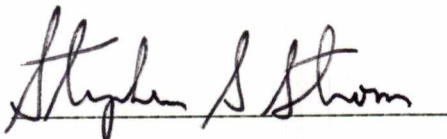


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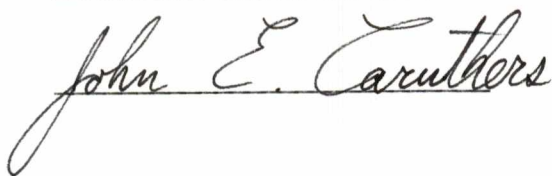
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L. Crawford, Major Professor

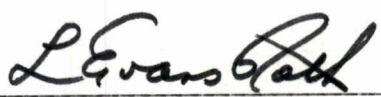
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PACKED TOWER DESIGN FOR CARBON DIOXIDE ABSORPTION
INTO POTASSIUM CARBONATE SOLUTIONS

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Michèle Gay Macaraeg

August 1980

3044815

To My Parents,
Lyn and Roger

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ABSTRACT

Much experimental work has been conducted through the years concerning carbon dioxide (CO_2) absorption into various media. Removing CO_2 from synthesis gases is desirable since it can act as an unwanted diluent or as a catalyst poison. The following study involved an in depth analysis of experimental data collected by the U.S. Bureau of Mines (USBM) for CO_2 removal from a hot potassium carbonate (K_2CO_3) solution. Mass transfer theory coupled with statistical techniques resulted in an empirically substantiated equation for calculating the height of a tower necessary to accomplish a given CO_2 absorption into a K_2CO_3 solution. Utilization of these results were incorporated into a computer program applicable to a range of conditions commonly used in industrial operations.

PREFACE

In the pages which follow the application of mass transfer principles and data analysis will be utilized in developing an expression for tower height. Chapter III is a summary of the theoretical background used in the study. This chapter will develop a material balance expressing mass transfer through an absorption tower, followed by the development of a suitable rate expression for CO_2 absorption into a K_2CO_3 solution. Chapter IV discusses the methodology utilized in the mass transfer data analysis for determining the equilibrium relationship between temperature, partial pressure of CO_2 , and chemical composition of the liquid, and for expressing the mass transfer coefficient as a function of experimental variables. Discussion of results and application in the form of a computer program for calculating tower height will follow. The closing chapter will contain recommendations for further study.

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LIST OF SYMBOLS

C_0	Equivalent concentration of K_2CO_3 (moles/liter)
f	Fraction conversion of K_2CO_3 to $KHCO_3$
f^*	Equilibrium value of f
G	Gas velocity (moles/hr·ft ²)
K or % K_2CO_3	Percent equivalent weight of K_2CO_3
K_E	Equilibrium constant
k_g	Individual gas phase mass transfer coefficient
K_{Ga}	Overall mass transfer coefficient based on gas phase
k_l	Individual liquid phase mass transfer coefficient
K_{La}	Overall mass transfer coefficient based on liquid phase
K_0	Overall mass transfer coefficient defined by equation (10)
L	Liquid velocity (lb/hr·ft ²)
M_{CO_2}	Molecular weight of CO_2
P_{CO_2}	Partial pressure of CO_2 (psi)
W_0	Equivalent concentration of H_2O (moles/liter)
x	Liquid weight ratio of CO_2
x_1	Inlet CO_2 liquid weight ratio
x_2	Exiting CO_2 liquid weight ratio
x_{LB}	CO_2 liquid weight ratio in the bulk solution
x_{Li}	CO_2 liquid weight ratio at an interface
x^+	Mass of CO_2 absorbed at complete conversion of K_2CO_3 to $KHCO_3$, per unit mass of original, unreacted solution.
x^*	Equilibrium value of x
y	Gas mole ratio of CO_2

y_1	Exiting CO ₂ gas mole ratio
y_2	Inlet CO ₂ gas mole ratio
y_{GB}	CO ₂ gas mole ratio in the bulk gas phase
y_{Gi}	CO ₂ gas mole ratio at an interface
y^*	Equilibrium value of y
z	Height (ft)
	Density (gm/ml)

VARIABLES USED IN COMPUTER PROGRAM TO CALCULATE HEIGHT

Input:

QL	Liquid rate (lb/(hr·ft ²))
TT	Temperature at the top of the column (degrees F)
TB	Temperature at the column's bottom (degrees F)
VF	CO ₂ in (volume percent of total gas stream)
VS	CO ₂ out (volume percent of total gas stream)
G	Gas rate (moles/(hr·ft ²))
PK	Weight percent equivalent K ₂ CO ₃
FR	KHCO ₃ in (fraction KHCO ₃ in K ₂ CO ₃ solution)
FS	KHCO ₃ out (fraction KHCO ₃ in K ₂ CO ₃ solution)
P	System pressure (psi)
QLL	Liquid rate (gal/hr)
GG	gas rate (scf/hr)

Output:

OUT (1) = QL	
OUT (2) = TT	(degrees K)
OUT (3) = TB	(degrees K)

CHAPTER I

INTRODUCTION

Over the past few decades, the rapid growth in energy demands has necessitated increasing emphasis on energy resource conservation, utilization of new energy sources, and efforts to improve the efficiency of energy systems. Scientists and engineers have consequently directed their attention towards energy conversion systems which meet increasingly stringent demands for preservation of the environment.

Production and utilization of electrical energy has received much attention since electricity permits a broad range of functions to be performed conveniently in many areas of industry as well as in small scale applications. Until recently, electrical generating systems could reach only forty percent thermal efficiency. Detailed analysis has established that the coal-fired magnetohydrodynamics (MHD) process has the potential to increase the overall thermal efficiency to between fifty and sixty percent. MHD deals with the flow of an electrically conducting fluid in the presence of a magnetic field. In the MHD generator, the gas itself is a conductor which by expansion through a nozzle moves itself. The moving, electrically conductive fluid in an MHD generator accomplishes the same result as the copper armature in a conventional generator. The motion of a conductor through a magnetic field gives rise to an electromotive force and a flow of current. In order to impart the desired degree of electrical conductivity to the hot MHD working fluid, a readily ionizable seeding compound (e.g., an alkali salt) is necessary in the high temperature combustion products flowing through the MHD channel.

In terms of production levels, availability, and ionization potential, potassium salts are the most favored choice as seed. Experimental evidence, obtained from testing performed at The University of Tennessee Space Institute, has shown that utilizing potassium carbonate (K_2CO_3) as seed significantly lowers sulfur dioxide (SO_2) emissions since the potassium combines with the sulfur in the coal to form potassium sulfate (K_2SO_4).

The problem of maximum seed recovery and regeneration in the MHD process is a very important aspect in the design of an MHD plant. Its solution is necessitated by environmental as well as economic considerations. High seed cost merits its recovery, and following recovery, the potassium compound must be regenerated to a form capable of combining with sulfur.

Two processes commercially available for use in the pulp and paper industry are the Tomlinson (recovery boiler) Process and the Tampella Recovery Process. Both utilize a sodium instead of potassium base. A modification of these processes for MHD application to seed regeneration is given in Figure 1 [1]¹.

The study which follows will present a method for design of the carbonation tower, or carbonator as labelled in Figure 1, by constructing a mathematical model of the carbonation reaction, which is the absorption of carbon dioxide (CO_2) into a K_2CO_3 solution to form potassium bicarbonate ($KHCO_3$). The chemical reactions associated with the unit operations given in the diagram are summarized below.

¹Numbers in brackets refer to numbered references in the bibliography.

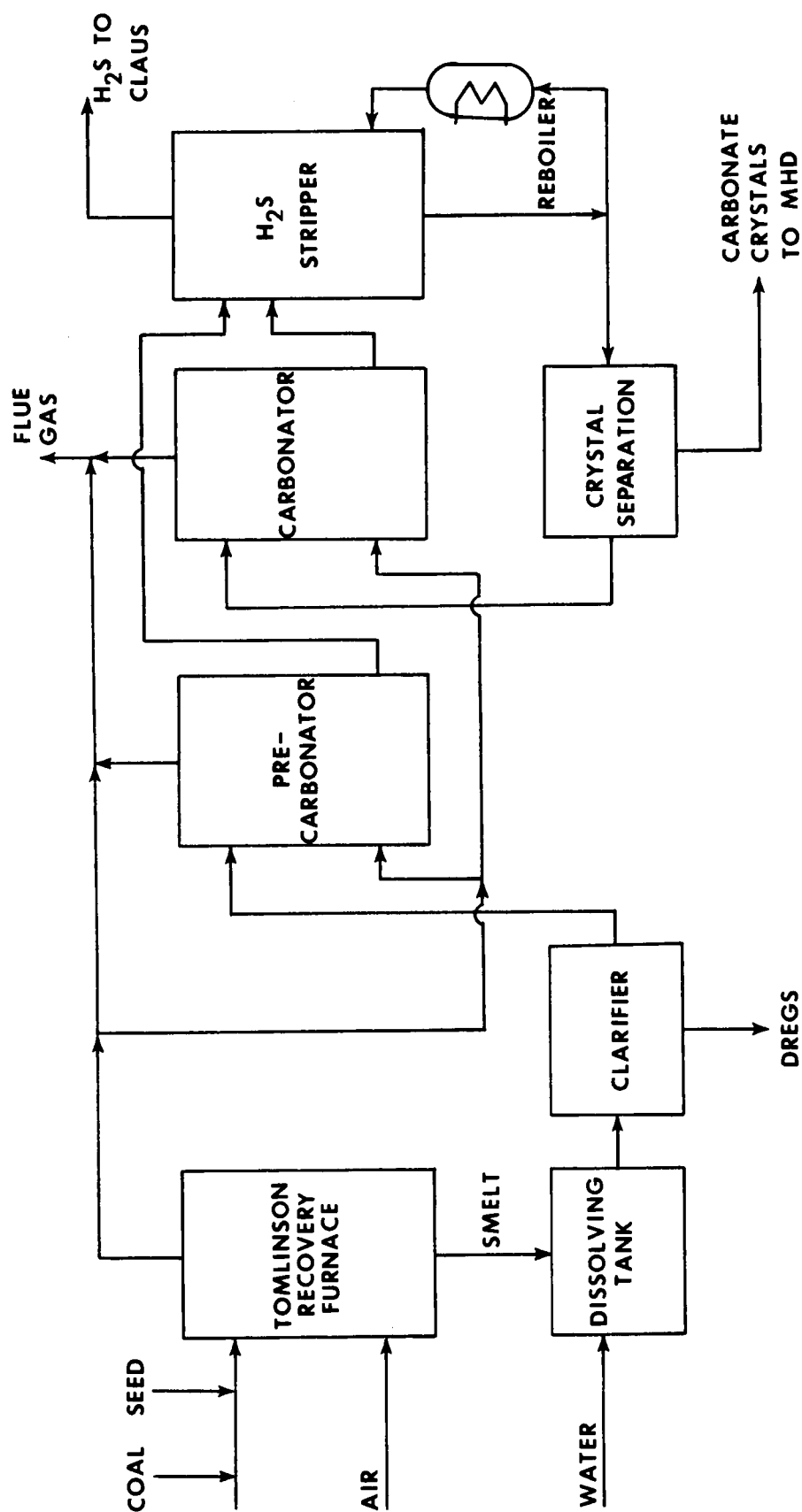


Figure 1. The Tomlinson Tampella Process

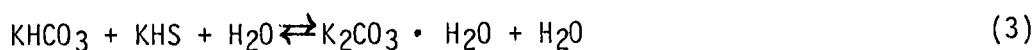
In the Tomlinson Tampella Process, coal, spent seed, and approximately 65 percent stoichiometric air are combined in the Tomlinson Recovery Furnace where the following reaction takes place:



These products form a molten mixture (smelt) of K_2S , K_2CO_3 , and K_2SO_4 which enters a dissolving tank where it is quenched and dissolved in water. Next, ash introduced from the coal used in the reduction furnace is removed in the clarifier. The liquor is then contacted with flue gas in a precarbonation step represented by the following reaction:



These products then enter a stripping column where they are mixed with potassium bicarbonate (KHCO_3) solution. Here the liquor is heated in a reboiler so that H_2S removal and potassium carbonate hydrate recrystallization may take place as represented by the following reaction:



This H_2S gas is converted to elemental sulfur in a Claus reactor. The $\text{K}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ crystals are separated from the mother liquor and recycled for use in the MHD system. The mother liquor is converted to KHCO_3 in a carbonation tower where it is contacted with flue gas as shown in the reaction below:

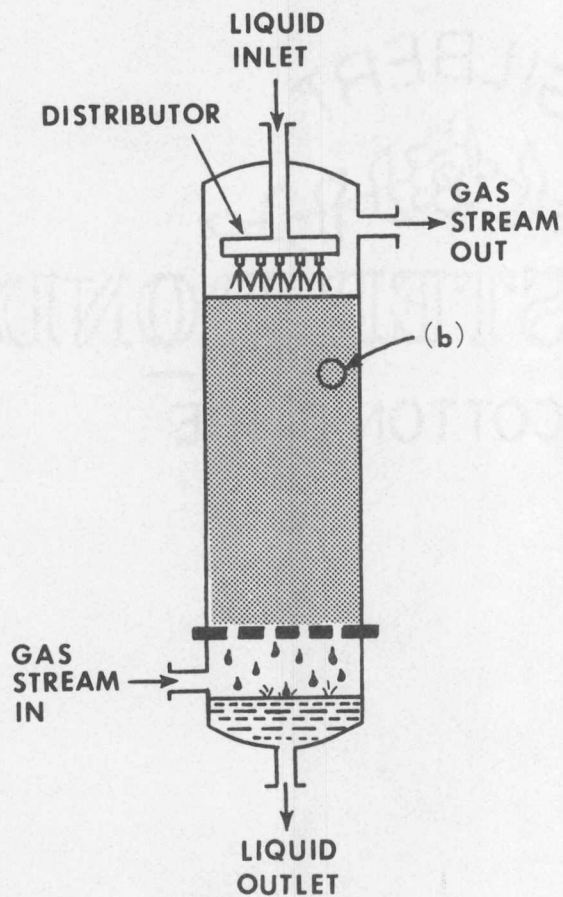


The KHCO_3 is then used in the H_2S stripping column previously described.

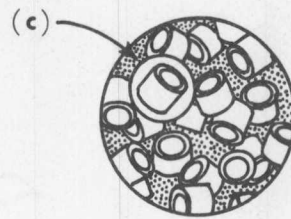
In this study, a method for designing a carbonation tower needed to accomplish a given absorption of CO_2 into K_2CO_3 is given by mathematically modelling the carbonation reaction given in equation (4). Though the Tomlinson-Tampella Process is a commercially available process, the unknown step for MHD application is the effect of changing from sodium to potassium. Fortunately, experimental work has been done on several unit operations of the process, in particular, the carbonation step using a packed tower.

Packed columns, or "towers", have found extensive application in liquid-gas contact systems, primarily in the case of absorption operations (Figure 2). The column is a vertical pipe filled with half-inch to two-inch rings, called Raschig rings, randomly dispersed throughout the tower. A liquid distributor is set above the packing and designed to provide effective irrigation of the packing. The liquid absorbent is fed at the top and trickles over the surfaces of these small rings, while the gas passes countercurrently through the solid-liquid matrix.

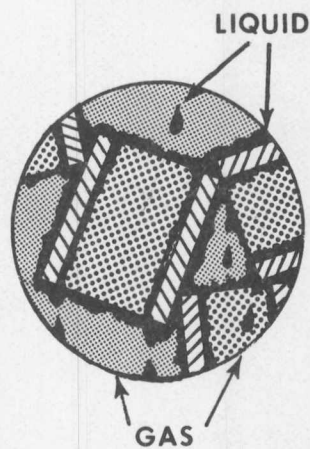
The study which follows involves an analysis of data collected from experiments conducted by the United States Bureau of Mines (USBM) for CO_2 absorption into K_2CO_3 using packed towers as described above. The results of the study are incorporated into a computer program which will compute a tower height for accomplishing a given absorption corresponding to the operating conditions specified.



(a) Packed Column (schematic).



(b) Close-up view of Raschig rings randomly packed.



(c) Flow over individual packing particles.

Figure 2. Packed Column Apparatus

CHAPTER II

REVIEW OF PREVIOUS CO₂ ABSORPTION STUDIES

The literature surveyed contained much experimentation and analysis on CO₂ absorption for a variety of reasons. Removing CO₂ from synthesis gases such as those of oil gas, refinery hydrogen, coal derived Lurgi gas, and ammonia synthesis gas is desirable since CO₂ can act as an unwanted diluent and, in some processes, is considered to be a catalyst poison. Aqueous solutions of potassium or sodium carbonate-bicarbonate, as well as ethanolamine solutions, have been liquid absorption media commonly employed.

Furnas and Bellinger [2] studied operating characteristics of packed towers. They correlated gas absorption data with mass transfer coefficients of CO₂ in sodium carbonate (Na₂CO₃) solutions for a twelve-inch diameter tower using three different types of packing. A mass transfer coefficient is the ratio between the mass or molar flux of the substance of interest and the driving force for mass transfer, ordinarily a concentration or pressure difference of some type. Mass transfer coefficients usually are functions of the geometry of the system involved, fluid properties, species present, and flow variables. Mass transfer coefficients are defined in terms of moles transferred per unit time, per unit interfacial area. Frequently, the interfacial area is rather ill-defined and for that reason, the quantity $K_x a$ (where x will either be L or G depending upon whether the mass transfer driving force is in the liquid or gas phase, and " a " is the column's area per unit volume) is calculated from experiment rather than K_x and " a " separately calculated. In the article

by Furnas and Bellinger, an approximate calculation of K_{Ga} (overall transfer coefficient using gas film units) was made. Their results were summarized by an analytical expression for K_{Ga} as a function of liquid velocity, carbonate concentration, fraction conversion to the bicarbonate, temperature, and parameters associated with the type of packing used.

Harte and Baker [3] used experimental data to formulate an equilibrium relationship between temperature, partial pressure of CO_2 , and carbonate concentration for a variety of operating conditions. Here again, the system under study was absorption of CO_2 into a Na_2CO_3 solution.

Comstock and Dodge [4] have studied CO_2 absorption into K_2CO_3 solutions for a three-inch packed tower. They found that the absorption rate was independent of the gas rate but did vary as a function of the liquor rate, pH, and viscosity of the solution.

A search stimulated by high capital and operating costs for removing CO_2 and H_2S from synthesis gas used in producing liquid fuels was conducted by the USBM [5]. A purification process utilizing a hot potassium carbonate solution was developed. Absorption takes place at an elevated pressure near the atmospheric boiling point of the solution. The solution is regenerated by pressure letdown and steam stripping. Heat exchange between the absorption and regeneration steps is eliminated, and the steam requirements for regeneration are appreciably lower than those of mono-ethanolamine systems. The report includes pilot plant studies to determine economically and technically feasible operating conditions, as well as equilibrium studies [6] on the hot carbonate process. Such data are necessary for establishing limits of purification and are used in

designing absorption and regeneration towers.

All literature searched concerning absorption of CO_2 in K_2CO_3 solutions have used an overall coefficient based on partial pressures of the acid gas; however, absorption of CO_2 in carbonate solutions is controlled by conditions in the liquid phase. This study, therefore, employs an overall coefficient based on liquid phase driving forces ($K_L a$), rather than one based on partial pressures ($K_G a$).

CHAPTER III

THEORETICAL DEVELOPMENT FOR MASS TRANSFER STUDY

Techniques for calculating the height of a tower needed for a given absorption are based on the use of rate expressions which represent mass transfer at a point on the interface and on material balances which express changes in the bulk composition in the two phases that pass each other. The rate expressions are based on the two-film concept [7], which will be discussed below. The following paragraphs will establish a material balance which expresses the relationship between distance along the column and the amount of solute absorbed.

Material Balance

Consider the change in gas and liquid composition in the differential section of packing, dz , labelled in Figure 3. The symbol y represents the mole ratio of CO_2 in the gas to all other inert gas components, and x is the mass ratio of absorbed CO_2 in the liquid to all other liquid components. G represents the gas flux in pound-moles per hour per square foot ($\text{lb moles}/(\text{hr}\cdot\text{ft}^2)$) of inert gas (i.e., all gases excluding CO_2), while L is the liquid flux in pounds per hour per square foot ($\text{lb}/(\text{hr}\cdot\text{ft}^2)$) of all components except absorbed CO_2 . Defining G and L in this way allows the quantities to remain constant throughout the column. The variables are subscripted to indicate entering and exiting quantities.

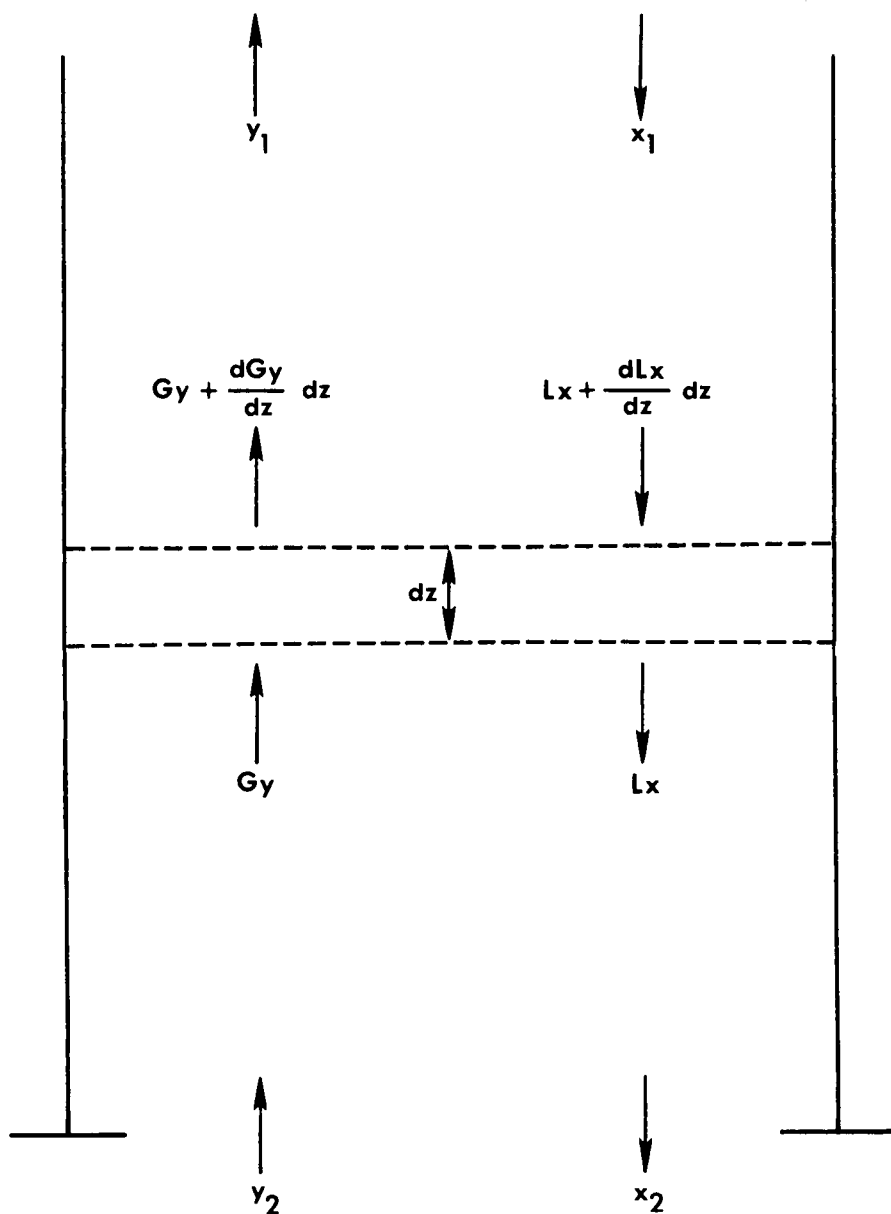


Figure 3. Diagrammatic Sketch of a Packed Column.

By applying the mass conservation law and assuming steady state one can write:

$$Lx + (dLx/dz) (dz) + (Gy) (M_{CO_2}) = Lx + (Gy + (dGy/dz) (dz)) M_{CO_2} \quad (5)$$

After cancellation,

$$dLx = M_{CO_2} (dGy), \quad (6)$$

and since L and G are constant,

$$dy = (L/(G \cdot M_{CO_2})) dx \quad (7)$$

or

$$y-y_2 = (L/(G \cdot M_{CO_2})) (x-x_2). \quad (8)$$

This is the equation for the operating line which is a material balance giving the relationship between the compositions of the gas and liquid streams at any point in the column. Figure 4 shows a plot of the operating line equation.

Development of Rate Expressions

The principles behind the defining of mass transfer coefficients (or rate expressions) are incorporated in the two-film concept which assumes additivity of the gas and liquid phase resistances in order to obtain an overall resistance. The additivity concept assumes no resistance to transport at the interface, or in other words, the phases are in equilibrium at the actual points of contact at the interface. This "interface

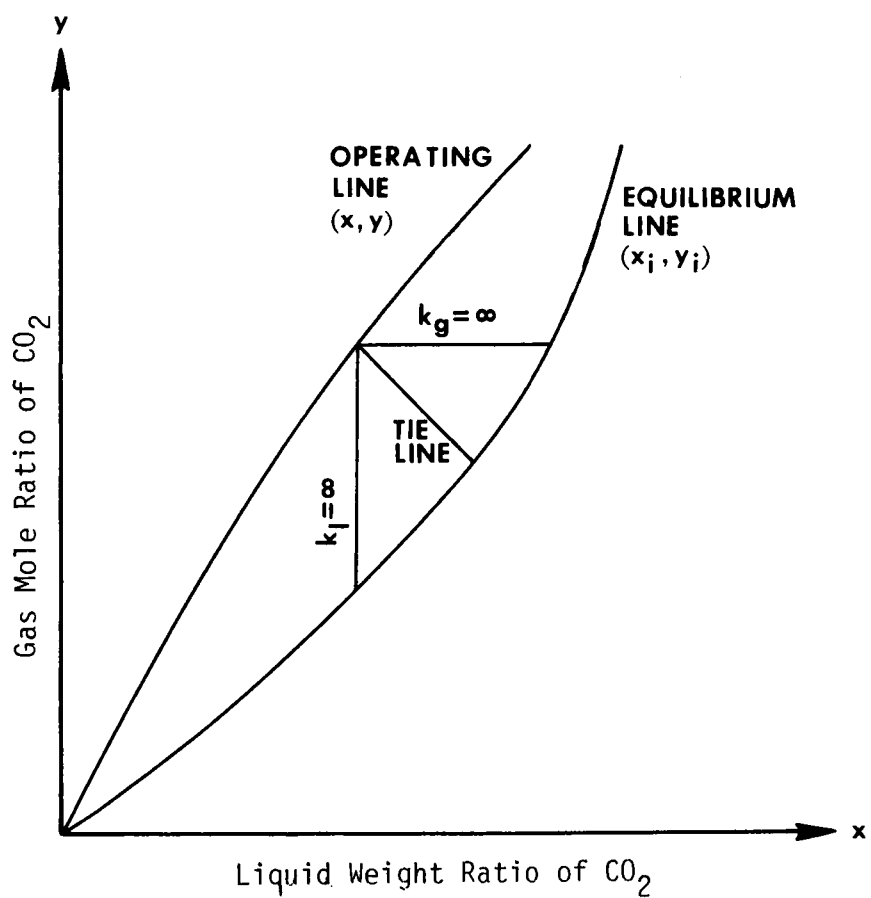


Figure 4. Diagram Depicting Relationship Between Operating and Equilibrium Line. (The symbols k_1 and k_g denote individual phase transfer coefficients. Subscript i indicates interfacial compositions).

equilibrium" assumption is one usually made in mathematical analysis of mass transfer [7].

In Figure 5, solute is being transported from the bulk gas phase to the phase boundary, or interface, and then from the interface to the bulk liquid phase. Symbols x and y are weight and mole ratios respectively, as defined in the previous section. The concentration gradient existing between the bulk and interface (equilibrium) composition is the driving force in mass transfer. The driving force of each phase defines an individual mass transfer coefficient as follows:

$$\begin{aligned} N_A &= \text{molar flux of solute} = k_g(y_{GB} - y_{Gi}) \\ &= k_l(x_{Li} - x_{LB}) \end{aligned} \quad (9)$$

These equations may be written separately as:

$$N_A/k_g = y_{GB} - y_{Gi}, \text{ and} \quad (10)$$

$$N_A/k_l = x_{Li} - x_{LB}. \quad (11)$$

Figure 6 has a plot of a straight operating line, and straight and curved equilibrium lines. For a straight equilibrium line, equation (12) holds:

$$y_{Gi} = y_0 + m \cdot x_{Li}, \quad (12)$$

where $m = d(y_{Gi})/d(x_{Li})$, and y_0 is the value of y_{Gi} at $x_{Li} = 0$. Then one may write by substitution:

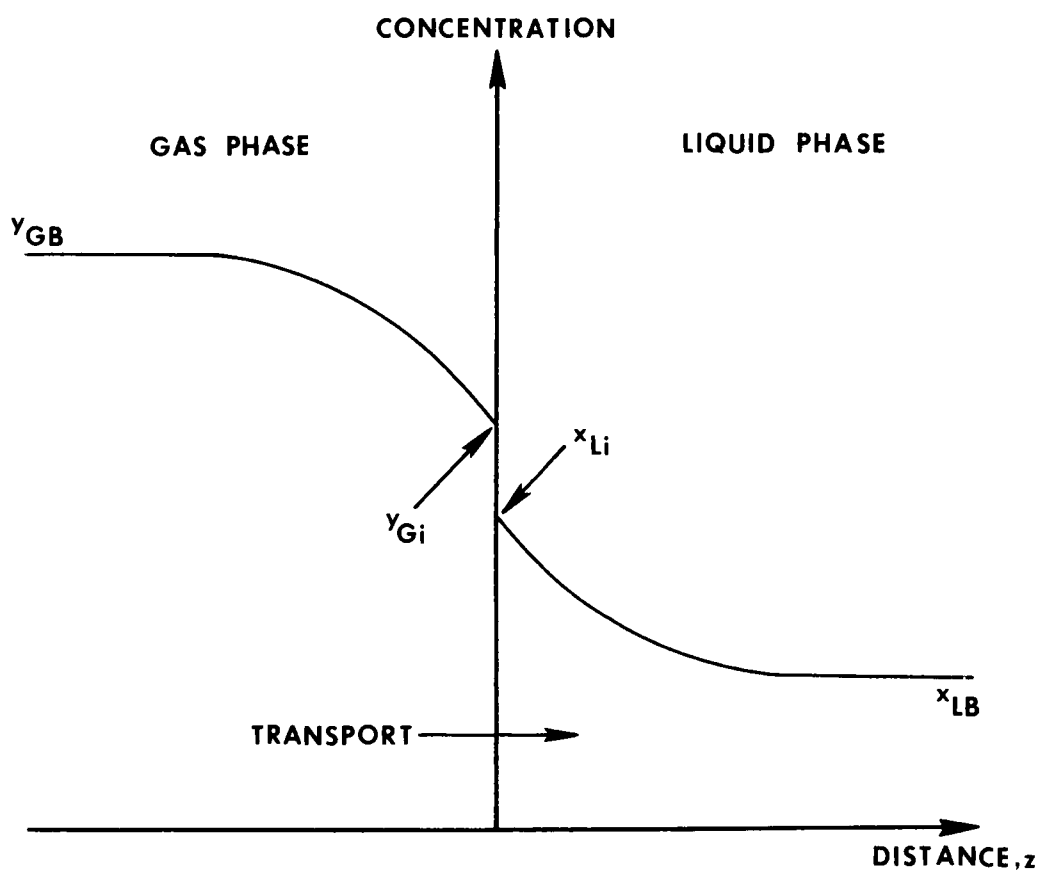


Figure 5. Concentration Gradients Near a Phase Boundary.

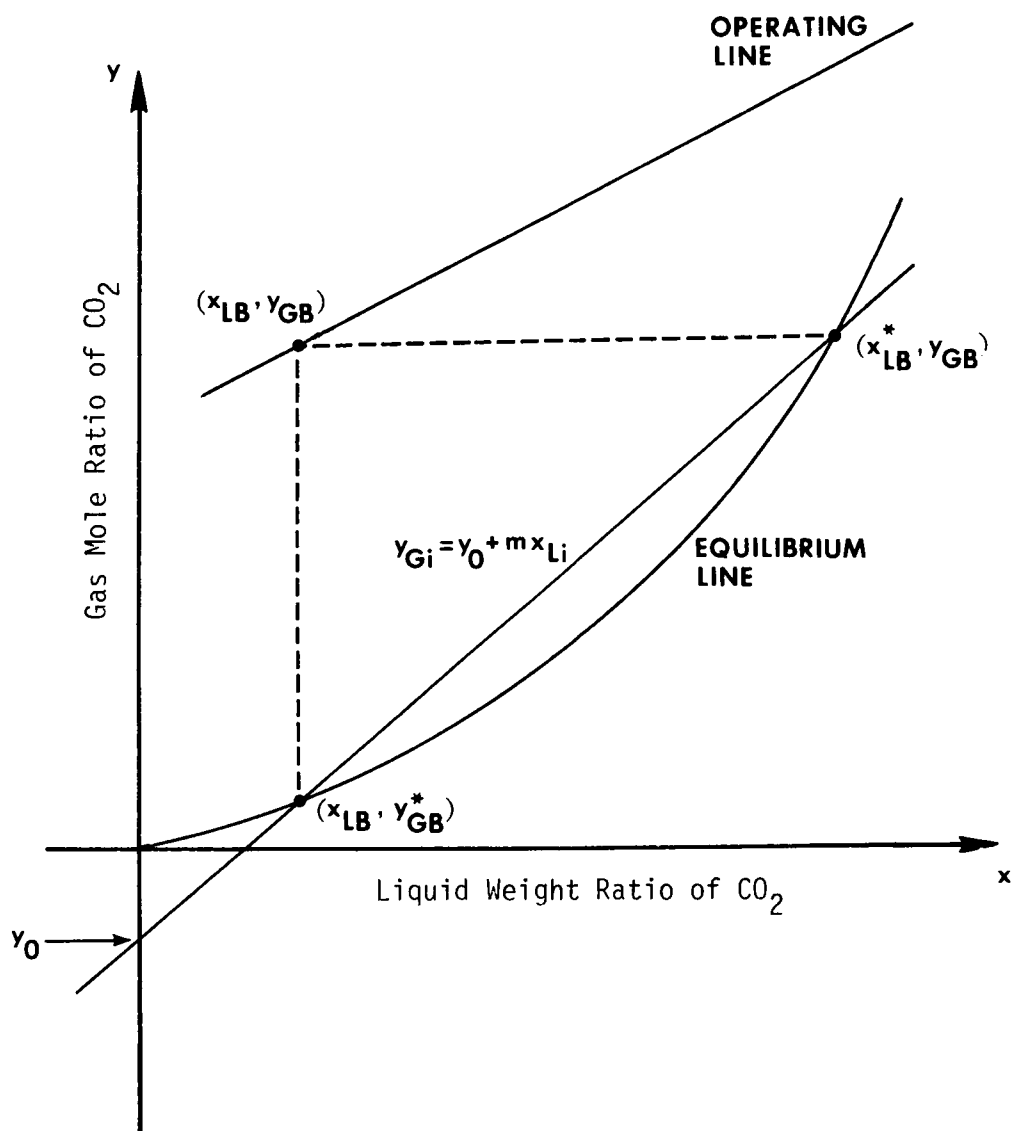


Figure 6. Diagram Depicting Straight Equilibrium Line for Deriving Equation (16).

$$\begin{aligned}
N_A / (k_g \cdot m) &= (y_{GB}/m) - (y_{Gi}/m) \\
&= (y_{GB}/m) - (y_0 + m \cdot x_{Li})/m \\
&= (y_{GB}/m) - (y_0/m) - x_{Li} \\
&= x_{LB} - x_{Li}
\end{aligned} \tag{13}$$

Combining equations (11) and (13), one may write:

$$\begin{aligned}
N_A (1/(m \cdot k_g) + 1/k_1) &= (y_{GB}/m) - (y_{Gi}/m) + x_{Li} - x_{LB} \\
&= x_{LB} - x_{LB}
\end{aligned} \tag{14}$$

For practical purposes of process design, transport rates are expressed in terms of the bulk phase concentrations. Overall transfer coefficients for the liquid and gas phase respectively are defined as follows:

$$N_A = K_G (y_{GB} - y_{GB}) = K_L (x_{LB} - x_{LB}) \tag{15}$$

Combining equations (14) and (15), one obtains:

$$1/K_L = (1/(m \cdot k_g)) + (1/k_1) = 1/(K_G \cdot m). \tag{16}$$

If k_1 is large, K_G is approximately k_g . In this case, the liquid side resistance is negligible. If the gas side resistance, $1/k_g$, is negligible in comparison to the liquid side resistance, m/k_1 , then K_L is approximately k_1 .

In most situations, neither phase resistance is exactly zero, though assuming that one is negligible is often a good approximation. The ratio between the individual mass transfer coefficients is indicative of what phase offers the greatest resistance. This can be seen if equation (9) is rewritten as follows:

$$y_{GB} - y_{Gi} = (k_1/k_g) (x_{Li} - x_{LB}). \quad (17)$$

The ratio, $-k_1/k_g$, is the slope of a tie line which connects the equilibrium and operating lines. (The equilibrium line, depicted in Figure 4, gives the interfacial relationship between y_i and x_i , assumed to be in equilibrium. Once y is known as a function of x along the operating line, y_i can be found at corresponding points from the equilibrium line.) As k_g approaches infinity, the tie line becomes horizontal or ($y_{GB} - y_{Gi}$) approaches zero. In this case the liquid phase resistance is controlling. Similarly, a vertical tie line indicates a large k_1 or high gas phase resistance to mass transfer.

A hypothetical, perfect solvent having no liquid phase resistance and having infinite chemical reactivity has a K_Ga (overall coefficient based on gas phase resistance) value of 24.0 (lb mole)/(hr·ft³ atm) [8]. Values of K_Ga for CO₂ absorption into K₂CO₃ reported by the USBM are all much less than one, which is strong evidence that resistance to mass exchange is primarily in the liquid.

Therefore, using an overall mass transfer coefficient based on a liquid phase driving force, K_La for CO₂ absorption can be written as:

$$\text{moles transferred}/(\text{hr} \cdot \text{ft}^2) = K_La (x^* - x) dz, \quad (18)$$

where the driving force, $(x^* - x)$, is the difference in the equilibrium weight ratio of CO₂, x^* , and the CO₂ weight ratio in the bulk solution, x .

Defining the liquid velocity (L) in lb/(hr·ft²), one can rewrite equation (18) as:

$$L \, dx/M_{CO_2} = K_L a \, (x^* - x) \, dz. \quad (19)$$

Solving for z one obtains:

$$z = L/(M_{CO_2} \cdot K_L a) \int (dx/(x^* - x)). \quad (20)$$

If, in the integration interval, x^* equals x , the tower height goes to infinity. This situation, known as a pinch point, is illustrated in Figure 7. It occurs when the operating line crosses the equilibrium line at the exact CO_2 weight fraction desired in the separation, or as in rare cases, where it is tangent to the equilibrium line. This point establishes a minimum slope, $L/(G \cdot M_{CO_2})$, for an operating line.

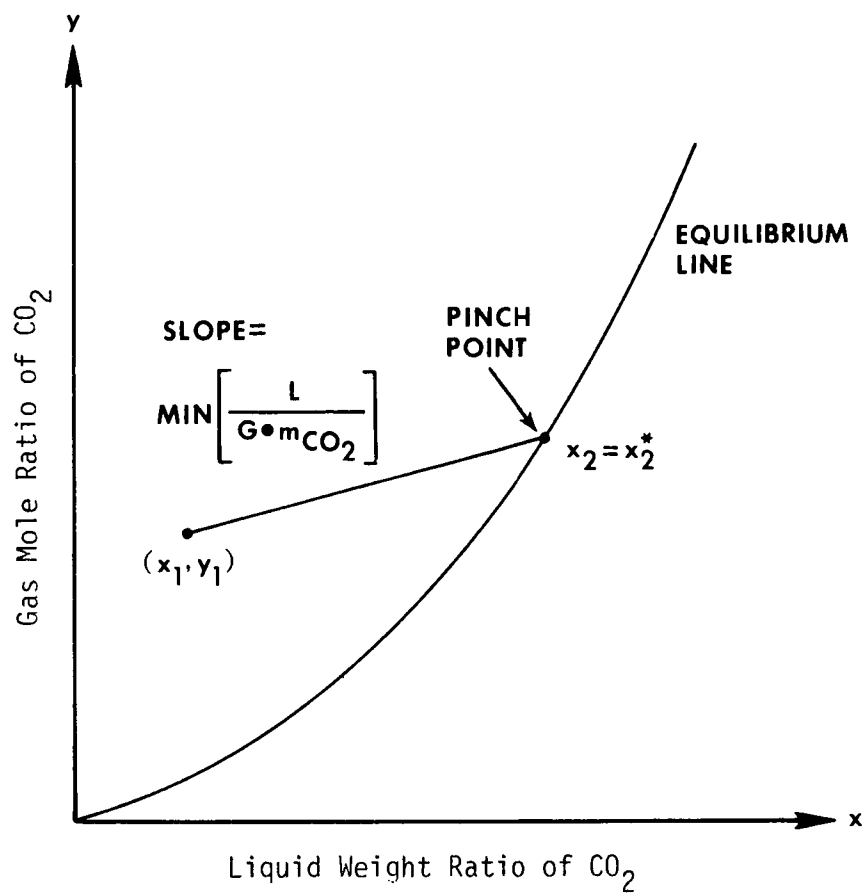


Figure 7. Diagram Depicting Occurrence of the Minimum Operating Line.

CHAPTER IV

METHODOLOGY FOR MASS TRANSFER DATA ANALYSIS

Equation (20) for tower height requires knowledge of the driving force, $(x^* - x)$, and the mass transfer coefficient representative of CO_2 absorption. The extensive data provided by the USBM was utilized in developing the relationship between equilibrium gas and liquid concentrations for CO_2 absorption into K_2CO_3 , and for correlating K_La with experimental variables. Statistical techniques used in establishing these correlations involved use of a regression analysis computer program discussed in Appendix A.

Expression for Equilibrium Correlation

Harte and Baker [3] developed an equilibrium relationship between temperature, partial pressure of CO_2 , and chemical composition in the liquid for absorption into Na_2CO_3 , over a range of conditions approximating those encountered in large scale processes. By utilizing equilibrium data from the USBM equilibrium study, an expression for CO_2 absorption into K_2CO_3 was derived for a temperature range of 363 to 403 degrees Kelvin and a 20 to 40 percent equivalent weight K_2CO_3 ¹. The development

¹Percent equivalent weight K_2CO_3 (% K_2CO_3) is in units of equivalent mass percent. An equivalent mass of K_2CO_3 contains, by weight, all potassium present in solution plus half as many gram ions of carbonate. An equivalent mass of water includes all the water and an equivalent mass used in the formation of KHCO_3 , so that % K_2CO_3 = 100 (equivalent mass of K_2CO_3)/equivalent mass of $(\text{H}_2\text{O} + \text{K}_2\text{CO}_3)$. Defining K_2CO_3 concentration in this way avoids the difficulty of dealing with moles in a reversible reaction where the species exist in a dissociated form as well as intact molecules.

of this expression will now be discussed.

In order to develop an expression for equilibrium concentrations of reactants and products, the equilibrium constant (K_E) for the CO_2 absorption reaction is defined as follows:

$$\begin{aligned} K_E &= [\text{KHCO}_3]^2 / ([\text{K}_2\text{CO}_3] [\text{H}_2\text{O}] \cdot P_{\text{CO}_2}) \\ &= 2f^2 C_0^2 / ((1 - f) \cdot C_0 \cdot [\text{H}_2\text{O}] \cdot P_{\text{CO}_2}) \end{aligned} \quad (21)$$

for the reaction:



where P_{CO_2} is the partial pressure of CO_2 , f is the fraction conversion to potassium bicarbonate (KHCO_3), C_0 is the equivalent concentration of K_2CO_3 in moles/liter and $[]$ signifies the concentration of a given species in moles per liter.

Due to reaction, $[\text{H}_2\text{O}]$ may be written as:

$$[\text{H}_2\text{O}] = W_0 (1 - C_0/W_0), \quad (23)$$

where W_0 is equivalent concentration of H_2O in moles per liter. Since W_0 is large (55 moles/liter), C_0/W_0 may be neglected so that equation (21) becomes:

$$K_E = 2f^2 C_0 / ((1 - f) W_0 (P_{\text{CO}_2})). \quad (24)$$

The equivalent concentration of K_2CO_3 , (C_0), can be written as follows:

$$C_0 = K(p) (1000\text{ml/l}) / ((138.2\text{gm/mole}) 100) \quad (25)$$

where $K = \%K_2CO_3$, $138.2 =$ the molecular weight of K_2CO_3 , and ρ is the density² of K_2CO_3 in gm/ml.

Substituting into equation (24) one obtains:

$$K_E = 2f^2 K (\rho) (1000)/((1-f) W_0 (138.2) (P_{CO_2}) 100) \quad (26)$$

or

$$P_{CO_2} (1-f)/(f^2 K) = \text{a constant, proportional to } 1/K_E. \quad (27)$$

It was hypothesized that K_E obeys an Arrhenius-type relationship, i.e., an equation involving an exponential expression for temperature (T), and since P_{CO_2} and f are dependent on K , one may write:

$$\ln (P_{CO_2} (1-f)/(f^2 K)) = F(T, K, f). \quad (28)$$

An analytical expression of the form:

$$\ln (P_{CO_2} (1-f)/(K^{.75} f^2)) = a_0 + a_1/T + b_1 (K/T) + c_1 K + d_1 \ln T + e_1 \ln K + f_1 f \quad (29)$$

was hypothesized. The exponent on K , .75, was chosen after plots of $\ln f$ versus $\ln (P_{CO_2} K^u)$ for 20, 30, and 40 percent K_2CO_3 solutions at a given temperature were found to satisfactorily fit a line for $u = .75$. The best coefficients, in a least squares sense, were sought by use of the regression analysis program discussed in Appendix A.

²Densities were obtained by plotting values of densities obtained from The International Critical Tables [9] and interpolating for the particular K_2CO_3 solution desired.

Expressing K_La as a Function of Experimental Variables

As stated in Chapter III, the liquid phase mass transfer coefficient (K_La) is representative of CO_2 absorption into K_2CO_3 , and the defining equation can be written as:

$$K_La = \text{moles of } \text{CO}_2 \text{ transferred } / (\text{hr} \cdot \text{ft}^3) \quad (30)$$

$$= L / (M_{\text{CO}_2} \cdot z) \int dx / (x^* - x) \quad (31)$$

$$= L / (M_{\text{CO}_2} \cdot z) \int df / (f^* - f) \quad (32)^3$$

where, recall, f = fraction conversion of K_2CO_3 to KHCO_3 , $L = (\text{lb}) / (\text{hr} \cdot \text{ft}^2)$, and the integrated expression is the mass transfer driving force.

As a first approximation, a straight equilibrium line was assumed so that the integral in equation (32) could be equated to a log mean term. These values were improved upon by performing a numerical integration, so that a straight equilibrium line was no longer assumed. It was this set of K_La values that were correlated with experimental data by again using the regression analysis program. The variables with which K_La was correlated were liquid velocity (L), average CO_2 partial pressure (P), equivalent percent K_2CO_3 (K), average fraction conversion to KHCO_3 (f), and average temperature in the column (T).

The first expression for K_La as a function of experimental variables assumed the mass transfer coefficient to be constant throughout

³For the relationship between x and f , see Appendix D.

the tower corresponding to a given set of inlet and exit conditions.

This equation was of the form:

$$K_L a = (GAV) f^A L^B K^C (T/383)^{Dp} E (1-f)^F, \quad (33)$$

where GAV is a constant. The experimental variables were taken as averages of their inlet and exit values.

Equation (33) was incorporated into (32), but this time the experimental variables were allowed to vary with position along the tower. The degree of generality of the resulting expression was measured by how constant GAV remained for the range of data utilized in the correlation.

Substituting equation (33) and (32) and solving for GAV, one obtains:

$$GAV = L/(M_{CO_2}(z)) \int df / ((f^*-f) f^A L^B K^C (T/383)^{Dp} E (1-f)^F), \quad (34)$$

where all experimental parameters were allowed to vary with f except for liquid velocity (L), and K_2CO_3 concentration (K). The exponents were varied systematically to find the set of values which would minimize the standard deviation on GAV. Each exponent was made to vary a given increment in a positive and negative direction until the standard deviation increased on either side of a given set of exponential values. At this point, at least a relative minimum standard deviation will have been reached. Results of the analysis are in the following chapter.

CHAPTER V

RESULTS OF DATA ANALYSIS

Results of Equilibrium Correlation

Results from application of the regression analysis program to the equilibrium data utilized in equation (29) were as follows: $a_0=0$, $a_1=1388$, $b_1=17487$, $c_1=44.9$, $d_1=e_1=f_1=0$. The percent errors on a_1 , b_1 , and c_1 were 1.72, 3.2, and 3.1, respectively. The standard deviation of the fit was .154, the covariance was .163; the variance of the actual data was .185; the variance of the curve fitted data was .166; and the correlation coefficient was .934. The largest percent difference in y , as determined from the least squares fit, was 12.9. Application of this result for predicting equilibrium partial pressures of CO_2 is given in Table 1. Also shown are experimental values obtained from the USBM study. The experimental values of P_{CO_2} versus those calculated are shown in Figure 8.

Results of $K_L a$ Correlation

Results from minimizing the standard deviation on the constant GAV of equation (34), obtained from the $K_L a$ correlations of Chapter IV, were as follows: $A=0$, $B=.55$, $C=-.6$, $D=6.25$, $E=-.05$, $F=-1.65$, and $\text{GAV}=.015079$. The local minimum standard deviation on GAV was found to be 31.9 percent. The sensitivity of this minimum to perturbations of .05 on the exponents was negligible, i.e., less than .2 percent.

Table 1. Equilibrium Partial Pressure of CO₂ (P_{CO₂})
Calculated and Obtained from Experiments

Equivalent Weight Percent of K ₂ CO ₃ (%)	T (°K)	Fraction Conversion	Experimental P _{CO₂} (psi)	Calculated P _{CO₂} (psi)
20	363	0.2	0.33	0.3556
20	363	0.502	2.93	3.599
20	363	0.797	15.6	22.3
20	383	0.202	0.49	0.493
20	383	0.507	5.11	3.023
20	383	0.817	30.9	35.1
20	403	0.201	0.79	0.64
20	403	0.5	7.41	6.33
20	403	0.792	40.4	38.2
30	363	0.199	0.35	0.344
30	363	0.489	3.45	3.25
30	363	0.786	19.6	20.1
30	383	0.198	0.59	0.592
30	383	0.483	5.5	5.46
30	383	0.761	28.4	29.3
30	403	0.198	0.86	0.976
30	403	0.473	9.03	8.47
30	403	0.735	38.4	40.7
40	363	0.1	0.08	0.07
40	363	0.2	0.34	0.311
40	363	0.419	2.49	1.38
40	383	0.2	0.71	0.696
40	383	0.485	7.89	6.36
40	383	0.809	50.5	47.7
40	393	0.295	1.81	2.49
40	393	0.588	18.5	17.0
40	393	0.835	83.5	85.4
40	403	0.199	1.36	1.42
40	403	0.34	20.5	18.3
40	403	0.814	104.4	102.6

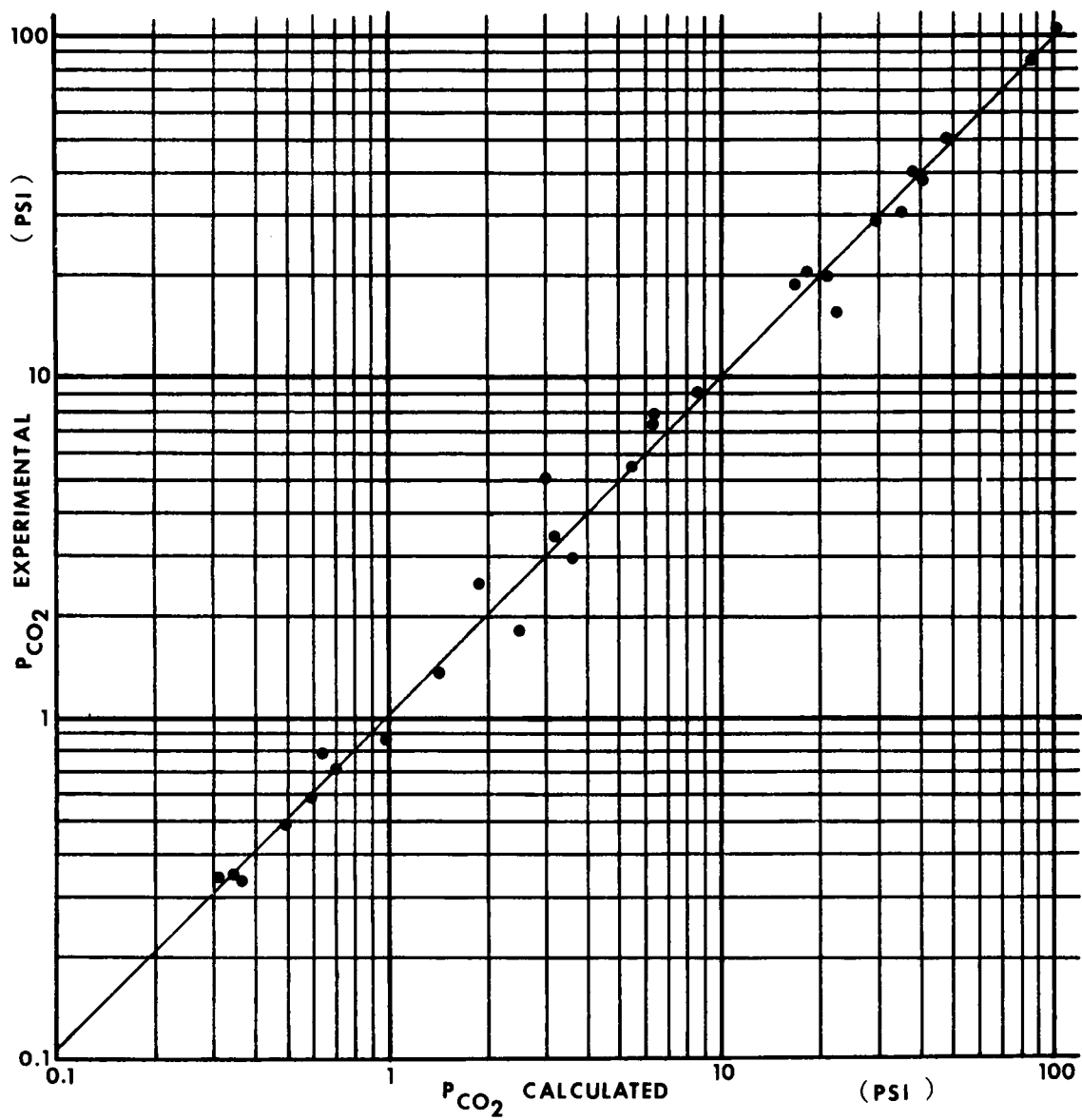


Figure 8. Plot of P_{CO_2} , Experimental, Versus P_{CO_2} , Calculated From Equilibrium Relationship Derived.

The formulation of this result used data encompassing a temperature range of 200 to 260 degrees F for thirty-, nine-, and four-foot towers having either one-inch or half-inch Raschig rings. The absorption pressure for these experiments was at 300 psi for most sets of data and at 100 psi for others.

CHAPTER VI

COMPUTER PROGRAM FOR TOWER HEIGHT DETERMINATION

The preceding results from the data analysis were incorporated into a computer program which calculates a height by solving equation (34) for z . The derived equilibrium relationship was written as a subroutine for calculating f^* values necessary to obtain the driving force. A simple flow chart indicating the order of calculations performed in the program is given in Figure 9.

The input variables in the order necessary for program utilization are given in the List of Symbols. The variable names are as they appear in the program. Also listed in the List of Symbols are the output quantities the program will return. Note that VS , the fraction of CO_2 in the outlet gas stream, is a calculated quantity. It is obtained from the operating line equation, with CO_2 weight fraction in the liquid (x) written in terms of fraction converted to $KHCO_3$ (FR and FS):

$$(L/m_{CO_2}) (FR-FS)x^+ = G(y_2-y_1). \quad (35)$$

This is an equation in six unknowns. Five of the variables must be specified; the sixth is calculated. The choice of this sixth variable is arbitrary. In the program, VS , which is a function of y_2 , is calculated. VS is related to y_2 by:

$$y_2 = VS/(1-VS). \quad (36)$$

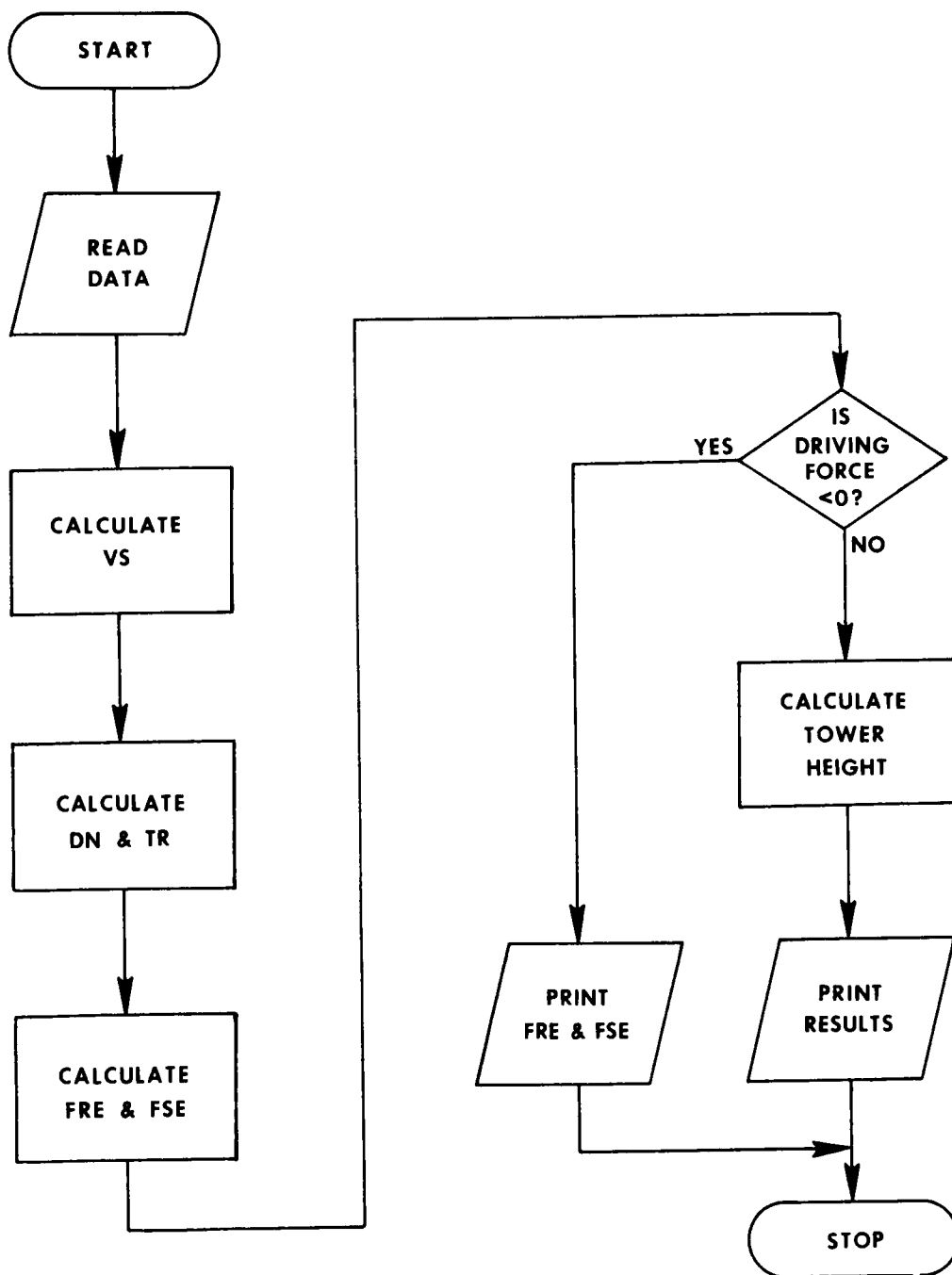


Figure 9. Flowchart of Basic Functions Performed in Computer Program for Tower Height Calculation.

Three examples using actual experimental data from the USBM are given in Table 2. The output shown in Table 3 includes the actual tower height used in the study for purposes of comparison with the program's calculation. The three cases are taken from the four-, nine-, and thirty-foot column experiments. The bad agreement between actual and calculated tower height for case 3 is expected since for this run, the standard deviation on GAV was near 35 percent, which is about the maximum discrepancy obtained in the data analysis.

Table 2. Input for Computer Program to Calculate Tower Height Utilizing Actual Experimental Data

CASE	QL $\frac{\text{lb}}{\text{hr} \cdot \text{ft}^2}$	TT (°F)	TB (°F)	VF	VS	G $\frac{\text{moles}}{\text{hr} \cdot \text{ft}^2}$	PK (%)	FR	FS	P (psi)	QLL $\frac{\text{gal}}{\text{hr}}$	GG $\frac{\text{SCF}}{\text{hr}}$
1.	16869	230	230	11.9	3.4	23.0	39.5	0.32	0.36	314.7	27.2	1494
2.	3875	264	277	28.3	12.5	17.4	35.8	0.3	0.61	317.7	27.2	500
3.	3433	232	248	20.3	2.4	18.8	35.0	0.33	0.67	314.7	18.8	1220

Table 3. Output from Computer Program to Calculate Tower Height Utilizing Actual Experimental Data

CASE	QL <u>lb</u> hr-ft ²	TT (°K)	TB	VF <u>100</u>	VS <u>100</u>	G <u>moles</u> hr-ft ²	PK <u>100</u>	FR	FS	P (psi)	HT (ft)	TR moles of CO ₂ trans- ferred	DN <u>gm</u> ml
1.	16869	383	383	0.119	0.0383	23.0	0.395	0.32	0.36	314.7	4.28 (4)	0.349	1.40809
2.	3875	401.9	409.1	0.283	0.1268	17.4	0.358	0.30	0.61	317.7	10.3 (9)	0.249	1.36496
3.	3433	384.1	393	0.203	0.0128	18.8	0.35	0.33	0.74	314.7	23.27 (30)	0.6445	1.35496

¹Entries in brackets refer to the actual column height.

CHAPTER VII

RECOMMENDATIONS

The following recommendations for further work, or extension of the preceding study, are listed below.

1. In an application where a given tower height is specified, one may want to determine its performance level for purifying a CO_2 gas stream. This would entail a simple program modification. Utilizing the equations derived in the study and solving for a variable corresponding to the amount of CO_2 absorbed (since height would now be a known quantity) would be indicative of a given tower's performance.

2. In equation (35), the flexibility in choosing the experimental parameter for which to solve could be incorporated into a program modification which would allow one to choose this unknown. This could be accomplished by a branching Fortran command giving one several alternatives for the variable one wants the program to solve.

3. The derived equation for tower height (34), was based on parameters obtained by finding a local minimum standard deviation for GAV. This may not be the absolute minimum, so further investigation might improve the accuracy of the tower height calculation.

4. If the conditions with which one is working fall outside of the range utilized in the study, the exact analysis may be applied to the new set of data.

5. The precarbonation step in the Tomlinson Tampella Process is very similar to the carbonation reaction, the difference being that CO_2 is absorbed into a K_2S solution instead of a K_2CO_3 solution. Design of

this tower is probably very similar to the carbonation tower design, so that the preceding analysis would apply. Experimental verification is merited to investigate this possibility.

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BIBLIOGRAPHY

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APPENDICES

APPENDIX A

LINEAR LEAST SQUARES REGRESSION ANALYSIS

The least squares regression analysis program used in the study performed a correlation for a maximum of six independent variables. The program and a sample output are displayed in Appendices B and C, respectively. The sample utilized the regression analysis on the dependent variable, $\ln(K_L a)$, and three dependent variables, $\ln(\text{CO}_2 \text{ inlet pressure})$, $\ln((1-f)/f)$, and $\ln(L)$. A general explanation of the statistical theory is outlined below.

The program takes a systems of equations

$$\begin{aligned}
 F_1 &= A_0 + A_1x_1 + A_2y_1 + \dots \\
 F_2 &= A_0 + A_1x_2 + A_2y_2 + \dots \\
 &\cdot \\
 &\cdot \\
 &\cdot \\
 F_N &= A_0 + A_1x_N + A_2y_N + \dots
 \end{aligned} \tag{37}$$

which can be written in the form $F = XA$, where

$$F = \begin{bmatrix} F_1 \\ F_2 \\ \cdot \\ \cdot \\ \cdot \\ F_N \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 & \cdot & \cdot & \cdot \\ 1 & x_2 & y_2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_N & y_N & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

and solves for the A matrix. These entries, or coefficients, are solved by the following standard matrix operations:

$$X^T F = X^T X A \quad (39)$$

$$(X^T X)^{-1} = A. \quad (40)$$

The matrix $X^T F$ is called the Z matrix in the program's output.

The program prints a standard deviation of fit ($\sigma_{F,C}$), covariance, variance of actual data (σ_F^2), variance of curve fitted data (σ_C^2), and a correlation coefficient. These quantities are calculated according to the equations below:

$$\sigma_{F,C} = \sum^N ((F(N) - \text{CAL}(N))^2 / (NPTS - NN))^{1/2} \quad (41)$$

where $F(N)$ is the dependent variable inputted, $\text{CAL}(N)$ is the calculated dependent variable for the N^{th} point, $NPTS$ is the number of data points entered, and NN is the total number of coefficients.

The covariance was calculated by equation (42).

$$\text{covariance} = \sum^N ((F(N) - \bar{F}) (\text{CAL}(N) - \overline{\text{CAL}}) / (NPTS - NN)) \quad (42)$$

where $\overline{\text{CAL}}$ is the average of all $\text{CAL}(N)$, and $\bar{F}$ is the average of all $F(N)$.

The variance of the actual data is

$$\sigma_F^2 = \sum^N (F(N) - \bar{F})^2 / (NPTS - NN), \quad (43)$$

and the variance of the calculated data is

$$\sigma_C^2 = \sum^N (\text{CAL}(N) - \overline{\text{CAL}})^2 / (NPTS - NN). \quad (44)$$

The correlation coefficient is calculated as follows:

$$\text{correlation coefficient} = \sigma_{F,C}^2 / \sigma_F \sigma_C. \quad (45)$$

The last portion of the program calculates a variance-covariance and correlation matrix, which indicate the degree of intercorrelation between independent variables. Entries in the variance-covariance matrix are obtained by the following equation:

$$\text{the variance-covariance matrix} = \sigma_{F,C}^2 (X^T X)^{-1} \quad (46)$$

The correlation matrix is a normalized form of the variance-covariance matrix. Its entries are calculated in equation (47):

$$c_{ij} = v_{ij} / (v_{ii}^{1/2} v_{jj}^{1/2}), \quad (47)$$

where c_{ij} are the elements of the correlation matrix, and v_{ij} are the elements of the variance-covariance matrix.

The output displays the data followed by three columns labeled FCAL, DIFFERENCE, and % ERROR. These are, respectively, the calculated dependent variable, the difference between the calculated and experimental dependent variable, and one-hundred times this difference divided by the calculated value.

The least squares coefficients are next printed out with a standard deviation (labelled ERROR, and % ERROR, which is one-hundred times the error divided by the coefficient. The standard deviation of the least squares coefficients is the square root of the diagonal elements of the variance-covariance matrix.

As a general rule one 1) rejects all curve fits where a coefficient is less than its standard deviation, 2) minimizes the standard deviation of the fit, and 3) maximizes (.9 or better) the correlation coefficient.

REM

APPENDIX B

1

REM

REGRESSION ANALYSIS COMPUTER PROGRAM

REM

(CBASIC)

REM U T S I GAS DIAGNOSTICS DIVISION JANUARY 25, 1980
REM MULTIVARIATE LINEAR REGRESSION OF UP TO 6 VARIABLES
REM THE FILE NAME FOR THIS CBASIC PROGRAM IS "CREG6.BAS"
REM WRITTEN BY J. O. HORNKOHL AND REVISED BY R. D. MORRIS

DIM X(600),F(100),A(15),XTX(15,16),Z(15),EX(15),AA(15)
DIM LOCATE(15,3),B(15,15),TEST(15,15),VC(15,15),LOC(15),CK(15)
DIM ID\$(10),PRNT(7)

10 IF PRINT\$="YES" THEN LPRINTER :PRINT CHR\$(12) :CONSOLE
PRINT\$=" " :GOSUB 900

REM CLEAR INPUT DATA ARRAY
FOR I=1 TO 600
X(I)=0.0
NEXT I

REM PRINT INTRODUCTORY MESSAGE ON CONSOLE
PRINT TAB(2);"M U L T I V A R I A T E P O L Y N O M I A L R E G R
E S S I O N"
PRINT
PRINT TAB(6);"THIS PROGRAM FITS DATA TO POLYNOMIALS OF THE FORM"
PRINT
PRINT TAB(10);"F=A0 + A1*X + A2*X**2 + . . . + AN*X**N"
PRINT TAB(10);" + B1*Y + B2*Y**2 + . . . + BN*Y**N"
PRINT TAB(10);" + C1*Z + C2*Z**2 + . . . + CN*Z**N"
PRINT TAB(10);" + D1*U + D2*U**2 + . . . + DN*U**N"
PRINT TAB(10);" + E1*V + E2*V**2 + . . . + EN*V**N"
PRINT TAB(10);" + F1*W + F2*W**2 + . . . + FN*W**N"
PRINT
PRINT "FREE SPACE =";FRE

REM ENTER COMMENTS TO BE PRINTED ON THE OUTPUT
PRINT "ENTER ID STRINGS"
NID=-1

1

NOTE THAT IN ORDER TO OBTAIN THE REQUIRED MARGINS, SOME STATEMENTS WERE
PRINTED ON MORE THAN ONE LINE. IN THE ACTUAL PROGRAM, EACH OF THESE WOULD BE
LISTED ON ONE LINE OR BE WRITTEN WITH THE APPROPRIATE CONTINUATION MARKS.

```

10.5  NID=NID+1
      INPUT LINE ID$(NID)
      IF LEN(ID$(NID)) > 0 THEN 10.5
      NID=NID-1 :PRINT
REM   ENTER DESCRIPTION OF THE CURVE FITTED EQUATION
      INPUT "NUMBER OF INDEPENDENT VARIABLES =";NVARI
      INPUT "HIGHEST EXPONENT OF X =";HEX
      IF NVARI=1 THEN 11
      INPUT "HIGHEST EXPONENT OF Y =";HEY
      IF NVARI=2 THEN 11
      INPUT "HIGHEST EXPONENT OF Z =";HEZ
      IF NVARI=3 THEN 11
      INPUT "HIGHEST EXPONENT OF U =";HEU
      IF NVARI=4 THEN 11
      INPUT "HIGHEST EXPONENT OF V =";HEV
      IF NVARI=5 THEN 11
      INPUT "HIGHEST EXPONENT OF W =";HEW
11    I=1 :NX=0 :NY=0 :NZ=0 :NU=0 :NV=0 :NW=0
      FOR N=0 TO HEX
      PRINT "IS THE COEFFICIENT OF X**";N;"CONSTRAINED TO 0";
      INPUT C$
      IF C$="YES" THEN 12
      EX(I)=N :I=I+1
      NX=NX+1
12    NEXT N
      IF NVARI=1 THEN 20
      FOR N=1 TO HEY
      PRINT "IS THE COEFFICIENT OF Y**";N;"CONSTRAINED TO 0";
      INPUT C$
      IF C$="YES" THEN GOTO 13
      EX(I)=N :I=I+1
      NY=NY+1
13    NEXT N
      IF NVARI=2 THEN 20
      FOR N=1 TO HEZ
      PRINT "IS THE COEFFICIENT OF Z**";N;"CONSTRAINED TO 0";
      INPUT C$
      IF C$="YES" THEN GOTO 14
      EX(I)=N :I=I+1
      NZ=NZ+1
14    NEXT N
      IF NVARI=3 THEN 20
      FOR N=1 TO HEU
      PRINT "IS THE COEFFICIENT OF U**";N;"CONSTRAINED TO 0";
      INPUT C$
      IF C$="YES" THEN GOTO 15
      EX(I)=N :I=I+1
      NU=NU+1
15    NEXT N
      IF NVARI=4 THEN 20
      FOR N=1 TO HEV

```

```

PRINT "IS THE COEFFICIENT OF V**";N;"CONSTRAINED TO 0";
INPUT C$
IF C$="YES" THEN GOTO 16
EX(I)=N :I=I+1
NV=NV+1
16 NEXT N
IF NVARI=5 THEN 20
FOR N=1 TO HEW
PRINT "IS THE COEFFICIENT OF W**";N;"CONSTRAINED TO 0";
INPUT C$
IF C$="YES" THEN GOTO 17
EX(I)=N :I=I+1
NW=NW+1
17 NEXT N
20 NN=NX+NY+NZ+NU+NV+NW
INPUT "ARE THE DATA ON DISK ";FY$
IF FY$<>"YES" THEN 30

REM READ THE INPUT DATA FROM THE DISK
INPUT "ENTER THE FILE NAME ";FILENAME$
FILE FILENAME$
READ #1; NPTS
FOR N=1 TO NPTS
READ #1; X(N),X(N+NPTS),X(N+2*NPTS),X(N+3*NPTS),X(N+4*NPTS),X(N+5*NPTS
),F(N)
NEXT N
CLOSE 1
GOTO 40

REM ENTER NEW INPUT DATA IF IT IS NOT ON DISK
30 INPUT "ENTER THE NUMBER OF DATA POINTS ";NPTS
FOR N=1 TO NPTS
IF NVARI=1 THEN PRINT "N=";N;" ENTER X AND F(X) ";
IF NVARI=2 THEN PRINT "N=";N;" ENTER X, Y, AND F(XY) ";
IF NVARI=3 THEN PRINT "N=";N;" ENTER X, Y, Z, AND F(XYZ) ";
IF NVARI=4 THEN PRINT "N=";N;" ENTER X, Y, Z, U, AND F(XYZU) ";
IF NVARI=5 THEN PRINT "N=";N;" ENTER X, Y, Z, U, V, AND F(XYZUV) ";
IF NVARI=6 THEN PRINT "N=";N;" ENTER X, Y, Z, U, V, W, AND F(XYZUVW) ";
IF NVARI=1 THEN INPUT X(N),F(N)
IF NVARI=2 THEN INPUT X(N),X(N+NPTS),F(N)
IF NVARI=3 THEN INPUT X(N),X(N+NPTS),X(N+2*NPTS),F(N)
IF NVARI=4 THEN INPUT X(N),X(N+NPTS),X(N+2*NPTS),X(N+3*NPTS),F(N)
IF NVARI=5 THEN INPUT X(N),X(N+NPTS),X(N+2*NPTS),X(N+3*NPTS),X(N+4*NPT
S),F(N)
IF NVARI=6 THEN INPUT X(N),X(N+NPTS),X(N+2*NPTS),X(N+3*NPTS),X(N+4*NPT
S),X(N+5*NPTS),F(N)
NEXT N

REM THE NEW INPUT DATA MAY NOW BE STORED ON DISK
INPUT "DO YOU WANT TO SAVE THESE DATA ";FY$
IF FY$<>"YES" THEN 40

```

```

      INPUT "ENTER THE FILENAME ";FILENAME$
      FILE FILENAME$
      PRINT #1;NPTS
      FOR N=1 TO NPTS
      PRINT #1; X(N),X(N+NPTS),X(N+2*NPTS),X(N+3*NPTS),X(N+4*NPTS),X(N+5*NPTS),F(N)
      NEXT N
      CLOSE 1

REM   THIS ROUTINE ESTABLISHES THE ORIGIN OF THE INPUT DATA
40    X0=0 :Y0=0 :Z0=0 :U0=0 :V0=0 :W0=0
      INPUT "DO YOU WANT TO TRANSLATE THE ORIGIN ";K$
      IF K$<>"YES" THEN 50
      INPUT "X0 =";X0
      IF NVARI>1 THEN INPUT "Y0 =";Y0
      IF NVARI>2 THEN INPUT "Z0 =";Z0
      IF NVARI>3 THEN INPUT "U0 =";U0
      IF NVARI>4 THEN INPUT "V0 =";V0
      IF NVARI>5 THEN INPUT "W0 =";W0
      FOR N=1 TO NPTS
      X(N)=X(N)-X0
      X(N+NPTS)=X(N+NPTS)-Y0
      X(N+2*NPTS)=X(N+2*NPTS)-Z0
      X(N+3*NPTS)=X(N+3*NPTS)-U0
      X(N+4*NPTS)=X(N+4*NPTS)-V0
      X(N+5*NPTS)=X(N+5*NPTS)-W0
      NEXT N

REM   DO YOU WANT TO OUTPUT THE XTX AND IDENTITY MATRICES?
50    INPUT "DO YOU WANT TO PRINT THE MATRICES ";MATRIX$
      INPUT "DO YOU WANT THE PRINTER ON ";PRINT$
      IF PRINT$="YES" THEN LPRINTER
      FOR N=0 TO NID
      PRINT ID$(N)
      NEXT N
      IF FY$="YES" THEN PRINT "DATA FROM FILE - ";FILENAME$
      QY=NX+NY
      QZ=NX+NY+NZ
      QU=NX+NY+NZ+NU
      QV=NX+NY+NZ+NU+NV

REM   COMPUTE THE ELEMENTS OF THE XTX MATRIX
      FOR I=1 TO NN
      IF I<=NX THEN QI=0
      IF I>NX AND I<=QY THEN QI=NPTS
      IF I>QY AND I<=QZ THEN QI=2*NPTS
      IF I>QZ AND I<=QU THEN QI=3*NPTS
      IF I>QU AND I<=QV THEN QI=4*NPTS
      IF I>QV THEN QI=5*NPTS
      FOR J=1 TO NN
      IF J<=NX THEN QJ=0

```

```

      IF J>NX AND J<=QY THEN QJ=NPTS
      IF J>QY AND J<=QZ THEN QJ=2*NPTS
      IF J>QZ AND J<=QU THEN QJ=3*NPTS
      IF J>QU AND J<=QV THEN QJ=4*NPTS
      IF J>QV THEN QJ=5*NPTS
      XTX(I,J)=0.0
      FOR K=1 TO NPTS
REM      RAISE X(K+QI) TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRXI=1: GOTO 51
      PWRXI=X(K+QI)
      IF EX(I)=1 THEN GOTO 51
      FOR M=2 TO EX(I)
      PWRXI=PWRXI*X(K+QI)
      NEXT M
REM      RAISE X(K+QJ) TO THE EX(J) POWER
51      IF EX(J)=0 THEN PWRXJ=1: GOTO 52
      PWRXJ=X(K+QJ)
      IF EX(J)=1 THEN GOTO 52
      FOR M=2 TO EX(J)
      PWRXJ=PWRXJ*X(K+QJ)
      NEXT M
52      XTX(I,J)=XTX(I,J)+PWRXI*PWRXJ
      NEXT K
      XTX(J,I)=XTX(I,J)
      NEXT J
      NEXT I

REM      COMPUTE THE Z MATRIX WHICH IS THE XTX MATRIX TIMES THE A MATRIX
      FOR I=1 TO NN
      Z(I)=0
      IF I<=NX THEN QI=0
      IF I>NX AND I<=QY THEN QI=NPTS
      IF I>QY AND I<=QZ THEN QI=2*NPTS
      IF I>QZ AND I<=QU THEN QI=3*NPTS
      IF I>QU AND I<=QV THEN QI=4*NPTS
      IF I>QV THEN QI=5*NPTS
      FOR K=1 TO NPTS
REM      RAISE X(K+QI) TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRXI=1: GOTO 53
      PWRXI=X(K+QI)
      IF EX(I)=1 THEN GOTO 53
      FOR M=2 TO EX(I)
      PWRXI=PWRXI*X(K+QI)
      NEXT M
53      Z(I)=Z(I)+PWRXI*F(K)
      NEXT K
      NEXT I

REM      DUPLICATE THE XTX MATRIX
      FOR I=1 TO NN
      FOR J=1 TO NN

```

```

      B(I,J)=XTX(I,J)
    NEXT J
  NEXT I
  IF MATRIX$<>"YES" THEN 190

REM   DISPLAY THE MATRICES
  IF PRINT$<>"YES" THEN GOSUB 900
  PRINT TAB(6);"THIS IS THE XT TIMES X MATRIX"
  FOR I=1 TO NN
    FOR J=1 TO NN
      PRNT(J)=XTX(I,J)
    NEXT J
    GOSUB 5000      REM   SELECT THE PROPER PRINT FORMAT
  NEXT I
  PRINT
  PRINT TAB(6);"THIS IS THE Z MATRIX"
  FOR I=1 TO NN
    PRINT USING "-#.#####^"; Z(I)
  NEXT I
  PRINT

REM   INVERT THE MATRIX
  GOSUB 3000
  IF MATRIX$<>"YES" THEN 200

REM   DISPLAY THE INVERTED MATRIX
  PRINT TAB(6);"THIS IS THE INVERSE OF THE ABOVE MATRIX"
  FOR I=1 TO NN
    FOR J=1 TO NN
      PRNT(J)=XTX(I,J)
    NEXT J
    GOSUB 5000      REM   SELECT THE PROPER PRINT FORMAT
  NEXT I
  PRINT

REM   COMPUTE THE PRODUCT OF THE MATRIX AND ITS INVERSE
  FOR I=1 TO NN
    FOR J=1 TO NN
      TEST(I,J)=0
      FOR K=1 TO NN
        TEST(I,J)=TEST(I,J) + XTX(I,K)*B(K,J)
      NEXT K
    NEXT J
  NEXT I

REM   PRINT THE MATRIX WHICH SHOULD BE THE IDENTITY MATRIX
  PRINT TAB(6);"THIS SHOULD BE THE IDENTITY MATRIX"
  FOR I=1 TO NN
    FOR J=1 TO NN
      PRNT(J)=TEST(I,J)
    NEXT J

```

```

      GOSUB 5000      REM  SELECT THE PROPER PRINT FORMAT
      NEXT I
      PRINT

REM    COMPUTE THE COEFFICIENTS
200   FOR I=1 TO NN
      A(I)=0.0
      FOR K=1 TO NN
        A(I)=A(I) + XTX(I,K) * Z(K)
      NEXT K
    NEXT I

REM    PRINT THE PROPER HEADING FOR THE DATA LISTING
      IF NVARI=1 THEN PRINT TAB(6);"X";TAB(19);"F(X)";TAB(34);"FCAL";TAB(44)
; "DIFFERENCE";TAB(57);"% ERROR"
      IF NVARI=2 THEN PRINT TAB(6);"X";TAB(19);"Y";TAB(31);"F(X,Y)";TAB(47);
"FCAL";TAB(57);"DIFFERENCE";TAB(70);"% ERROR"
      IF NVARI=3 THEN PRINT TAB(6);"X";TAB(19);"Y";TAB(32);"Z";TAB(43);"F(X,
Y,Z)";TAB(60);"FCAL";TAB(70);"DIFFERENCE";TAB(83);"% ERROR"
      IF NVARI=4 THEN PRINT TAB(6);"X";TAB(19);"Y";TAB(32);"Z";TAB(45);"U";T
AB(55);"F(X,Y,Z,U)";TAB(73);"FCAL";TAB(83);"DIFFERENCE";TAB(96);"% ERROR"
      IF NVARI=5 THEN PRINT TAB(6);"X";TAB(19);"Y";TAB(32);"Z";TAB(45);"U";T
AB(58);"V";TAB(67);"F(X,Y,Z,U,V)";TAB(86);"FCAL";TAB(96);"DIFFERENCE";TAB(109)
; "% ERROR"
      IF NVARI=6 THEN PRINT TAB(6);"X";TAB(19);"Y";TAB(32);"Z";TAB(45);"U";T
AB(58);"V";TAB(71);"W";TAB(79);"F(X,Y,Z,U,V,W)";TAB(99);"FCAL";TAB(109);"DIFFE
RENCE";TAB(122);"% ERROR"
      IF NVARI=1 THEN FOR$="-#.##### -#.##### -#.##### -#.##
#^ ^ ^ ^ -#.##^ ^ ^ ^"
      IF NVARI=2 THEN FOR$="-#.##### -#.##### -#.##### -#.####
##^ ^ ^ ^ -#.##### -#.##^ ^ ^ ^"
      IF NVARI=3 THEN FOR$="-#.##### -#.##### -#.##### -#.#####
^ ^ ^ ^ -#.##### -#.##### -#.##^ ^ ^ ^"
      IF NVARI=4 THEN FOR$="-#.##### -#.##### -#.##### -#.#####
^ ^ -#.##### -#.##### -#.##### -#.##^ ^ ^ ^"
      IF NVARI=5 THEN FOR$="-#.##### -#.##### -#.##### -#.#####
^ ^ -#.##### -#.##### -#.##### -#.##### -#.##^ ^ ^ ^"
      IF NVARI=6 THEN FOR$="-#.##### -#.##### -#.##### -#.#####
^ ^ -#.##### -#.##### -#.##### -#.##### -#.##^ ^ ^ ^"
      ^ ^ ^ ^"

REM    COMPUTE THE VARIANCE-COVARIANCE MATRIX
      SUMSIGMA=0.0
      SUMCAL=0.0
      SUMF=0.0
      FOR K=1 TO NPTS
        CAL=0
        FOR I=1 TO NN
          IF I<=NX THEN QI=0
          IF I>NX AND I<=QY THEN QI=NPTS
          IF I>QY AND I<=QZ THEN QI=2*NPTS

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      IF I>QZ AND I<=QU THEN QI=3*NPTS
      IF I>QU AND I<=QV THEN QI=4*NPTS
      IF I>QV THEN QI=5*NPTS
REM   RAISE X(K+QI) TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRXI=1: GOTO 210
      PWRXI=X(K+QI)
      IF EX(I)=1 THEN GOTO 210
      FOR M=2 TO EX(I)
      PWRXI=PWRXI*X(K+QI)
      NEXT M
210   CAL=CAL+A(I)*PWRXI
      NEXT I
      SUMSIGMA=SUMSIGMA + (F(K)-CAL) * (F(K)-CAL)

REM   PRINT THE DATA LISTING
      IF NVARI=1 THEN PRINT USING FOR$;X(K)+X0,F(K),CAL,CAL-F(K),100*(CAL-F(
K))/F(K)
      IF NVARI=2 THEN PRINT USING FOR$;X(K)+X0,X(K+NPTS)+Y0,F(K),CAL,CAL-F(K
),100*(CAL-F(K))/F(K)
      IF NVARI=3 THEN PRINT USING FOR$;X(K)+X0,X(K+NPTS)+Y0,X(K+2*NPTS)+Z0,F
(K),CAL,CAL-F(K),100*(CAL-F(K))/F(K)
      IF NVARI=4 THEN PRINT USING FOR$;X(K)+X0,X(K+NPTS)+Y0,X(K+2*NPTS)+Z0,X
(K+3*NPTS)+U0,F(K),CAL,CAL-F(K),100*(CAL-F(K))/F(K)
      IF NVARI=5 THEN PRINT USING FOR$;X(K)+X0,X(K+NPTS)+Y0,X(K+2*NPTS)+Z0,X
(K+3*NPTS)+U0,X(K+4*NPTS)+V0,F(K),CAL,CAL-F(K),100*(CAL-F(K))/F(K)
      IF NVARI=6 THEN PRINT USING FOR$;X(K)+X0,X(K+NPTS)+Y0,X(K+2*NPTS)+Z0,X
(K+3*NPTS)+U0,X(K+4*NPTS)+V0,X(K+5*NPTS)+W0,F(K),CAL,CAL-F(K),100*(CAL-F(K))/F
(K)
      SUMCAL=SUMCAL+CAL
      SUMF=SUMF+F(K)
      NEXT K
REM   CALCULATE THE STANDARD DEVIATION OF FIT
      SIGMAFIT=SQR(SUMSIGMA/ (NPTS-NN))
      AVCAL=SUMCAL/NPTS
      AVF=SUMF/NPTS

REM   CALCULATE THE ELEMENTS OF THE VARIANCE-COVARIANCE MATRIX
      FOR I=1 TO NN
      FOR J=1 TO NN
      VC(I,J)=XTX(I,J) * (SIGMAFIT * SIGMAFIT)
      NEXT J
      NEXT I
      PRINT

REM   COMPUTE VARIANCE OF ACTUAL AND CALCULATED DATA
      SUMDV=0.0
      SUMCV=0.0
      SUMSIGMA=0.0
      FOR K=1 TO NPTS
      CAL=0
      FOR I=1 TO NN

```

```

      IF I<=NX THEN QI=0
      IF I>NX AND I<=QY THEN QI=NPTS
      IF I>QY AND I<=QZ THEN QI=2*NPTS
      IF I>QZ AND I<=QU THEN QI=3*NPTS
      IF I>QU AND I<=QV THEN QI=4*NPTS
      IF I>QV THEN QI=5*NPTS
REM   RAISE X(K+QI) TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRXI=1: GOTO 215
      PWRXI=X(K+QI)
      IF EX(I)=1 THEN GOTO 215
      FOR M=2 TO EX(I)
      PWRXI=PWRXI*X(K+QI)
      NEXT M
215   CAL=CAL+A(I)*PWRXI
      NEXT I
      SUMDV=SUMDV+(F(K)-AVF)*(F(K)-AVF)
      SUMCV=SUMCV+(CAL-AVCAL)*(CAL-AVCAL)
      SUMSIGMA=SUMSIGMA+(F(K)-AVF)*(CAL-AVCAL)
      NEXT K
      DATVAR=SUMDV/(NPTS-NN)
      CALVAR=SUMCV/(NPTS-NN)
REM   COMPUTE THE COVARIANCE
      COVARIANCE=SUMSIGMA/(NPTS-NN)
REM   COMPUTE THE CORRELATION COEFFICIENT
      CORCOEF=COVARIANCE/(SQR(DATVAR)*SQR(CALVAR))

REM   DISPLAY THE RESULTS OF THE CURVE FIT
220  PRINT TAB(6);"THESE ARE THE LEAST SQUARES COEFFICIENTS"
      PRINT TAB(42);"ERROR";TAB(60);"% ERROR"
      FOR I=1 TO NN
REM   CALCULATE THE ERROR FOR EACH COEFFICIENT
      SIGMA=SQR(ABS(VC(I,I)))
REM   CALCULATE THE PERCENT ERROR FOR EACH COEFFICIENT
      PERCENT=ABS(SIGMA/A(I)) * 100.0
      IF I<=NX THEN PRINT "COEFFICIENT A";EX(I);" =";A(I);TAB(37);SIGMA;TAB(
57);PERCENT
      IF I>NX AND I<=QY THEN PRINT "COEFFICIENT B";EX(I);" =";A(I);TAB(37);S
IGMA;TAB(57);PERCENT
      IF I>QY AND I<=QZ THEN PRINT "COEFFICIENT C";EX(I);" =";A(I);TAB(37);S
IGMA;TAB(57);PERCENT
      IF I>QZ AND I<=QU THEN PRINT "COEFFICIENT D";EX(I);" =";A(I);TAB(37);S
IGMA;TAB(57);PERCENT
      IF I>QU AND I<=QV THEN PRINT "COEFFICIENT E";EX(I);" =";A(I);TAB(37);S
IGMA;TAB(57);PERCENT
      IF I>QV THEN PRINT "COEFFICIENT F";EX(I);" =";A(I);TAB(37);SIGMA;TAB(5
7);PERCENT
      NEXT I
      PRINT
      PRINT TAB(6);"STANDARD DEVIATION OF FIT =";SIGMAFIT
      PRINT TAB(6);"COVARIANCE = ";COVARIANCE
      PRINT TAB(6);"VARIANCE OF ACTUAL DATA = ";DATVAR

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PRINT TAB(6);"VARIANCE OF CURVE FITTED DATA = ";CALVAR
PRINT TAB(6);"CORRELATION COEFFICIENT = ";CORCOEF
PRINT

REM    COMPUTE CORRELATION MATRIX
FOR I=1 TO NN
FOR J=1 TO NN
IF J=I THEN 225
XTX(I,J)=XTX(I,J) / SQR(ABS(XTX(I,I)*XTX(J,J)))
225  NEXT J
NEXT I
FOR I=1 TO NN
XTX(I,I)=1.0
NEXT I
IF MATRIX$ <> "YES" THEN 226

REM    PRINT THE VARIANCE-COVARIANCE MATRIX
PRINT TAB(6);"THIS IS THE VARIANCE-COVARIANCE MATRIX"
FOR I=1 TO NN
FOR J=1 TO NN
PRNT(J)=VC(I,J)
NEXT J
GOSUB 5000      REM    SELECT THE PROPER PRINT FORMAT
NEXT I
PRINT

REM    PRINT THE CORRELATION MATRIX
226  PRINT TAB(6);"THIS IS THE CORRELATION MATRIX"
FOR I=1 TO NN
FOR J=1 TO NN
PRNT(J)=XTX(I,J)
NEXT J
GOSUB 5000      REM    SELECT THE PROPER PRINT FORMAT
NEXT I
PRINT

REM    DO GAUSS-JORDON SOLUTION FOR COMPARISON
FOR I=1 TO NN
FOR J=1 TO NN
XTX(I,J)=B(I,J)
NEXT J
NEXT I
NP=NN+1
FOR I=1 TO NN
XTX(I,NP)=Z(I)
NEXT I
GOSUB 4000      REM GAUSS-JORDAN ROUTINE
PRINT TAB(6);"COEFFICIENTS FROM GAUSS-JORDAN ROUTINE"
FOR I=1 TO NN
IF I<=NX THEN PRINT "COEFFICIENT A";EX(I);" =";AA(I)
IF I>NX AND I<=QY THEN PRINT "COEFFICIENT B";EX(I);" =";AA(I)

```

```

IF I>QY AND I<=QZ THEN PRINT "COEFFICIENT C";EX(I);" =";AA(I)
IF I>QZ AND I<=QU THEN PRINT "COEFFICIENT D";EX(I);" =";AA(I)
IF I>QU AND I<=QV THEN PRINT "COEFFICIENT E";EX(I);" =";AA(I)
IF I>QV THEN PRINT "COEFFICIENT F";EX(I);" =";AA(I)
NEXT I
PRINT

REM      DO INTERPOLATION IF DESIRED
230      CONSOLE
      INPUT "DO YOU WANT TO INTERPOLATE ";K$
      IF K$<>"YES" THEN GOTO 10      REM 10 RESTARTS THE PROGRAM
      IF PRINT$="YES" THEN LPRINTER
      INPUT "VALUE OF X =";XX
      IF NVARI>1 THEN INPUT "VALUE OF Y =";YY
      IF NVARI>2 THEN INPUT "VALUE OF Z =";ZZ
      IF NVARI>3 THEN INPUT "VALUE OF U =";UU
      IF NVARI>4 THEN INPUT "VALUE OF V =";VV
      IF NVARI>5 THEN INPUT "VALUE OF W =";WW
      XX=XX-X0
      YY=YY-Y0
      ZZ=ZZ-Z0
      UU=UU-U0
      VV=VV-V0
      WW=WW-W0
      CAL=0.0
      FOR I=1 TO NX
REM      RAISE XX TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRXX=1: GOTO 231
      PWRXX=XX
      IF EX(I)=1 THEN GOTO 231
      FOR M=2 TO EX(I)
      PWRXX=PWRXX * XX
      NEXT M
231      CAL=CAL+A(I)*PWRXX
      NEXT I
      IF NVARI=1 THEN GOTO 235
      FOR I=NX+1 TO QY
REM      RAISE YY TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRYY=1: GOTO 232
      PWRYY=YY
      IF EX(I)=1 THEN GOTO 232
      FOR M=2 TO EX(I)
      PWRYY=PWRYY * YY
      NEXT M
232      CAL=CAL+A(I)*PWRYY
      NEXT I
      IF NVARI=2 THEN GOTO 235
      FOR I=QY+1 TO QZ
REM      RAISE ZZ TO THE EX(I) POWER
      IF EX(I)=0 THEN PWRZZ=1: GOTO 233
      PWRZZ=ZZ

```

```

        IF EX(I)=1 THEN GOTO 233
        FOR M=2 TO EX(I)
        PWRZZ=PWRZZ * ZZ
        NEXT M
233    CAL=CAL+A(I)*PWRZZ
        NEXT I
        IF NVARI=3 THEN GOTO 235
        FOR I=QZ+1 TO QU
        REM    RAISE UU TO THE EX(I) POWER
        IF EX(I)=0 THEN PWRUU=1: GOTO 234
        PWRUU=UU
        IF EX(I)=1 THEN GOTO 234
        FOR M=2 TO EX(I)
        PWRUU=PWRUU * UU
        NEXT M
234    CAL=CAL+A(I)*PWRUU
        NEXT I
        IF NVARI=4 THEN GOTO 235
        FOR I=QU+1 TO QV
        REM    RAISE VV TO THE EX(I) POWER
        IF EX(I)=0 THEN PWRVV=1: GOTO 234.1
        PWRVV=VV
        IF EX(I)=1 THEN GOTO 234.1
        FOR M=2 TO EX(I)
        PWRVV=PWRVV*VV
        NEXT M
234.1  CAL=CAL+A(I)*PWRVV
        NEXT I
        IF NVARI=5 THEN GOTO 235
        FOR I=QV TO NN
        REM    RAISE WW TO THE EX(I) POWER
        IF EX(I)=0 THEN PWRWW=1: GOTO 234.2
        PWRWW=WW
        IF EX(I)=1 THEN GOTO 234.2
        FOR M=2 TO EX(I)
        PWRWW=PWRWW*WW
        NEXT M
234.2  CAL=CAL+A(I)*PWRWW
        NEXT I

        REM    PRINT THE RESULTS OF THE INTERPOLATION
235    IF NVARI=1 THEN PRINT "INTERPOLATED VALUE FOR X =";XX;"IS";CAL
        IF NVARI=2 THEN PRINT "INTERPOLATED VALUE FOR X =";XX;" Y =";YY;"IS";
        CAL
        IF NVARI=3 THEN PRINT "INTERPOLATED VALUE FOR X =";XX;" Y =";YY;" Z
        =";ZZ;"IS";CAL
        IF NVARI=4 THEN PRINT "INTERPOLATED VALUE FOR X =";XX;" Y =";YY;" Z
        =";ZZ;" U =";UU;"IS";CAL
        IF NVARI=5 THEN PRINT "INTERPOLATED VALUE FOR X =";XX;" Y =";YY;" Z
        =";ZZ;" U =";UU;" V =";VV;"IS";CAL
        IF NVARI=6 THEN PRINT "INTERPOLATED VALUE FOR X =";XX;" Y =";YY;" Z

```

```
=";ZZ;"; U=";UU;"; V=";VV;"; W=";WW;"IS";CAL
GOTO 230
```

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900    REM  COME HERE TO CLEAR THE TERMINAL SCREEN
      PRINT CHR$(12)
      FOR N=1 TO 20
      NEXT N
      RETURN
```

```
3000   REM    MATRIX INVERSION SUBROUTINE
      SUM=0
      FOR N=1 TO NN
      LOCATE (N,3)=0
      SUM=SUM + XTX(N,N)
      NEXT N
      ZERO=1E-20 * NN / SUM
      FOR N=1 TO NN
      AMAX=0
      FOR I=1 TO NN
      IF LOCATE(I,3) <> 0 THEN 3020
      FOR J=1 TO NN
      IF LOCATE(J,3) <> 0 THEN 3010
      IF ABS(XTX(I,J)) < AMAX THEN 3010
      AMAX=ABS(XTX(I,J))
      IROW=I
      JCOL=J
3010   NEXT J
3020   NEXT I
      IF AMAX < ZERO THEN PRINT "SINGULAR MATRIX" : RETURN
      LOCATE(N,1)=IROW
      LOCATE(N,2)=JCOL
      LOCATE(JCOL,3)=1
      IF IROW=JCOL THEN 3030
      FOR J=1 TO NN
      SWAP=XTX(IROW,J)
      XTX(IROW,J)=XTX(JCOL,J)
      XTX(JCOL,J)=SWAP
      NEXT J
3030   PIVOT=XTX(JCOL,JCOL)
      XTX(JCOL,JCOL)=1.0
      FOR J=1 TO NN
      XTX(JCOL,J)=XTX(JCOL,J) / PIVOT
      NEXT J
      FOR I=1 TO NN
      IF I=JCOL THEN 3040
      FF=XTX(I,JCOL)
      XTX(I,JCOL)=0
      FOR J=1 TO NN
      XTX(I,J)=XTX(I,J) - FF*XTX(JCOL,J)
      NEXT J
3040   NEXT I
```

```

NEXT N
FOR N=1 TO NN
L=NN-N+1
IF LOCATE(L,1)=LOCATE(L,2) THEN 3050
IROW=LOCATE(L,1)
JCOL=LOCATE(L,2)
FOR K=1 TO NN
SWAP=XTX(K,IROW)
XTX(K,IROW)=XTX(K,JCOL)
XTX(K,JCOL)=SWAP
NEXT K
3050 NEXT N
RETURN

REM GAUSS-JORDAN ROUTINE
4000 FOR I=1 TO NN
CK(I)=0
NEXT I
FOR I=1 TO NN
IP=I+1
AMAX=0
FOR K=1 TO NN
IF AMAX>ABS(XTX(K,I)) THEN 4010
IF CK(K)<>0 THEN 4010
LOC(I)=K
AMAX=ABS(XTX(K,I))
4010 NEXT K
IF AMAX<1E-20 THEN PRINT "NO SOLUTION" :RETURN
L=LOC(I)
CK(L)=1
FOR J=1 TO NN
IF L=J THEN 4020
FG=-XTX(J,I) / XTX(L,I)
FOR K=IP TO NP
XTX(J,K)=XTX(J,K) + FG*XTX(L,K)
NEXT K
4020 NEXT J
NEXT I
FOR I=1 TO NN
L=LOC(I)
AA(I)=XTX(L,NP) / XTX(L,I)
NEXT I
RETURN

REM MATRIX PRINT SUBROUTINE
5000 FOR$ = "-#.#####^***"
IF NN=1 THEN PRINT USING FOR$;PRNT(1)
IF NN=2 THEN PRINT USING FOR$;PRNT(1),PRNT(2)
IF NN=3 THEN PRINT USING FOR$;PRNT(1),PRNT(2),PRNT(3)
IF NN=4 THEN PRINT USING FOR$;PRNT(1),PRNT(2),PRNT(3),PRNT(4)
IF NN=5 THEN PRINT USING FOR$;PRNT(1),PRNT(2),PRNT(3),PRNT(4),PRNT(5)

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```
      IF NN=6 THEN PRINT USING FOR$;PRNT(1),PRNT(2),PRNT(3),PRNT(4),PRNT(5),  
PRNT(6)  
      IF NN=7 THEN PRINT USING FOR$;PRNT(1),PRNT(2),PRNT(3),PRNT(4),PRNT(5),  
PRNT(6),PRNT(7)  
      RETURN  
      END
```

APPENDIX C

REGRESSION ANALYSIS COMPUTER PROGRAM OUTPUT

MULTIVARIATE POLYNOMIAL REGRESSION

THIS PROGRAM FITS DATA TO POLYNOMIALS OF THE FORM

$$F = A_0 + A_1X + A_2X^2 + \dots + A_NX^N + B_1Y + B_2Y^2 + \dots + B_NY^N + C_1Z + C_2Z^2 + \dots + C_NZ^N + D_1U + D_2U^2 + \dots + D_NU^N + E_1V + E_2V^2 + \dots + E_NV^N + F_1W + F_2W^2 + \dots + F_NW^N$$

FREE SPACE = 6836

ENTER ID STRINGS

? 200S.

? N = 0.75

? {LN (KLA) - N * LN (L)} vs LN (PFEED), LN {(1-F)/F}, and LN (L).

? JANUARY 26, 1980.

?

NUMBER OF INDEPENDENT VARIABLES = 3

HIGHEST EXPONENT OF X = 1

HIGHEST EXPONENT OF Y = 1

HIGHEST EXPONENT OF Z = 1

IS THE COEFFICIENT OF X** 0 CONSTRAINED TO 0? NO

IS THE COEFFICIENT OF X** 1 CONSTRAINED TO 0? NO

IS THE COEFFICIENT OF Y** 1 CONSTRAINED TO 0? NO

IS THE COEFFICIENT OF Z** 1 CONSTRAINED TO 0? NO

ARE THE DATA ON DISK NO

ENTER THE NUMBER OF DATA POINTS 8

N= 1 ENTER X, Y, Z, AND F(XYZ) ? 3.39,0.597,8.98,-5.1

N= 2 ENTER X, Y, Z, AND F(XYZ) ? 3.09,0.479,7.6,-4.04

N= 3 ENTER X, Y, Z, AND F(XYZ) ? 4.12,0.641,8.98,-4.28

N= 4 ENTER X, Y, Z, AND F(XYZ) ? 2.95,0.777,8.97,-5.139

N= 5 ENTER X, Y, Z, AND F(XYZ) ? 3.31,0.241,8.98,-4.783

N= 6 ENTER X, Y, Z, AND F(XYZ) ? 2.66,0.437,7.57,-4.414

N= 7 ENTER X, Y, Z, AND F(XYZ) ? 2.69,0.847,7.97,-4.865

N= 8 ENTER X, Y, Z, AND F(XYZ) ? 3.56,0.777,9.61,-5.314

DO YOU WANT TO SAVE THESE DATA YES

1

NOTE THAT IN ORDER TO OBTAIN THE REQUIRED MARGINS, THE PRINTOUT VALUES FOR THE X, Y, AND Z DATA WERE TYPED WITHOUT THEIR ORIGINAL SCIENTIFIC NOTATION (i.e. 5.9700E-01 = .59700).

ENTER THE FILENAME 200S7PFL.DAT

DO YOU WANT TO TRANSLATE THE ORIGIN NO

DO YOU WANT TO PRINT THE MATRICES YES

DO YOU WANT THE PRINTER ON YES

200S.

N = 0.75

{LN (KLA) - N * LN (L)} vs LN (PFEED), LN {(1-F)/F}, and LN (L).

JANUARY 26, 1980.

DATA FROM FILE - 200S7PFL.DAT

THIS IS THE XT TIMES X MATRIX

8.00000E 00	2.57700E 01	4.79600E 00	6.86600E 01
2.57700E 01	8.46585E 01	1.54417E 01	2.22896E 02
4.79600E 00	1.54417E 01	3.17065E 00	4.14172E 01
6.86600E 01	2.22896E 02	4.14172E 01	5.93320E 02

THIS IS THE Z MATRIX

-3.79350E 01

-1.22144E 02

-2.30476E 01

-3.27240E 02

THIS IS THE INVERSE OF THE ABOVE MATRIX

1.85437E 01	4.80689E-01	-5.53515E-03	-2.32610E 00
4.80689E-01	1.15913E 00	4.82952E-01	-5.24795E-01
-5.53515E-03	4.82952E-01	3.78146E 00	-4.44761E-01
-2.32610E 00	-5.24795E-01	-4.44761E-01	4.99066E-01

THIS SHOULD BE THE IDENTITY MATRIX

1.00000E 00	0.00000E 00	1.00000E-12	1.00000E-10
0.00000E 00	1.00000E 00	-1.00000E-12	1.00000E-11
-3.00000E-12	-7.00000E-12	1.00000E 00	0.00000E 00
0.00000E 00	0.00000E 00	0.00000E 00	1.00000E 00

X	Y	Z	F(X,Y,Z)	FCAL	DIFFERENCE	% ERROR
3.3900	.59700	8.9800	-5.100000E 00	-4.895117E 00	2.049E-01	-4.02E 00
3.0900	.47900	7.6000	-4.040000E 00	-4.088496E 00	-4.850E-02	1.20E 00
4.1200	.64100	8.9800	-4.280000E 00	-4.337025E 00	-5.702E-02	1.33E 00
2.9500	.77700	8.9700	-5.139000E 00	-5.304750E 00	-1.657E-01	3.23E 00
3.3100	.24100	8.9800	-4.783000E 00	-4.819437E 00	-3.644E-02	7.62E-01
2.6600	.43700	7.5700	-4.414000E 00	-4.389294E 00	2.471E-02	-5.60E-01
2.6900	.84700	7.9700	-4.865000E 00	-4.814413E 00	5.059E-02	-1.04E 00
3.5600	.77700	9.6100	-5.314000E 00	-5.286467E 00	2.753E-02	-5.18E-01

THESE ARE THE LEAST SQUARES COEFFICIENTS

		ERROR	%ERROR
COEFFICIENT A 0	==0.84581431732	0.610168179055	72.1397316835
COEFFICIENT A 1	= 0.78799648424	0.152551663426	19.359434525
COEFFICIENT B 1	==0.38966176524	0.275538120871	70.7121266315
COEFFICIENT C 1	==0.7224925289	0.10009919764	13.8547034933

STANDARD DEVIATION OF FIT = 0.141694112725

COVARIANCE = 0.340822497168
 VARIANCE OF ACTUAL DATA = 0.36089971875
 VARIANCE OF CURVE FITTED DATA = 0.340822497167
 CORRELATION COEFFICIENT = 0.971786485889

THIS IS THE VARIANCE-COVARIANCE MATRIX

3.72305E-01	9.65089E-03	-1.11130E-04	-4.67016E-02
9.65089E-03	2.32720E-02	9.69634E-03	-1.05364E-02
-1.11130E-04	9.69634E-03	7.59213E-02	-8.92956E-03
-4.67016E-02	-1.05364E-02	-8.92956E-03	1.00198E-02

THIS IS THE CORRELATION MATRIX

1.00000E 00	1.03681E-01	-6.61000E-04	-7.64631E-01
1.03681E-01	1.00000E 00	2.30680E-01	-6.89994E-01
-6.61000E-04	2.30680E-01	1.00000E 00	-3.23756E-01
-7.64631E-01	-6.89994E-01	-3.23756E-01	1.00000E 00

COEFFICIENTS FROM GAUSS-JORDAN ROUTINE

COEFFICIENT A 0 = -0.845814317292
 COEFFICIENT A 1 = 0.787996484242
 COEFFICIENT B 1 = -0.389661765247
 COEFFICIENT C 1 = -0.722492528903

DO YOU WISH TO INTERPOLATE YES
 VALUE OF X = 4.0
 VALUE OF Y = 0.5
 VALUE OF Z = 8.0
 INTERPOLATED VALUE FOR X = 4 ; Y = 0.5 ; Z = 8 IS -3.66859949418
 DO YOU WISH TO INTERPOLATE NO

APPENDIX D

RELATIONSHIP BETWEEN x and f

The relationship between x , the weight ratio of CO_2 in the liquid, and f , the fraction conversion to KHCO_3 , can be expressed in terms of x^+ , the mass of CO_2 absorbed at complete conversion of K_2CO_3 to KHCO_3 , per unit mass of original, unreacted solution. x^+ is a function of the equivalent weight percent of K_2CO_3 (K) by the following argument. In one milliliter of K_2CO_3 solution, of density ρ ,

$$\text{the mass of } \text{K}_2\text{CO}_3 = (K) \rho / 100, \quad (48)$$

and moles of K_2CO_3 equal this quantity divided by the molecular weight of K_2CO_3 , 138.2 gm/mole, so that the mass of CO_2 which can be absorbed is equal to:

$$K \rho (\text{molecular weight of } \text{CO}_2) / (100)(138.2). \quad (49)$$

Utilizing these quantities one can write x^+ as:

$$\begin{aligned} x^+ &= (K) (\rho) (\text{molecular weight of } \text{CO}_2) / ((100) (138.2) (\rho)) \\ &= (K) (\text{molecular weight of } \text{CO}_2) / ((100) (138.2)) \end{aligned} \quad (50)$$

The original weight ratio of CO_2 in solution, x^+ , times whatever fraction enters into solution (i.e., converted to KHCO_3), f , will equal the weight ratio of CO_2 in solution, x . Mathematically this is expressed in equation (51):

$$x = (f) (x^+). \quad (51)$$

For $f=1$, x^+ corresponds to all of the K_2CO_3 going to $KHCO_3$, so that $x = x^+$.

APPENDIX E

COMPUTER PROGRAM FOR HEIGHT CALCULATION

(FORTRAN)

THIS PROGRAM CALCULATES A TOWER HEIGHT NECESSARY FOR THE
PURIFICATION LEVEL OF CO2 SPECIFIED.
THE PROGRAM WAS WRITTEN BY DR. LLOYD CRAWFORD, AND REVISED
BY MICHELE MACARAEG.

```

PARAMETER LNG=100,NXP=6
REAL NUM
DIMENSION DAT(12),OUT(13),QL(LNG),TT(LNG),TB(LNG),VF(LNG),
1VS(LNG),G(LNG),PK(LNG),FR(LNG),FS(LNG),HT(LNG),
2FRE(LNG),FSE(LNG),P(LNG),ZERO(13),QLL(LNG),GG(LNG)
3,F(0:10),Y(0:10),YMOL(0:10),EMOL(0:10),T(0:10),YE(0:10)
4,TR(LNG),DN(LNG),DATA(12),XP(NXP)
LOGICAL MORE,TMORE,LG(LNG)
EQUIVALENCE (A,XP(1)),(B,XP(2)),(CFEXP,XP(3))
1,(EXPK,XP(4)),(CTT,XP(5)),(PEXP,XP(6))
DATA ZERO/13*0./
II=0
JJ=II
OPEN(UNIT=1,NAME='TOWER.DAT',TYPE='OLD',READONLY)
OPEN(UNIT=2,NAME='CALC.DAT',CARRIAGECONTROL='LIST')
READ (1,*,END=2) A,B,CFEXP,EXPK,CTT,PEXP
WRITE (2,32) A,B,CFEXP,EXPK,CTT,PEXP
32 FORMAT(1X,F8.2,F8.2,4F8.2)
MORE=.FALSE.
3 READ(1,*,END=2) DAT
IF(DAT(1).EQ.0.) MORE=.TRUE.
TMORE=MORE
IF(MORE) GO TO 2
II=II+1

INPUT DATA

QL(II)=DAT(1)
TT(II)=((DAT(2)-32.)/1.8)+273.
TB(II)=((DAT(3)-32.)/1.8)+273.
IF(DAT(3).EQ.0.) TB(II)=TT(II)
VF(II)=DAT(4)/100.
VS(II)=DAT(5)/100.

```

```

G(II)=DAT(6)
PK(II)=DAT(7)/100.
FR(II)=DAT(8)
FS(II)=DAT(9)
P(II)=DAT(10)
Y(10)=VF(II)/(1.-VF(II))
NUM=((QL(II)*(FS(II)-FR(II))*(.31845*PK(II)))/(44.*G(II)*(1.-
?VF(II))))-Y(10)
C
C CALCULATE EXIT CO2 MOLE RATIO
C
VS(II)=NUM/(NUM-1.)
QLL(II)=DAT(11)
GG(II)=DAT(12)
DAT(3)=0.
GO TO 3
2 CONTINUE
IF(II.EQ.JJ) STOP 'ABNORMAL ENDING'
JJP1=JJ+1
DO 4 I=JJP1,II
LG(I)=.FALSE.
C
C CALCULATE EQUILIBRIUM VALUES FOR FRACTION CONVERSION TO KHC03
C
CALL FE(P(I),VS(I),PK(I),TT(I),FRE(I))
CALL FE(P(I),VF(I),PK(I),TB(I),FSE(I))
C
C CALCULATE MOLES OF CO2 TRANSFERRED , AND K2CO3 SOLUTION'S
C DENSITY.
C
TRAN=GG(I)*(VF(I)-VS(I)*(1.-VF(I))/(1.-VS(I)))/359.
DEN=.9982+PK(I)*(.87625+PK(I)*.40875)
DN(I)=DEN
TR(I)=TRAN
IF (FS(I).GT.1.)LG(I)=.TRUE.
D1=FRE(I)-FR(I)
D2=FSE(I)-FS(I)
C
C CHECK FOR NEGATIVE DRIVING FORCE.
C
IF ((D1.GE.0.).AND.(D2.GE.0.)) GO TO 199
WRITE (2,99) FRE(I),FSE(I)
99 FORMAT (1X,F8.4,5X,F8.4)
199 IF(D1.LE.0..OR.D2.LE.0.) LG(I)=.TRUE.
IF(LG(I)) GO TO 4
TEMP=D2/D1
IF(TEMP.LT..9.OR.TEMP.GT.1.1) GO TO 5
DRIVE=.5*(D1+D2)
GO TO 6
5 DRIVE=(D2-D1)/LOG(TEMP)
6 CONTINUE
4 CONTINUE
C
C OUTPUT

```

C

```
DO 7 I=JJP1,II
OUT(1)=QL(I)
QL(I)=OUT(1)
OUT(2)=TT(I)
OUT(3)=TB(I)
OUT(4)=VF(I)
OUT(5)=VS(I)
OUT(6)=G(I)
OUT(7)=PK(I)
OUT(8)=FR(I)
OUT(9)=FS(I)
OUT(10)=P(I)
OUT(11)=OUT(10)
IF (LG(I)) GO TO 23
```

C

C

C

CALCULATE TOWER HEIGHT.

CALL

```
1HTCAL(HT,VS,VF,FS,FR,TB,TT,P,PK,QL,TR,XP,I,LNG,NXP)
OUT(11)=HT(I)
23 OUT(12)=TR(I)
OUT(13)=DN(I)
WRITE(2,8) OUT,LG(I)
7 CONTINUE
WRITE(2,8) ZERO,.TRUE.
9 FORMAT(F8.6,F8.4)
8 FORMAT(F8.2,2(1XF6.1),2(1XF6.4),1XF7.1,3(1XF6.4),1XF6.1,1(1XF8.2),
11XF7.4,1XF7.5,
21XL1)
STOP
END
```

C

C

C

C

SUBROUTINE FOR CALCULATING EQUILIBRIUM VALUES OF FRACTION
CONVERSION TO KHC03.

```
SUBROUTINE FE(P,V,PK,T,X)
TEMP=((1388.-17487.*PK)/T)+44.9*PK
TEMP=(P*V/(PK**.75))*EXP(-TEMP)
X=-TEMP+SQRT(TEMP*(4.+TEMP))
X=.5*X
RETURN
END
```

C

C

C

SUBROUTINE TO CALCULATE ABSORPTION TOWER HEIGHT.

SUBROUTINE

```
1HTCAL(HT,VS,VF,FS,FR,TB,TT,P,PK,QL,TR,XP,I,LNG,NXP)
DIMENSION QL(LNG),TT(LNG),TB(LNG),VF(LNG),
1VS(LNG),PK(LNG),FR(LNG),FS(LNG),HT(LNG),
2P(LNG),ZERO(13)
3,F(0:10),Y(0:10),YMOL(0:10),EMOL(0:10),T(0:10),YE(0:10)
4,TR(LNG),DATA(12),XP(NXP)
GAV=.015079
```

```

A=XP(1)
B=XP(2)
CFEXP=XP(3)
EXPK=XP(4)
CTT=XP(5)
PEXP=XP(6)
Y(0)=VS(I)/(1.-VS(I))
IF(Y(0).GE.0.)GOTO 555
WRITE (2,55) VS(I)
55 FORMAT (1X,F8.4)
555 Y(10)=VF(I)/(1.-VF(I))
DELY=(Y(10)-Y(0))/10.
DELF=(FS(I)-FR(I))/10.
DELT=(TB(I)-TT(I))/10.
DO 14 J=0,10
AJ=J
Y(J)=Y(0)+AJ*DELY
F(J)=FR(I)+AJ*DELF
T(J)=TT(I)+AJ*DELT
YMOL(J)=Y(J)/(1.+Y(J))
CALL FE(P(I),YMOL(J),PK(I),T(J),EMOL(J))
14 CONTINUE
SUMM=0.
PP=P(I)*YMOL(0)
CC=1.-F(0)
TTT=T(0)/383.
T2=GAV*(F(0)**(A))*(TTT**(CTT))/((PP**(PEXP))*(CC**(CFEXP)))
T2=1./((EMOL(0)-F(0))*T2)
DO 22 J=1,10
T1=T2
CC=1.-F(J)
PP=P(I)*YMOL(J)
TTT=T(J)/383.
T2=GAV*(F(J)**(A))*(TTT**(CTT))/((PP**(PEXP))*(CC**(CFEXP)))
T2=1./((EMOL(J)-F(J))*T2)
SUMM=SUMM+(T1+T2)*.5
22 CONTINUE
SUMM=SUMM*DELF/44.
HT(I)=(SUMM*(PK(I)**(EXPK)))/(QL(I)**(B-1.))
RETURN
END

```

APPENDIX F

DATA UTILIZED IN THE MASS TRANSFER STUDY

The data from the USBM study (6) utilized in minimizing the standard deviation on GAV is displayed in Table 4. The entries correspond to the following quantities: liquid rate (QL) in gal/hr, temperature at the top of the column (TT) in degrees F, temperature at the bottom of the column (TB) in degrees F, volume percent of CO₂ (VF) at the entrance, volume percent of CO₂ (VS) at the exit, gas rate (GG) in SCF/hr, weight percent of K₂CO₃ (PK), fraction conversion of K₂CO₃ to KHCO₃ at the column entrance (FR), fraction conversion of K₂CO₃ to KHCO₃ at the column exit (FS), system pressure (P) in psi, and identification of the table number and particular run as cited in the USBM report. Notation for this last entry lists the table number followed by a dash and the particular run as labelled in the USBM study. For example, 17-S12 refers to Table 17, and case S12. The two numbers at the start of the table and between sets of data are cross-sectional area in square feet, and total volume of the column in cubic feet. Double commas indicate repetition of the preceding value in that case. A double comma at the end of a case refers to the same system pressure as the preceding case. The variable names given in parentheses for the data entries described above are as they appear in the program.

The exponents on fraction conversion to KHCO₃, liquid rate, one minus fraction conversion to KHCO₃, percent equivalent KHCO₃, temperature divided by 383, and partial pressure of CO₂ are given at the start of the input as 0.00, -.55, 1.65, .6, -6.25, and .05, respectively. The

succeeding line lists five quantities (in this case all are $-.5$), which are the amounts that the exponents will be perturbed in order to test the effect on GAV.

Table 4. Data Utilized in GAV Calculation

.0,-.55,1.65,.6,-6.25,.05
 -.05,-.05,-.05,-.05,-.05,-.05
 .181,.664
 123.,230.,,3.15,1.1,1453.,39.,.22,.24,315.,'17-SII'
 123.,233.,,8.3,4.75,1517.,38.9,.43,.47,, '17-SI3'
 ,232.,,16.6,10.4,1512.,37.,.58,.65,, '17-SI4'
 ,231.,,28.95,19.35,1511.,37.5,.59,.71,, '17-SI5'
 ,200.,,1.3,.3,1491.,39.,.17,.18,, '17-SI6'
 ,199.,,9.9,5.,1549.,39.,.33,.38,, '17-SI7'
 31.,201.,,7.3,4.8,1980.,,32,.445,, '17-SI8'
 123.,199.,,6.4,3.,1477.,37.5,.3,.33,, '17-SI11'
 ,,,9.1,5.05,1524.,39.,.42,.46,, '17-SI12'
 ,,,37.5,30.1,1470.,37.,.6,.705,, '17-SI15'
 0.,,,,,,,,,,
 .181,.664
 31.,230.,,4.65,2.95,1493.,40.5,.33,.4,315.,'17-SII1'
 46.,230.,,4.9,3.2,1502.,39.,.32,.37,, '17-SII2'
 61.5,230.,,6.1,3.,1494.,37.3,.28,.35,, '17-SII3'
 93.,228.,,7.1,3.2,1487.,41.,.27,.32,, '17-SII4'
 123.,231.,,7.3,3.1,1516.,38.3,.29,.34,, '17-SII5'
 260.,230.,,11.9,3.4,1494.,39.5,.32,.36,, '17-SII6'
 154.,230.,,10.1,2.9,1004.,42.,.35,.39,, '17-SII7'
 231.,,11.7,3.,1020.,38.5,.33,.36,, '17-SII8'
 308.,,11.85,2.9,1009.,39.3,.35,.37,, '17-SII9'
 325.,,11.3,3.,1017.,40.5,.32,.34,, '17-SII10'
 31.,200.,,4.75,3.1,1501.,34.8,.35,.435,, '17-SII11'
 46.,,4.9,2.95,1507.,35.4,.27,.33,, '17-SII12'
 231.,201.,,11.7,3.8,1015.,38.5,.3,.33,, '17-SII13'
 61.5,260.,,6.3,2.8,1517.,37.5,.3,.38,, '17-SII15'
 231.,,11.6,3.,1030.,39.,.31,.35,, '17-SII16'
 0.,,,,,,,,,,
 .07986,.72
 26.2,244.,243.,27.7,16.3,494.3,36.2,.32,.56,317.7,'1-6A'
 25.8,259.,245.,30.3,20.3,512.6,38.9,.325,.57,317.7,'1-6B'
 29.9,246.,243.,28.1,12.9,486.4,40.5,.30,.51,317.7,'1-7A'
 22.2,262.,274.,28.9,16.8,501.6,38.4,.30,.56,317.7,'1-8A'
 27.2,264.,277.,28.3,12.5,500.1,35.8,.3,.61,317.7,'1-8B'
 17.9,239.,243.,9.4,5.1,450.9,34.9,.53,.68,319.7,'1-2B'
 21.66,231.,248.,9.8,3.3,462.3,34.8,.49,.64,322.7,'1-3A1'
 15.21,230.,242.,11.4,7.,450.7,36.5,.56,.7,322.7,'1-3C1'
 15.7,226.,230.,11.4,5.7,467.6,33.,.51,.7,323.7,'1-3C2'
 25.8,236.,242.,11.,3.7,467.2,33.4,.52,.68,327.7,'1-4A1'
 34.96,239.,237.,9.2,3.,468.5,32.7,.53,.66,323.7,'1-4A2'

Table 4 (continued)

21.8,235.,246.,11.,3.6,450.9,32.9,.52,.7,322.7,'1-4B'
25.8,234.,241.,11.2,2.4,240.9,32.6,.53,.63,314.7,'1-5A'
0.,,,,,,,,,,
.181,5.43
55.,235.,248.,20.,2.5,1183.,37.5,.39,.74,314.7,'6-19A'
55.,238.,253.,19.9,1.8,1166.,39.,.39,.69,,,'6-19B'
55.,252.,273.,21.,1.9,1166.,37.5,.34,.71,,,'6-19'
55.,275.,287.,20.,1.8,1169.,39.,.28,.65,,,'6-19C'
50.,252.,268.,20.1,2.6,1228.,38.,.32,.69,,,'6-12A1'
55.,232.,248.,20.3,2.4,1220.,35.,.33,.67,,,'6-26A'
36.,257.,268.,15.6,5.7,1220.,41.5,.36,.61,,,'6-36A'
36.,280.,283.,15.7,5.2,1210.,43.5,.31,.57,,,'6-37A'
50.,234.,244.,16.5,.8,1207.,40.,.37,.64,,,'6-31C'
50.,257.,270.,15.5,.9,1200.,40.,.28,.58,,,'6-36D'
50.,280.,283.,16.1,.9,1185.,42.,.26,.53,,,'6-37D'
55.,250.,268.,20.1,1.7,1223.,40.,.36,.71,,,'4-13A'
60.,252.,270.,20.,1.7,1220.,37.5,.38,.67,,,'4-14A'
50.,253.,275.,20.,.7,1236.,34.5,.3,.66,,,'4-12C'
55.,253.,271.,20.1,.7,1222.,40.5,.28,.64,,,'4-13B'
43.,232.,248.,16.8,2.,1216.,37.5,.33,.74,,,'4-28B'
46.,230.,245.,15.8,2.,1225.,38.5,.33,.62,,,'4-30A1'
46.,232.,243.,16.2,2.5,1186.,39.,.37,.71,,,'4-31A1'
46.,228.,235.,16.7,2.1,1200.,36.5,.32,.66,,,'4-50A'
57.,196.,204.,15.9,1.8,1216.,31.5,.44,.76,,,'4-83A'
49.,199.,209.,16.,2.1,1203.,32.,.41,.77,,,'4-83B'
43.,199.,212.,15.9,1.9,1196.,30.5,.385,.75,,,'4-83C'
38.,199.,212.,16.,1.9,1192.,30.5,.37,.76,,,'4-83D'
60.,202.,212.,15.5,1.95,1210.,32.5,.42,.66,,,'4-80B'
55.,238.,253.,19.9,1.8,1166.,39.,.69,.39,,,'10-10B'
55.,234.,243.,20.5,2.3,1213.,36.5,.68,.39,,,'10-21B'
55.,234.,238.,19.8,1.8,1208.,37.5,.67,.31,,,'10-21C'
50.,235.,254.,19.7,1.7,1206.,36.,.7,.3,,,'10-23A'
50.,235.,241.,20.,2.1,1202.,38.5,.63,.3,,,'10-22B'
64.,229.,246.,30.1,2.,903.,35.,.4,.79,,,'11-103A'
64.,219.,237.,29.8,2.1,893.,35.,.43,.81,,,'11-103B'
64.,201.,223.,29.8,2.,904.,35.,.39,.84,,,'11-103D'
55.,250.,268.,20.1,1.7,1223.,40.,.36,.71,,,'13-13A'
50.,252.,268.,20.1,3.4,1235.,36.5,.34,.71,,,'13-12B'
55.,253.,271.,20.1,.7,1222.,40.5,.28,.64,,,'13-13B'
50.,252.,266.,20.,.6,1230.,38.,.41,.63,,,'13-12D'
60.,252.,270.,20.,1.7,1220.,37.5,.38,.67,,,'13-14A'
60.,253.,270.,19.8,.9,1216.,36.8,.31,.6,,,'13-14B'

APPENDIX G

SAMPLE OUTPUT OF GAV CALCULATION

The output corresponding to the input data displayed in Table 4 is shown in Table 5. The exponents for the experimental variables are first printed out, followed by the column's cross-sectional area and total volume. The entries which follow are liquid rate in $\text{lb}/(\text{hr}\cdot\text{ft}^2)$, temperature at the column entrance in degrees K, temperature at the column exit in degrees K, volume fraction of CO_2 in the feed gas stream, volume fraction of CO_2 in the exiting gas stream, gas rate in $\text{moles}/(\text{hr}\cdot\text{ft}^2)$, weight fraction equivalent of K_2CO_3 solution, entering fraction conversion of K_2CO_3 to KHCO_3 , exiting fraction conversion of K_2CO_3 to KHCO_3 , system pressure in psi, K_{La} (assuming a straight equilibrium line) in $\text{moles}/(\text{hr}\cdot\text{ft}^3)$, GAV, moles of CO_2 transferred, density of the K_2CO_3 solution, a logical character indicating a negative driving force by printing "T" or a positive driving force by "F", and the case identification.

Table 5. Output for GAV Calculation

0.00	-0.55	1.65	0.60	-6.25	0.05					
0.181000	0.6640									
7946.47	383.0	383.0	0.0315	0.0110	22.4	0.3900	0.2200	0.2412	315.0	
4.269 1	0.0117	0.0839	1.40211	F 17-SI1						
7939.70	384.7	384.7	0.0830	0.0475	23.3	0.3890	0.4300	0.4710	315.0	
8.8338	0.0148	0.1575	1.40091	F 17-SI3						
7811.93	384.1	384.1	0.1660	0.1040	23.3	0.3700	0.5800	0.6622	315.0	
22.3045	0.0207	0.2914	1.37837	F 17-SI4						
7845.39	383.6	383.6	0.2895	0.1935	23.3	0.3750	0.5900	0.7292	315.0	
31.9516	0.0257	0.5010	1.38427	F 17-SI5						
7946.47	366.3	366.3	0.0130	0.0030	22.9	0.3900	0.1700	0.1805	315.0	
2.2938	0.0085	0.0417	1.40211	F 17-SI6						
7946.47	365.8	365.8	0.0990	0.0500	23.8	0.3900	0.3300	0.3871	315.0	
6.1909	0.0186	0.2226	1.40211	F 17-SI7						
2002.77	366.9	366.9	0.0730	0.0480	30.5	0.3900	0.3200	0.4672	315.0	
4.7376	0.0269	0.1448	1.40211	F 17-SI8						
7845.39	365.8	365.8	0.0640	0.0300	22.7	0.3750	0.3000	0.3388	315.0	
4.5121	0.0143	0.1442	1.38427	F 17-SI11						
7946.47	365.8	365.8	0.0910	0.0505	23.5	0.3900	0.4200	0.4669	315.0	
6.3370	0.0150	0.1811	1.40211	F 17-SI12						
7811.93	365.8	365.8	0.3750	0.3010	22.6	0.3700	0.6000	0.7226	315.0	
20.1719	0.0223	0.4335	1.37837	F 17-SI15						
0.00	0.0	0.0	0.0000	0.0000	0.0	0.0000	0.0000	0.0000	0.0	
0.0000	0.0000	0.0000	0.00000	T						
0.181000	0.6640									
2028.51	383.0	383.0	0.0465	0.0295	23.0	0.4050	0.3300	0.4006	315.0	
3.8407	0.0179	0.0728	1.42013	F 17-SI11						
2971.85	383.0	383.0	0.0490	0.0320	23.1	0.3900	0.3200	0.3703	315.0	
3.4817	0.0136	0.0735	1.40211	F 17-SI12						
3916.00	383.0	383.0	0.0610	0.0300	23.0	0.3730	0.2800	0.3518	315.0	
5.6058	0.0195	0.1330	1.38191	F 17-SI13						
6111.43	381.9	381.9	0.0710	0.0320	22.9	0.4100	0.2700	0.3226	315.0	
5.7034	0.0176	0.1669	1.42617	F 17-SI14						
7899.17	383.6	383.6	0.0730	0.0310	23.3	0.3830	0.2900	0.3378	315.0	
7.2197	0.0172	0.1830	1.39376	F 17-SI15						
16869.12	383.0	383.0	0.1190	0.0340	23.0	0.3950	0.3200	0.3636	315.0	
13.3972	0.0197	0.3662	1.40809	F 17-SI16						
10206.25	383.0	383.0	0.1010	0.0290	15.5	0.4200	0.3500	0.3887	315.0	
8.7274	0.0160	0.2074	1.43833	F 17-SI17						
14860.36	383.0	383.0	0.1170	0.0300	15.7	0.3850	0.3300	0.3654	315.0	
10.1498	0.0152	0.2548	1.39614	F 17-SI18						

Table 5 (continued)

19949.41	383.0	383.0	0.1185	0.0290	15.5	0.3930	0.3500	0.3763	315.0
10.8658	0.0133	0.2591	1.40570	F 17-SII9					
21266.59	383.0	383.0	0.1130	0.0300	15.7	0.4050	0.3200	0.3424	315.0
8.8936	0.0118	0.2424	1.42013	F 17-SII10					
1932.10	366.3	366.3	0.0475	0.0310	23.1	0.3480	0.3500	0.4340	315.0
3.1630	0.0171	0.0712	1.35264	F 17-SII11					
2881.78	366.3	366.3	0.0490	0.0295	23.2	0.3540	0.2700	0.3350	315.0
2.8580	0.0157	0.0843	1.35962	F 17-SII12					
14860.36	366.9	366.9	0.1170	0.0380	15.6	0.3850	0.3000	0.3321	315.0
6.2415	0.0140	0.2322	1.39614	F 17-SII13					
3922.70	399.7	399.7	0.0630	0.0280	23.3	0.3750	0.3000	0.3818	315.0
10.8332	0.0267	0.1522	1.38427	F 17-SII15					
14923.86	399.7	399.7	0.1160	0.0300	15.9	0.3900	0.3100	0.3447	315.0
13.5220	0.0161	0.2544	1.40211	F 17-SII16					
0.00	0.0	0.0	0.0000	0.0000	0.0	0.0000	0.0000	0.0000	0.0
0.0000	0.0000	0.0000	0.00000	T					
0.079860	0.7200								
3745.68	390.8	390.2	0.2770	0.1630	17.2	0.3620	0.3200	0.5682	317.7
6.0442	0.0143	0.1875	1.36897	F 1-6A					
3774.57	399.1	391.3	0.3030	0.2030	17.9	0.3890	0.3250	0.5446	317.7
5.3268	0.0127	0.1792	1.40091	F 1-6B					
4434.40	391.9	390.2	0.2810	0.1290	17.0	0.4050	0.3000	0.5366	317.7
6.8286	0.0166	0.2364	1.42013	F 1-7A					
3234.07	400.8	407.4	0.2890	0.1680	17.5	0.3840	0.3000	0.5935	317.7
7.6850	0.0159	0.2032	1.39495	F 1-8A					
3875.35	401.9	409.1	0.2830	0.1250	17.4	0.3580	0.3000	0.6245	317.7
11.4414	0.0184	0.2515	1.36428	F 1-8B					
2530.72	388.0	390.2	0.0940	0.0510	15.7	0.3490	0.5300	0.6481	319.7
8.4998	0.0137	0.0569	1.35380	F 1-2B					
3059.68	383.6	393.0	0.0980	0.0330	16.1	0.3480	0.4900	0.6383	322.7
13.1786	0.0189	0.0866	1.35264	F 1-3A1					
2180.09	383.0	389.7	0.1140	0.0700	15.7	0.3650	0.5600	0.6976	322.7
7.9745	0.0127	0.0594	1.37249	F 1-3C1					
2183.74	380.8	383.0	0.1140	0.0570	16.3	0.3300	0.5100	0.7092	323.7
8.5045	0.0145	0.0787	1.33188	F 1-3C2					
3600.93	386.3	389.7	0.1100	0.0370	16.3	0.3340	0.5200	0.6698	327.7
16.5580	0.0187	0.0987	1.33647	F 1-4A1					
4850.10	388.0	386.9	0.0920	0.0300	16.3	0.3270	0.5300	0.6260	323.7
21.5415	0.0209	0.0834	1.32844	F 1-4A2					
3029.58	385.8	391.9	0.1100	0.0360	15.7	0.3290	0.5200	0.6965	322.7
22.2643	0.0234	0.0964	1.33073	F 1-4B					
3576.22	385.2	389.1	0.1120	0.0240	8.4	0.3260	0.5300	0.6247	314.7

Table 5 (continued)

0.0000	0.0000	0.0605	1.32730	T	1-5A					
0.00	0.0	0.0	0.0000	0.0000		0.0	0.0000	0.0000	0.0000	0.0
0.0000	0.0000	0.0000	0.00000	T						
0.181000	5.4300									
3508.10	385.8	393.0	0.2000	0.0250		18.2	0.3750	0.3900	0.7493	314.7
11.0028	0.0102	0.5915	1.38427	F	6-19A					
3553.30	387.4	395.8	0.1990	0.0180		17.9	0.3900	0.3900	0.7358	314.7
17.4804	0.0125	0.5986	1.40211	F	6-19B					
3508.10	395.2	406.9	0.2100	0.0190		17.9	0.3750	0.3400	0.7219	314.7
21.4976	0.0133	0.6324	1.38427	F	6-19					
3553.30	408.0	414.7	0.2000	0.0180		18.0	0.3900	0.2800	0.6241	314.7
14.3227	0.0126	0.6035	1.40211	F	6-19C					
3202.83	395.2	404.1	0.2010	0.0260		18.9	0.3800	0.3200	0.7205	314.7
12.9257	0.0121	0.6146	1.39020	F	6-12A1					
3433.81	384.1	393.0	0.2030	0.0240		18.8	0.3500	0.3300	0.7405	314.7
8.4403	0.0097	0.6233	1.35496	F	6-26A					
2375.78	398.0	404.1	0.1560	0.0570		18.8	0.4150	0.3600	0.6494	314.7
4.8769	0.0088	0.3568	1.43224	F	6-36A					
2416.38	410.8	412.4	0.1570	0.0520		18.6	0.4350	0.3100	0.5928	314.7
6.2771	0.0113	0.3733	1.45671	F	6-37A					
3257.90	385.2	390.8	0.1650	0.0080		18.6	0.4000	0.3700	0.6965	314.7
0.0000	0.0000	0.5321	1.41410	T	6-31C					
3257.90	398.0	405.2	0.1550	0.0090		18.5	0.4000	0.2800	0.5788	314.7
17.3329	0.0231	0.4925	1.41410	F	6-36D					
3313.72	410.8	412.4	0.1610	0.0090		18.2	0.4200	0.2600	0.5474	314.7
0.0000	0.0000	0.5063	1.43833	T	6-37D					
3583.69	394.1	404.1	0.2010	0.0170		18.8	0.4000	0.3600	0.7152	314.7
31.8158	0.0166	0.6377	1.41410	F	4-13A					
3827.02	395.2	405.2	0.2000	0.0170		18.8	0.3750	0.3800	0.7319	314.7
59.5638	0.0205	0.6326	1.38427	F	4-14A					
3108.28	395.8	408.0	0.2000	0.0070		19.0	0.3450	0.3000	0.7922	314.7
0.0000	0.0000	0.6692	1.34916	T	4-12C					
3598.96	395.8	405.8	0.2010	0.0070		18.8	0.4050	0.2800	0.6409	314.7
0.0000	0.0000	0.6650	1.42013	T	4-13B					
2742.70	384.1	393.0	0.1680	0.0200		18.7	0.3750	0.3300	0.7247	314.7
8.2324	0.0106	0.5115	1.38427	F	4-28B					
2959.21	383.0	391.3	0.1580	0.0200		18.9	0.3850	0.3300	0.6651	314.7
5.4438	0.0091	0.4805	1.39614	F	4-30A1					
2971.85	384.1	390.2	0.1620	0.0250		18.3	0.3900	0.3700	0.6899	314.7
5.8309	0.0089	0.4642	1.40211	F	4-31A1					
2909.07	381.9	385.8	0.1670	0.0210		18.5	0.3650	0.3200	0.6918	314.7

Table 5 (continued)

5.2049	0.0089	0.4985	1.37249 F	4-50A						
3453.14	364.1	368.6	0.1590	0.0180	18.7	0.3150	0.4400	0.7965	314.7	
8.4088	0.0091	0.4863	1.31478 F	4-83A						
2981.31	365.8	371.3	0.1600	0.0210	18.5	0.3200	0.4100	0.8067	314.7	
7.6454	0.0092	0.4758	1.32046 F	4-83B						
2582.62	365.8	373.0	0.1590	0.0190	18.4	0.3050	0.3850	0.8631	314.7	
0.0000	0.0000	0.4754	1.30348 T	4-83C						
2282.31	365.8	373.0	0.1600	0.0190	18.3	0.3050	0.3700	0.9123	314.7	
0.0000	0.0000	0.4772	1.30348 T	4-83D						
3666.34	367.4	373.0	0.1550	0.0195	18.6	0.3250	0.4200	0.7314	314.7	
5.8712	0.0080	0.4658	1.32616 F	4-80B						
3553.30	387.4	395.8	0.1990	0.0180	17.9	0.3900	0.6900	1.0481	314.7	
0.0000	0.0000	0.5986	1.40211 T	10-10B						
3478.23	385.2	390.2	0.2050	0.0230	18.7	0.3650	0.6800	1.0885	314.7	
0.0000	0.0000	0.6294	1.37249 T	10-21B						
3508.10	385.2	387.4	0.1980	0.0180	18.6	0.3750	0.6700	1.0566	314.7	
0.0000	0.0000	0.6168	1.38427 T	10-21C						
3148.52	385.8	396.3	0.1970	0.0170	18.6	0.3600	0.7000	1.1476	314.7	
0.0000	0.0000	0.6151	1.36662 T	10-23A						
3216.53	385.8	389.1	0.2000	0.0210	18.5	0.3850	0.6300	1.0366	314.7	
0.0000	0.0000	0.6122	1.39614 T	10-22B						
3995.71	382.4	391.9	0.3010	0.0200	13.9	0.3500	0.4000	0.8113	314.7	
16.5064	0.0096	0.7212	1.35496 F	11-103A						
3995.71	376.9	386.9	0.2980	0.0210	13.7	0.3500	0.4300	0.8327	314.7	
16.3042	0.0092	0.7038	1.35496 F	11-103B						
3995.71	366.9	379.1	0.2980	0.0200	13.9	0.3500	0.3900	0.7970	314.7	
8.1593	0.0087	0.7143	1.35496 F	11-103D						
3583.69	394.1	404.1	0.2010	0.0170	18.8	0.4000	0.3600	0.7152	314.7	
31.8158	0.0166	0.6377	1.41410 F	13-13A						
3162.03	395.2	404.1	0.2010	0.0340	19.0	0.3650	0.3400	0.7490	314.7	
16.3755	0.0135	0.5947	1.37249 F	13-12B						
3598.96	395.8	405.8	0.2010	0.0070	18.8	0.4050	0.2800	0.6409	314.7	
0.0000	0.0000	0.6650	1.42013 T	13-13B						
3202.83	395.2	403.0	0.2000	0.0600	18.9	0.3800	0.4100	0.7460	314.7	
12.6612	0.0118	0.5103	1.39020 F	13-12D						
3827.02	395.2	405.2	0.2000	0.0170	18.8	0.3750	0.3800	0.7319	314.7	
59.5638	0.0205	0.6326	1.38427 F	13-14A						

Table 5 (continued)

3804.19	395.8	405.2	0.1980	0.0090	18.7	0.3680	0.3100	0.6751	314.7
0.0000	0.0000	0.6460	1.37601	T	13-14B				
0.00	0.0	0.0	0.0000	0.0000	0.0	0.0000	0.0000	0.0000	0.0
0.0000	0.0000	0.0000	0.00000	T					
0.015079	0.004804	0.318608							
0.015715	0.005010	0.318806							
-0.05	-0.55	1.65	0.60	-6.25	0.05				
0.009899	0.003160	0.319217							
0.00	-0.60	1.65	0.60	-6.25	0.05				
0.015581	0.004966	0.318696							
0.00	-0.55	1.60	0.60	-6.25	0.05				
0.015838	0.005046	0.318610							
0.00	-0.55	1.65	0.55	-6.25	0.05				
0.015074	0.004803	0.318611							
0.00	-0.55	1.65	0.60	-6.30	0.05				
0.012891	0.004137	0.320891							
0.00	-0.55	1.65	0.60	-6.25	0.00				

VITA

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