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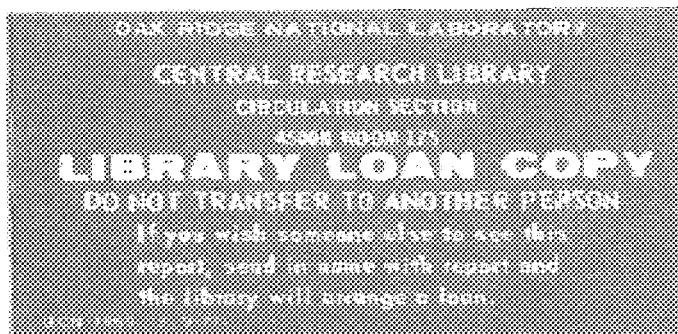
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ORNL/TM-10258

## Thermodynamic Properties of Aqueous Ternary Solutions Relevant to Chemical Heat Pumps

### Final Report

M. R. Ally



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MARTIN MARIETTA ENERGY SYSTEMS, INC.  
FOR THE UNITED STATES  
DEPARTMENT OF ENERGY

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Energy Division

THERMODYNAMIC PROPERTIES OF AQUEOUS TERNARY SOLUTIONS  
RELEVANT TO CHEMICAL HEAT PUMPS

FINAL REPORT

Moonis R. Ally

Date Published - March 1987

OAK RIDGE NATIONAL LABORATORY  
Oak Ridge, Tennessee 37831  
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MARTIN MARIETTA ENERGY SYSTEMS, INC.  
for the  
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**PREFACE**

This document was prepared for the U.S. Department of Energy (DOE) Office of Industrial Programs (OIP) as part of the OIP Chemical Heat Pump Study. The development of the correlations was performed at the Oak Ridge National Laboratory (ORNL), and the experimental data were provided by Energy Concepts, Inc., Annapolis, Maryland, an ORNL subcontractor.

Particular thanks are due to R. N. Chappell of DOE Idaho Operations Office; Scott Richlen of DOE/OIP, Washington, D.C.; and Stephen I. Kaplan of ORNL for their understanding and support.

The author wishes to thank Gil Farrell for typing the manuscript, Leroy Gilliam for the graphics, and Sharon McConathy for editing. Their skills are noteworthy.

**EXECUTIVE SUMMARY**

This report contains equations correlating vapor liquid equilibria (VLE) and specific enthalpy of solution (H-X-t) data on a new chemical heat pump fluid henceforth referred to as a ternary nitrate mixture. This fluid was developed by Energy Concepts, Inc., Annapolis, Maryland. The composition of the solute is 53 wt % LiNO<sub>3</sub>, 28 wt % KNO<sub>3</sub>, and 19 wt % NaNO<sub>3</sub>. The fluid mixture apparently is a competitor to existing chemical heat pump fluids and operates up to 260°C (500°F) without causing corrosion problems.

Computer simulation of heat pump cycles are facilitated if the VLE and H-X-t data can be represented by algebraic equations. Based on least-square-fit techniques, the appropriate equations are developed for the ternary nitrate mixture.

The results show that the maximum deviation between the correlations and experimental data is less than 3%; this accuracy is considered sufficient for heat pump cycle performance studies.

**ABSTRACT**

Polynomial expressions are developed that correlate experimental vapor-liquid-equilibrium (VLE) and specific enthalpy concentration data for a newly developed ternary absorption fluid. The development of these expressions are an important step toward using existing Oak Ridge National Laboratory computer software to evaluate heat pump performance. A canned least-square-fit program, POLFIT.BAS, was invoked to obtain the polynomial coefficients. The results show that the maximum deviation between correlated and actual values is less than 3% for vapor pressure and enthalpy. This is considered sufficiently accurate for heat pump cycle performance studies.



## 1. INTRODUCTION

A new absorption working fluid<sup>1</sup> developed by Energy Concepts Company, Annapolis, Maryland, is claimed to provide higher temperature capability (260°C) and higher lifts, without the attendant problems of corrosion and high pressures associated with banal fluids such as LiBr-H<sub>2</sub>O and NH<sub>3</sub>-H<sub>2</sub>O, respectively.

Using water as the refrigerant, the absorbent is a ternary mixture of 53 wt % LiNO<sub>3</sub>, 28 wt % KNO<sub>3</sub>, and 19 wt % NaNO<sub>3</sub>. The performance of a heat pump containing this new fluid can be calculated using data contained in the Duhring charts and specific enthalpy vs concentration diagrams. Computer codes that can perform such cycle calculations for a particular heat pump configuration and working fluid have been developed at Oak Ridge National Laboratory (ORNL).<sup>2</sup> These calculations are facilitated if the thermodynamic information contained in the Duhring charts and specific enthalpy vs concentration diagrams can be represented algebraically, by polynomial equations, like in the case of LiBr-H<sub>2</sub>O solutions.<sup>3</sup>

The thrust of this report is to correlate through polynomials, experimental data pertaining to equilibrium vapor pressures of the refrigerant and specific enthalpies of ternary solutions. The coefficients of the polynomials are obtained by invoking a canned program, POLFIT.BAS, which operates on the least-square-fit technique.

## 2. EQUATIONS DESCRIBING AQUEOUS TERNARY NITRATE SOLUTIONS

### 2.1 EQUATIONS DESCRIBING EQUILIBRIUM VAPOR PRESSURES OF AQUEOUS TERNARY SOLUTIONS (DUHRING CHART)

The measured vapor-liquid-equilibrium (VLE) data<sup>1</sup> for the equilibrium vapor pressures of refrigerant (H<sub>2</sub>O) over aqueous ternary solutions of various concentrations and temperatures are reproduced in Table 1. The same data appear graphically in Fig. 1 (Duhring chart). The relationship between the saturation temperature of the pure refrigerant and the temperature of the ternary solution of known concentration X can be represented by an equation of the form

$$t = A(X)t' + B(X) , \quad (1)$$

where t and t' are the solution and pure refrigerant saturation temperatures expressed in degrees Fahrenheit, respectively, and A and B are polynomial functions of the ternary concentration X.

The methodology for determining polynomial functions A(X) and B(X) is as follows. At a fixed concentration X, A and B have definite fixed values because they depend on X only. All that is required are two sets

Table 1. Measured VLE data

Concentration w/o salt	Temp. (°C)	Pressure (mm Hg)	Concentration w/o salt	Temp. (°C)	Pressure (mm Hg)
50	40	727	76	70	708
	50	704		80	679
	60	670		90	636
	70	621		100	582
	80	548		110	508
	90	450		120	413
	100	318		130	263
	110	142		140	104
	115.5	0		144	6
60	40	734	78	80.2	693
	50	715		90	657
	60	691		100	609
	70	653		110	544
	80	592		120	466
	90	504		130	353
	100	409		140	211
	110	269		151	-4
	120	84			
	123.8	0			
65	55	714	80	90	682
	60	701		100	642
	70	667		110	587
	80	619		120	515
	90	556		130	421
	100	470		140	302
	110	352		150	144
	120	190		157.6	0
	129	-4			
70	50	731.8	82.6	110	619
	60	712.4		120	549
	70	682.7		130	480
	80	644.1		140	367
	90	584.6		150	240
	100	507.3		160	80
	100	407.3		164	0
	120	277			
	130	94.1			
	133	0			

Table 1 (continued)

Concentration w/o salt	Temp. (°C)	Pressure (mm Hg)	Concentration w/o salt	Temp. (°C)	Pressure (mm Hg)
87	131.4	541	92.4	156	479
	140	460		160	450
	150	360		165	404
	160	237		170	354
	170	72		175	307
	174.5	-3		180	240
				185	16
				190	88
				195	3
				195.5	-9
88	130	560.6	94.1	170	453
	140	483.6		175	401
	150	392.6		180	356
	160	272.6		185	295
	170	108.6		190	241
	176.5	0.6		195	176
				200	108
				205	21
				206.7	3

Source: W. F. Davidson and D. C. Erickson, *New High Temperature Absorbent for Absorption Heat Pumps*, ORNL/Sub/85-22013/1, Oak Ridge National Laboratory, July 1986.

## TERNARY SALT COMPOSITION

53 wt % LiNO<sub>3</sub>28 wt % KNO<sub>3</sub>19 wt % NaNO<sub>3</sub>

○ CALCULATED FROM CORRELATIONS

— REPORTED DATA

$$t = At' + B$$

$$A = -1.06427 + 0.102088X - 1.62660 \times 10^{-3}X^2 + 8.93054 \times 10^{-6}X^3$$

$$B = 291.113 - 13.0305X + 0.187146X^2 - 7.87688 \times 10^{-4}X^3$$

$$\log P = C + \frac{D}{(t' + 459.67)} + \frac{E}{(t' + 459.67)^2}$$

$$C = 6.211$$

$$D = -2886.37$$

$$E = -337269.46$$

t' = REFRIGERANT TEMPERATURE (°F)

t = SOLUTION TEMPERATURE (°F)

X = wt % TERNARY SALT

P = psia

70 ≤ X ≤ 94.1

32 ≤ t' ≤ 450

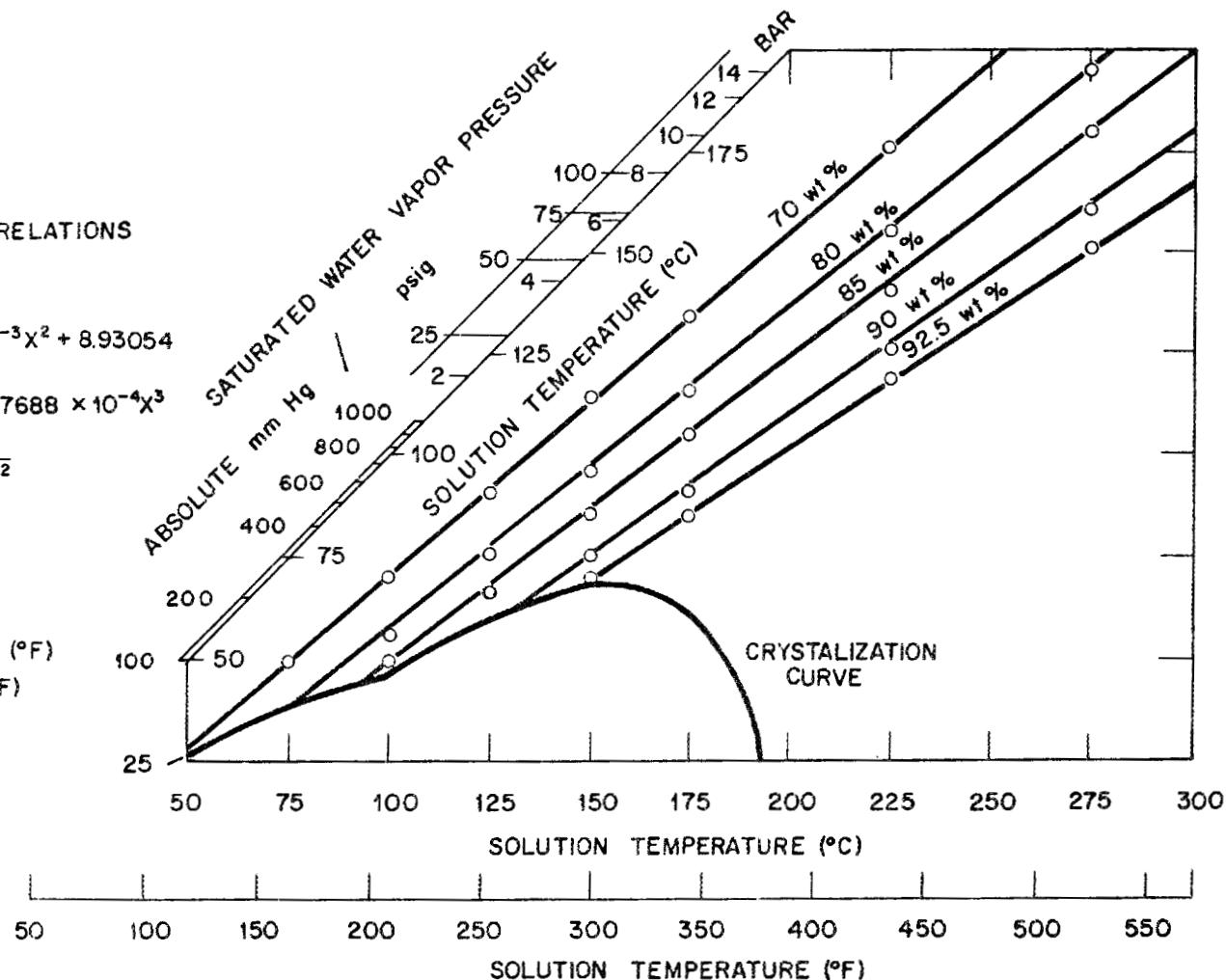


Fig. 1. Equilibrium vapor pressure of refrigerant (H<sub>2</sub>O) over aqueous ternary solutions (Duhring chart).

of ordered pairs  $(t, t')$ , which when substituted in Eq. 1 give two simultaneous equations whose solutions yield the required A and B values at that particular concentration. The ordered pairs  $(t, t')$  may be obtained from the VLE data of Table 1 and steam tables or directly from Fig. 1. The disadvantage of reading directly as in the latter case is that visual reading of numbers from a graph entails a greater compromise on accuracy. Repeating the procedure at other solution concentrations X enables one to tabulate A and B as functions of concentrations, as shown in Table 2. Since the dependence of A and B upon X is now established, it becomes a simple matter to correlate it.

A canned program, POLFIT.BAS, available at ORNL was used to obtain a least-squares fit to the data of Table 2. The output from POLFIT.BAS is shown in Appendix A. For  $A(X)$ , a third-degree polynomial provided a reasonably accurate fit as indicated by the standard error of estimate of  $2.037 \times 10^{-2}$ . Unfortunately, with POLFIT.BAS it was not possible to correlate  $B(X)$  to the same accuracy as  $A(X)$ , despite attempts at increasing the degree of the polynomial. In a bid to improve the fit, another canned software available on the PDP-11 computer was tried, but its results were identical with those from POLFIT.BAS up to six significant figures. Under the circumstances, the "best" fit for B appeared to be a third-degree polynomial.

The polynomial equations for  $A(X)$  and  $B(X)$  from POLFIT.BAS are as follows:

$$A(X) = -1.06427 + 0.102088(X) - 1.62660 \times 10^{-3}(X^2) \quad (2)$$

$$+ 8.93054 \times 10^{-6}(X^3),$$

$$B(X) = 291.113 - 13.0305(X) + 0.187146(X^2) - 7.87688 \times 10^{-4}(X^3), \quad (3)$$

valid between  $50\% \leq X \leq 94.1\%$ . Equations 2 and 3 when substituted in Eq. 1 give an expression for relating the pure refrigerant temperature  $t'$  to the solution temperature  $t$  whose concentration is X. The temperature difference,  $t - t'$ , is clearly the boiling point elevation.

The refrigerant vapor pressure above a ternary solution of concentration X and at temperature t can be described by a Van't Hoff type of equation,

$$\log P = C + \frac{D}{(t' + 459.67)} + \frac{E}{(t' + 459.67)^2}, \quad (4)$$

where C, D, E are constants and thus are independent of composition and temperature, and  $t' = (t - B)/A$  from Eq. 1. Since  $t'$  is the saturation

Table 2. Variation of coefficients A and B as a function  
of ternary solution concentration X  
calculated using POLFIT.BAS

A	B	X
1.09	8.89	50
1.13	12.9	60
1.15	18.5	65
1.17	25.8	70
1.22	35.9	76
1.24	39.5	78
1.26	43.1	80
1.3	47.7	82.6
1.39	55.3	87
1.41	56.9	88
1.53	63.5	92.4
1.58	65.7	94.1

temperature of the pure refrigerant and C, D, and E are independent of composition and temperature, P must be the saturation pressure of pure water. Further, it is noteworthy that C, D, E and t' are also independent of the nature of the solute. Under these circumstances, Eq. 4 does nothing more than provide a relationship between the saturation temperature and pressure of pure water. Therefore, it is obvious that Eq. 4, as applied to the ternary solution, should be identical to the one reported in the literature<sup>3</sup> for LiBr-H<sub>2</sub>O because both share a common refrigerant. A clarification to be noted is that although Eq. 4 gives the same value for the vapor pressure P at a given t' for the ternary and LiBr solutions, the corresponding solution temperatures will be different for the two through their respective relations t' = (t - B)/A. The constants<sup>3</sup> in Eq. 4 are therefore

$$C = 6.211 ,$$

$$D = -2886.37 ,$$

$$E = -337,269.26 .$$

An interactive computer program TERNRY (Appendix B) written in FORTRAN 77 incorporates Eqs. 1 through 4 and outputs in tabular form equilibrium vapor pressure, refrigerant temperatures, solution composition, and temperatures.

The computed values are plotted as dots in Fig. 1 for the purpose of comparing these results with the measured VLE data. The comparison shows that the maximum error (at certain points) is about 3% or better of the measured data.

## 2.2 EQUATIONS DESCRIBING SPECIFIC ENTHALPY-CONCENTRATION DATA OF TERNARY SOLUTIONS

The specific enthalpy-concentration data for ternary solutions was not measured calorimetrically by Energy Concepts Company but was calculated by the method proposed by McNeely<sup>4</sup> for LiBr-H<sub>2</sub>O solutions. The calculated values are shown in Table 3 and graphically in Fig. 2. It is proposed that the specific enthalpy-concentration data may be represented by the equation

$$H = \alpha(X) + \beta(X)t , \quad (5)$$

where  $\alpha$  and  $\beta$  are polynomials in the concentration X and t is the solution temperature.

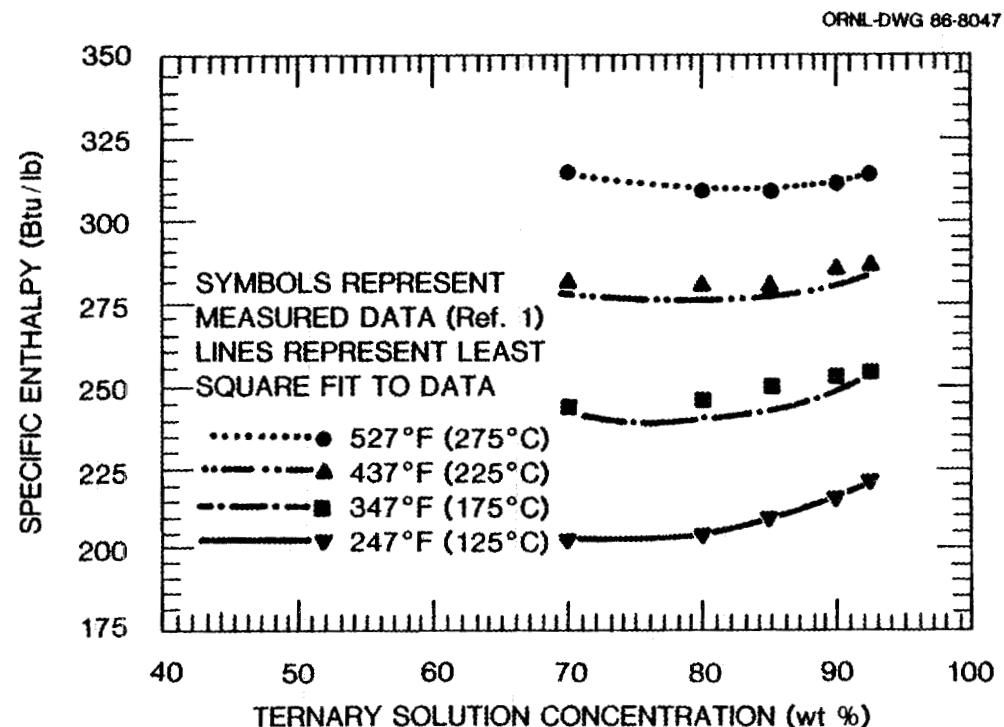
The data in Table 3 are used to obtain the polynomial expressions for  $\alpha$  and  $\beta$  as follows. At a fixed value of the concentration X, the specific enthalpy H is evaluated at two different solution temperatures

Table 3. Specific enthalpy-concentration data

Concentration, X (wt %)	Solution temperature, t [°C (°F)]	Specific enthalpy <sup>a</sup> [kJ/kg (Btu/lb)]
70	125 (257)	473.6 (203.6)
	175 (347)	571.0 (245.5)
	225 (437)	658.1 (283.0)
	275 (527)	733.9 (315.5)
80	125 (257)	476.5 (204.9)
	175 (347)	576.9 (248.0)
	225 (437)	658.1 (283.0)
	275 (527)	719.9 (309.5)
85	125 (257)	487.1 (209.4)
	175 (347)	583.4 (250.8)
	225 (437)	659.2 (283.4)
	275 (527)	719.6 (309.4)
90	125 (257)	503.8 (216.6)
	175 (347)	591.6 (254.4)
	225 (437)	665.4 (286.1)
	275 (527)	723.1 (310.9)
92.5	125 (257)	512.6 (220.4)
	175 (347)	596.1 (256.3)
	225 (437)	669.3 (287.8)
	275 (527)	730.1 (313.9)

<sup>a</sup>Reference temperature = 273 K (0°C).

Source: W. F. Davidson and D. C. Erickson, *New High Temperature Absorbent for Absorption Heat Pumps*, ORNL/Sub/85-22013/1, Oak Ridge National Laboratory, July 1986.



$$H(X,t) = \alpha(X) + \beta(X)t$$

$$\alpha(X) = 394.516 - 8.64996X + (6.28787 \times 10^{-2})X^2$$

$$\beta(X) = 0.388691 + (3.02719 \times 10^{-3})X - (3.80068 \times 10^{-5})X^2$$

*t* = SOLUTION TEMPERATURE (°F)

*H* = SPECIFIC ENTHALPY OF SOLUTION (Btu/lb)

Fig. 2. Specific enthalpy of ternary solutions.

t. Applying this to Eq. 5 provides two equations in two unknown constants,  $\alpha$  and  $\beta$ . Solution of the two equations simultaneously yields values of  $\alpha$  and  $\beta$  at that particular concentration X. The above calculation procedure is repeated to yield the next set of  $\alpha$  and  $\beta$  values at a new value of the concentration X. This procedure enables one to find how  $\alpha$  and  $\beta$  vary with X, as shown in Table 4. Since the dependence of  $\alpha$  and  $\beta$  on X is now established, it is correlated by invoking the canned program POLFIT.BAS. The results from POLFIT.BAS for correlating  $\alpha$  and  $\beta$  are shown in Appendix C. The resulting polynomial equations are

$$\alpha(X) = 394.516 - 8.64996(X) + 6.28787 \times 10^{-2}(X^2) \quad (6a)$$

and

$$\beta(X) = 0.388691 + 3.02719 \times 10^{-3}(X) - 3.80068 \times 10^{-5}(X^2), \quad (6b)$$

applicable between 70%  $\leq$  X  $\leq$  94.1%.

Equations 6a and 6b substituted in Eq. 5 give an expression for relating the specific enthalpy of a ternary solution to its concentration and temperature. Equations 5 and 6 are incorporated in a FORTRAN program called TERNRY.H, which is listed and executed in Appendix D. The goodness of the specific enthalpy correlation can be judged from Table 5 or graphically from Fig. 2, where the computed results of TERNRY.H are compared with the reported values.

### 3. ACCURACY AND SIGNIFICANT DIGITS

Since raw data are used extensively to obtain the required correlations, a few words should be said about the accuracy of the computed results. The approach is to first establish the intended accuracy of raw data as a necessary guide to the number of digits to retain in the computed result. The identification of significant digits (intended accuracy) is only possible through a knowledge of the circumstances under which the measurements were made. For example, in the VLE data of Table 1, the concentration (wt %) of 50, 60, 65, etc., is interpreted as having an accuracy of two significant digits only. It is the author's inference that researchers at Energy Concepts Company were unable to make measurements on concentrations better than the two significant digits that they reported. Similar argument applies to the other measured quantities. Therefore, in reading the computed values, it should be noted that a concentration of 50.0 wt % does not apply to three significant digits of accuracy, but rather only to two. What

Table 4. Coefficients  $\alpha$  and  $\beta$  as functions  
of ternary solution concentration X

Concentration, X (wt %)	$\alpha$	$\beta$
70	97.12	0.413
72.5	97.89	0.409
77.5	101.81	0.396
80	104.94	0.388
82.5	108.86	0.379
85	113.56	0.371
87.5	119.06	0.362
90	125.34	0.353
92.5	132.4	0.344

Table 5. Comparison between reported and correlated specific enthalpies of aqueous ternary solutions

Ternary solution concentration (wt %)	Solution temperature [°C (°F)]	Specific enthalpy <sup>a</sup> (kJ/kg)	
		Reported <sup>b</sup>	From correlation
70	125 (257)	473.6	473.52
	175 (347)	571.0	560.24
	225 (437)	658.1	646.97
	275 (527)	733.9	733.70
80	125 (257)	476.5	475.71
	175 (347)	576.9	556.85
	225 (437)	658.1	637.98
	275 (527)	719.9	719.11
85	125 (257)	487.1	486.08
	175 (347)	583.4	563.81
	225 (437)	659.2	639.09
	275 (527)	719.6	719.28
90	125 (257)	503.8	502.62
	175 (347)	591.6	576.56
	225 (437)	665.4	650.50
	275 (527)	723.1	724.45
92.5	125 (257)	512.6	513.20
	175 (347)	596.1	585.10
	225 (437)	669.3	657.00
	275 (527)	730.1	728.89

<sup>a</sup>Reference temperature = 273 K (0°C).

<sup>b</sup>From W. F. Davidson and D. C. Erickson, *New High Temperature Absorbent for Absorption Heat Pumps*, ORNL/Sub/85-22013/1, Oak Ridge National Laboratory, July 1986.

about the coefficients in  $A(X)$ ,  $B(X)$ ,  $\alpha(X)$ , and  $\beta(X)$ ? These coefficients can legitimately have several significant digits if the final computed value, after all the conversions have taken place, has an accuracy at best equal to the number of significant digits in the measured data.

#### 4. SUMMARY OF RESULTS

A summary of the equations describing the vapor pressure, composition, temperature (P-X-t) data and the enthalpy, concentration, temperature (H-X-t) data appears below.

##### 4.1 P-X-t CORRELATION (Ternary Salt Composition)

53 wt % LiNO<sub>3</sub>  
 28 wt % KNO<sub>3</sub>  
 19 wt % NaNO<sub>3</sub>

$$t = At' + B$$

$$A = -1.06427 + 0.102088X - 1.62660 \times 10^{-3}X^2 + 8.93054 \times 10^{-6}X^3$$

$$B = 291.113 - 13.0305X + 0.187146X^2 - 7.87688 \times 10^{-4}X^3$$

$$\log P = C + \frac{D}{(t' + 459.67)} + \frac{E}{(t' + 459.67)^2}$$

where

X = wt % ternary salt

70% ≤ X ≤ 94.1%

32 ≤ t' ≤ 450

C = 6.21147

D = -2886.373

E = -337269.46

t' = refrigerant temperature (°F)

t = solution temperature (°F)

P = psia

**4.2 H-X-t CORRELATION (Ternary Salt Composition)**

53 wt % LiNO<sub>3</sub>  
28 wt % KNO<sub>3</sub>  
19 wt % NaNO<sub>3</sub>

$$H(X, t) = \alpha(X) + \beta(X)t$$
$$\alpha(X) = 394.516 - 8.64996X + (6.28787 \times 10^{-2})X^2$$
$$\beta(X) = 0.388691 + (3.02719 \times 10^{-3})X - (3.80068 \times 10^{-5})X^2$$

where

t = solution temperature (°F)

H = specific enthalpy of solution (Btu/lb)

## REFERENCES

1. W. F. Davidson and D. C. Erickson, *New High Temperature Absorbent for Absorption Heat Pumps*, ORNL/Sub/85-22013/1, Oak Ridge National Laboratory, July 1986.
2. G. Grossman and E. Michelson, *Absorption Heat Pump Simulation and Studies Part 1: A Modular Computer Simulation of Absorption Systems*, ORNL/Sub/83-43337/2, Oak Ridge National Laboratory, April 1986.
3. ASHRAE, *1981 Fundamentals*, American Society of Heating, Refrigeration, and Air-Conditioning Engineers, pp. 17.71-17.72.
4. L. A. McNeely, "Thermodynamic Properties of Aqueous Solutions of Lithium Bromide," *ASHRAE Trans.* 85, 1979.

**Appendix A**

**COEFFICIENTS OF A(X) AND B(X)  
USING POLFIT.BAS**

R BASIC

READY, FOR HELP TYPE HELP.  
OLD BAS:POLFIT.BAS

READY  
RUN

BAS:POLFIT 10:07 06-OCT-86

THIS PROGRAM FITS LEAST-SQUARES POLYNOMIALS TO BIVARIATE DATA, USING AN ORTHOGONAL POLYNOMIAL METHOD. LIMITS ARE 11-TH DEGREE FIT AND A MAX OF 100 DATA POINTS. PROGRAM ALLOWS USER TO SPECIFY THE LOWEST DEGREE POLYNOMIAL TO BE FIT, AND THEN FITS THE POLYNOMIALS IN ORDER OF ASCENDING DEGREE. AT EACH STAGE, THE INDEX OF DETERMINATION IS PRINTED, AND THE USER HAS THE CHOICE OF GOING TO THE NEXT HIGHER DEGREE FIT, SEEING EITHER OF TWO SUMMARIES OF FIT AT THAT STAGE, OR OF STOPPING THE PROGRAM. TO USE, TYPE:

```
10 DATA N, D
      (WHERE N = NUMBER OF DATA POINTS TO BE READ
       AND D = INITIAL (LOWEST) DEGREE TO BE FIT)
100 DATA X(1),Y(1),X(2),Y(2),...,X(N),Y(N)
      (CONTINUATION ON LINES 101-299 AS NEEDED)
RUN
```

TIME: 0.25 SECS.

READY
10 DATA 12,3
100 DATA 50,1.09,60,1.13,65,1.17,70,1.15,76,1.21,78,1.27,80,1.26,82.6,1.3
101 DATA 87,1.4,88,1.4,92.4,1.5,94.1,1.6
RUN

BAS:POLFIT 10:10 06-OCT-86

## LEAST-SQUARES POLYNOMIALS

NUMBER OF POINTS = 12  
 MEAN VALUE OF X = 76.925  
 MEAN VALUE OF Y = 1.29  
 STD ERROR OF Y = 0.157191

NOTE: CODE FOR 'WHAT NEXT?' IS:

0 = STOP PROGRAM  
 1 = COEFFICIENTS ONLY  
 2 = ENTIRE SUMMARY  
 3 = FIT NEXT HIGHER DEGREE

POLYFIT OF DEGREE 3 INDEX OF DETERM = 0.4d3207      WHAT NEXT ??

TERM	COEFFICIENT
0	-1.06427
1	0.102088
2	-1.62660E-3
3	8.93054E-6

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
50	1.09	1.08992	7.71880E-5	7.08197E-3
60	1.13	1.13421	-4.21494E-3	-0.371618
65	1.17	1.15158	1.84208E-2	1.59961
70	1.15	1.17469	-2.46859E-2	-2.10149
76	1.21	1.21942	-9.42490E-3	-0.772897
78	1.27	1.24032	2.96807E-2	2.39299
80	1.26	1.26492	-4.91880E-3	-0.388863
82.6	1.3	1.30314	-3.14234E-3	-0.241136
87	1.4	1.38638	1.36159E-2	0.982118
88	1.4	1.40894	-8.94170E-3	-0.634639
92.4	1.5	1.52629	-2.62868E-2	-1.72227
94.1	1.6	1.58018	1.98219E-2	1.25441

STD ERROR OF ESTIMATE FOR Y = 2.03703E-2

WHAT NEXT ?0

TIME: 0.42 SECS.

READY  
 BYE

Job 180, User [6421,324] Logged off TTY220 1013 6-Oct-86  
 Saved all files (2580 blocks)

R BASIC

READY, FOR HELP TYPE HELP.  
OLD BAS:POLFIT.BAS

READY  
RUN

BAS:POLFIT 10:19 06-OCT-86

THIS PROGRAM FITS LEAST-SQUARES POLYNOMIALS TO BIVARIATE DATA, USING AN ORTHOGONAL POLYNOMIAL METHOD. LIMITS ARE 11-TH DEGREE FIT AND A MAX OF 100 DATA POINTS. PROGRAM ALLOWS USER TO SPECIFY THE LOWEST DEGREE POLYNOMIAL TO BE FIT, AND THEN FITS THE POLYNOMIALS IN ORDER OF ASCENDING DEGREE. AT EACH STAGE, THE INDEX OF DETERMINATION IS PRINTED, AND THE USER HAS THE CHOICE OF GOING TO THE NEXT HIGHER DEGREE FIT, SEEING EITHER OF TWO SUMMARIES OF FIT AT THAT STAGE, OR OF STOPPING THE PROGRAM. TO USE, TYPE:

```
10 DATA N, D
      (WHERE N = NUMBER OF DATA POINTS TO BE READ
      AND D = INITIAL (LOWEST) DEGREE TO BE FIT)
100 DATA X(1),Y(1),X(2),Y(2),...,X(N),Y(N)
      (CONTINUATION ON LINES 101-299 AS NEEDED)
RUN
```

TIME: 0.27 SECS.

READY
10 DATA 12,3
100 DATA 50,8.89,60,13.7,65,16.9,70,27.6,76,34.7,78,35.3,80,47.8
101 DATA 82.6,49,87,57,88,53,92.4,64,94.1,66
RUN

BAS:POLFIT 10:22 06-OCT-86

#### L E A S T - S Q U A R E S P O L Y N O M I A L S

NUMBER OF POINTS = 12
MEAN VALUE OF X = 76.925
MEAN VALUE OF Y = 39.4908
STD ERROR OF Y = 19.6464

NOTE: CODE FOR 'WHAT NEXT?' IS:

0 = STOP PROGRAM
1 = COEFFICIENTS ONLY
2 = ENTIRE SUMMARY
3 = FIT NEXT HIGHER DEGREE

2 = ENTIRE SUMMARY  
 3 = FIT NEXT HIGHER DEGREE

POLYFIT OF DEGREE 3 INDEX OF DETERM = 0.977957      WHAT NEXT ?2

TERM      COEFFICIENT

0	291.113
1	-13.0305
2	0.187146
3	-7.87688E-4

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
50	8.89	8.98885	-9.88497E-2	-1.09969
60	13.7	12.8638	0.836158	6.50006
65	16.9	18.4989	-1.59885	-8.64298
70	27.6	25.8112	1.78884	6.93047
76	34.7	35.9682	-1.26821	-3.52593
78	35.3	39.5251	-4.22514	-10.6898
80	47.8	43.1047	4.69531	10.8928
82.6	49	47.7297	1.27027	2.66138
87	57	55.2653	1.73469	3.13884
88	53	56.8928	-3.89282	-6.84237
92.4	64	63.4959	0.504076	0.793871
94.1	66	65.7456	0.254379	0.386914

STD ERROR OF ESTIMATE FOR Y = 2.91691

WHAT NEXT ?3

POLYFIT OF DEGREE 4 INDEX OF DETERM = 0.974808      WHAT NEXT ?2

TERM      COEFFICIENT

0	293.909
1	-13.1932
2	0.190629
3	-8.20276E-4
4	1.12501E-7

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
50	8.89	8.99018	-0.100181	-1.11434
60	13.7	12.8598	0.840171	6.5333
65	16.9	18.4985	-1.59847	-8.6411
70	27.6	25.8136	1.7864	6.92037
76	34.7	35.9707	-1.27069	-3.53258
78	35.3	39.5268	-4.22685	-10.6936
80	47.8	43.1053	4.69468	10.8912
82.6	49	47.7288	1.27123	2.66345
87	57	55.2624	1.73759	3.14426
88	53	56.8898	-3.88983	-6.83747
92.4	64	63.4957	0.504259	0.794162
94.1	66	65.7485	0.251505	0.382526

STD ERROR OF ESTIMATE FOR Y = 3.1183

POLYFIT OF DEGREE 5 INDEX OF DETERM = 0.971641      WHAT NEXT ??

## TERM      COEFFICIENT

0	-4291.77
1	315.925
2	-9.13076
3	0.129507
4	-9.00096E-4
5	2.45929E-6

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
50	8.89	8.88025	9.75096E-3	0.109805
60	13.7	13.588	0.111987	0.824162
65	16.9	17.9407	-1.04074	-5.80096
70	27.6	25.1403	2.45968	9.78381
76	34.7	36.098	-1.39802	-3.87285
78	35.3	39.8721	-4.57213	-11.467
80	47.8	43.547	4.253	9.76647
82.6	49	48.0686	0.931396	1.93764
87	57	54.9616	2.03839	3.70875
88	53	56.4331	-3.43311	-6.0835
92.4	64	63.1467	0.853333	1.35135
94.1	66	66.2142	-0.214233	-0.323546

STD ERROR OF ESTIMATE FOR Y = 3.30846

WHAT NEXT ?3

POLYFIT OF DEGREE 6 INDEX OF DETERM = 0.966684      WHAT NEXT ??

## TERM      COEFFICIENT

0	28191.
1	-2465.09
2	89.0793
3	-1.70241
4	1.81435E-2
5	-1.02188E-4
6	2.37574E-7

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
50	8.89	8.90137	-1.13672E-2	-0.127702
60	13.7	13.2764	0.423633	3.19088
65	16.9	18.5085	-1.60855	-8.69082
70	27.6	24.9929	2.60708	10.4313
76	34.7	35.6694	-0.969434	-2.71783
78	35.3	39.6853	-4.3853	-11.0502
80	47.8	43.6685	4.13154	9.46116
82.6	49	48.4995	0.500488	1.03194
87	57	55.1008	1.89917	3.44672
88	53	56.3523	-3.35229	-5.94882
92.4	64	62.564	1.43604	2.29531
94.1	66	66.5789	-0.578857	-0.869431

STD ERROR OF ESTIMATE FOR Y = 3.58599

WHAT NEXT ?0

TIME: 0.89 SECS.

**Appendix B**

**LISTING AND EXECUTION OF  
COMPUTER PROGRAM, TERNRY**

```

TY TERNRY
00020 C      PROGRAM TO CALCULATE VAPOR PRESSURE OF WATER ABOVE AQUEOUS TERNARY
00040 C      SOLUTION.
00060 C      RELEVANT EMPIRICAL EQUATIONS ARE BASED UPON DATA FROM ENERGY
00080 C      CONCEPT'S REPORT, FEBRUARY 1986.
00100 C
00120      C=6.21147
00140      D=-2886.373
00160      E=-337269.46
00180 C
00200      WRITE(6,21)
00220      21  FORMAT(/,3X,'SOLUTION',7X,'REFRIGERANT',10X,'REFRIGERANT',15X,
00240      C'TERNARY')
00260      WRITE(6,31)
00280      31  FORMAT(3X,'TEMPERATURE',4X,'TEMPERATURE',10X,'PRESSURE',9X)
00300      WRITE(6,41)
00320      41  FORMAT(4X,'(F)',3X,'(K)',6X,'(F)',3X,'(K)',6X,'(PSIA)',3X,
00340      C'(PA)',7X,'(MM HG)',6X,'(WT.%)')
00360 C
00380      TSOLN=527.0
00400 C
00420      DO 99 XX=50.0,92.5,2.5
00440      X=XX
00460      TSOLNK=KELVN(TSOLN)
00480 C      CHOOSE VALUE FOR SOLUTION CONCENTRATION, WT % TERNARY,X
00500      A=-1.064 +0.1021*X -(1.627E-03)*(X**2.) +(8.931E-06)*(X**3.)
00520      B=291.1 - 13.03*X + 0.1871*X**2. -(7.877E-04)*X**3.
00540 C
00560 C      CALCULATE REFRIGERANT TEMP (F), TREFG
00580      TREFG=(TSOLN-B)/A
00600      TREFGK=KELVN(TREFG)
00620 C
00640 C      CALCULATE REFRIGERANT VAPOR PRESSURE (PSIA),P
00660      P=C+D/(TREFG+459.67)+E/(TREFG+459.67)**2.0
00680      P=10.0**P
00700 C
00720 C
00740 C      XR=FRAC(X)
00760      TSOLNK=KELVN(TSOLN)
00780      PRES=PASCAL(P)
00800      PMMHG=MMHG(P)
00820      WRITE(6,51)TSOLN,TSOLNK,TREFG,TREFGK,P,PRES,PMMHG,X
00840      51  FORMAT(/,2X,2(F6.1),4X,F5.1,X,F5.1,5X,F6.2,2X,E9.3,2X,E9.3,
00860      C6X,F4.1)
00880      99  CONTINUE
00900      STOP
00920      END
00940 C
00960      FUNCTION KELVN(T)
00980      KELVN=(T+459.72)/1.8
01000      RETURN
01020      END
01040 C
01060      FUNCTION PASCAL(P)
01080      PASCAL=6.8947E+03*P
01100      RETURN
01120      END
01140 C
01160      FUNCTION FRAC(X)
01180      FRAC=((100.-X)/18.0)/((100.-X)/18.0+X/86.85)
01200      RETURN
01220      END
01240 C
01260      FUNCTION MMHG(P)
01280      MMHG=P/14.696*760.
01300      RETURN
01320      END

```

EX  
 LINK: Loading  
 [LNKXCT TERNARY execution]

SOLUTION TEMPERATURE (F)	REFRIGERANT TEMPERATURE (F)	REFRIGERANT PRESSURE (PSIA)	REFRIGERANT PRESSURE (PA)	TERNARY (MM HG)	TERNARY (WT.%)
167.0 348.0	145.1 335.0	3.28	.226E+05	.169E+03	50.0
167.0 348.0	143.3 335.0	3.14	.217E+05	.162E+03	52.5
167.0 348.0	141.3 333.0	2.98	.206E+05	.154E+03	55.0
167.0 348.0	138.9 332.0	2.80	.193E+05	.144E+03	57.5
167.0 348.0	136.1 330.0	2.61	.180E+05	.134E+03	60.0
167.0 348.0	132.8 329.0	2.39	.165E+05	.123E+03	62.5
167.0 348.0	129.2 327.0	2.17	.150E+05	.112E+03	65.0
167.0 348.0	125.0 324.0	1.94	.134E+05	.100E+03	67.5
167.0 348.0	120.4 322.0	1.71	.118E+05	.880E+02	70.0
167.0 348.0	115.4 319.0	1.49	.103E+05	.760E+02	72.5
167.0 348.0	110.0 316.0	1.27	.879E+04	.650E+02	75.0
167.0 348.0	104.2 313.0	1.08	.743E+04	.550E+02	77.5
167.0 348.0	98.2 309.0	0.90	.621E+04	.460E+02	80.0
167.0 348.0	92.1 306.0	0.75	.514E+04	.380E+02	82.5
167.0 348.0	85.9 303.0	0.61	.422E+04	.310E+02	85.0
167.0 348.0	79.7 299.0	0.50	.346E+04	.250E+02	87.5
167.0 348.0	73.7 296.0	0.41	.283E+04	.210E+02	90.0
167.0 348.0	67.9 293.0	0.34	.233E+04	.170E+02	92.5
STOP					

END OF EXECUTION  
 CPU TIME: 0.17 ELAPSED TIME: 11.40  
 EXIT

EX  
 LINK: Loading  
 [LNKXCT TERNRY execution]

SOLUTION TEMPERATURE (F)	SOLUTION TEMPERATURE (K)	REFRIGERANT TEMPERATURE (F)	REFRIGERANT TEMPERATURE (K)	REFRIGERANT PRESSURE (PSIA)	REFRIGERANT PRESSURE (PA)	TERNARY (MM HG)	TERNARY (WT.%)
212.0	373.0	186.4	358.0	8.62	.594E+05	.445E+03	50.0
212.0	373.0	184.1	357.0	8.20	.566E+05	.424E+03	52.5
212.0	373.0	181.6	356.0	7.77	.536E+05	.401E+03	55.0
212.0	373.0	178.9	354.0	7.31	.504E+05	.378E+03	57.5
212.0	373.0	175.8	353.0	6.82	.470E+05	.352E+03	60.0
212.0	373.0	172.2	351.0	6.30	.434E+05	.325E+03	62.5
212.0	373.0	168.3	348.0	5.75	.396E+05	.297E+03	65.0
212.0	373.0	163.8	346.0	5.18	.357E+05	.267E+03	67.5
212.0	373.0	158.8	343.0	4.60	.317E+05	.237E+03	70.0
212.0	373.0	153.2	340.0	4.02	.277E+05	.207E+03	72.5
212.0	373.0	147.2	337.0	3.46	.239E+05	.179E+03	75.0
212.0	373.0	140.7	333.0	2.94	.203E+05	.152E+03	77.5
212.0	373.0	133.8	329.0	2.46	.170E+05	.127E+03	80.0
212.0	373.0	126.7	325.0	2.03	.140E+05	.105E+03	82.5
212.0	373.0	119.3	321.0	1.66	.115E+05	.850E+02	85.0
212.0	373.0	111.9	317.0	1.35	.929E+04	.690E+02	87.5
212.0	373.0	104.5	313.0	1.09	.750E+04	.560E+02	90.0
212.0	373.0	97.4	309.0	0.88	.604E+04	.450E+02	92.5

STOP

END OF EXECUTION  
 CPU TIME: 0.19 ELAPSED TIME: 11.47  
 EXIT

:X  
 -INK: Loading  
 [LNKXCT TERNRY execution]

SOLUTION TEMPERATURE (F) (K)	REFRIGERANT TEMPERATURE (F) (K)	REFRIGERANT PRESSURE (PSIA) (PA)	REFRIGERANT PRESSURE (MM HG) (WT.%)	TERNARY
302.0 423.0	268.9 404.0	41.18	.284E+06 .213E+04	50.0
302.0 423.0	265.6 402.0	38.95	.269E+06 .201E+04	52.5
302.0 423.0	262.3 401.0	36.84	.254E+06 .191E+04	55.0
302.0 423.0	259.8 399.0	34.75	.240E+06 .180E+04	57.5
302.0 423.0	255.1 397.0	32.61	.225E+06 .169E+04	60.0
302.0 423.0	251.0 394.0	30.37	.209E+06 .157E+04	62.5
302.0 423.0	246.4 392.0	28.01	.193E+06 .145E+04	65.0
302.0 423.0	241.3 389.0	25.53	.176E+06 .132E+04	67.5
302.0 423.0	235.4 386.0	22.96	.158E+06 .119E+04	70.0
302.0 423.0	228.9 382.0	20.33	.140E+06 .105E+04	72.5
302.0 423.0	221.6 378.0	17.71	.122E+06 .915E+03	75.0
302.0 423.0	213.7 374.0	15.16	.105E+06 .784E+03	77.5
302.0 423.0	205.1 369.0	12.76	.880E+05 .660E+03	80.0
302.0 423.0	195.9 364.0	10.56	.728E+05 .546E+03	82.5
302.0 423.0	186.3 358.0	8.61	.593E+05 .445E+03	85.0
302.0 423.0	176.4 353.0	6.91	.477E+05 .357E+03	87.5
302.0 423.0	166.3 347.0	5.49	.379E+05 .284E+03	90.0
302.0 423.0	156.3 342.0	4.33	.298E+05 .223E+03	92.5

STOP

END OF EXECUTION  
 CPU TIME: 0.18 ELAPSED TIME: 10.00  
 EXIT

•

EX TERNRY  
 LINK: Loading  
 [LNKXCT TERNRY execution]

SOLUTION TEMPERATURE (F)	SOLUTION TEMPERATURE (K)	REFRIGERANT TEMPERATURE (F)	REFRIGERANT TEMPERATURE (K)	REFRIGERANT PRESSURE (PSIA)	REFRIGERANT PRESSURE (PA)	TERNARY (MM HG)	TERNARY (WT.%)
527.0	548.0	475.4	519.0	548.13	.378E+07	.283E+05	50.0
527.0	548.0	469.4	516.0	517.45	.357E+07	.268E+05	52.5
527.0	548.0	463.9	513.0	490.91	.338E+07	.254E+05	55.0
527.0	548.0	458.8	510.0	466.60	.322E+07	.241E+05	57.5
527.0	548.0	453.6	507.0	443.02	.305E+07	.229E+05	60.0
527.0	548.0	448.0	504.0	418.98	.289E+07	.217E+05	62.5
527.0	548.0	441.9	500.0	393.60	.271E+07	.204E+05	65.0
527.0	548.0	435.0	497.0	366.32	.253E+07	.189E+05	67.5
527.0	548.0	427.1	492.0	336.89	.232E+07	.174E+05	70.0
527.0	548.0	418.0	487.0	305.44	.211E+07	.158E+05	72.5
527.0	548.0	407.7	481.0	272.43	.188E+07	.141E+05	75.0
527.0	548.0	396.0	475.0	238.61	.165E+07	.123E+05	77.5
527.0	548.0	383.1	468.0	204.95	.141E+07	.106E+05	80.0
527.0	548.0	368.9	460.0	172.48	.119E+07	.892E+04	82.5
527.0	548.0	353.7	451.0	142.19	.980E+06	.735E+04	85.0
527.0	548.0	337.5	442.0	114.86	.792E+06	.594E+04	87.5
527.0	548.0	320.7	433.0	91.03	.628E+06	.471E+04	90.0
527.0	548.0	303.5	424.0	70.89	.489E+06	.367E+04	92.5

STOP

END OF EXECUTION  
 CPU TIME: 0.18 ELAPSED TIME: 10.37  
 EXIT

**Appendix C**

COEFFICIENTS OF  $\alpha(X)$ ,  $\beta(X)$   
USING POLFIT.BAS

R BASIC

READY, FOR HELP TYPE HELP.  
OLD BAS:POLFIT.BAS

READY  
RUN

BAS:POLFIT 13:25 06-OCT-86

THIS PROGRAM FITS LEAST-SQUARES POLYNOMIALS TO BIVARIATE DATA, USING AN ORTHOGONAL POLYNOMIAL METHOD. LIMITS ARE 11-TH DEGREE FIT AND A MAX OF 100 DATA POINTS. PROGRAM ALLOWS USER TO SPECIFY THE LOWEST DEGREE POLYNOMIAL TO BE FIT, AND THEN FITS THE POLYNOMIALS IN ORDER OF ASCENDING DEGREE. AT EACH STAGE, THE INDEX OF DETERMINATION IS PRINTED, AND THE USER HAS THE CHOICE OF GOING TO THE NEXT HIGHER DEGREE FIT, SEEING EITHER OF TWO SUMMARIES OF FIT AT THAT STAGE, OR OF STOPPING THE PROGRAM. TO USE, TYPE:

```
10 DATA N, D
      (WHERE N = NUMBER OF DATA POINTS TO BE READ
       AND D = INITIAL (LOWEST) DEGREE TO BE FIT)
100 DATA X(1),Y(1),X(2),Y(2),...,X(N),Y(N)
      (CONTINUATION ON LINES 101-299 AS NEEDED)
RUN
```

TIME: 0.25 SECS.

READY
10 DATA 9,2
100 DATA 70.0,97.0878,72.5,98.296,77.5,101.152,80.,105.336,82.5,107.959,
101 DATA 85.,114.215,87.5,118.718,90.,126.840,92.5,131.402
RUN

BAS:POLFIT 13:28 06-OCT-86

#### LEAST-SQUARES POLYNOMIALS

NUMBER OF POINTS = 9
MEAN VALUE OF X = 81.9444
MEAN VALUE OF Y = 111.223
STD ERROR OF Y = 12.3989

NOTE: CODE FOR 'WHAT NEXT?' IS:

0 = STOP PROGRAM
1 = COEFFICIENTS ONLY
2 = ENTIRE SUMMARY
3 = FIT NEXT HIGHER DEGREE

POLYFIT OF DEGREE 2 INDEX OF DETERM = 0.994198 WHAT NEXT ??

POLYFIT OF DEGREE 2 INDEX OF DETERM = 0.994198      WHAT NEXT ?2

TERM            COEFFICIENT

0	394.516
1	-8.64996
2	6.28787E-2

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
70	97.0878	97.1246	-3.68223E-2	-3.79124E-2
72.5	98.296	97.9003	0.395747	0.404235
77.5	101.152	101.809	-0.657463	-0.645778
80	105.336	104.943	0.392954	0.374445
82.5	107.959	108.863	-0.903613	-0.830049
85	114.215	113.568	0.646839	0.56956
87.5	118.718	119.06	-0.341692	-0.286992
90	126.84	125.337	1.50279	1.199
92.5	131.402	132.401	-0.998711	-0.754309

STD ERROR OF ESTIMATE FOR Y = 0.944468

WHAT NEXT ?3

POLYFIT OF DEGREE 3 INDEX OF DETERM = 0.993907      WHAT NEXT ?2

TERM            COEFFICIENT

0	944.077
1	-29.1229
2	0.315831
3	-1.03672E-3

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
70	97.0878	97.4533	-0.365523	-0.375075
72.5	98.296	97.6847	0.611316	0.625805
77.5	101.152	101.438	-0.286133	-0.282076
80	105.336	104.766	0.570154	0.544218
82.5	107.959	108.931	-0.972312	-0.892592
85	114.215	113.837	0.377705	0.331793
87.5	118.718	119.387	-0.668627	-0.560052
90	126.84	125.482	1.35787	1.08212
92.5	131.402	132.027	-0.624603	-0.473089

STD ERROR OF ESTIMATE FOR Y = 0.967813

WHAT NEXT ?0

TIME: 0.51 SECS.

R BASIC

READY, FOR HELP TYPE HELP.  
OLD BAS:POLFIT.BAS

READY  
RUN

BAS:POLFIT 13:32 06-OCT-86

THIS PROGRAM FITS LEAST-SQUARES POLYNOMIALS TO BIVARIATE DATA, USING AN ORTHOGONAL POLYNOMIAL METHOD. LIMITS ARE 11-TH DEGREE FIT AND A MAX OF 100 DATA POINTS. PROGRAM ALLOWS USER TO SPECIFY THE LOWEST DEGREE POLYNOMIAL TO BE FIT, AND THEN FITS THE POLYNOMIALS IN ORDER OF ASCENDING DEGREE. AT EACH STAGE, THE INDEX OF DETERMINATION IS PRINTED, AND THE USER HAS THE CHOICE OF GOING TO THE NEXT HIGHER DEGREE FIT, SEEING EITHER OF TWO SUMMARIES OF FIT AT THAT STAGE, OR OF STOPPING THE PROGRAM. TO USE, TYPE:

```
10 DATA N, D
      (WHERE N = NUMBER OF DATA POINTS TO BE READ
       AND D = INITIAL (LOWEST) DEGREE TO BE FIT)
100 DATA X(1),Y(1),X(2),Y(2),...,X(N),Y(N)
      (CONTINUATION ON LINES 101-299 AS NEEDED)
RUN
```

TIME: 0.27 SECS.

READY
10 DATA 9,2
100 DATA 70.,.41444,72.5,.407407,77.5,.396296,80.,.387407,82.5,.381482
101 DATA 85.,.37037,87.5,.362963,90.,.349259,92.5,.346296
RUN

BAS:POLFIT 13:34 06-OCT-86

#### L E A S T - S Q U A R E S   P O L Y N O M I A L S

NUMBER OF POINTS = 9
MEAN VALUE OF X = 81.9444
MEAN VALUE OF Y = 0.379547
STD ERROR OF Y = 2.42951E-2

NOTE: CODE FOR 'WHAT NEXT?' IS:

0 = STOP PROGRAM
1 = COEFFICIENTS ONLY
2 = ENTIRE SUMMARY

POLYFIT OF DEGREE 2 INDEX OF DETERM = 0.9913 WHAT NEXT ?2

TERM COEFFICIENT

0	0.388691
1	3.02719E-3
2	-3.80068E-5

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
70	0.41444	0.414361	7.89091E-5	1.90436E-2
72.5	0.407407	0.408389	-9.82121E-4	-0.240486
77.5	0.396296	0.39502	1.27607E-3	0.32304
80	0.387407	0.387623	-2.15705E-4	-5.56483E-2
82.5	0.381482	0.37975	1.73160E-3	0.455985
85	0.37037	0.371403	-0.001033	-0.278136
87.5	0.362963	0.362581	3.82476E-4	0.105487
90	0.349259	0.353283	-4.02395E-3	-1.13902
92.5	0.346296	0.34351	2.78569E-3	0.810949

STD ERROR OF ESTIMATE FOR Y = 2.26605E-3

WHAT NEXT ?3

POLYFIT OF DEGREE 3 INDEX OF DETERM = 0.991308 WHAT NEXT ?2

TERM COEFFICIENT

0	-1.13752
1	5.98835E-2
2	-7.40493E-4
3	2.87912E-6

X-ACTUAL	Y-ACTUAL	Y-CALC	DIFF	PCT-DIFF
70	0.41444	0.413448	9.91739E-4	0.23987
72.5	0.407407	0.408988	-1.58082E-3	-0.38652
77.5	0.396296	0.396051	2.44834E-4	6.18187E-2
80	0.387407	0.388115	-7.07824E-4	-0.182375
82.5	0.381482	0.37956	1.92237E-3	0.506473
85	0.37037	0.370656	-2.85584E-4	-7.70485E-2
87.5	0.362963	0.361673	1.29045E-3	0.3568
90	0.349259	0.352881	-3.62151E-3	-1.02627
92.5	0.346296	0.344549	1.74673E-3	0.506961

STD ERROR OF ESTIMATE FOR Y = 2.26505E-3

WHAT NEXT ?0

TIME: 0.52 SECS.



Appendix D

LISTING AND EXECUTION OF  
COMPUTER PROGRAM TERNRY.H

```

TY TERNRY.H
00020 C      PROGRAM TO CALCULATE SPECIFIC ENTHALPIES OF EC'S TERNARY
00040 C      SOLUTION.
00060 C
00080 C      DOUBLE PRECISION A,B,C,H,T
00100 C
00120      WRITE(6,11)
00140      11 FORMAT(/,3X,'SOLUTION TEMPERATURE, F = ')
00160      READ(5,21)T
00180      21 FORMAT(F6.2)
00200 C
00220      DEGC=CENT(T)
00240      DEBK=KELVN(T)
00260 C
00280      WRITE(6,31)T,DEGC,DEBK
00300      31 FORMAT(/,2X,'SOLUTION TEMPERATURE =',F9.2,'(F)',F9.2,'(C)',,
00320                  CF9.2,'(K)')
00340 C
00360      WRITE(6,41)
00380      41 FORMAT(/,2X,'TERNARY SALT CONC.', 10X,'ENTHALPY',/,7X,'(WT.%)',11X
,
00400      C'(BTU/LB)',2X,'(KJ/KG)',/,2X,'-----'
00420      C-----')
00440      DO 99 XX=70,92.5,2.5
00460      X=XX
00542      A=394.516 - 8.64996*(X) + 6.2878E-02*(X**2)
00560 C
00622      B=0.388691 + 3.02719E-03*(X) - 3.80068E-05*(X**2)
00640 C
00720 C
00740 C      H=200.
00760      H=A + B*T
00780      HKJKG=HKJ(H)
00800 C      WRITE(6,900)A,B,C,T
00820      900 FORMAT(/,X,'A=',E9.3,'B=',F7.3,'C=',E11.4,'T=',F6.2)
00840 C
00860      WRITE(6,51)X,H,HKJKG
00880      51 FORMAT(/,7X,F5.1,11X,F8.2,4X,F8.2)
00900 C
00920      99 CONTINUE
00940 C
00960      STOP
00980      END
01000 C
01020      FUNCTION CENT(T)
01040      CENT=(T+459.67)/1.8 - 273.15
01060      RETURN
01080      END
01100 C
01120      FUNCTION KELVN(T)
01140      KELVN=(T+459.67)/1.8
01160      RETURN
01180      END
01200 C
01220      FUNCTION HKJ(H)
01240      HKJ=H/0.4300
01260      RETURN
01280      END

```

EX TERNRY.H

LINK: Loading

[LNKXCT TERNRY execution]

SOLUTION TEMPERATURE, F =  
257.0

SOLUTION TEMPERATURE = 257.00(F) 125.00(C) 398.00(K)

TERNARY SALT CONC. (WT.%)	ENTHALPY (BTU/LB)	ENTHALPY (KJ/KG)
------------------------------	----------------------	---------------------

70.0	203.61	473.52
72.5	202.85	471.75
75.0	202.76	471.53
77.5	203.33	472.85
80.0	204.56	475.71
82.5	206.45	480.12
85.0	209.01	486.08
87.5	212.24	493.58
90.0	216.13	502.62
92.5	220.68	513.20

STOP

END OF EXECUTION  
CPU TIME: 0.13 ELAPSED TIME: 10.43  
EXIT



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