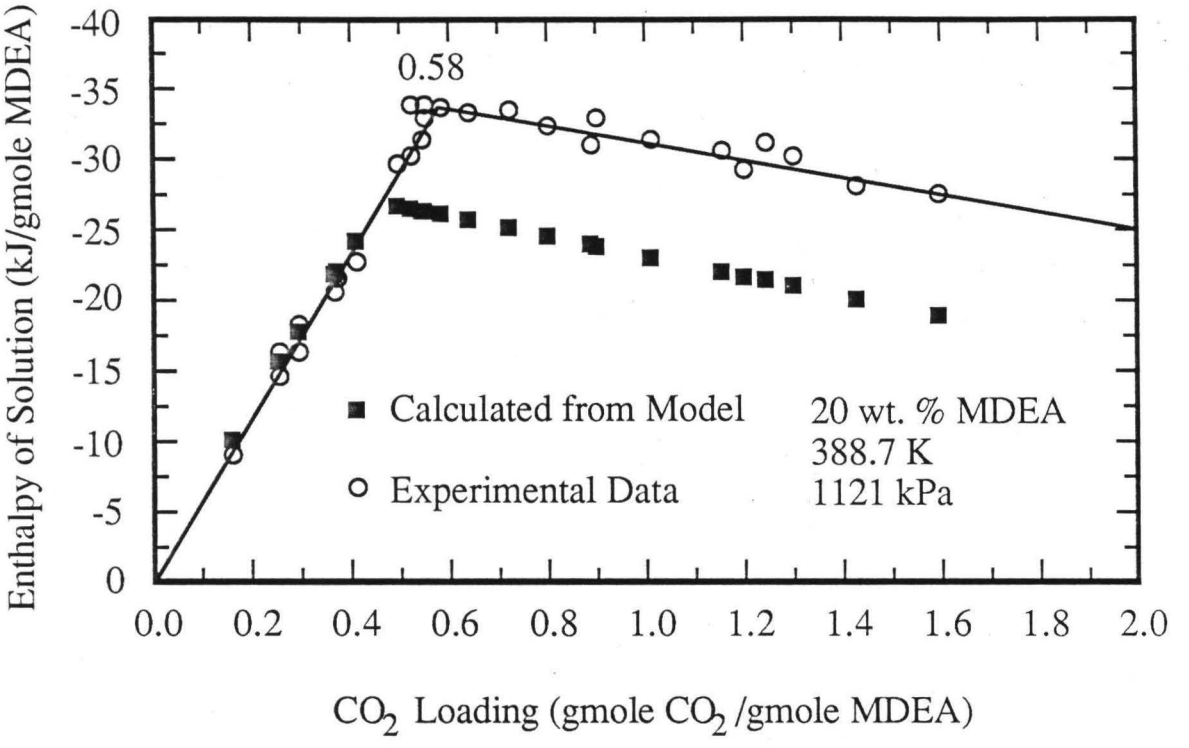

20 wt. % MDEA
333.2 K
156 kPa
0.71
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

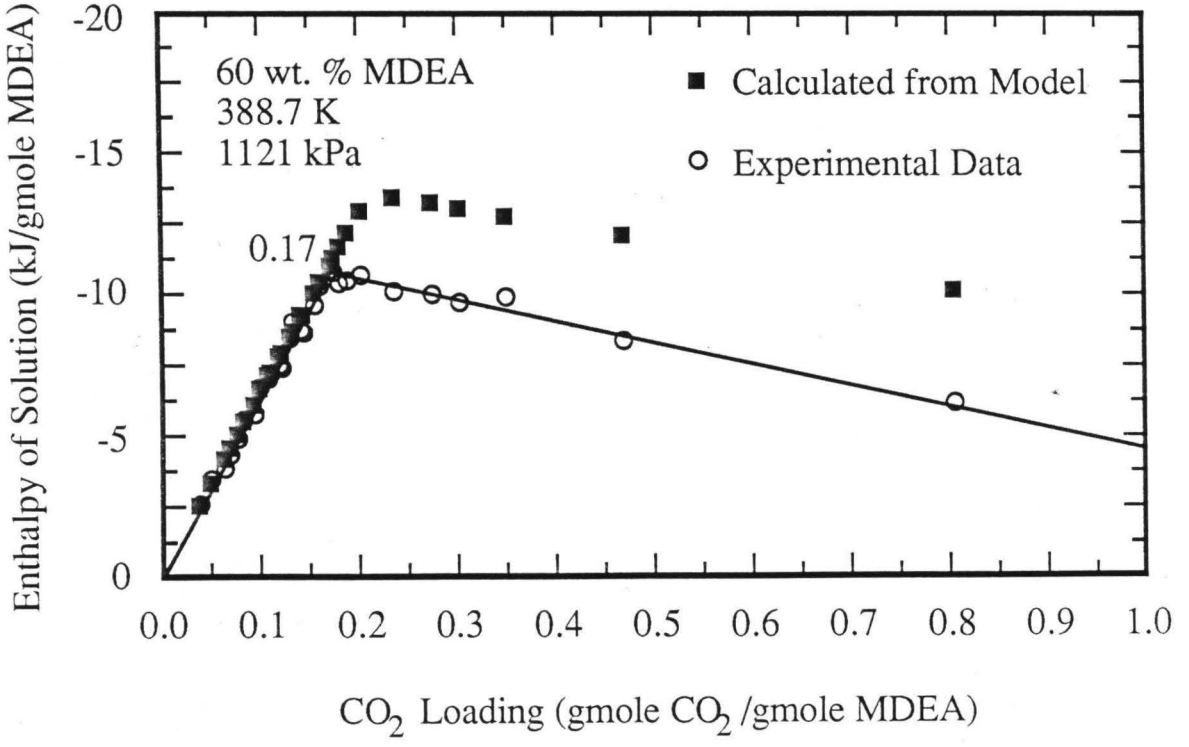

40 wt. % MDEA
333.2 K
1121 kPa
0.94
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)

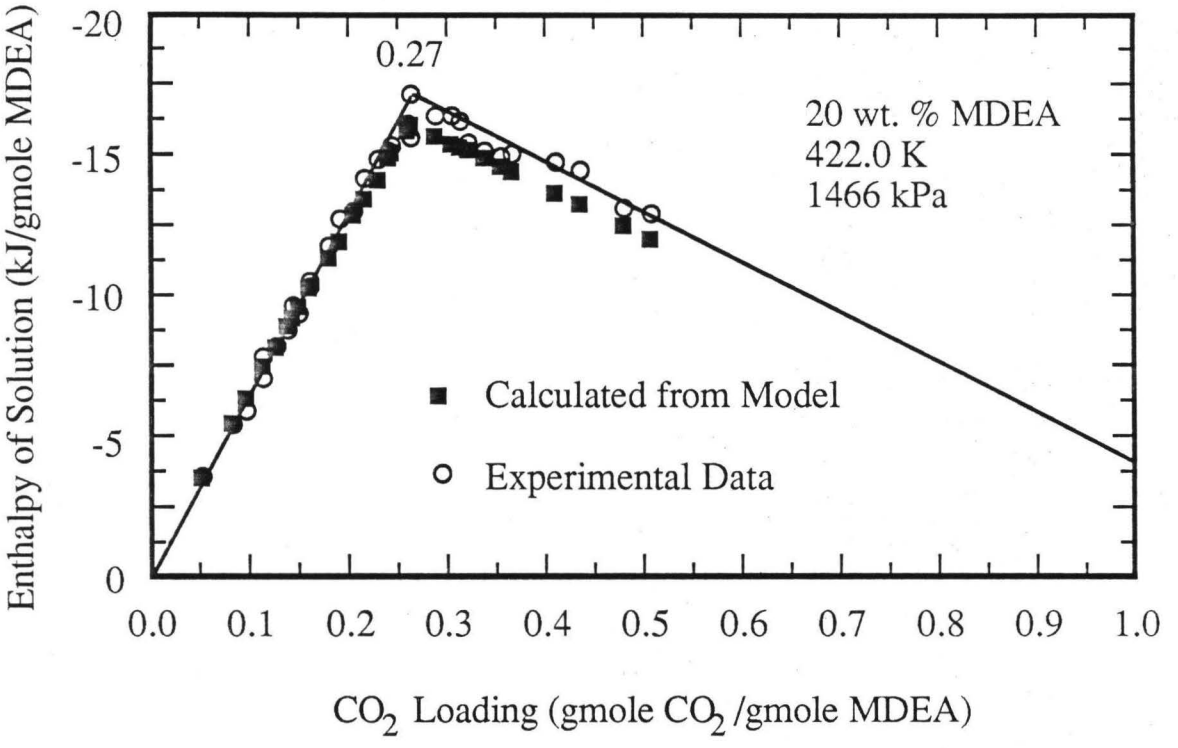

40 wt. % MDEA
333.2 K
156 kPa
0.70
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


60 wt. % MDEA
333.2 K
1121 kPa
0.81
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-80
-70
-60
-50
-40
-30
-20
-10
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


60 wt. % MDEA
333.2 K
156 kPa
0.36
Calculated from Model
Experimental Data
Enthalpy of Solution (kJ/gmole MDEA)
-40
-35
-30
-25
-20
-15
-10
-5
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


Enthalpy of Solution (kJ/gmole MDEA)
-40
-35
-30
-25
-20
-15
-10
-5
0
0.58
Calculated from Model
Experimental Data
20 wt. % MDEA
388.7 K
1121 kPa
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
CO2 Loading (gmole CO2 /gmole MDEA)


Enthalpy of Solution (kJ/gmole MDEA)
-20
-15
-10
-5
0
60 wt. % MDEA
388.7 K
1121 kPa
Calculated from Model
Experimental Data
0.17
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
CO2 Loading (gmole CO2 /gmole MDEA)


-20
-15
-10
-5
0
0.27
20 wt. % MDEA
422.0 K
1466 kPa
Calculated from Model
Experimental Data
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Enthalpy of Solution (kJ/gmole MDEA)
CO2 Loading (gmole CO2 /gmole MDEA)