AN ABSTRACT OF THE THESIS OF

STUART AMES EIDE for the degree of DOCTOR OF PHILOSOPHY

in PHYSICS presented on December 10, 1976

Title: THE EFFECT OF ULTRA-HIGH PRESSURE ON THE EMF OF THERMOCOUPLES

Abstract approved: Redacted for Privacy

Olaf A Boedtker

The effect of ultra-high pressure on the thermal emf of a chromel/alumel thermocouple is investigated using an indirect method which does not require a direct knowledge of the temperature of the pressurized junction. The unknown temperature is written parametrically as a function of a directly measured quantity, the electrical power delivered to the internal furnace. The emf of the pressurized thermocouple is then written as a function of the temperature and a set of unknown coefficients. Combining the two functions to eliminate the unknown junction temperature, the pressurized emf is given as a function of the furnace power. The coefficients of both the temperature-versus-power function and the pressure-corrected emf-versus-temperature function are then obtained simultaneously by performing a nonlinear least-squares fit to the directly measured emf-versus-furnace power data. Results for the temperature correction

due to pressure are compared with estimates obtained by other methods for pressures between 25.0 kbar and 60.6 kbar and temperatures up to approximately 900°C.

The Effect of Ultra-High Pressure on the emf of Thermocouples

by

Stuart Ames Eide

A THESIS

submitted to

Oregon State University

in partial fulfillment of
the requirements for the
degree of

Doctor of Philosophy

June 1977

APPROVED:

Redacted for Privacy

Associate Professor of Physics

in charge of major

Redacted for Privacy

Chairman of Department of Physics

Redacted for Privacy

Dean of Graduate School

Date thesis is presented December 10, 1976

Typed by Clover Redfern for Stuart Ames Eide

ACKNOWLEDGMENTS

The author wishes to express special thanks to Dr. Olaf A. Boedtker for his guidance and encouragement during the course of this work. Thanks are also due the Albany Metallurgy Research Center, U.S. Bureau of Mines, Albany, Oregon for financial support during the early stages of the project and for the use of the 300-ton tetrahedral press throughout the work.

TABLE OF CONTENTS

	Page
INTRODUCTION	1
Statement of the Problem	1
Review of Previous Work	2
Theoretical Considerations	21
The Present Study	26
EXPERIMENTAL APPARATUS AND TECHNIQUE	28
The Tetrahedral Press	28
The High Pressure Cell	31
Thermocouple Circuitry	36
Collection of Data	40
Pressure Calibration	41
COMPUTATIONS	49
RESULTS	54
General Remarks	54
Effect of Pressure on Thermal Emf	58
Temperature Corrections	59
Effect of Pressure on Relative Seebeck, Peltier and Thomson Coefficients	71
SUMMARY AND CONCLUSIONS	76
BIBLIOGRAPHY	78
APPENDICES	86
Appendix A: Computer Program and Subroutines	86
Appendix B: Sample Computer Output	131

LIST OF FIGURES

Figure		Page
1.	Single-wire configuration.	3
2.	Externally-heated thermocouple configuration.	6
3.	Externally-heated differential thermocouple configuration.	8
4.	Internally-heated thermocouple configuration.	11
5.	Comparison of current estimates of temperature correction for chromel/alumel thermocouples at 40 kbar.	18
6.	The 300-ton tetrahedral-anvil press.	29
7.	Detail view of pyrophyllite pressure seal.	30
8.	The pyrophyllite tetrahedron.	32
9.	Interior detail of high-temperature, high-pressure cell.	34
10.	Thermocouple assembly detail.	35
11.	The tetrahedral pressure cell. Exploded view.	37
12.	Tetrahedral cell, before and after pressure run.	38
13.	High-temperature, high-pressure instrumentation.	39
14.	Pressure calibration cell. Interior detail.	43
15.	Pressure calibration circuit.	44
16.	Pressure calibration. Bismuth I-II transformation.	45
17.	Pressure calibration. Thallium II-III transformation.	46
18.	Pressure calibration. Barium I-II transformation.	47
19.	Pressure calibration curve. True cell pressure versus hydraulic oil pressure.	48
20.	Data processing flow chart.	52

Figure		Page
21.	Typical furnace temperature versus furnace power curve.	55
22.	Temperature correction. Comparison of results at 25.0 kbar.	65
23.	Temperature correction. Comparison of results at 35.2 kbar.	66
24.	Temperature correction. Comparison of results at 44.6 kbar.	67
25.	Temperature correction. Comparison of results at 53.0 kbar.	68
26.	Temperature correction. Comparison of results at 60.6 kbar.	69
27.	Effect of pressure on relative Seebeck coefficient.	72
28.	Effect of pressure on relative Peltier coefficient.	74
29.	Effect of pressure on relative Thomson coefficient.	75

LIST OF TABLES

Table		Page
1.	Coefficients of eighth-degree linear least-squares fit to NBS chromel/alumel tables, 0-900°C.	53
2.	Summary of results at 25.0 kbar.	60
3.	Summary of results at 35.2 kbar.	61
4.	Summary of results at 44.6 kbar.	62
5.	Summary of results at 53.0 kbar.	63
6.	Summary of results at 60.6 kbar.	64

THE EFFECT OF ULTRA-HIGH PRESSURE ON THE EMF OF THERMOCOUPLES

INTRODUCTION

Statement of the Problem

The accurate measurement of high temperatures presents a challenging experimental problem in a high-pressure environment. Such conditions are routinely encountered in the study of phase transformations in solids, where temperatures exceeding 2000° C and pressures of more than 100 kilobars are not uncommon (1 kilobar = 14,504 pounds/inch^2 = 10^8 newtons/m^2). When the temperatures involved are no more than a few hundred degrees Celsius, an entire pressure vessel may be heated externally, often by immersing the vessel in a heated fluid. Under such conditions when the system attains thermal equilibrium the temperature within the vessel may be conveniently determined externally with considerable accuracy by conventional means, such as a calibrated thermocouple or resistance thermometer, at atmospheric pressure. At temperatures above approximately 400° C the strength of the material of which the pressure vessel is constructed begins to decrease rapidly with increasing temperature, thus limiting the maximum safe operating pressure. This difficulty is commonly circumvented by heating only a relatively small, thermally-insulated high-pressure region by means of an

internal electric furnace, while the pressure vessel itself remains safely cool. Because of their simplicity, ruggedness and small size, thermocouples have become the principal means of determining the internal temperature of the pressurized region in such high-pressure devices. The absolute accuracy of such temperature measurements is in question, however, since the thermal emf produced in a thermocouple is itself dependent on the ambient pressure. As an example, for the commonly-used platinum-10% rhodium/platinum thermocouple (Pt10%Rh/Pt) the pressure effect at 1200°C and 50 kbar is believed to produce readings approximately 50°C lower than the true temperature (39,40).

Review of Previous Work

Before reviewing in detail the efforts of previous investigators we present a few necessary introductory remarks concerning the experimental configurations commonly used in this field of research. Attempts to experimentally determine the effect of pressure on the thermal emf of metals and alloys have generally employed either of two configurations: a single-wire method or a thermocouple approach. In the single-wire method a single, continuous, homogeneous wire of the material under investigation is passed through pressure and temperature gradients as shown schematically in Figure 1. Also shown in Figure 1 are the temperature and pressure as a function of position

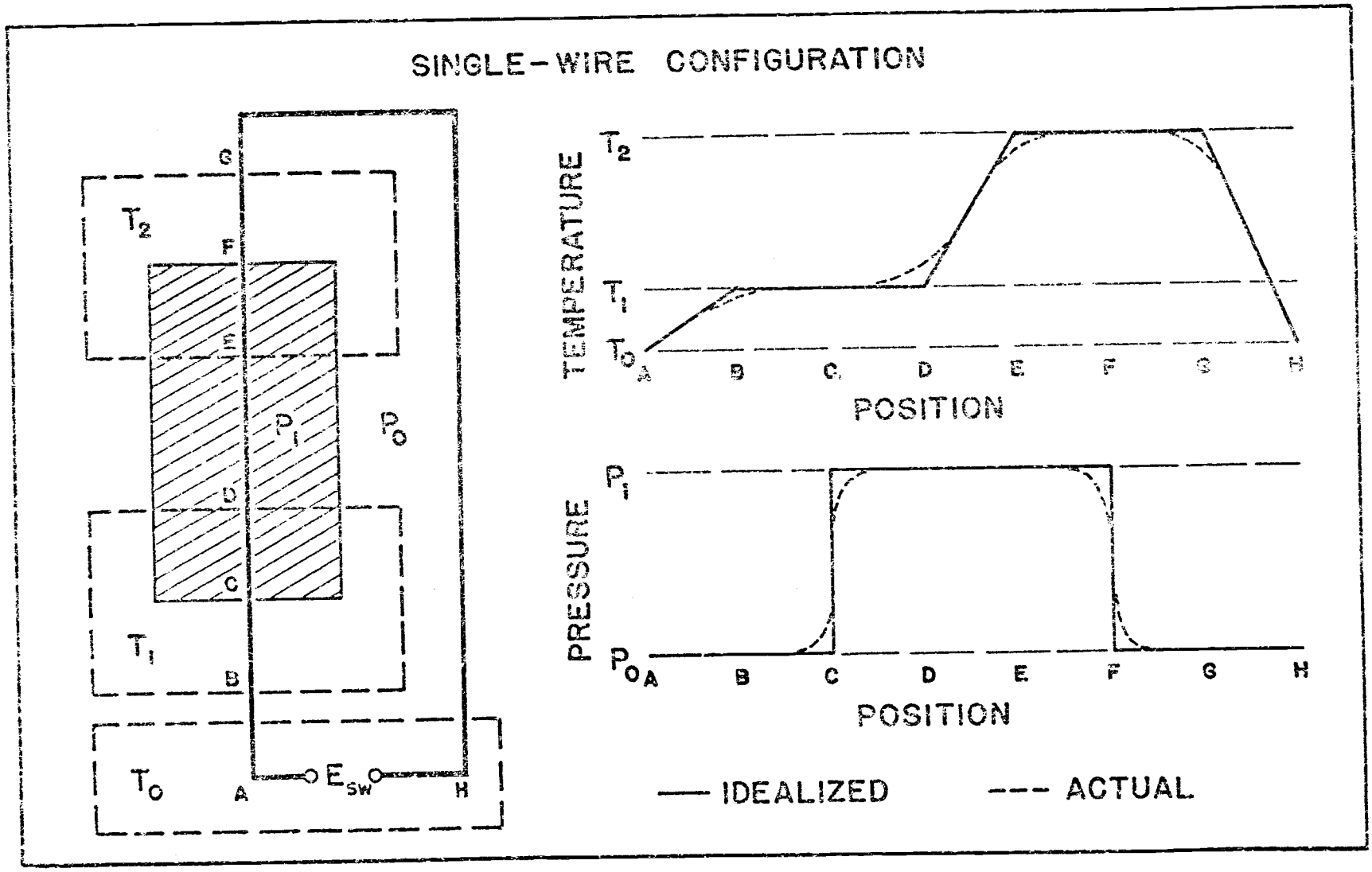


Figure 1. Single-wire configuration.

along the wire, both for the idealized case of isothermal pressure seals and for a more physically realistic case which might be encountered in an actual laboratory situation. Under atmospheric pressure ($p_0 \doteq 0.001$ kbar) the wire passes from the reference temperature T_0 (typically an ice point bath at 0° C) to the pressure seal at temperature $T_1 > T_0$. The wire then passes isothermally (in the idealized case) into the high-pressure region at pressure p_1. After leaving the pressurized region through another isothermal pressure seal at some temperature $T_2 > T_1$, the wire returns under atmospheric pressure, p_0, to the reference temperature, T_0. Denoting by $S(p, T)$ the Seebeck coefficient or thermoelectric power (also referred to as the "thermopower") at pressure p and temperature T, the total thermal emf generated in the circuit is determined by summing the contributions from each segment around the circuit.

$$E_{sw} = \oint S(p, T)dT$$

$$= \int_{T_0}^{T_1} S(p_0, T)dT + \int_{T_1}^{T_2} S(p_1, T)dT + \int_{T_2}^{T_0} S(p_0, T)dT$$

$$E_{sw} = \int_{T_1}^{T_2} [S(p_1, T)-S(p_0, T)]dT \qquad (1-1)$$

The alternative method most commonly used exposes a thermocouple composed of two dissimilar metals, denoted here by subscripts a and b, to pressures and temperatures as depicted schematically in Figure 2. Both wires pass from reference temperature T_0 at atmospheric pressure, p_0, to the pressure seal at temperature $T_1 > T_0$. The wires then pass through an (ideally) isothermal pressure seal into the pressurized region at high pressure p_1. Under pressure p_1, the wires then increase in temperature from T_1 to T_2, the temperature at the thermocouple junction. Again, evaluating the total thermal emf around the circuit we have

$$E_{tc} = \oint S(p, T)dT$$

$$= \int_{T_0}^{T_1} S_a(p_0, T)dT + \int_{T_1}^{T_2} S_a(p_1, T)dT + \int_{T_2}^{T_1} S_b(p_1, T)dT + \int_{T_1}^{T_0} S_b(p_0, T)dT$$

$$E_{tc} = \int_{T_0}^{T_1} [S_a(p_0, T) - S_b(p_0, T)]dT + \int_{T_1}^{T_2} [S_a(p_1, T) - S_b(p_1, T)]dT \qquad (1\text{-}2)$$

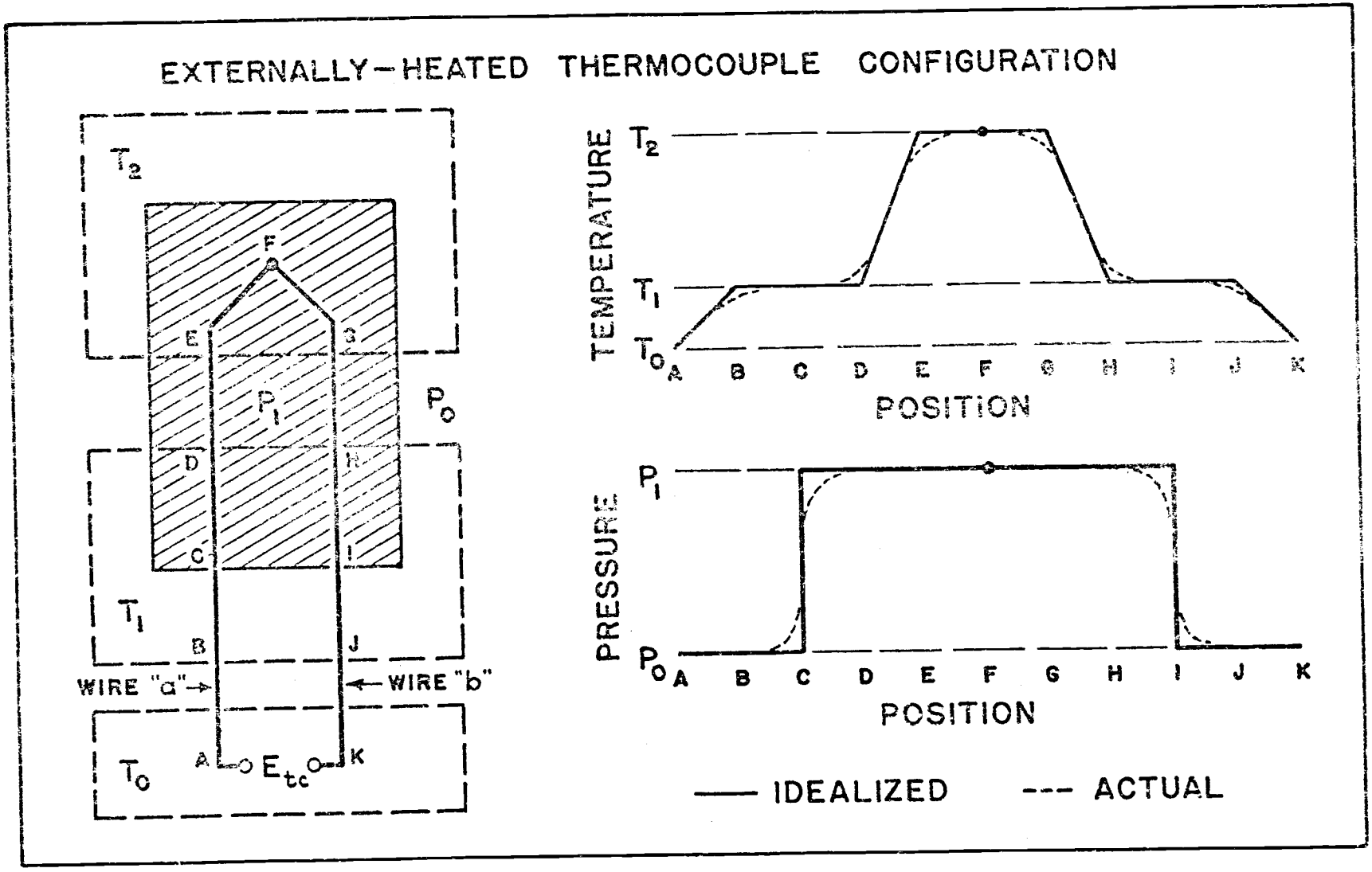


Figure 2. Externally-heated thermocouple configuration.

or

$$E_{tc} = \int_{T_0}^{T_1} S_{ab}(p_0, T)dT + \int_{T_1}^{T_2} S_{ab}(p_1, T)dT \qquad (1-3)$$

where

$$S_{ab}(p, T) \equiv S_a(p, T) - S_b(p, T) \qquad (1-4)$$

is defined as the relative Seebeck coefficient. The first term in Equation (1-3) is simply the contribution due to the unpressurized portion of the circuit between the reference temperature, T_0, and the pressure seal temperature, T_1. For $T_0 = 0°C$ and a known temperature T_1, this first term may be evaluated for standard thermocouple pairs using published reference tables (71) for use at atmospheric pressure

One modification of this thermocouple configuration consists of connecting two identical thermocouples in a differential mode with one thermocouple under pressure and the other at atmospheric pressure, with both hot junctions at temperature T_2, as shown schematically in Figure 3.

Evaluating the total thermal emf around the circuit we find

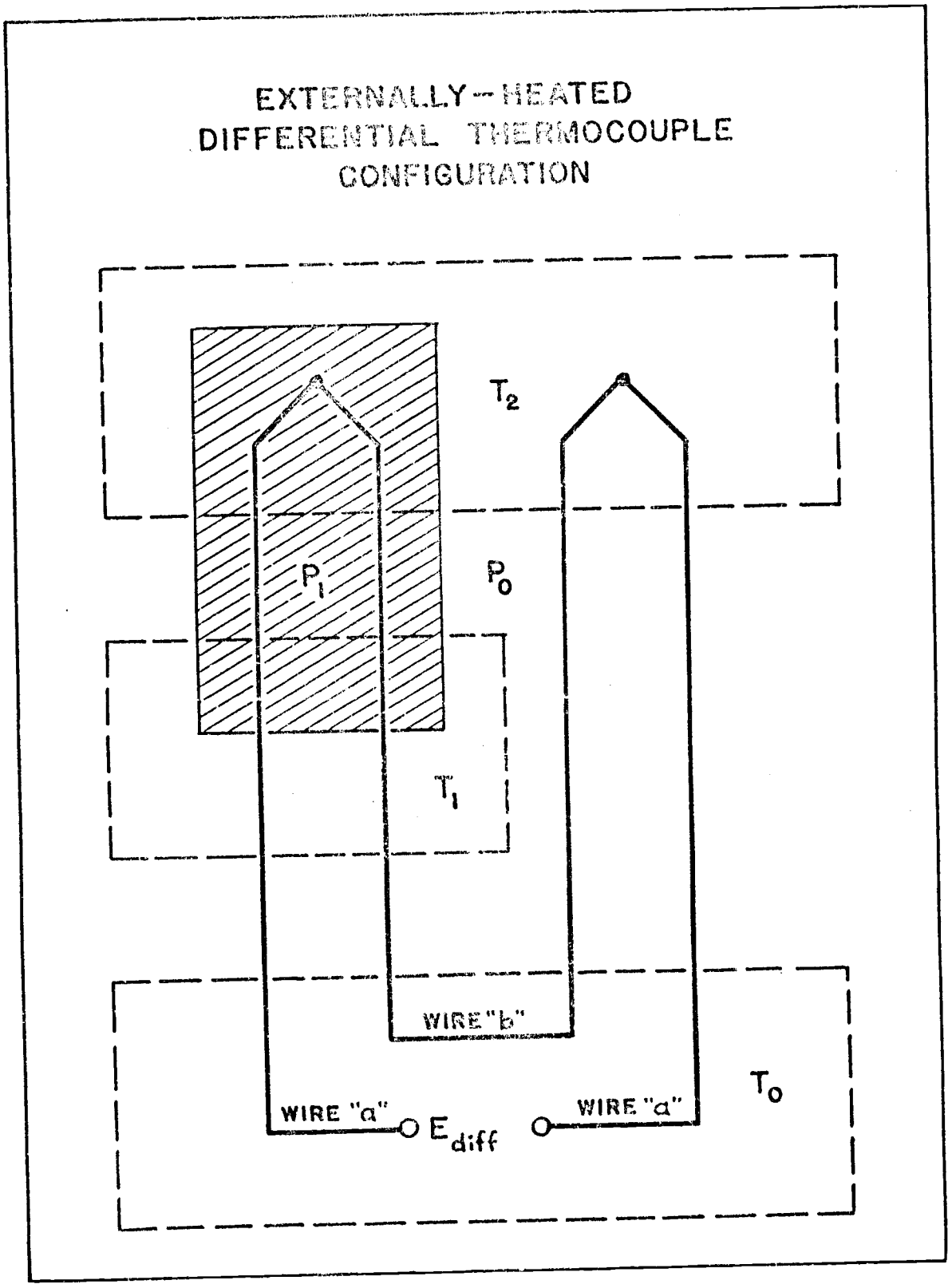


Figure 3. Externally-heated differential thermocouple configuration.

$$E_{diff} = \int_{T_0}^{T_1} S_a(p_0, T)dT + \int_{T_1}^{T_2} S_a(p_1, T)dT + \int_{T_2}^{T_1} S_b(p_1, T)dT$$

$$+ \int_{T_1}^{T_0} S_b(p_0, T)dT + \int_{T_0}^{T_2} S_b(p_0, T)dT + \int_{T_2}^{T_0} S_a(p_0, T)dT$$

$$= \int_{T_1}^{T_2} [S_a(p_1, T) - S_b(p_1, T)]dT$$

$$- \int_{T_1}^{T_2} [S_a(p_0, T)dT - S_b(p_0, T)]dT \qquad (1-5)$$

$$E_{diff} = \int_{T_1}^{T_2} [S_{ab}(p_1, T) - S_{ab}(p_0, T)]dT \qquad (1-6)$$

which gives directly the change in thermal emf which results from placing the thermocouple under pressure. This quantity can also be obtained using the absolute corrections from single-wire experiments. Rewriting Equation (1-5) we obtain

$$E_{diff} = \int_{T_1}^{T_2} [S_a(p_1, T) - S_a(p_0, T)]dT - \int_{T_1}^{T_2} [S_b(p_1, T) - S_b(p_0, T)]dT \qquad (1-7)$$

which demonstrates that E_{diff} is also equal to the difference between the single-wire corrections for each of the individual

materials, represented by subscripts a and b, which constitute the thermocouple; that is, from Equations (1-1) and (1-7)

$$E_{diff} = (E_{sw})_a - (E_{sw})_b \tag{1-8}$$

Finally, a common variation of the thermocouple configuration used in ultra-high-pressure systems which employ a solid pressure-transmitting medium is illustrated in Figure 4. The pressurized junction is heated by means of an internal electrical resistance furnace. The total thermal emf for this configuration is also given by Equation (1-3),

$$E_{tc} = \int_{T_0}^{T_1} S_{ab}(p_0, T)dT + \int_{T_1}^{T_2} S_{ab}(p_1, T)dT . \tag{1-9}$$

Proceeding with a review of this field one finds that high-pressure research falls generally into two pressure ranges. Studies done under truly hydrostatic conditions requiring the use of a liquid or gas as the pressure-transmitting medium have generally been limited to pressures up to 12 kbar and temperatures of no more than a few hundred degrees Celsius. To attain higher pressures and temperature one must be satisfied with quasi-hydrostatic conditions using a solid pressure-transmitting medium.

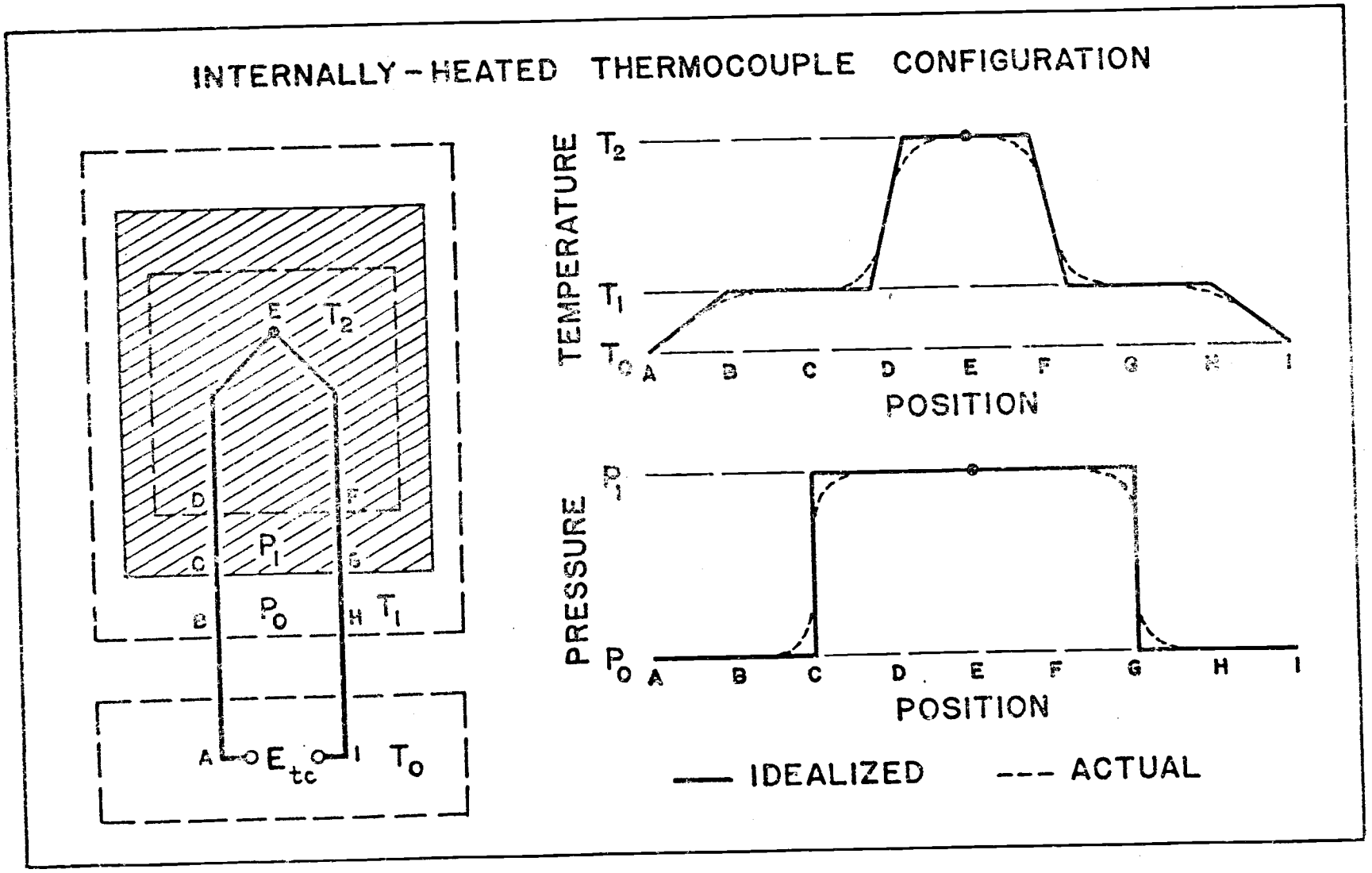


Figure 4. Internally-heated thermocouple configuration.

Within the hydrostatic pressure range the first significant study of the effect of pressure on the thermal emf of metals and alloys was that of Bridgman (16), whose extraordinary pioneering efforts laid the foundations of modern high-pressure physics. Using a single-wire approach (Figure 1), Bridgman studied 18 metallic elements and two alloys under pressures up to 12 kbar and temperatures up to 100°C, concluding that even over this rather limited range of pressure and temperature the results were "unexpectedly complicated". Unfortunately, Bridgman did not study most of the thermocouple materials in common use today.

Birch (10), using a thermocouple configuration (Figure 2), studied Pt10%Rh/Pt and chromel/alumel thermocouples at pressures up to 4 kbar and hot junction temperatures (T_2 in Equation (1-3)) up to 470°C. His results for Pt10%Rh/Pt indicated an emf pressure correction of +15 μV at 470°C and 4 kbar, corresponding to a temperature correction of approximately +15°C. (Note: According to convention the "emf pressure correction" is the voltage which must be added to the emf of the pressurized thermocouple in order to obtain the true temperature using standard atmospheric pressure thermocouple reference tables. The corresponding "temperature correction" is the number of degrees which must be added to the uncorrected temperature indicated by the pressurized thermocouple to obtain the true temperature.) Birch found the thermal emf of the chromel/alumel

thermocouple to be essentially independent of pressure to within 10 μV. However, he did not record the temperature of the pressure seal (T_1 in Equation (1-3)), which implies that the actual temperature gradient under pressure was somewhat smaller than otherwise indicated.

Bloch and Chaissé (11) employed a thermocouple configuration (Figure 2) to study the effect of pressure up to 5 kbar on copper/constantan thermocouples at low temperatures from -196°C to +89°C. They found a linear positive correction of 0.048°C/kbar at 89°C which agrees with the results of Bridgman (16) and Bundy (21) over the mutual range of measurement.

Bell, Boyd and England (8) employed a differential thermocouple arrangement (Figure 3) to study the effect of pressure on Pt10%Rh/Pt thermocouples under hydrostatic conditions up to 10 kbar and temperatures up to 509°C. Their results indicate that pressure decreases the thermal emf of a Pt10%Rh/Pt thermocouple, thus requiring the addition of a positive correction at pressures above atmospheric. An emf pressure correction of 20 μV was determined at 509°C and 3.5 kbar, corresponding to a temperature correction of approximately 2°C, values which compare favorably with results extrapolated from solid-media experiments at much higher pressures.

Freud and LaMori (32) conducted single-wire (Figure 1) hydrostatic studies on chromel, alumel, copper and constantan at pressures

up to 8 kbar and temperatures from -195°C to +290°C. Results computed for the copper/constantan thermocouple (Equation (1-8)) agree within experimental error with those of Bloch and Chaissé (11) and Bridgman (16). For chromel/alumel at 8 kbar the emf pressure correction was found to be essentially zero between -83°C and +27°C, increasing to approximately +1 μV between 100°C and 200°C, then decreasing and changing sign between 200°C and 300°C. This behavior agrees essentially with the results of Getting and Kennedy (34) for chromel/alumel extrapolated to these lower pressures.

Using hydrostatic pressures up to 7 kbar and an internal furnace to produce temperatures from 500°C to 980°C, Lazarus, Jeffrey and Weiss (56) employed a thermocouple approach (Figure 4) to compare differences between temperatures indicated by a pressurized chromel/alumel thermocouple as compared to a pressurized Pt10%Rh/Pt thermocouple. Their results indicate that the chromel/alumel thermocouple is definitely pressure dependent above 720°C with the correction reversing sign (becoming negative) above this temperature in agreement with higher-pressure results of Getting and Kennedy (34). Lack of knowledge of the precise temperature of the internal furnace precluded the quantitative evaluation of emf pressure corrections for the individual thermocouples.

Lallemand, et al. (53), using a Pt10%Rh/Pt thermocouple, studied the effect of pressure on the fusion curves of gold and silver.

By comparison with thermodynamic calculations they concluded that for pressures up to 8 kbar and temperatures between 960°C and 1100°C, the thermal emf of the Pt10%Rh/Pt thermocouple decreases with increasing pressure resulting in a temperature correction of approximately 0.5°C/kbar. This value is consistent with results of Lazarus et al. (56) and Getting and Kennedy (34).

Using a differential thermocouple arrangement (Figure 3), Cheng, Allen and Lazarus (23) have studied the effect of hydrostatic pressures up to 2 kbar and temperatures up to 950°C on chromel/alumel and Pt10%Rh/Pt thermocouples. Results indicate positive emf pressure corrections for Pt10%Rh/Pt in general agreement with Getting and Kennedy (34), while the corrections for chromel/alumel thermocouples may be even more negative than those indicated by Getting and Kennedy. The pressure dependence of the difference between indicated temperatures of the two thermocouples is generally in good agreement with the earlier work of Lazarus, et al. (56).

The most recent hydrostatic determinations are those of Diatschenko and Chu (30) for a chromel/alumel thermocouple (Figure 2) at pressures up to 22 kbar and temperatures between -269°C and +27°C, which indicate extremely small emf pressure corrections of no more than ±1 μV over the entire range of temperatures studied. This result is consistent with previous studies at temperature above 0°C (34, 40, 56).

Within the relatively limited pressure range of hydrostatic studies the results have generally agreed within experimental error. In the ultra-high pressure range above approximately 20 kbar, however, the currently available thermal emf corrections due to pressure are only approximate because of several inherent experimental difficulties (41):

(1) uncertainty in the absolute pressure in the nonhydrostatic solid pressure-transmitting medium,

(2) lack of precise knowledge of the true temperature within the pressurized region,

(3) pressure seals which are not isothermal,

(4) plastic deformation of the thermocouple wires, and

(5) environmental problems including chemical contamination and electrical shunting of the thermocouples at high temperatures.

In spite of these difficulties a number of significant results have been obtained in this higher pressure range using solid-media systems. Bundy (21) employed a single-wire method to study the effect of pressure on the thermal emf of eight metals and alloys at pressures up to 72 kbar and a temperature difference of 100°C. Taking differences between the single-wire corrections (Equation (1-8)) to determine the appropriate thermocouple emf pressure corrections Bundy found corresponding temperature corrections of nearly +5°C

at 100°C and 40 kbar for Pt10%Rh/Pt and slightly more than +1°C at 100°C and 40 kbar for chromel/alumel. The extrapolated results for chromel/alumel are shown in Figure 5 for a pressure of 40 kbar. Bundy also conducted common-junction thermocouple experiments which compared chromel/alumel against Pt10%Rh/Pt at pressures to 42 kbar and temperatures to 1200°C. The difference was found to first increase to as much as +15°C at 42 kbar and approximately 500°C; then to decrease, eventually changing sign at temperatures above 800°C. Bundy thus clearly demonstrated the danger inherent in extrapolating thermocouple corrections far beyond actual measured temperature and pressure ranges, a warning that has often been ignored in practice presumably for lack of better information.

Hanneman and Strong (39) used a thermocouple approach to determine relative temperature corrections for several thermocouples including chromel/alumel against Pt10%Rh/Pt. Their results differ from those of Bundy at high temperature, the relative temperature correction reaching +47°C at 1200°C and 50 kbar. Comparing experimental results with theoretical thermodynamic calculations for single-component phase transformations and for diffusion at high pressures, Hanneman and Strong were able to estimate the true temperature of the internally-heated pressurized region, thus determining the absolute temperature corrections for the individual thermocouples. Their results for chromel/alumel at 40 kbar are shown in Figure 5.

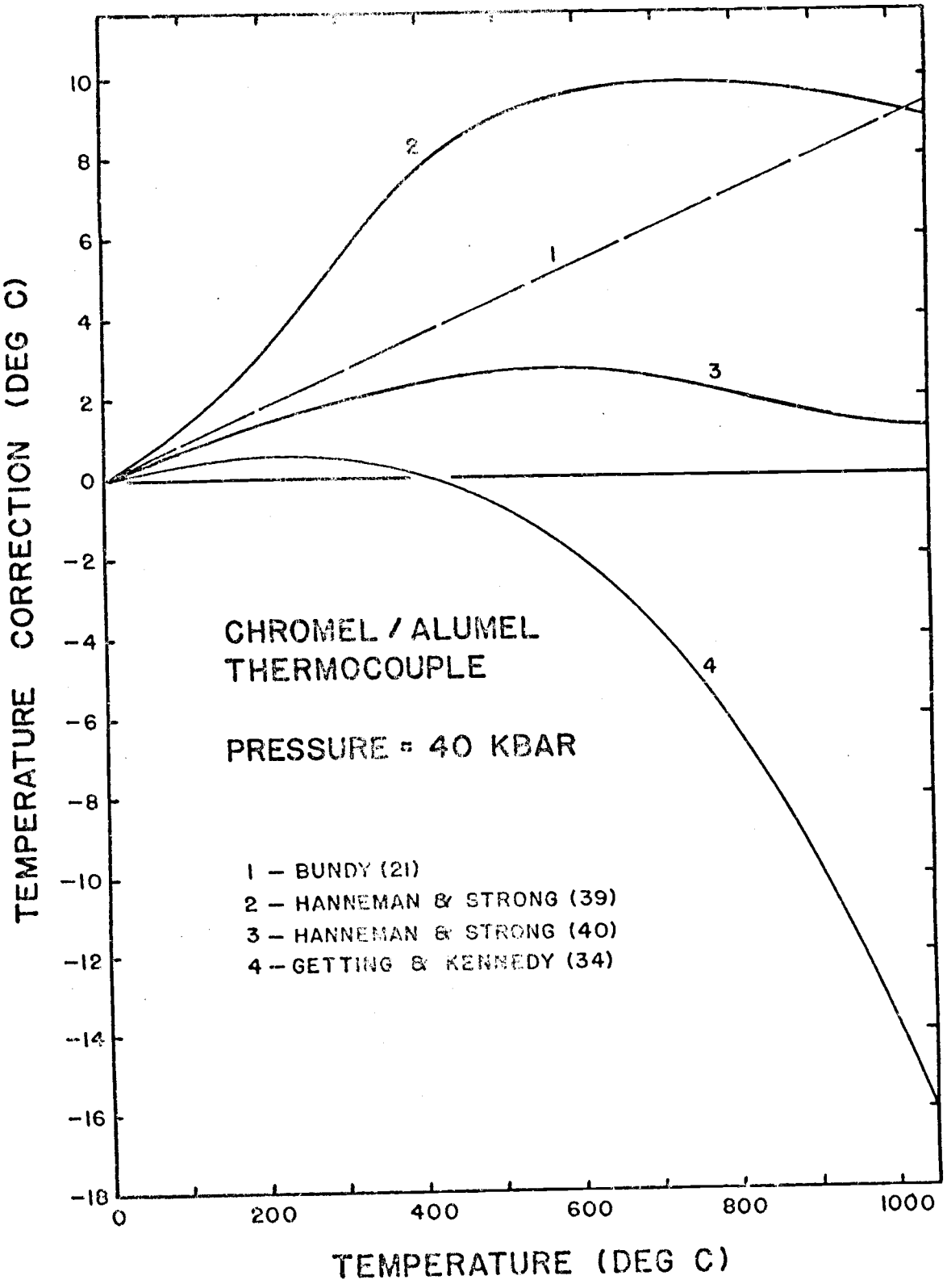


Figure 5. Comparison of current estimates of temperature correction for chromel/alumel thermocouples at 40 kbar.

Later work by the same investigators (40) using different high pressure cell materials and attempting to correct for temperature and pressure gradients in the pressure seal region resulted in a downward revision of their previous estimate for the temperature correction in chromel/alumel, also shown in Figure 5. Peters and Ryan (65) also measured relative temperature corrections for Pt10%Rh/Pt against chromel/alumel at 40 kbar and temperatures from 200°C to 1000°C, but found values exceeding those of Hanneman and Strong (39,40) by as much as 35% at 1000°C.

Getting and Kennedy (33, 34) have used a single-wire method to determine absolute thermal emf corrections for Pt, Pt10%Rh, chromel and alumel for pressures up to 35 kbar and temperatures up to 1000°C. Thermocouple corrections obtained from differences in the appropriate single-wire corrections indicate temperature corrections for Pt10%Rh/Pt of approximately half those of Hanneman and Strong (40) at 35 kbar and 1000°C. For chromel/alumel the temperature corrections differ considerably from previous work, becoming large and negative with increasingly negative slope at the higher temperatures (Figure 5). Freud and LaMori (32) also performed single-wire measurements on the same materials for pressures up to 40 kbar and temperatures from 30°C to 380°C. Their single-wire results agree with those of Getting and Kennedy for Pt, Pt10%Rh and alumel. For chromel, however, the results of Getting and Kennedy are lower

by about 30% at 20 kbar and 400°C. Freud and LaMori attribute the difference to possible strain effects on the chromel used by Getting and Kennedy.

A totally different approach has been attempted by Wentorf (75) using a Pt10%Rh/Pt thermocouple at pressures of 40 kbar and 50 kbar and temperatures up to about 1400°C. The true temperature of the thermocouple junction is estimated by measuring the minute fluctuating voltage ("thermal noise") generated within a small carbon resistor by thermal agitation of the charge carriers (48). The technique is quite difficult experimentally, requiring extremely low noise electronics, but the rather sparse data available indicate temperature corrections which agree with those of Hanneman and Strong (40).

Most recently Stokes (68) has employed Mössbauer effect studies to estimate the true temperature of a chromel/alumel thermocouple at pressures of 27 kbar, 50 kbar and 75 kbar at temperatures up to 600°C. Results for the temperature correction agree within rather large (±3°C) experimental error with the results of Hanneman and Strong (40) and Getting and Kennedy (34) at 27 kbar and 50 kbar up to 600°C. However, at higher pressure (75 kbar) the Mössbauer estimates give much larger positive temperature corrections than even the early results of Hanneman and Strong (39), suggesting corrections of the order of +25°C at 600°C.

The considerable uncertainty in the corrections for thermal emf and temperature measured with chromel/alumel thermocouples under ultra-high pressure is evident in Figure 5. It was hoped that the new approach employed in the present work might help to resolve this discrepancy.

Theoretical Considerations

Although the theoretical understanding of thermoelectric phenomena is currently inadequate to allow reliable calculations of a quantitative nature for the effect of high pressure on thermal emf, it is nonetheless instructive to attempt to determine at least the order of magnitude for the pressure effect which might be considered physically reasonable. From formal Boltzmann transport theory we obtain a general expression for the absolute thermopower of a metal, due to electron diffusion (6,61,78)

$$S = -\frac{\pi^2 k^2 T}{3|e|}\left[\frac{\partial(\ln \sigma(\varepsilon))}{\partial \varepsilon}\right]_{\varepsilon=\varepsilon_F} \qquad (1\text{-}10)$$

where

$\sigma(\varepsilon)$ = electrical conductivity

e = electronic charge

$= -1.60 \times 10^{-19}$ coulomb

k = Boltzmann constant

$= 1.38 \times 10^{-23}$ joule/°K

T = absolute temperature (degrees Kelvin)

ε_F = Fermi energy

The thermopower can also be written in the form

$$S = -\frac{\pi^2 k^2 T}{3|e|\varepsilon_F}\left[\frac{\partial \ln \sigma(\varepsilon)}{\partial \ln \varepsilon}\right]_{\varepsilon=\varepsilon_F} \tag{1-11}$$

$$= -\frac{\pi^2 k^2 T}{3|e|\varepsilon_F}\,\xi \tag{1-12}$$

where the dimensionless parameter ξ is commonly referred to as the thermoelectric parameter. The magnitude of ξ is generally taken to be of order unity. Values of ξ from 1.5 to 3 are common, depending upon the energy dependence of the electron scattering mechanisms contributing to the resistivity of the material.

We wish to derive an expression which will allow us to estimate the magnitude of the effect of pressure on the thermopower for simple metals, and further, to estimate the magnitude of the pressure correction for the thermal emf of such a metal under idealized high-temperature, high-pressure conditions. For the pressure derivative of the thermopower we write

$$\frac{\partial S}{\partial p} = \left(\frac{\partial S}{\partial \varepsilon_F}\right)\left(\frac{\partial \varepsilon_F}{\partial V}\right)\left(\frac{\partial V}{\partial p}\right) \tag{1-13}$$

Since the Fermi energy may be expressed in terms of the number of free electrons per unit volume we write (6)

$$\varepsilon_F = \frac{\hbar^2}{2m} (3\pi^2 N/V)^{2/3} \tag{1-14}$$

where

N = number of free electrons in volume V

$\hbar$ = Planck's constant/2π

= 1.054×10^{-34} joule-sec

m = electron rest mass

= 9.11×10^{-31} kg

thus

$$\frac{\partial \varepsilon_F}{\partial V} = -\frac{2}{3} \left(\frac{\hbar^2}{2m}\right)(3\pi^2 N)^{2/3} V^{-5/3}$$

$$= -\frac{2}{3} \frac{\varepsilon_F}{V}$$

Using the expression for S in Equation (1-12) we have

$$\frac{\partial S}{\partial p} = \left(\frac{\pi^2 k^2 T \xi}{3|e|\varepsilon_F^2}\right)\left(-\frac{2}{3}\frac{\varepsilon_F}{V}\right)\left(\frac{\partial V}{\partial p}\right) \tag{1-15}$$

which on re-arranging may be written as

$$\frac{\partial S}{\partial p} = \frac{2\pi^2 k^2 T \xi}{9|e|\varepsilon_F} \left(-\frac{1}{V}\frac{\partial V}{\partial p}\right) \tag{1-16}$$

where the factor in parentheses is just the isothermal cubic compressibility of the metal

$$\beta = -\frac{1}{V}\frac{\partial V}{\partial p} \tag{1-17}$$

Finally,

$$\frac{\partial S}{\partial p} = \frac{2\pi^2 k^2 T \xi \beta}{9|e|\varepsilon_F} \tag{1-18}$$

To obtain an expression for estimating the magnitude of the pressure correction for the thermal emf we expand the pressurized thermopower S' in a Taylor series to first order in pressure.

$$S' = S + (\frac{\partial S}{\partial p})p + \ldots \tag{1-19}$$

Thus, the emf measured in a single-wire experiment, Equation (1-1) yields

$$E_{sw} = \int_{T_1}^{T_2} (S'-S)dT$$

$$= \int_{T_1}^{T_2} (\frac{\partial S}{\partial p})p(T)dT, \tag{1-20}$$

where $p(T)$ describes the pressure-temperature profile of the pressurized wire. This is possible since both p and T can be expressed parametrically in terms of position. We may in principle

eliminate the position parameter between p and T, and express p as a function of T. For an idealized single-wire configuration with isothermal pressure seals, Equation (1-20) becomes

$$E_{sw} = p \int_{T_1}^{T_2} \left(\frac{\partial S}{\partial p}\right) dT$$

$$= \frac{\pi^2 k^2 \xi \beta p}{9|e|\varepsilon_F} (T_2^2 - T_1^2) \qquad (1\text{-}21)$$

where we have assumed the temperature dependence enters only through the explicit dependence of S on T in this approximation. Substituting typical values

$$p \doteq 60 \text{ kbar}$$

$$T_1 \doteq 0°C = 273°K$$

$$T_2 \doteq 1000°C = 1273°K$$

$$\varepsilon_F \doteq 5 \text{ eV}$$

$$\beta \doteq 10^{-3}/\text{kbar}$$

$$\xi \doteq 3 \quad \text{(for free electrons (6))}$$

in Equations (1-18) and (1-21) we find

$$\frac{\partial S}{\partial p} \simeq 0.013 \ \mu V/°K\text{-kbar}$$

and

$$E_{sw} \simeq 0.45 \text{ mV}$$

These results compare favorably with experimental single-wire values for platinum and platinum-10% rhodium (34). Single-wire corrections for chromel and for alumel are found (34) to be greater by factors of approximately 4 and 2, respectively.

For studies involving composite thermocouples we would reasonably expect the pressure corrections to be of this order or smaller since the composite thermocouple correction has been shown to be essentially equivalent to the difference between the two corresponding single-wire values. Thus, we might physically expect the pressure correction for Pt10%Rh/Pt thermocouples at 60 kbar and 1000°C to be 0.5 mv or less, while that for a chromel/alumel thermocouple in similar conditions might be of the order of 1-2 mv, corresponding to a temperature correction of 25°C or less.

The Present Study

Previous attempts to determine the pressure correction for the emf of thermocouples using solid pressure-transmitting media and internal electric furnaces have been limited by a lack of precise knowledge concerning the true temperature of the pressurized junction. In each case the true junction temperature has been estimated by some indirect means. In the present study a method is employed which requires no such initial estimate of the true temperature. The unknown temperature is written parametrically as a function of a

directly measured quantity, the electrical power delivered to the internal furnace. The emf of the pressurized thermocouple is then written as a function of the true (as yet unknown) junction temperature and a set of unknown coefficients. The temperature-versus-power function is then substituted into the pressurized emf-versus-temperature relationship to obtain an expression which gives the pressure-corrected thermocouple emf in terms of the furnace power. The coefficients for both the temperature-versus-power function and the pressure-corrected emf-versus-temperature function are then obtained simultaneously by performing a nonlinear least-squares fit to the directly measured emf-versus-furnace power data. The technique, first proposed by Waxman and Hastings (74), has been successfully used for determining coefficients in highly nonlinear equations of state for gases (73, 74). The present work represents the first attempt to apply this approach to actual experimental data for pressurized thermocouples.

EXPERIMENTAL APPARATUS AND TECHNIQUE

The Tetrahedral Press

The ultra-high pressures employed in this study were generated using a tetrahedral-anvil press designed by Hall (35, 38) and constructed by McCartney Manufacturing Company, Inc., Baxter Springs, Kansas. The press consists essentially of four tungsten carbide anvils with 1.0-inch triangular faces which are driven together by four hydraulic rams, each capable of exerting a force of up to 300 tons against the faces of a sample holder having the form of a regular tetrahedron (Figures 6 and 7). The anvils are electrically insulated from each other and from the main frame of the press, thus allowing electrical power and signals to be transmitted to and from the pressurized region through the anvils themselves. Each anvil is equipped with channels through which a fluid may be circulated to heat or cool the anvil. In the present study cold water was circulated through these channels to maintain the temperature in the pressure seal region at approximately 10°C. The oil pressure in the hydraulic rams is measured by means of a 0-12,000 psi Heise gauge of the Bourdon tube type. A common hydraulic system together with a series of sliding anvil guide rods ensure that all four anvils move simultaneously in proper alignment with each other toward a common center. Three 1/2-inch thick Plexiglas safety shields surround the pressurized

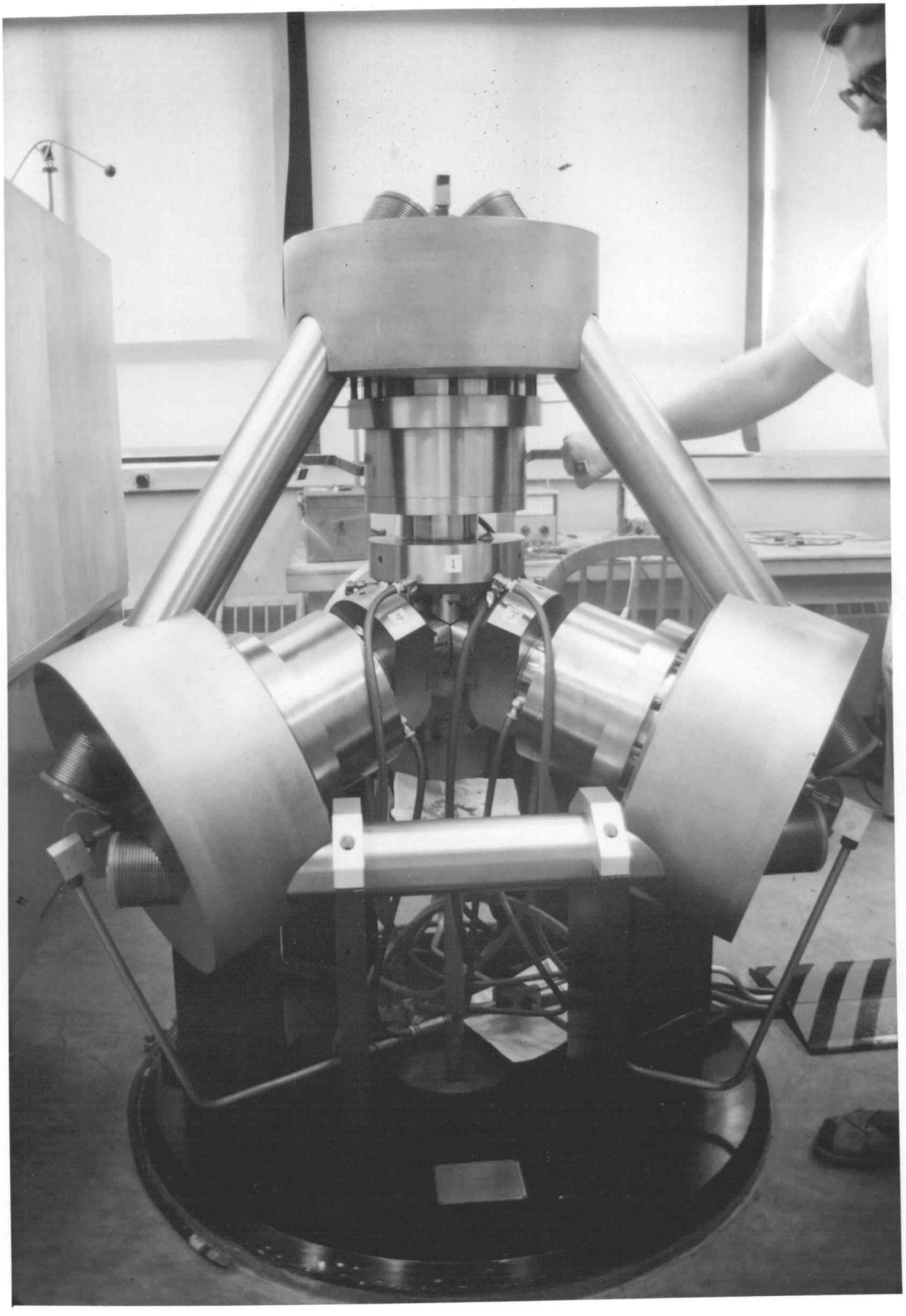


Figure 6. The 300-ton tetrahedral-anvil press.

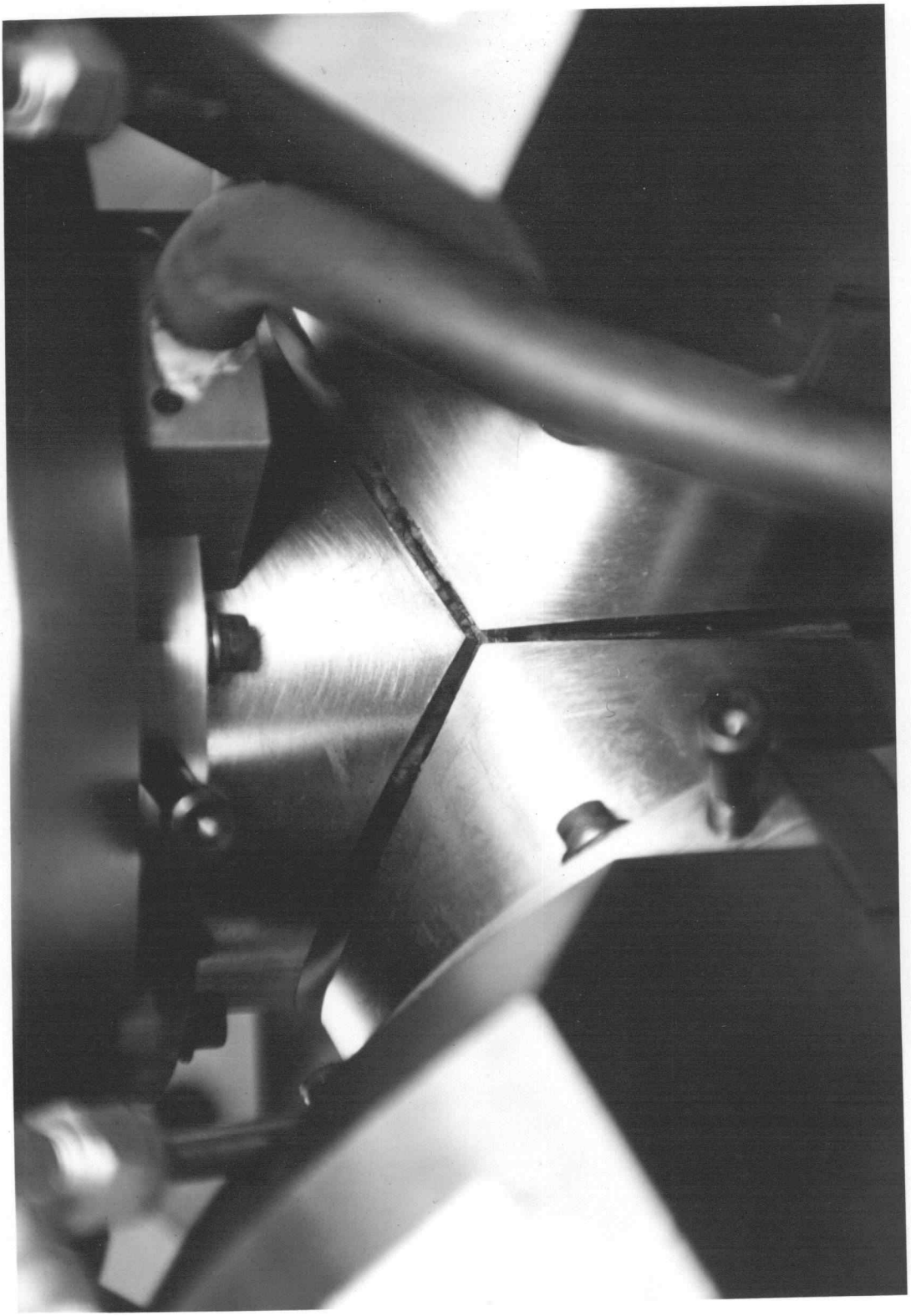


Figure 7. Detail view of pyrophyllite pressure seal.

region to protect the operator from flying debris in the event of sudden failure of the pressure seal.

The High Pressure Cell

The tetrahedral high-pressure sample holders, or "cells", were cut from 1" x 1" x 12" bars of pyrophyllite supplied by the American Lava Company, Chatanooga, Tennessee. Pyrophyllite, a soft, gray mineral resembling talc, is the most widely used solid pressure-transmitting medium. The blank tetrahedra were cut with a 1.25-inch (3.175 cm) edge length for use with the 1.0-inch anvils. When these oversized tetrahedra are placed under pressure, the excess pyrophyllite is extruded between the anvils to form the high-pressure seal, or "gasket". The 25% oversize factor has been found to provide the most efficient transmission of anvil pressure to the interior of the pyrophyllite cell (1, 57). The blank tetrahedra were machined as shown in Figure 8 to accommodate an internal graphite furnace and the thermocouple assembly. The internal furnace was made of spectroscopic graphite rod (37), 0.180 inch in diameter. Before being inserted in the tetrahedra, the graphite rod was coated with a thin layer (approximately 0.005 inch) of a 1:1 mixture (by volume) of finely divided boron nitride and Duco cement. The mixture was diluted with acetone until it had a watery consistency. The graphite rod was then dipped briefly in the dilute mixture to apply a

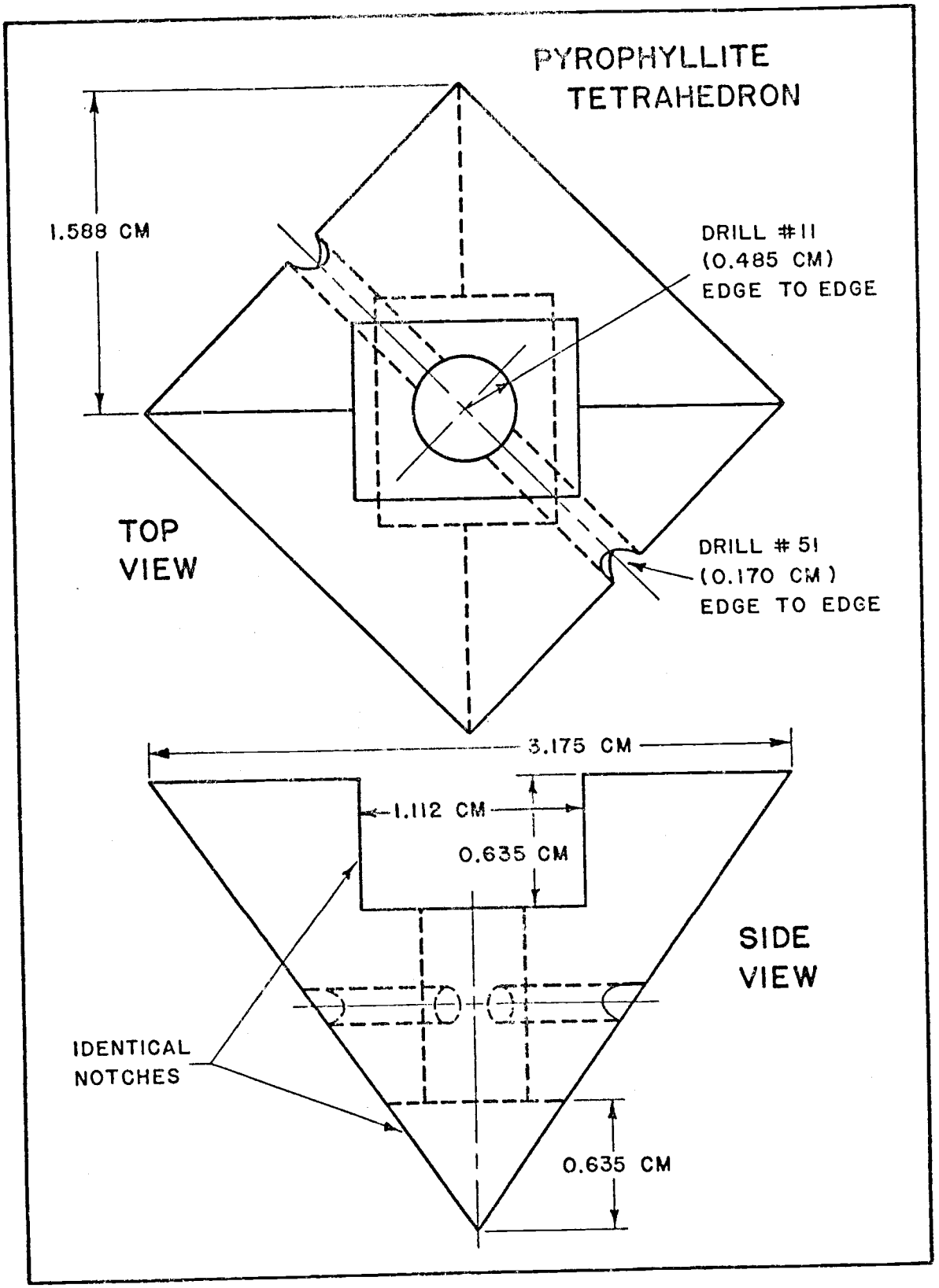


Figure 8. The pyrophyllite tetrahedron.

fairly uniform coating of the boron nitride. Early high-temperature, high-pressure cells were found to suffer from intrusions of apparently molten pyrophyllite in the graphite furnace region, which often increased the furnace resistance enough that furnace temperatures were limited to less than 200°C. The boron nitride seems to effectively prevent the formation of these intrusions. The furnace was inserted into the pyrophyllite tetrahedron, trimmed to proper length and drilled for the insertion of the thermocouple assembly. The interior detail of the assembled high-temperature, high-pressure cell is shown in Figure 9. The chromel/alumel thermocouples were prepared by spot-welding the two #36 AWG wires together and inserting the resulting junction in standard two-hole mullite ceramic thermocouple insulator (0.160 cm O.D.) prepared as shown in Figure 10. Both the thermocouple wires and the ceramic insulator were supplied by Omega Engineering, Inc., Stamford, Connecticutt. Kern Ceram Cement, an inorganic two-component refractory cement from Electronic Space Products, Inc., Los Angeles, California, was used in the preparation of the thermocouple assembly. With the thermocouple inserted, two wafers of pyrophyllite were cemented on either side of the mullite insulator where the insulator emerged from the tetrahedron. This produced a pre-formed gasket which minimized the pinching-off of thermocouple wires during the extrusion of the pyrophyllite pressure seal. A copper strip was placed across each

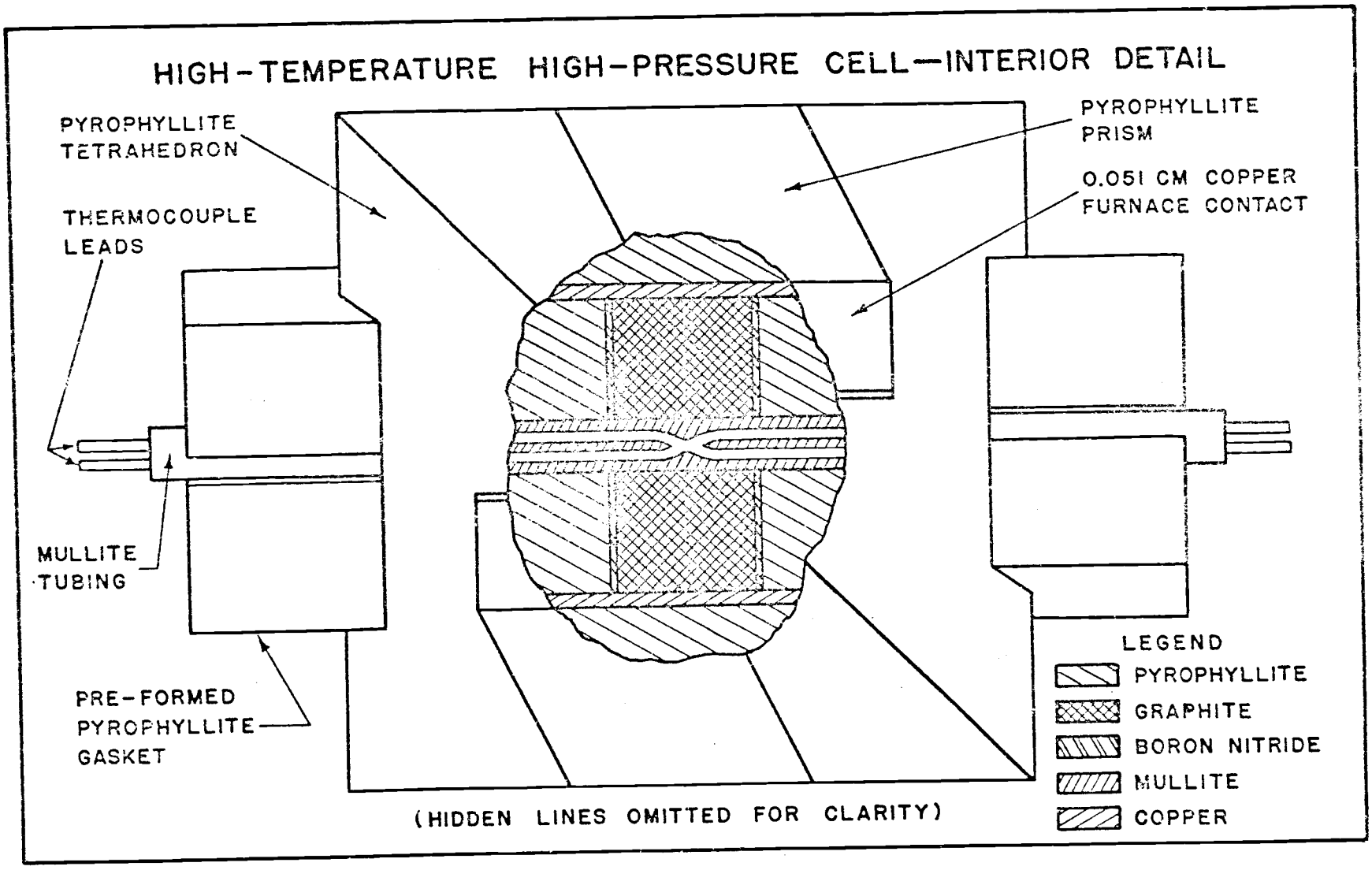


Figure 9. Interior detail of high-temperature, high-pressure cell.

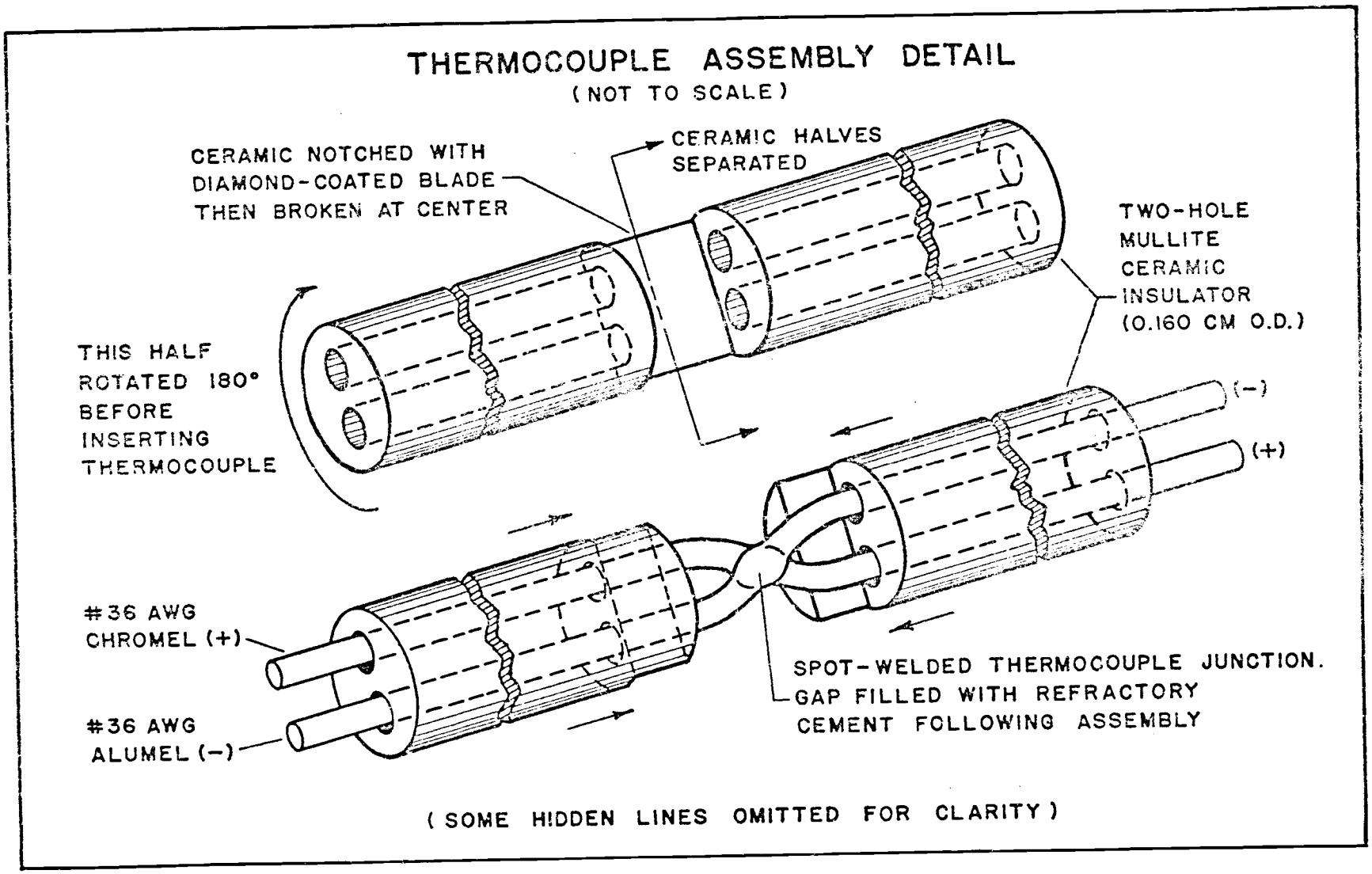


Figure 10. Thermocouple assembly detail.

end of the graphite furnace and topped with a pyrophyllite prism on each end. The copper furnace contacts were connected to a 6 VDC, 500 ampere power supply through the opposing pairs of anvils (Figure 9). An exploded view of the complete cell is shown in Figure 11. An example of a typical pyrophyllite gasket is shown in Figure 12.

Thermocouple Circuitry

The instrumentation and circuitry used in making the thermocouple readings is shown in Figure 13. The four thermocouple leads emerging from the tetrahedral pressure cell could be connected in four possible pairings. This minimized the risk of total failure should one, or even two, of the thermocouple wires be sheared in the process of gasket formation. The thermocouple extension leads which connected the pressurized thermocouple with the ice point reference junctions were of the same chromel/alumel material. All other circuitry, including the switches, were of copper. The ice point bath was surrounded by a Bayley Model 118 constant temperature bath kept at 1.0°C. The distilled water-and-ice mixture was constantly agitated by bubbling pre-chilled air up from the bottom of the bath.

Measurements of the furnace voltage were made with #30 AWG copper wires soldered directly to the copper furnace contacts, while measurements of furnace current were made by measuring the voltage drop across a standard high-current resistance (0.0002 ohm)

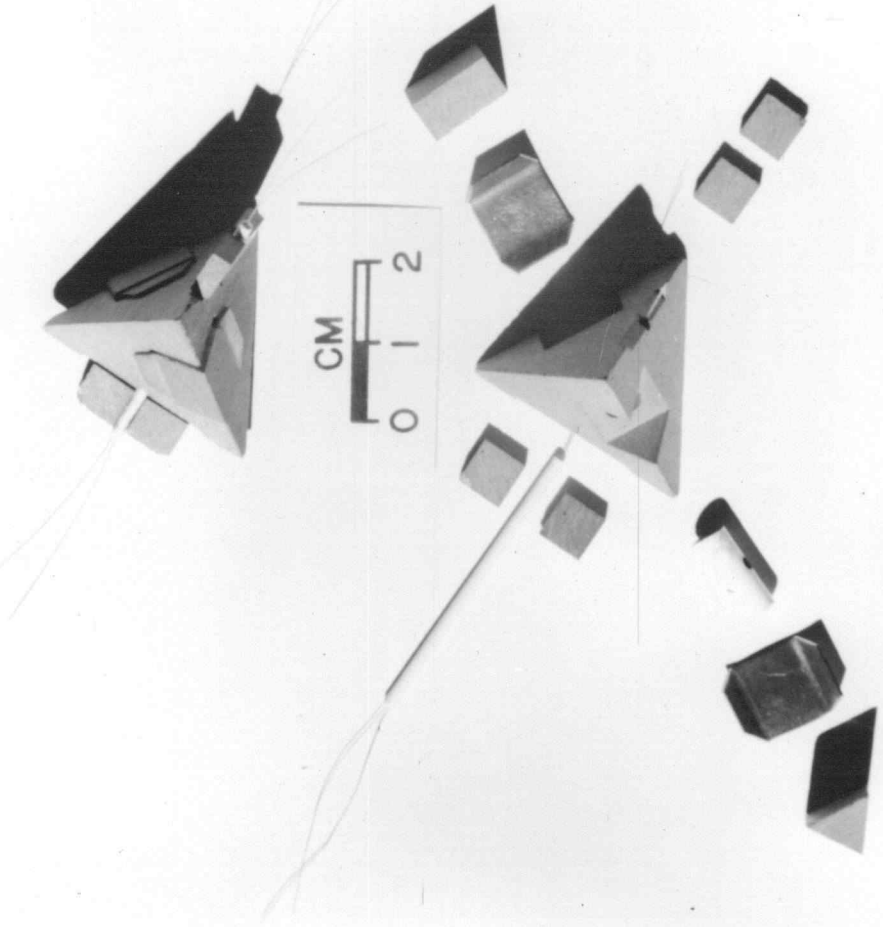


Figure 11. The tetrahedral pressure cell. Exploded view.

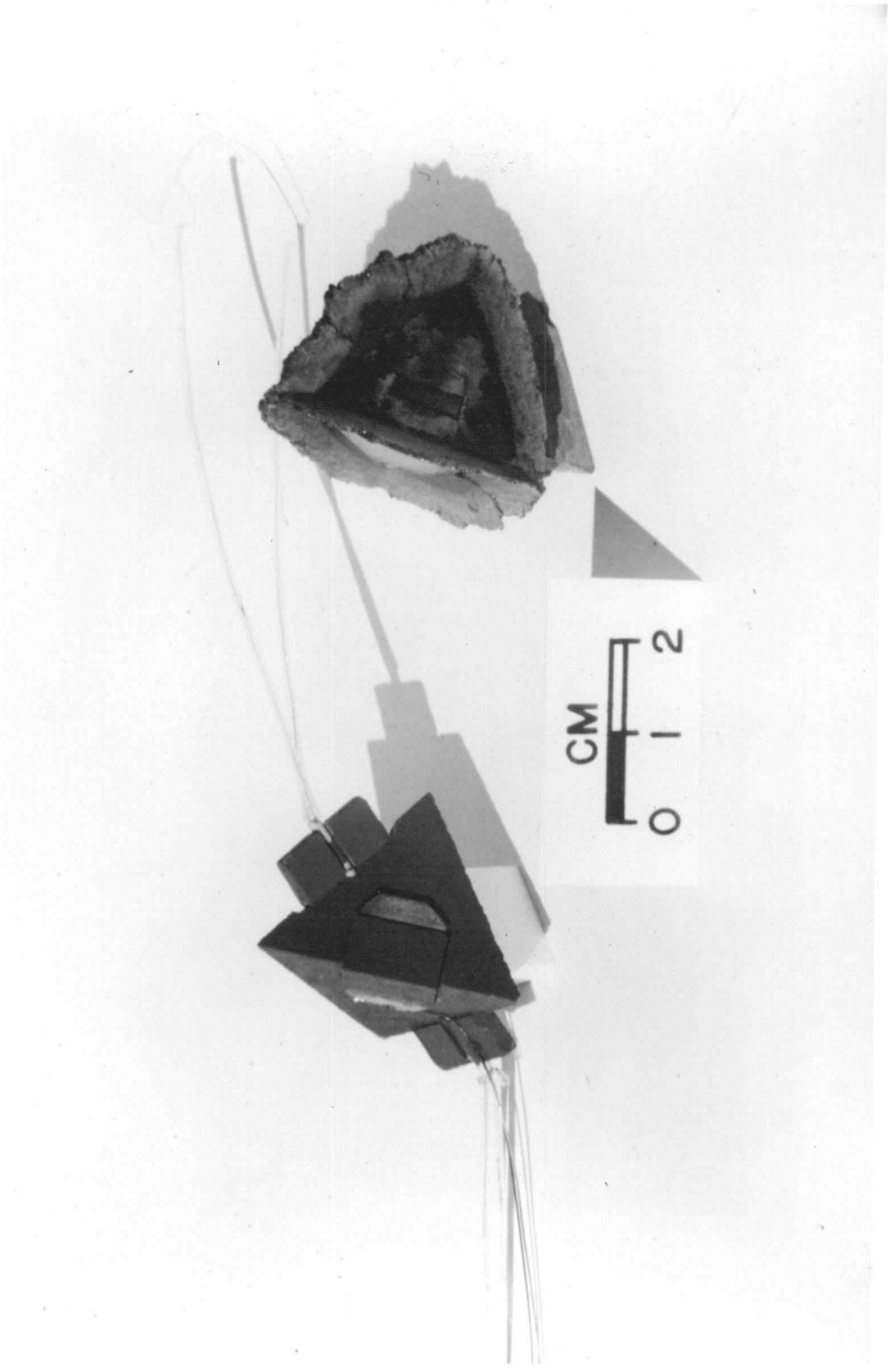


Figure 12. Tetrahedral cell, before and after pressure run.

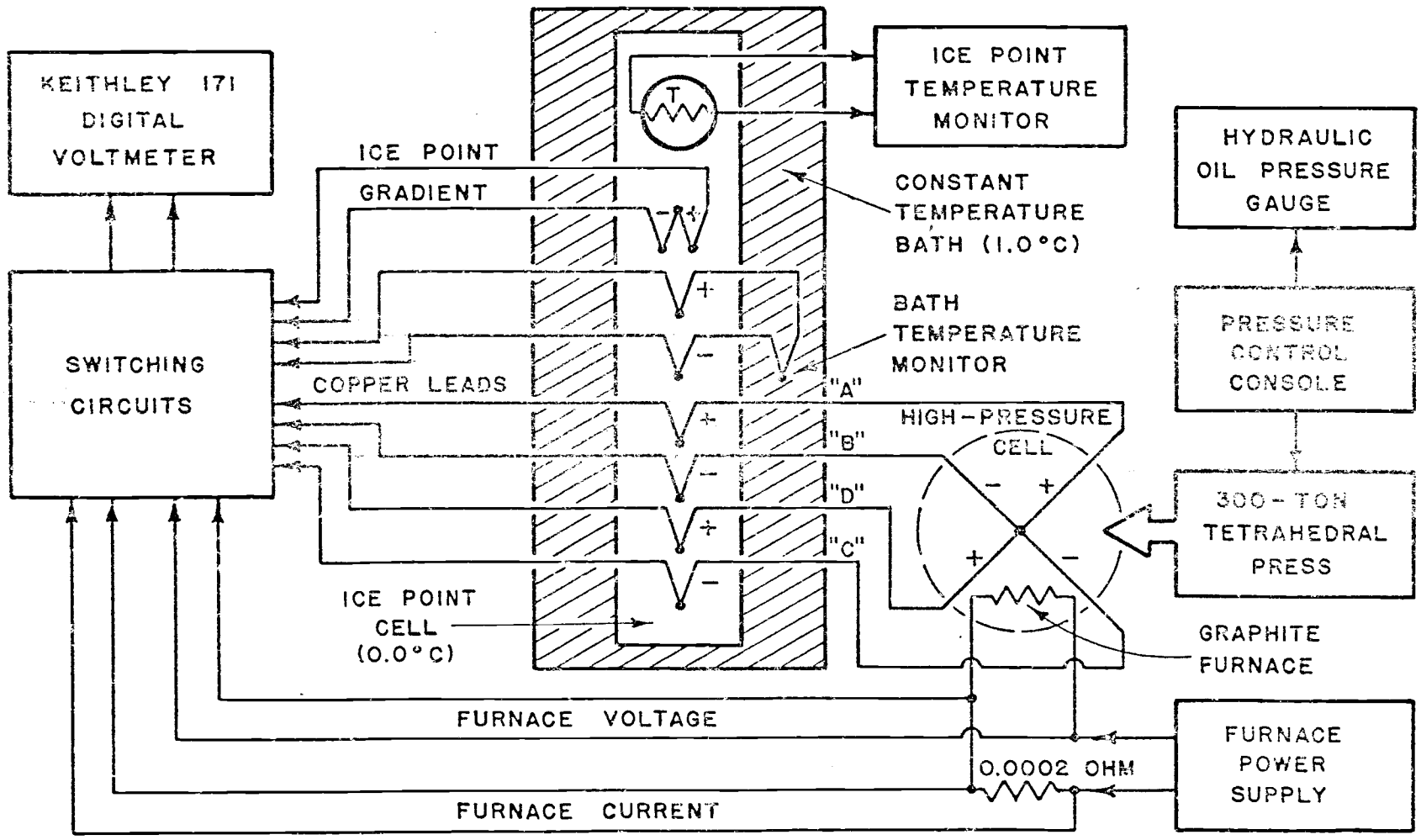


Figure 13. High-temperature, high-pressure instrumentation.

in series with the power supply.

Collection of Data

The steps involved in a typical experimental run were as follows:

1. The assembled tetrahedral cell was coated with a mixture of jeweler's rouge in methanol to increase friction between tetrahedron and anvils, thus minimizing amount of pyrophyllite extruded during gasket formation.
2. Tetrahedral cell was dryed at approximately 70°C-80°C for 24 hours prior to run.
3. Tetrahedral cell was connected (soldered) to extension leads.
4. Anvils were advanced to make contact with cell.
5. Coolant (water) was allowed to flow through anvils until system came to thermal equilibrium.
6. Thermocouple emf with power off was recorded.
7. Pressure increased slowly to form gasket, then increased to desired working pressure.
8. Thermocouple emf with power off was again recorded and compared with low pressure reading. (In all cases the difference was no more than a few microvolts, quite small for this thermocouple.)
9. The furnace power was increased; the system allowed to attain thermal equilibrium (as indicated by the stabilizing of

the emf of the pressurized thermocouple), usually requiring about 2-3 minutes.

10. Readings were then taken in the following order:
    a. furnace voltage (five readings)
    b. furnace current (five readings)
    c. thermocouple emf (five readings for each pair of thermocouple leads still intact)
    d. furnace voltage (five readings)
    e. furnace current (five readings)
    f. thermocouple emf (five readings for each pair)
    g. furnace voltage (five readings)
    h. furnace current (five readings)

    (Average values were used in the final computations.)
11. The run was terminated when the chromel/alumel thermocouple began to drift (usually at temperatures over 800°C).

Pressure Calibration

The pressure in solid-media high-pressure systems is generally determined by calibrating the hydraulic oil pressure gauge using well-established phase transformation in certain materials. Intermediate values of pressure are then obtained by interpolation. For the present study the tetrahedral press was calibrated using three well-established room-temperature transitions: bismuth I → II at 25.5 kbar

(13, 18, 29, 43, 50, 51, 72); thallium II → III at 36. 7 kbar (13, 17, 20, 29, 50, 51, 72); and barium I → II at 55. 0 kbar (19, 20, 29, 42, 47, 54, 72, 76). The lack of hydrostatic conditions within the solid pressure-transmitting medium requires that the calibration be carried out using an internal cell configuration which conforms as closely as possible to that used in the actual thermocouple cell. The calibration cell used is shown in Figure 14. The calibration assembly is simply inserted in place of the usual thermocouple, the remainder of the tetrahedral cell being unchanged. The electrical resistance of the calibrant shorting link is recorded (Figure 15) as a function of hydraulic oil pressure as the pressure is gradually increased. The results are plotted (Figures 16, 17 and 18), the onset of the phase transition being taken as the calibration point in solid-media systems (28, 77). We obtain hydraulic oil pressures of 4100 psi, 6300 psi and 10, 500 psi for the transitions in Bi, Tl and Ba respectively. (Though our calibrants are of high purity; 99. 9999%, 99, 999% and 99. 5%, respectively, the purity of the material is fortunately not extremely critical to reliable calibration (77).) Fitting the three calibration points with a quadratic function we obtain the pressure calibration curve of Figure 19. The hydraulic oil pressures of 4000, 6000, 8000, 10, 000 and 12, 000 psi correspond to cell pressure of 25. 0, 35. 2, 44. 6, 53. 0 and 60. 6 kbar, respectively.

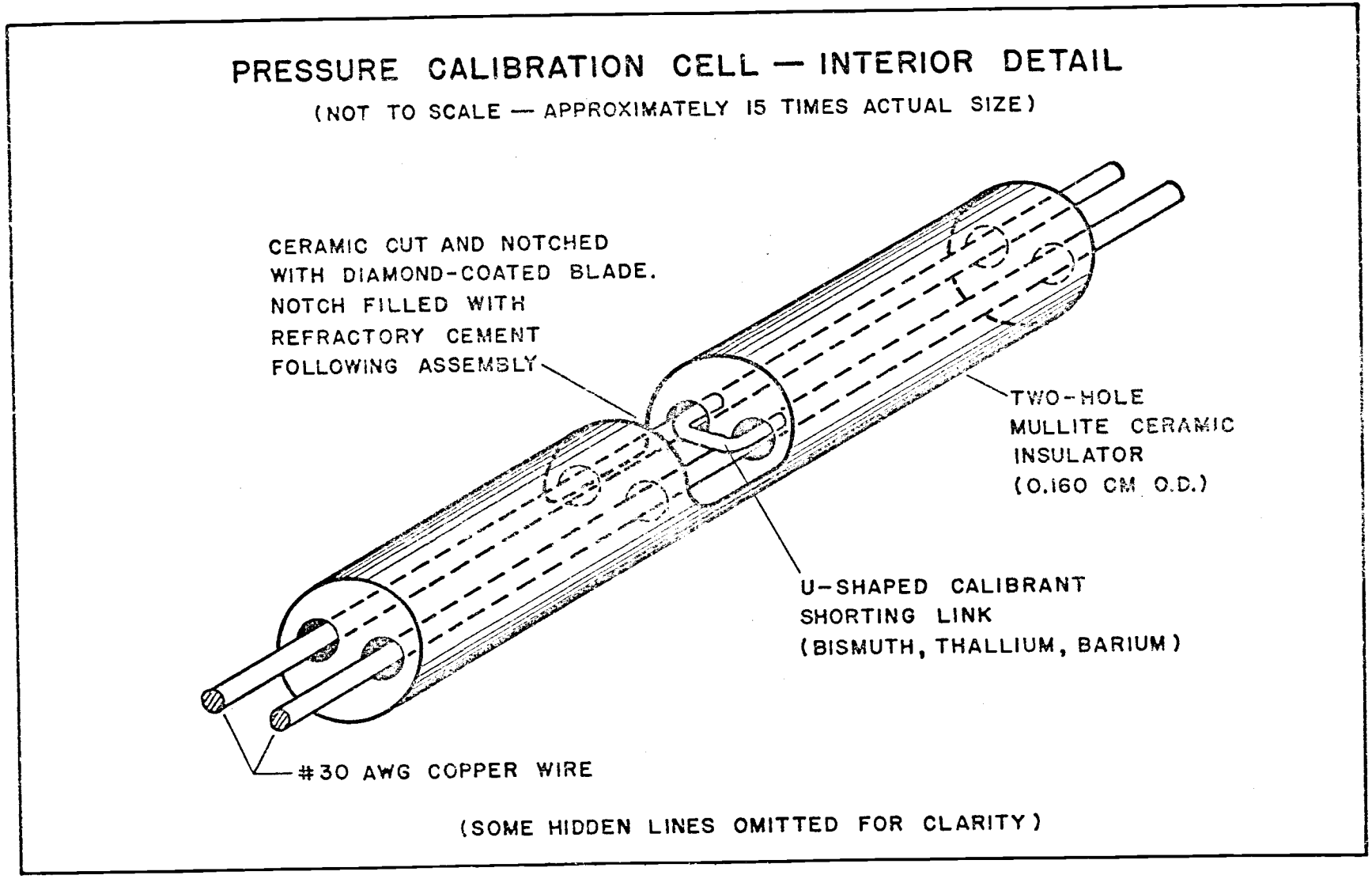


Figure 14. Pressure calibration cell. Interior detail.

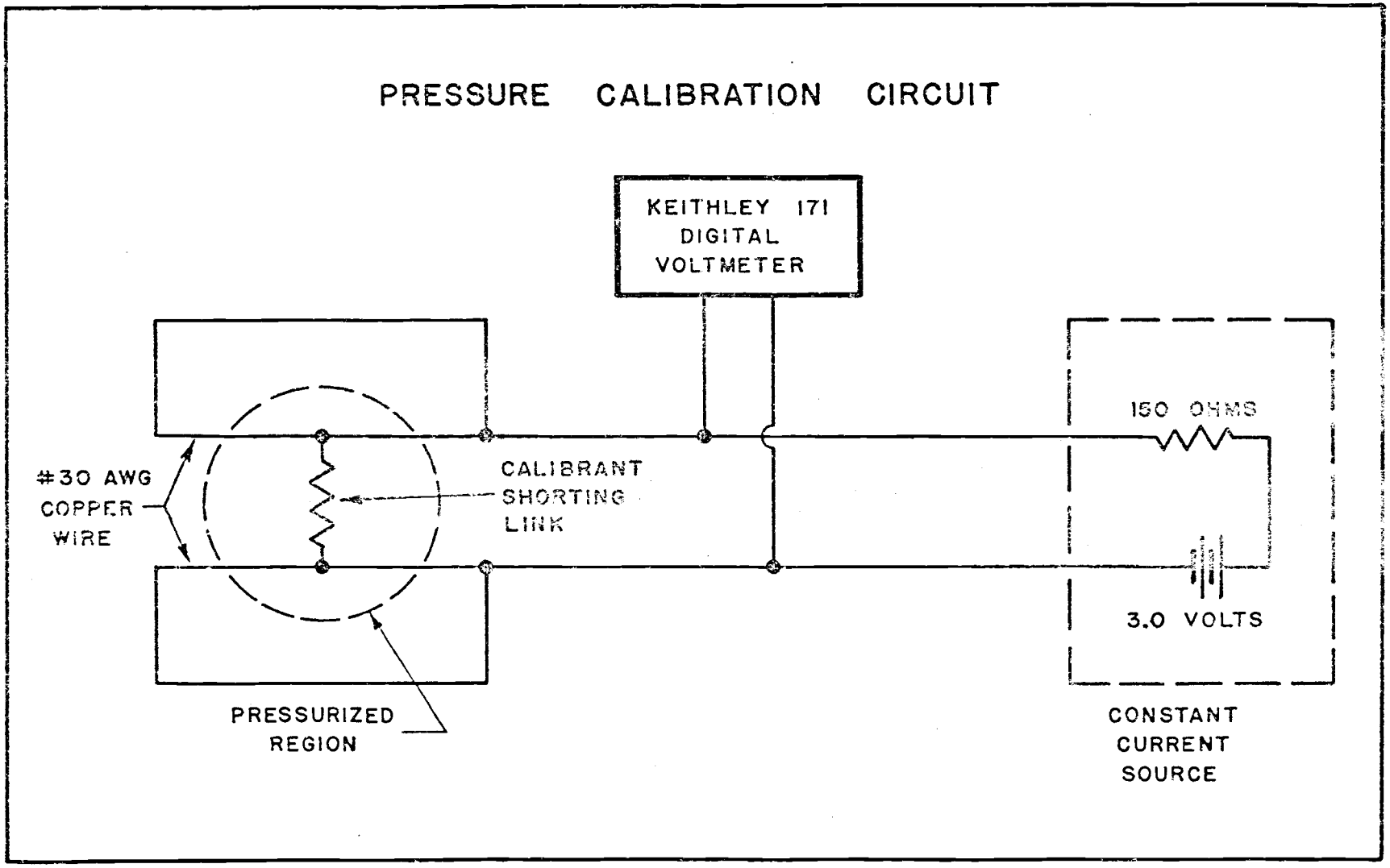


Figure 15. Pressure calibration circuit.

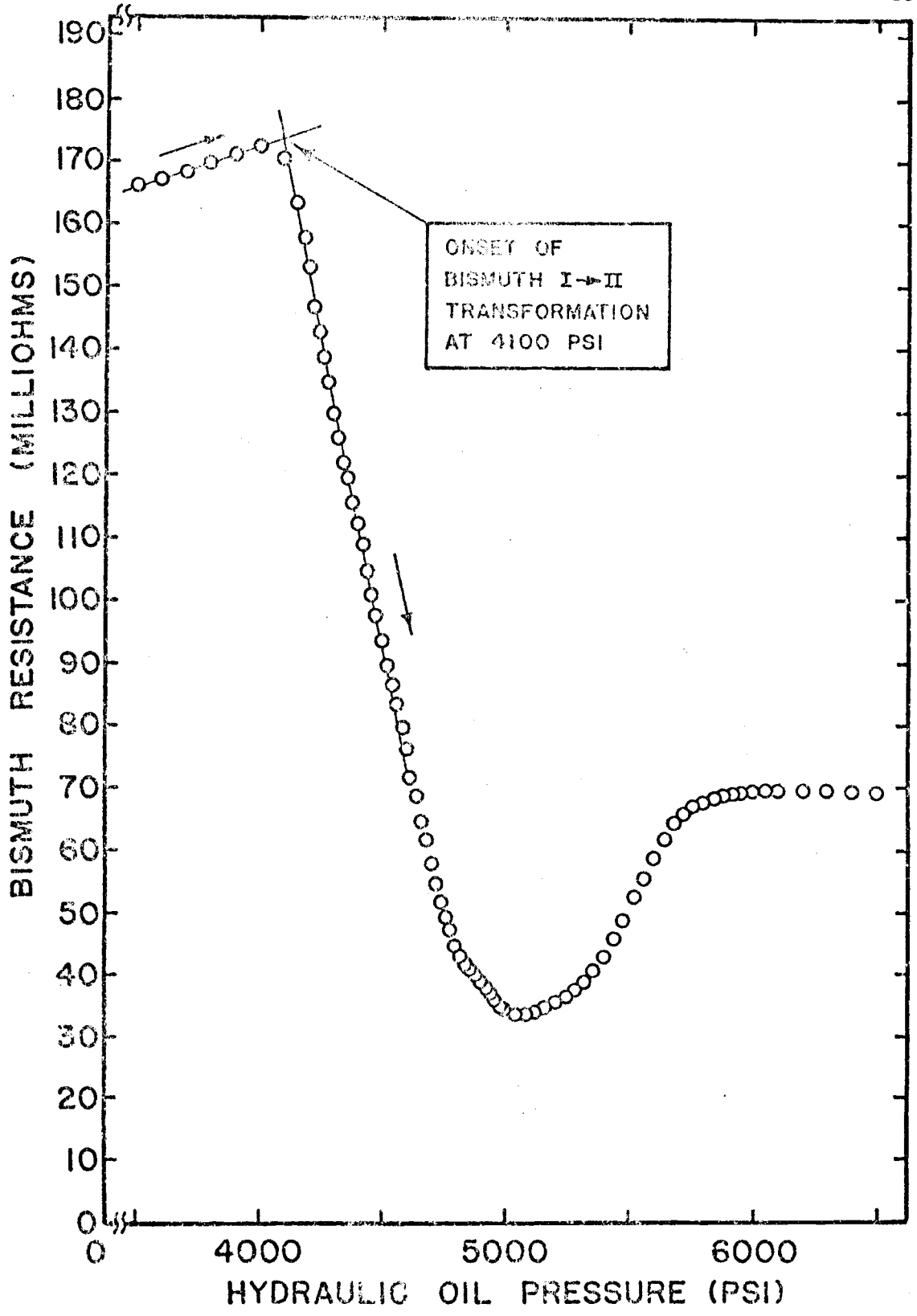


Figure 16. Pressure calibration. Bismuth I-II transformation.

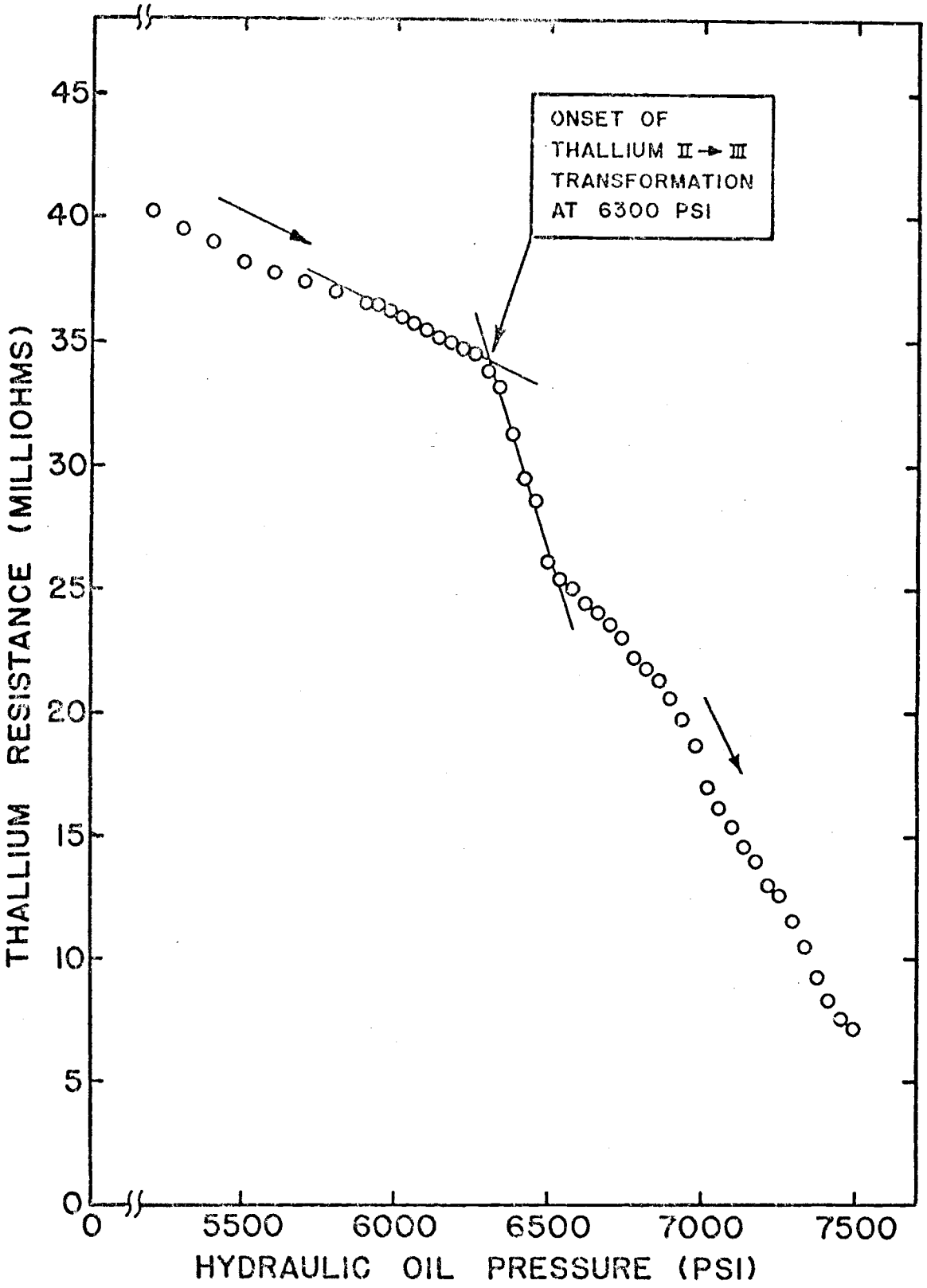


Figure 17. Pressure calibration. Thallium II-III transformation.

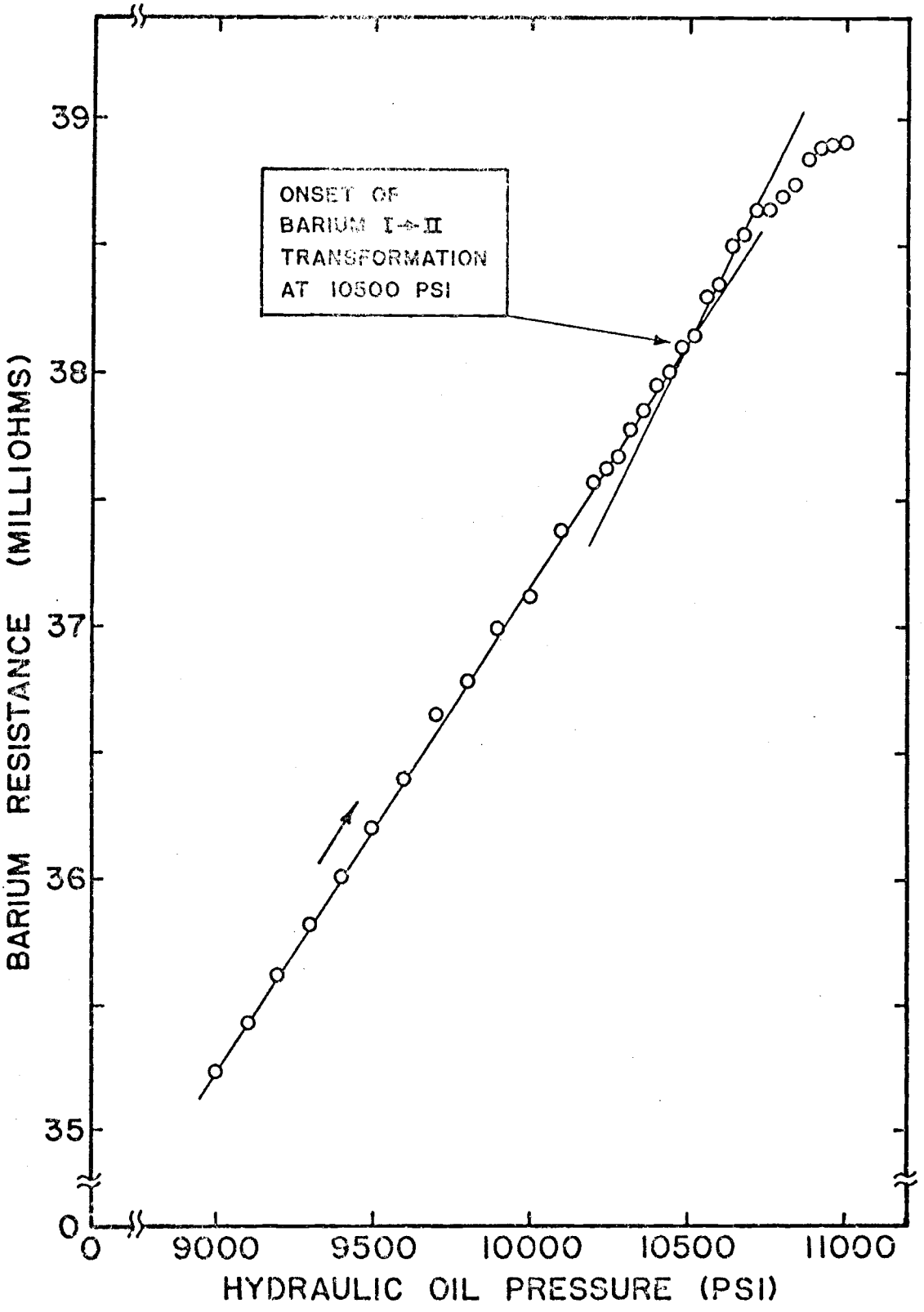


Figure 18. Pressure calibration. Barium I-II transformation.

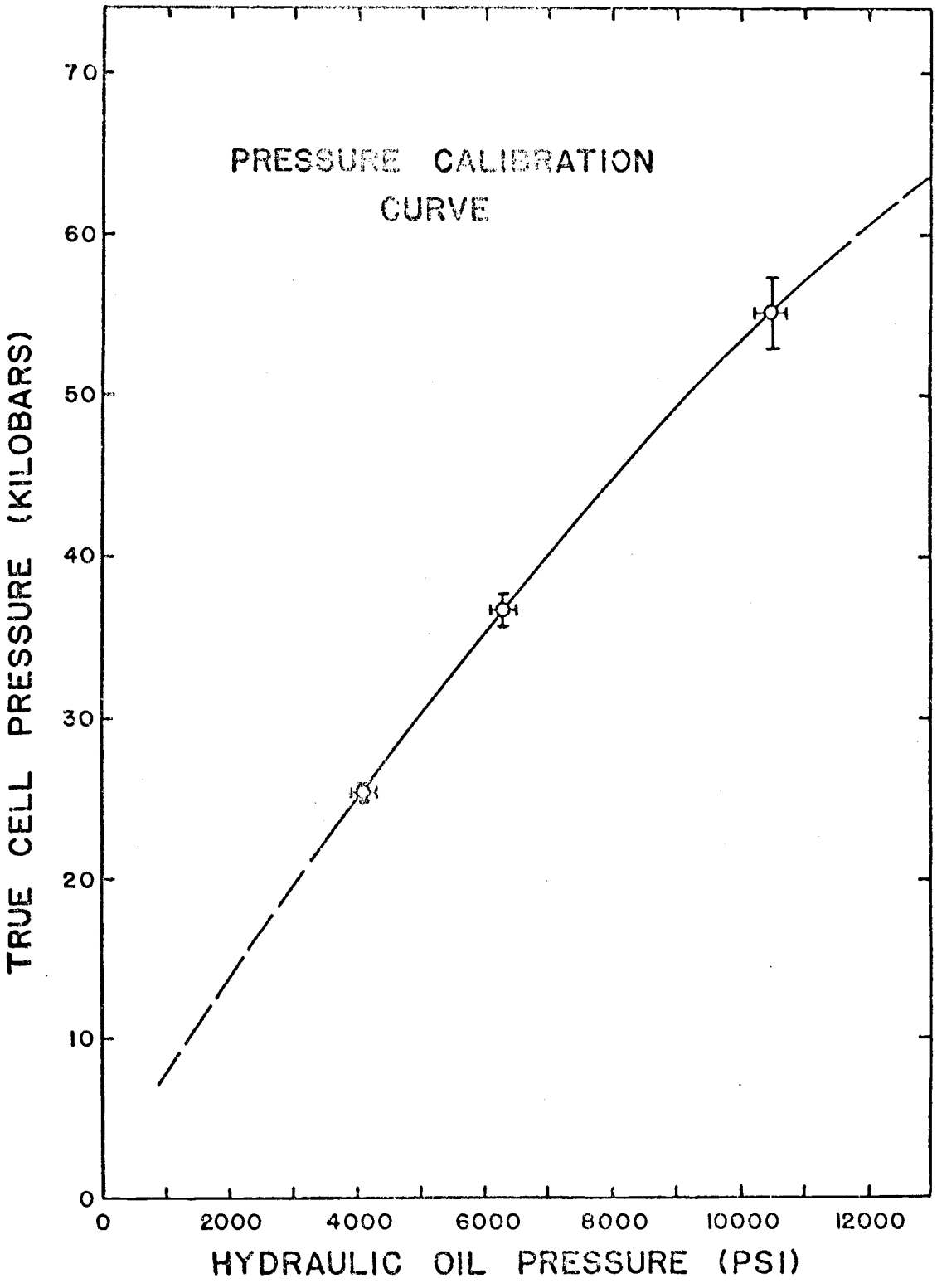


Figure 19. Pressure calibration curve. True cell pressure versus hydraulic oil pressure.

COMPUTATIONS

As mentioned earlier in this work, the principal advantage to be gained from this method is a determination of the effect of pressure on the thermal emf of the chromel/alumel thermocouple without actually having to measure the pressurized junction temperature directly. The unknown junction temperature is written parametrically as a function of the electrical power delivered to the pressurized furnace. In our case we have used a quadratic function for the temperature-versus-power function since this is the simplest function which gives an acceptable fit to the uncorrected temperature-versus-furnace power data, as will be seen in the chapter dealing with the results of this work. The pressurized emf is then expressed as a function of the (as yet unknown) junction temperature, the form of this function being determined by the thermocouple emf-versus-temperature data at atmospheric pressure. In the case of the chromel/alumel thermocouple, emf values for 66 equally-spaced temperatures between 0-900°C were taken from standard thermocouple reference tables (71) and fit with power series of the form

$$E = \sum_{n=1}^{k} c_n T^n$$

using linear least-squares methods. The maximum deviation of the

fitting function dropped by a factor of 3 to less than 10 μV (corresponding to a temperature error of less than one-fourth of a degree Celsius) on passing from $k = 7$ to $k = 8$. Thus, the eighth-degree power series was chosen for the form of our pressurized emf-versus-temperature function. Then, substituting

$$T = \sum_{m=0}^{2} a_m w^m \qquad (^\circ C) \tag{3-1}$$

into

$$E = \sum_{n=1}^{8} c_n T^n \qquad (mV) \tag{3-2}$$

where w = furnace power in watts, we eliminate the unknown temperature T, and obtain

$$E = \sum_{n=1}^{8} c_n \left(\sum_{m=0}^{2} a_m w^m \right)^n \tag{3-3}$$

expressing the pressurized emf E as a function of the furnace power, w, both of which are directly measured quantities. The problem is then to solve the nonlinear function in Equation (3-3) for the unknown coefficients a_m and c_n, which will then provide us with expressions for the junction temperature and pressurized emf (Equations (3-1) and (3-2)).

The iterative method ultimately chosen for the nonlinear least-squares fit is known as the damped least-squares method (60, 63). The particular form of the method we have used is an algorithm due to Marquardt (62), which is globally convergent, that is, if a minimum exists for the objective function (sum of the squares of the residuals), Marquardt's algorithm will converge to the minimum no matter what starting values are given. The method claims to combine the most attractive features of both Taylor series methods and steepest-decent methods while avoiding the pitfalls of each. The computer program which incorporates this algorithm for the specific problem under study is given in Appendix A. A typical output listing is presented in Appendix B. The computational procedures are summarized in Figure 20. The starting values for the coefficients a_1 and a_2 were determined from a linear least-squares fit of the uncorrected temperature-versus-furnace power data. The value of a_0, which was held constant throughout the nonlinear fit, was determined by direct measurement of the pressurized thermocouple emf with the furnace power off, neglecting the pressure correction since a_0 is of the order of 10°C. All estimates give pressure corrections of less than 5 μV at this temperature for the range of pressures treated here; and 5 μV is approximately the magnitude of the fluctuations in our emf readings.

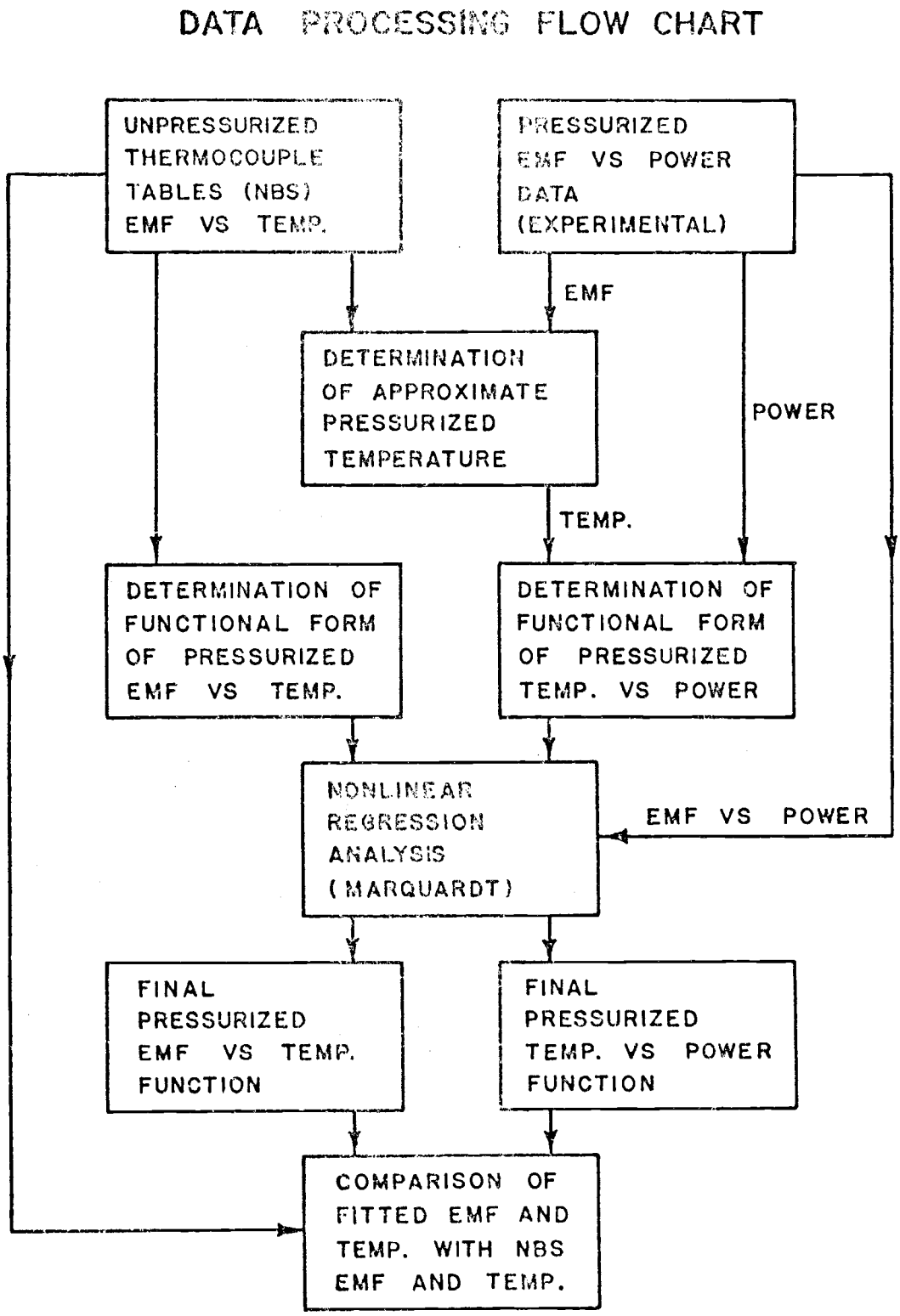


Figure 20. Data processing flow chart.

The initial values of the emf-versus-temperature coefficients are given in Table 1.

Table 1. Coefficients of eighth-degree linear least-squares fit to NBS chromel/alumel tables, 0-900°C.

c_1	3.893861×10^{-2}
c_2	5.117805×10^{-5}
c_3	-4.755624×10^{-7}
c_4	2.042506×10^{-9}
c_5	$-4.625686 \times 10^{-12}$
c_6	5.780822×10^{-15}
c_7	$-3.784051 \times 10^{-18}$
c_8	1.014250×10^{-21}

The convergence criterion found most satisfactory was to require that all of the coefficients change by less than some small fraction $\varepsilon > 0$ at any given iteration. Values of ε between 10^{-5} and 10^{-7} proved generally strict enough to ensure that the sum of squares also changed by a fractional amount less than ε.

RESULTS

General Remarks

A program of nonlinear regression analysis using Marquardt's algorithm was carried out at each of five pressures: 25.0 kbar, 35.2 kbar, 44.6 kbar, 53.0 kbar and 60.6 kbar (corresponding to hydraulic oil pressures of 4000, 6000, 8000, 10000 and 12000 pounds/inch^2). In each case, as previously mentioned, the initial values for the coefficients of the temperature-versus-power function were determined by direct measurement (a_0) or by linear least-squares analysis of the uncorrected thermocouple temperature (measured emf referred to standard thermocouple tables) as a quadratic function of the measured furnace power. The initial estimates of the coefficients of the pressurized emf-versus-temperature function were obtained from a linear least-squares eighth-degree polynomial fit to standard atmospheric pressure thermocouple reference tables (71) for type K (chromel/alumel) thermocouples between 0°C and 900°C.

A typical graph of uncorrected temperature versus furnace power is shown in Figure 21. Each data point shown represents a mean value of 20 to 40 individual thermocouple readings. The solid curve represents the linear least-squares fit of a quadratic function to those points lying below the point of inflection of the experimental

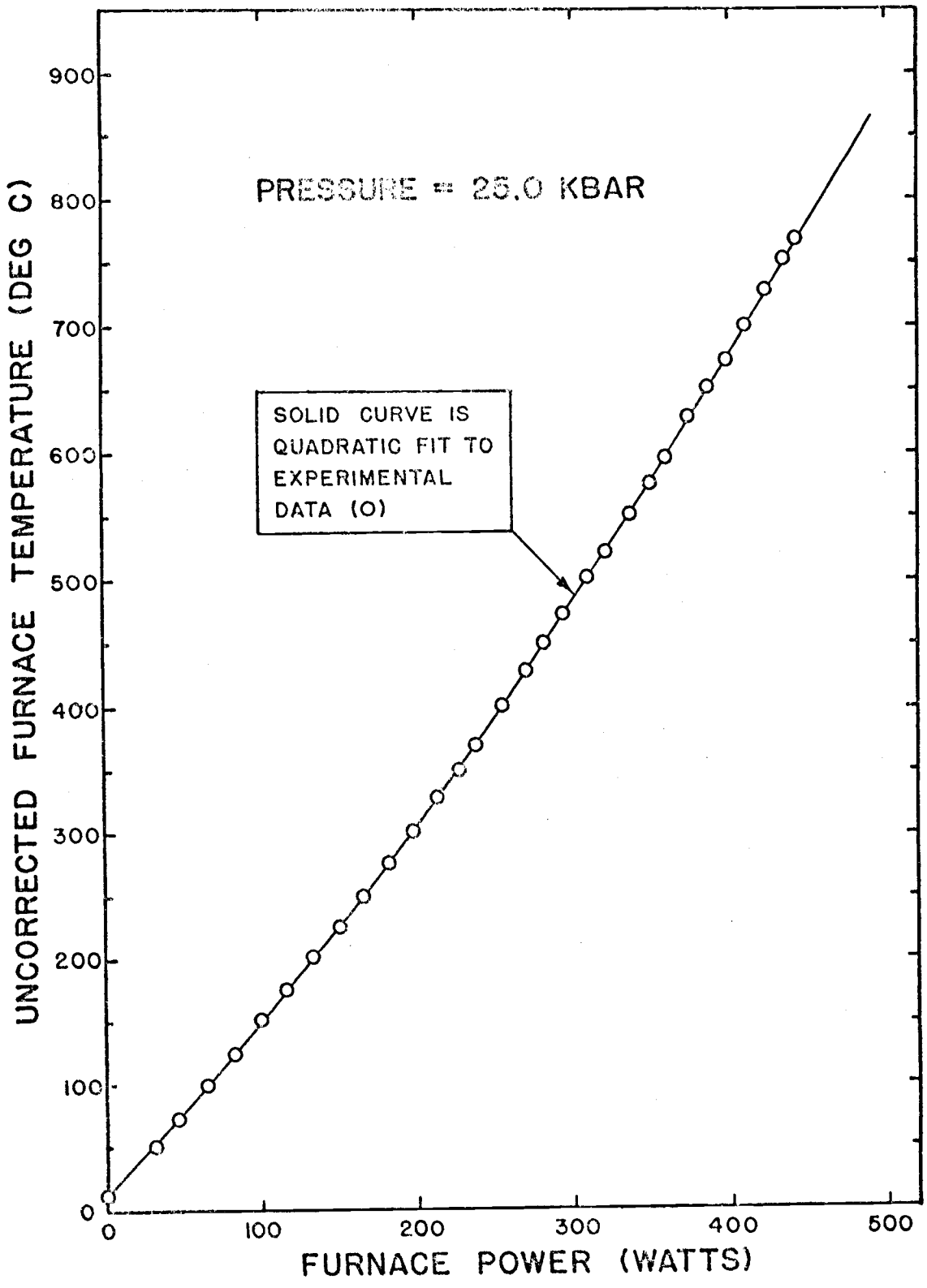


Figure 21. Typical furnace temperature versus furnace power curve.

curve. It is the measured emf-versus-furnace power data corresponding to these points which are subsequently used in the nonlinear regression.

Empirically it was found that the hypersurface (representing the sum of the squares of the residuals for the fit of the nonlinear model to the data) possesses multiple local minima. The Marquardt algorithm, in common with all other methods currently available, cannot distinguish between a local minimum and the global or absolute minimum (3). Thus, if the initial estimates of the coefficients are not sufficiently close to the "physically correct" final values, the algorithm may converge to a local minimum that will generally produce results which are obviously physically unreasonable (52); for example, temperature corrections of hundreds of degrees at temperatures of only a few hundred degrees Celsius. Predictably this becomes more of a problem at the higher pressures where the pressurized coefficients would logically be expected to differ from the unpressurized initial values by amounts increasing with increasing pressure. It was found that convergence to a physically acceptable minimum was most rapid when the data were equally weighted. Weighting the data with the reciprocal of the variance of the mean value for each data point often resulted in extremely slow convergence to physically unsatisfactory minima, the algorithm seemingly trapped in a deep valley, slowly changing only one coefficient while the rest of

the coefficients remained essentially unchanged over many iterations. This may have been a manifestation of the "ridge paralysis" phenomenon referred to by Zwart (79).

Since we have no means available for including the effect of multiple minima in our estimate of experimental error, we will assume that the algorithm has converged to a physically acceptable solution and base our estimate of the limits of experimental error on the more tangible aspects of the experimental configuration. The uncertainties associated with the final values of the pressurized emf-versus-temperature coefficients are taken to be an indication of the precision with which the final minimum is defined and contribute very little to the experimental uncertainty. The uncertainty in the absolute pressure within the pressurized region due to calibration error may be as great as ten percent at the highest pressures studied here due principally to hysteresis effects. However, since the thermoelectric power of the chromel/alumel thermocouple is not strongly pressure-dependent the net uncertainty introduced in the emf and temperature corrections by the uncertainty in pressure is probably not more than five percent. Errors due to uncertainty in determining the temperature of the pressure seal should be quite small for chromel/alumel thermocouples since both the magnitude and slope of the emf pressure corrections are extremely small for temperatures in the range between 10°C and 15°C (34). The effect of plastic deformation

of the thermocouple wires should also be quite small since deformation is chiefly confined to the pressure seal region where the temperature gradient should be very small. Temperature and pressure gradients within the pressure seal region are extremely difficult to measure in solid-media systems, but uncertainties of as much as ten percent are not unreasonable (40). The lack of specific temperature calibration data at atmospheric pressure for each individual thermocouple used requires that we consider the manufacturer's limits of error, which could introduce an additional uncertainty of the order of ten percent in the pressure corrections for emf and temperature. Errors in the measurement of the thermocouple emf are generally quite small, much less than one percent for the temperature range studied. Thus, we consider the overall limits of experimental error for the present work to be of the order of 25% to 30% for the emf pressure correction and for the corresponding temperature correction.

Effect of Pressure on Thermal Emf

The results of the nonlinear regression are summarized for each of the five pressures studied in Tables 2-6. The final values of the fitted coefficients are given for both the temperature-versus-furnace power function

$$T = \sum_{m=0}^{2} a_m w^m \qquad (°C) \qquad (4-1)$$

and the pressurized emf-versus-temperature function,

$$E = \sum_{n=1}^{8} c_n T^n \qquad (mV). \qquad (4-2)$$

Also given are the initial values of the temperature-versus-power coefficients, number of data points used in the nonlinear regression, number of iterations required to meet the convergence criterion, total running time of central processing unit (CPU) of computer (Digital Equipment Corporation PDP-15/30) and the maximum and standard deviations for the fit.

Temperature Corrections

The temperature corrections for the pressurized chromel/alumel thermocouple are plotted as a function of the true temperature in Figures 22-26. At 25.0 kbar (Figure 22) present results indicate temperature corrections which rise initially at temperatures below 400°C in the manner of the early estimates of Hanneman and Strong (39) but are approximately twice as great as their values at 400°C. Decreasing above 400°C and becoming negative at approximately

Table 2. Summary of results at 25.0 kbar.

Pressure	= 25.0 kbar
Data points used	= 31
Iterations required	= 23
CPU time required	= 5 min. 41.5 sec.
Maximum deviation of fit	= 0.095 mV
Standard deviation of fit	= 0.036 mV

Temperature-versus-power function

Initial values (linear least-squares)

$a_0 = 10.6567$ (fixed)

$a_1 = 1.305072$

$a_2 = 8.992534 \times 10^{-4}$

Final values (nonlinear regression)

$a_0 = 10.6567$ (fixed)

$a_1 = 1.357304(\pm 0.000048)$

$a_2 = 8.088715(\pm 0.001323) \times 10^{-4}$

Pressurized emf-versus-temperature function

Final values (nonlinear regression)

$c_1 = 3.836105(\pm 0.000123) \times 10^{-2}$

$c_2 = 4.835669(\pm 0.000200) \times 10^{-5}$

$c_3 = -4.742510(\pm 0.000030) \times 10^{-7}$

$c_4 = 2.051190(\pm 0.000004) \times 10^{-9}$

$c_5 = -4.622069(\pm 0.000006) \times 10^{-12}$

$c_6 = 5.770335(\pm 0.000008) \times 10^{-15}$

$c_7 = -3.799801(\pm 0.000012) \times 10^{-18}$

$c_8 = 1.031922(\pm 0.000016) \times 10^{-21}$

Table 3. Summary of results at 35.2 kbar.

Pressure	= 35.2 kbar
Data points used	= 31
Iterations required	= 35
CPU time required	= 8 min. 23.8 sec.
Maximum deviation of fit	= -0.080 mV
Standard deviation of fit	= 0.035 mV

Temperature-versus-power function

Initial values (linear least-squares)

$a_0 = 10.9421$ (fixed)

$a_1 = 1.298049$

$a_2 = 8.494781 \times 10^{-4}$

Final values (nonlinear regression)

$a_0 = 10.9421$ (fixed)

$a_1 = 1.381652(\pm 0.000151)$

$a_2 = 6.594274(\pm 0.004157) \times 10^{-4}$

Pressurized emf-versus-temperature function

Final values (nonlinear regression)

$c_1 = 3.824104(\pm 0.000405) \times 10^{-2}$

$c_2 = 4.574962(\pm 0.000674) \times 10^{-5}$

$c_3 = -4.686723(\pm 0.000102) \times 10^{-7}$

$c_4 = 2.056860(\pm 0.000015) \times 10^{-9}$

$c_5 = -4.624962(\pm 0.000021) \times 10^{-12}$

$c_6 = 5.756365(\pm 0.000029) \times 10^{-15}$

$c_7 = -3.813415(\pm 0.000040) \times 10^{-18}$

$c_8 = 1.058906(\pm 0.000054) \times 10^{-21}$

Table 4. Summary of results at 44.6 kbar.

Pressure	= 46.6 kbar
Data points used	= 44
Iterations required	= 55
CPU time required	= 16 min. 45.8 sec.
Maximum deviation of fit	= 0.067 mV
Standard deviation of fit	= 0.029 mV

Temperature-versus-power function

Initial values (linear least-squares)

$a_0 = 10.6757$ (fixed)

$a_1 = 1.309262$

$a_2 = 7.708974 \times 10^{-4}$

Final values (nonlinear regression)

$a_0 = 10.6757$ (fixed)

$a_1 = 1.283038(\pm 0.000412)$

$a_2 = 1.008781(\pm 0.001011) \times 10^{-4}$

Pressurized emf-versus-temperature function

Final values (nonlinear regression)

$c_1 = 3.985510(\pm 0.000932) \times 10^{-2}$

$c_2 = 5.864072(\pm 0.001254) \times 10^{-5}$

$c_3 = -6.227969(\pm 0.000154) \times 10^{-7}$

$c_4 = 2.593573(\pm 0.000018) \times 10^{-9}$

$c_5 = -5.537769(\pm 0.000021) \times 10^{-12}$

$c_6 = 6.461893(\pm 0.000024) \times 10^{-15}$

$c_7 = -3.923298(\pm 0.000026) \times 10^{-18}$

$c_8 = 9.692577(\pm 0.000295) \times 10^{-21}$

Table 5. Summary of results at 53.0 kbar.

Pressure	= 53.0 kbar
Data points used	= 21
Iterations required	= 31
CPU time required	= 5 min. 51.1 sec.
Maximum deviation of fit	= -0.044 mV
Standard deviation of fit	= 0.028 mV

Temperature-versus-power function

Initial values (linear least-squares)

a_0 = 11.1700 (fixed)

a_1 = 1.288227

a_2 = 7.592047×10^{-4}

Final values (nonlinear regression)

a_0 = 11.1700 (fixed)

a_1 = 1.331208(±0.000525)

a_2 = $6.630124(\pm 0.011824) \times 10^{-4}$

Pressurized emf-versus-temperature function

Final values (nonlinear regression)

c_1 = $3.880417(\pm 0.001375) \times 10^{-2}$

c_2 = $4.377894(\pm 0.001826) \times 10^{-5}$

c_3 = $-4.516860(\pm 0.000220) \times 10^{-7}$

c_4 = $1.962530(\pm 0.000026) \times 10^{-9}$

c_5 = $-4.457024(\pm 0.000029) \times 10^{-12}$

c_6 = $5.678940(\pm 0.000033) \times 10^{-15}$

c_7 = $-3.841081(\pm 0.000036) \times 10^{-18}$

c_8 = $1.068597(\pm 0.000040) \times 10^{-21}$

Table 6. Summary of results at 60.6 kbar.

Pressure	= 60.6 kbar
Data points used	= 22
Iterations required	= 44
CPU time required	= 8 min. 29.2 sec.
Maximum deviation of fit	= 0.038 mV
Standard deviation of fit	= 0.026 mV

Temperature-versus-power function

Initial values (linear least-squares)

a_0 = 11.1748 (fixed)

a_1 = 1.247312

a_2 = 7.380479 x 10^{-4}

Final values (nonlinear regression)

a_0 = 11.1748 (fixed)

a_1 = 1.312159(±0.000179)

a_2 = 8.495842(±0.004359) x 10^{-4}

Pressurized emf-versus-temperature function

Final values (nonlinear regression)

c_1 = 3.869921(±0.000433) x 10^{-2}

c_2 = 4.129931(±0.000609) x 10^{-5}

c_3 = -4.711172(±0.000077) x 10^{-7}

c_4 = 2.053068(±0.000009) x 10^{-9}

c_5 = -4.623358(±0 000011) x 10^{-12}

c_6 = 5.774496(±0.000013) x 10^{-15}

c_7 = -3.797166(±0.000015) x 10^{-18}

c_8 = 1.024677(±0.000017) x 10^{-21}

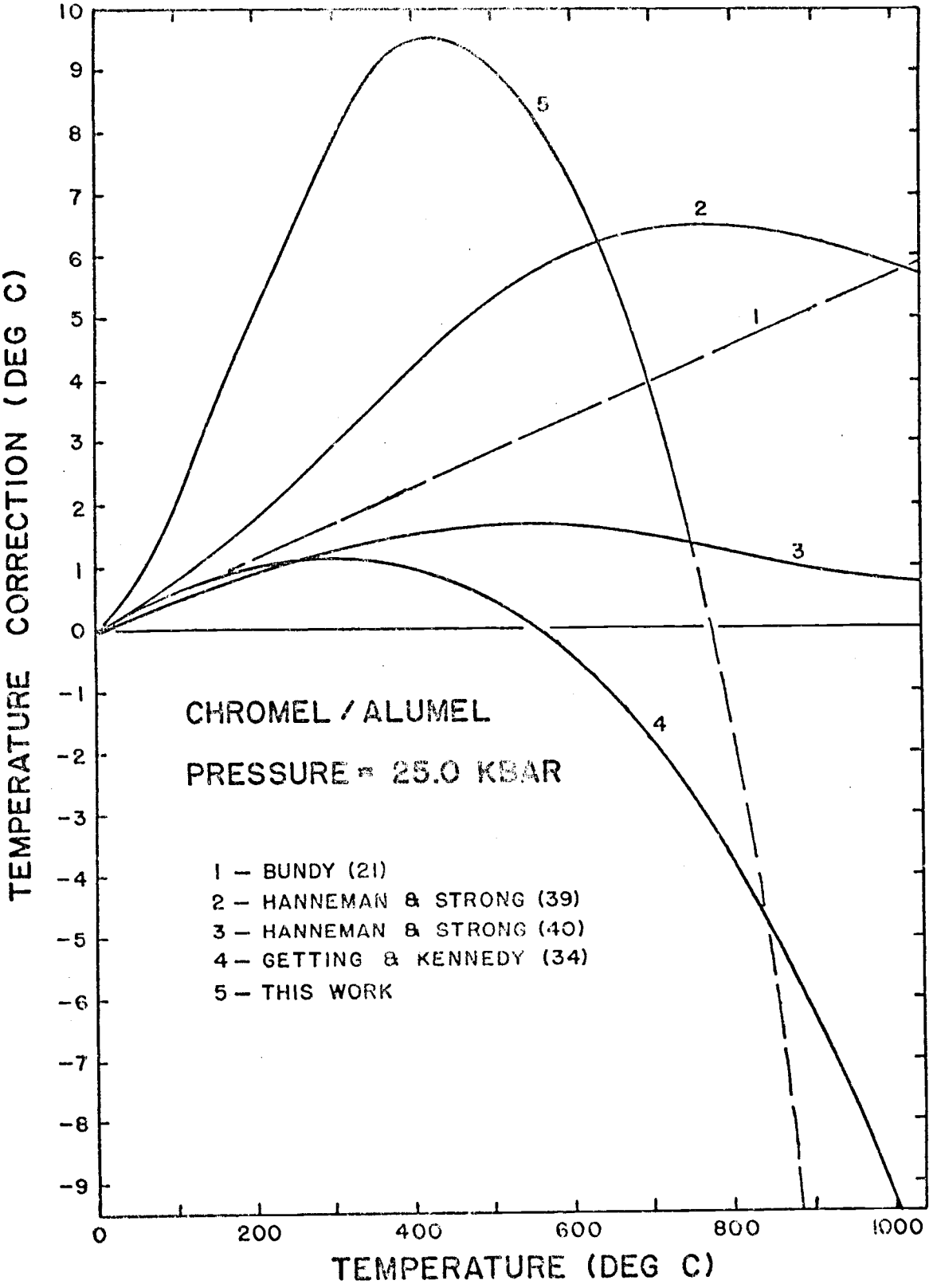


Figure 22. Temperature correction. Comparison of results at 25.0 kbar.

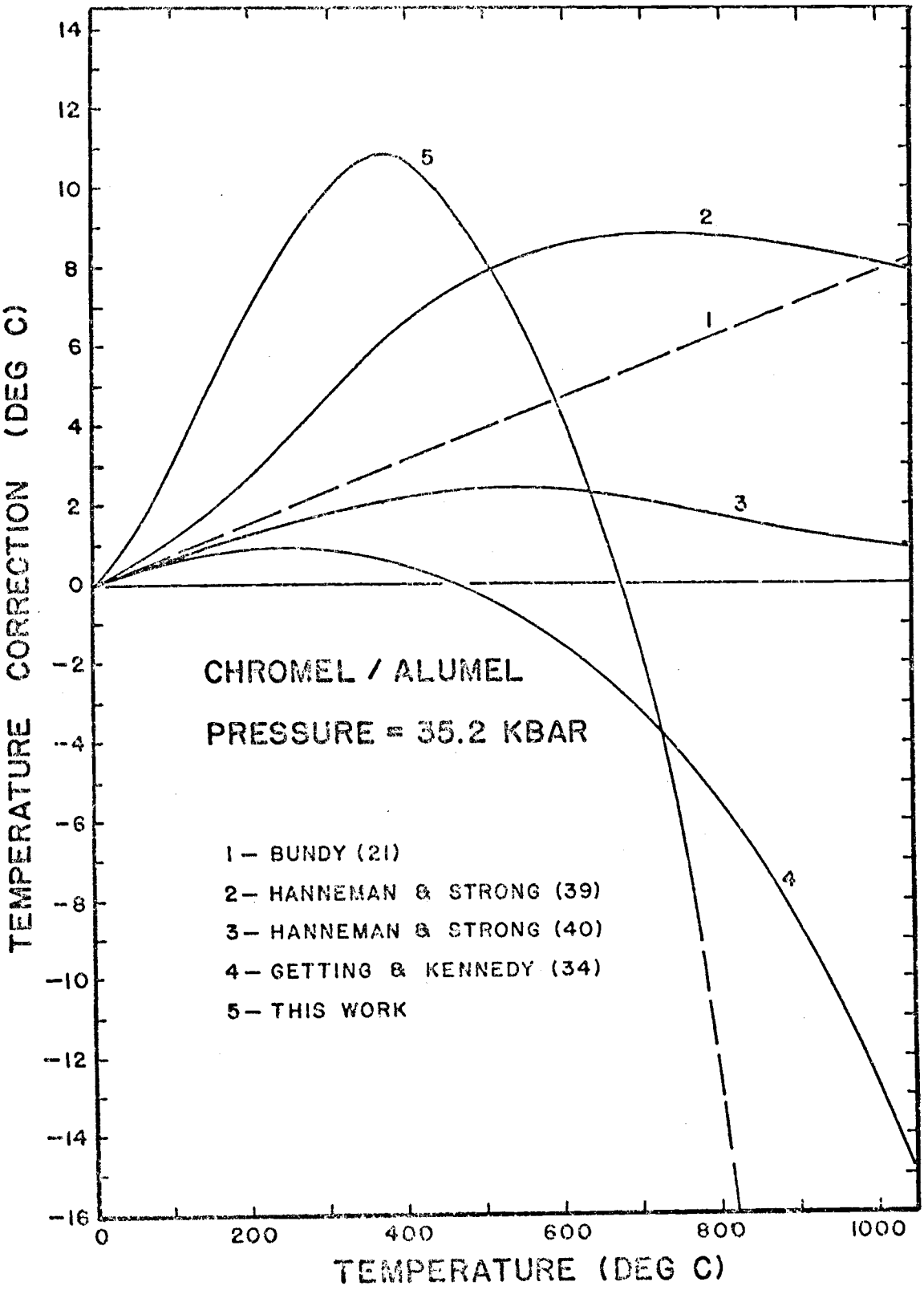


Figure 23. Temperature correction. Comparison of results at 35.2 kbar.

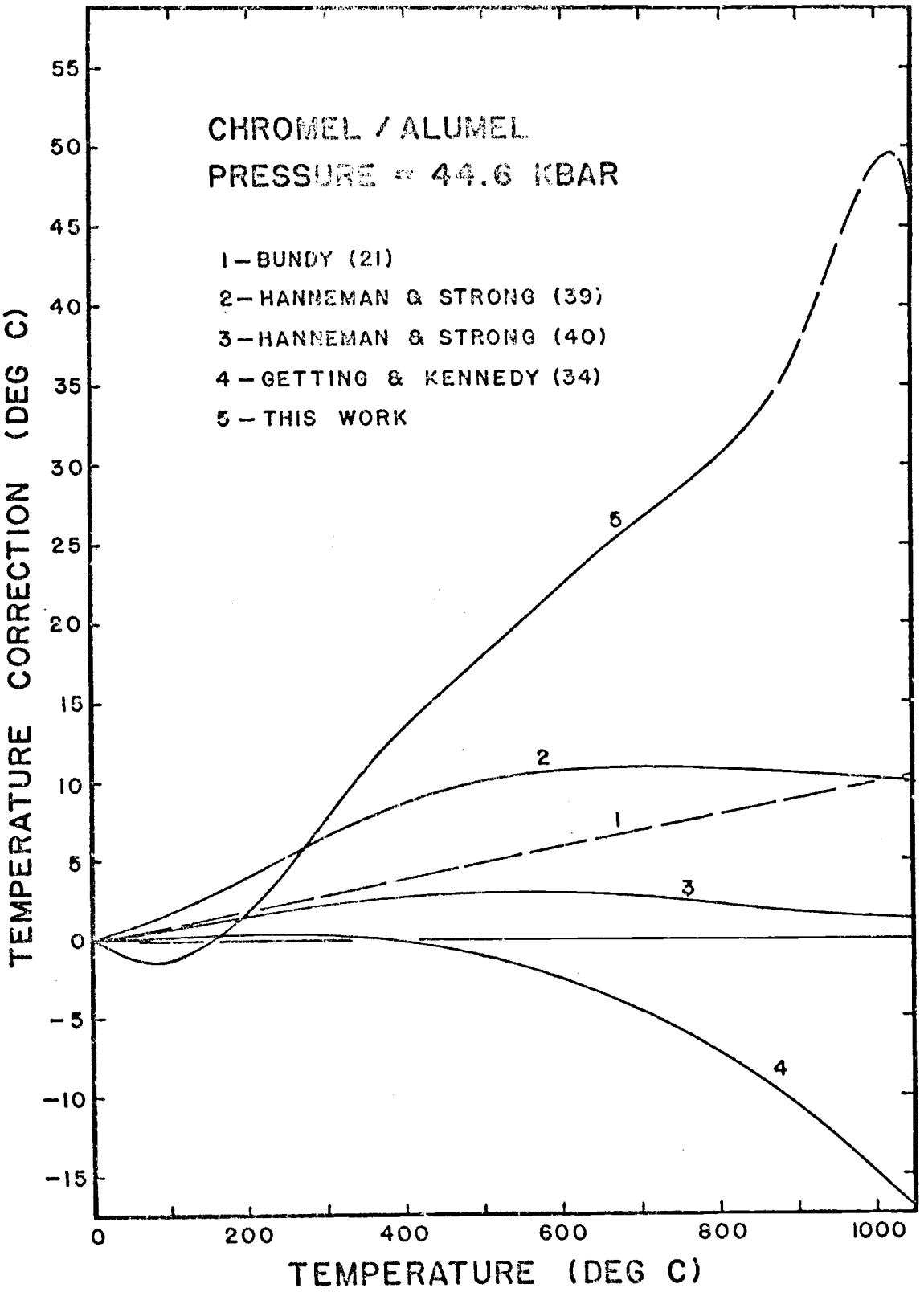


Figure 24. Temperature correction. Comparison of results at 44.6 kbar.

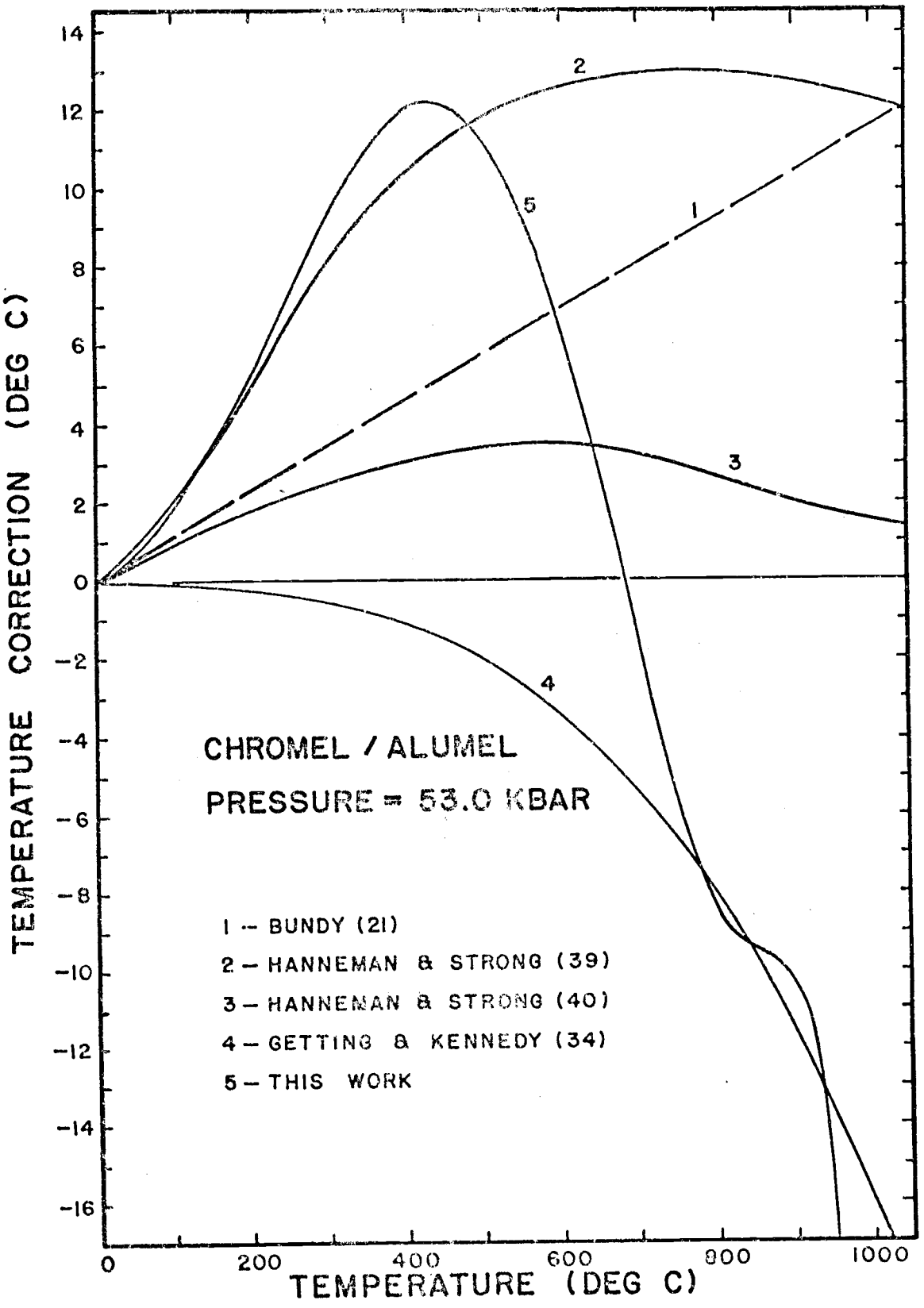


Figure 25. Temperature correction. Comparison of results at 53.0 kbar.

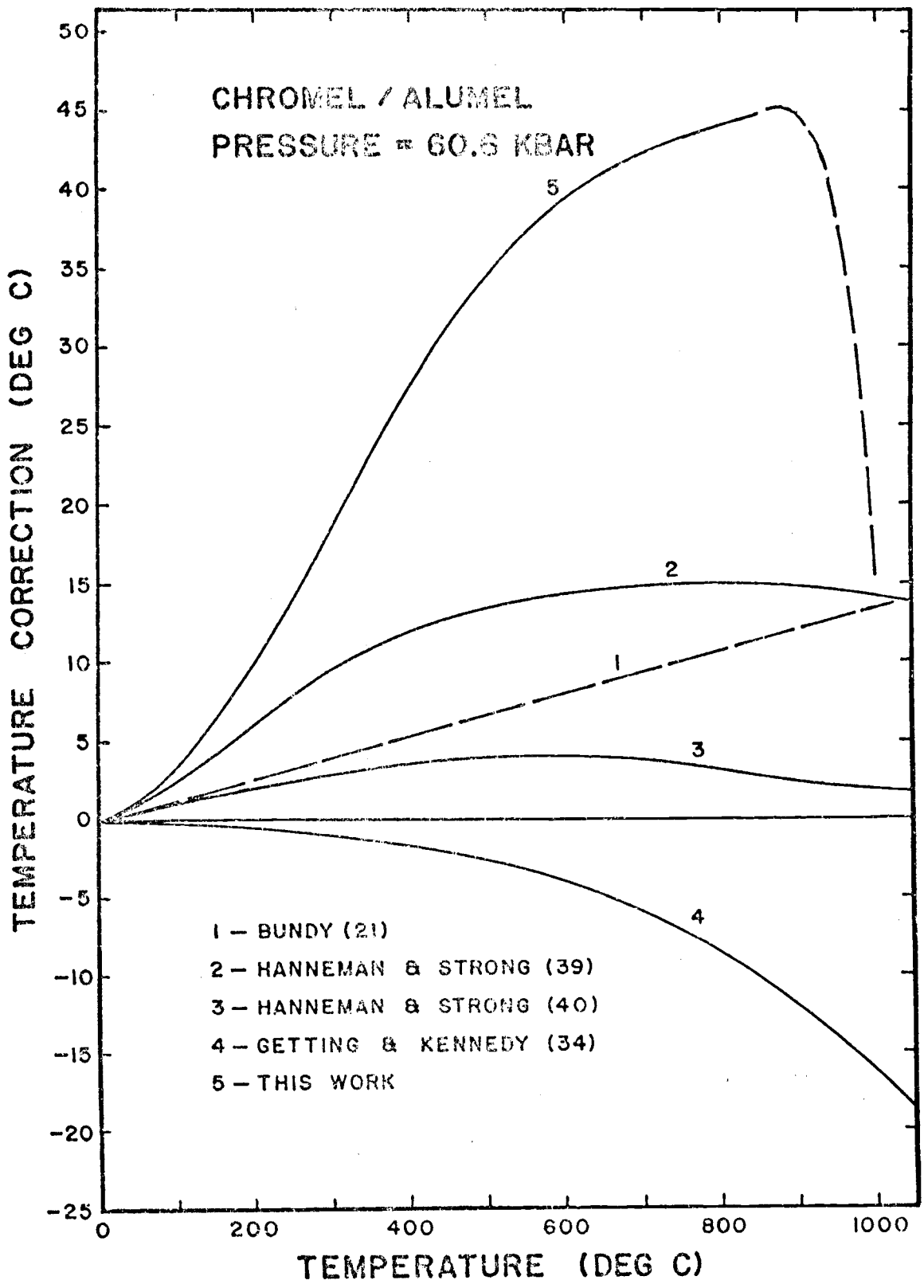


Figure 26. Temperature correction. Comparison of results at 60.6 kbar.

800°C, the curve more closely resembles the results of Getting and Kennedy (33, 34) at these higher temperatures. Similar results are seen at 35.2 kbar in Figure 23 with a maximum positive temperature correction of +10.9°C at 370°C, finally becoming negative at 680°C. At 44.6 kbar (Figure 24) the temperature correction curve takes a different form entirely, indicating a negative correction below 160°C, then rising to what appears to be inordinately large values at higher temperatures (+30°C at 800°C), suggesting the likelihood that the nonlinear algorithm has converged to one of the local minima discussed previously. At 53.0 kbar the indicated temperature correction follows the values of Hanneman and Strong (39) very closely at temperatures below 500°C, reaching a peak of +12.2°C at 430°C, then dropping rapidly between 500°C and 750°C to follow the estimated corrections of Getting and Kennedy (34) above 750°C. Finally, at 60.6 kbar the temperature correction rises rapidly above 100°C to rather large positive values (+44°C at 800°C), two to three times the magnitude of the Hanneman and Strong results (39). Though it is tempting to suppose this large positive correction is again due to convergence to a local minimum, it must be pointed out that recent Mössbauer effect studies by Stokes (68) suggest a temperature correction of as much as +25°C at 600°C for this thermocouple at 75 kbar.

Effect of Pressure on Relative Seebeck, Peltier and Thomson Coefficients

Although it is not specifically the goal of this study to evaluate any pressure corrections except those for the thermal emf of the chromel/alumel thermocouple, the fact that the model used expresses the thermal emf, E, as an analytic function of the temperature, T, permits the direct calculation of the effect of pressure on the relative Seebeck, Peltier and Thomson coefficients, defined as follows:

1. Relative Seebeck coefficient (thermoelectric power)

$$S_{ab} = \frac{\partial E_{ab}}{\partial T} \qquad (\mu V / ^\circ K)$$

where E_{ab} = thermal emf of thermocouple (a,b)

2. Relative Peltier coefficient

$$\pi_{ab} = TS_{ab} \qquad (mV)$$

3. Relative Thomson coefficient

$$\sigma_{T_{ab}} = T \frac{\partial S_{ab}}{\partial T} \qquad (\mu V / ^\circ K)$$

The relative Seebeck coefficient is shown in Figure 27 as a function of true temperature for six different pressures. With the

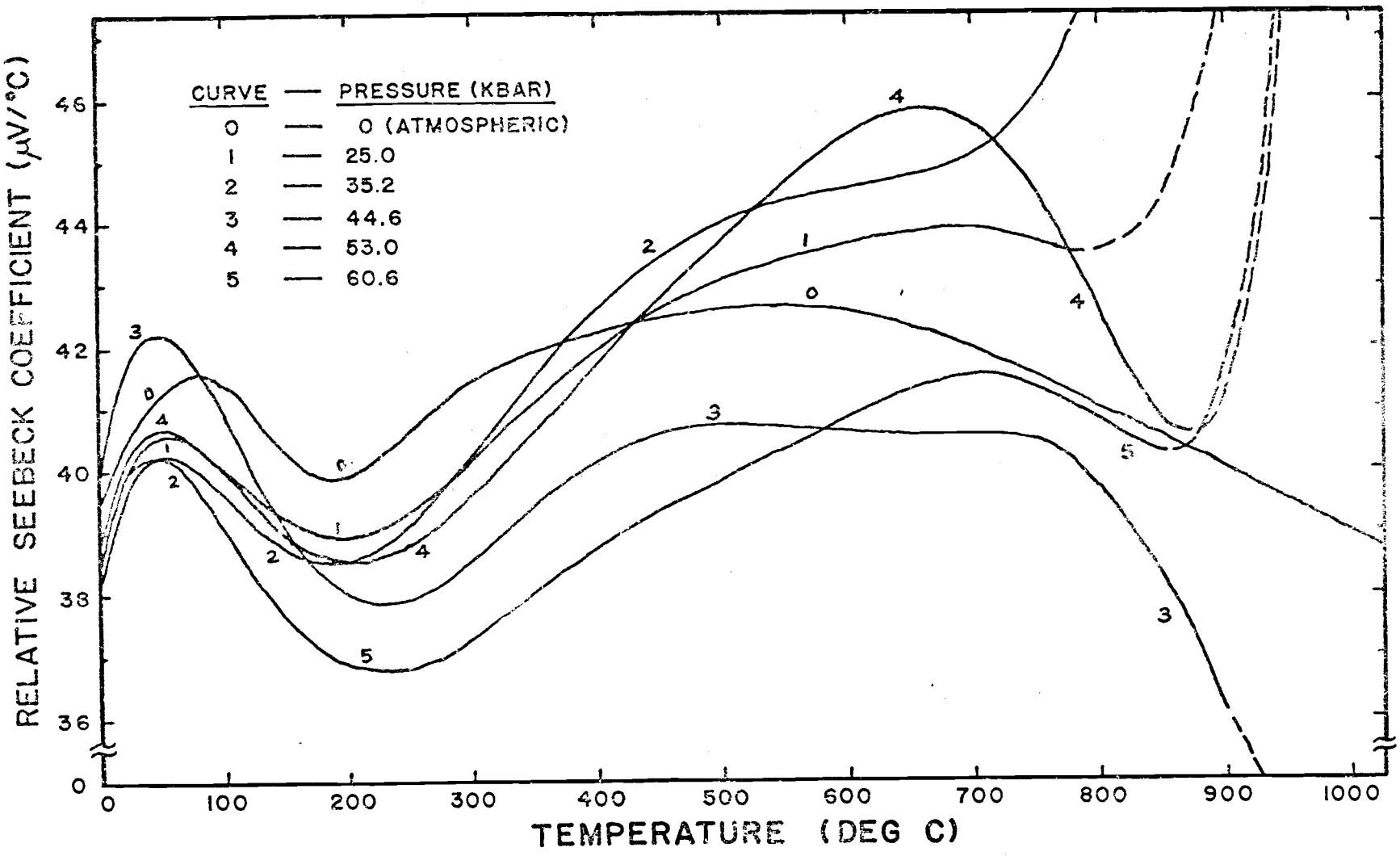


Figure 27. Effect of pressure on relative Seebeck coefficient.

exception of the curve for 44.6 kbar, the effect of pressure is to decrease the relative thermoelectric power at temperatures below 375°C compared to its value at atmospheric pressure. Near 400°C, three of the five high-pressure curves become greater than the corresponding value at atmospheric pressure.

The differences between the pressurized and unpressurized values of the relative Peltier coefficient and relative Thomson coefficient are shown in Figures 28 and 29, respectively. No attempt is made to interpret the individual curves. As Bridgman observed (16) from his study of similar properties under a much more limited range of temperatures (0-100°C) and pressures (0-12 kbar), the results are "unexpectedly complicated".

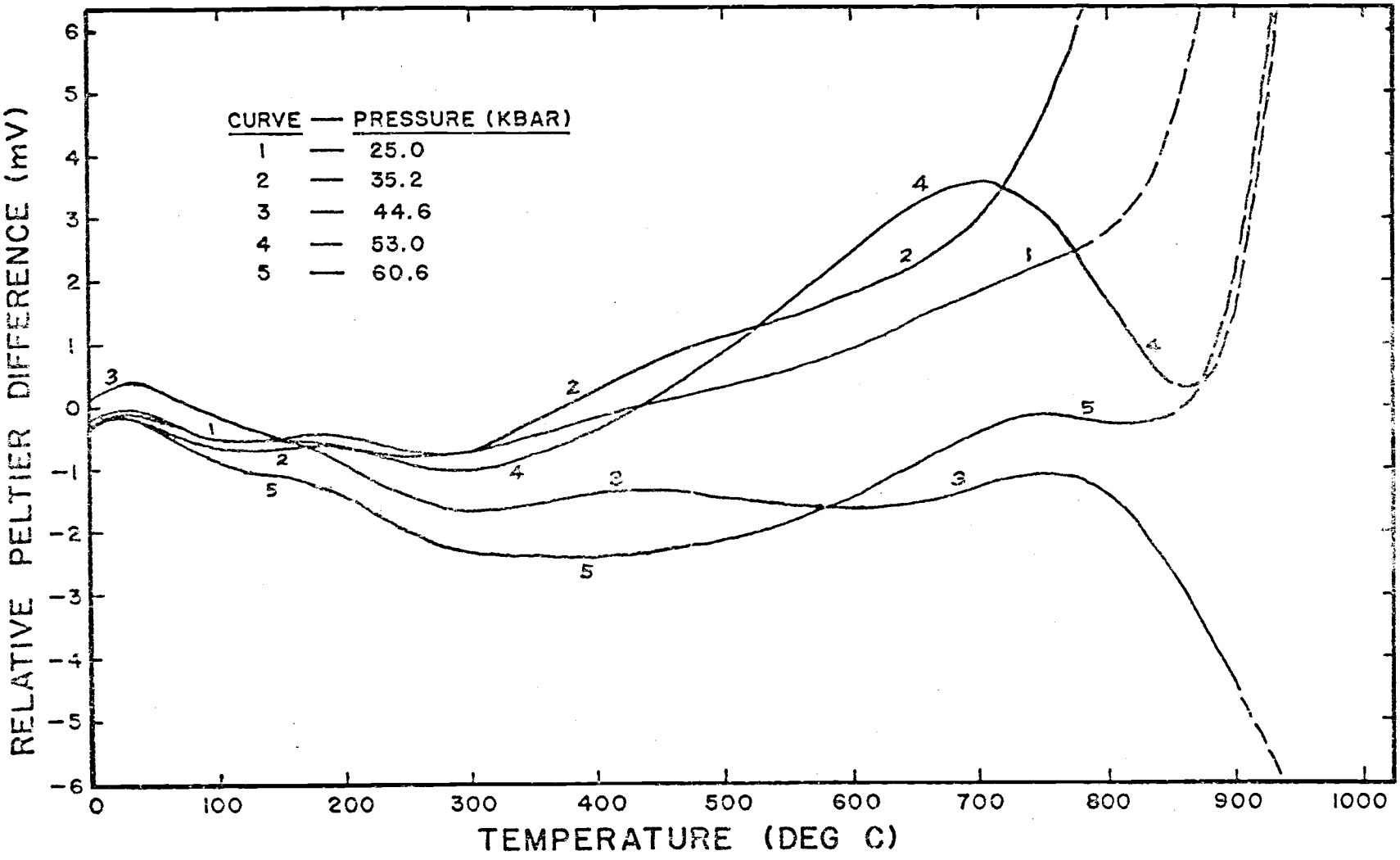


Figure 28. Effect of pressure on relative Peltier coefficient.

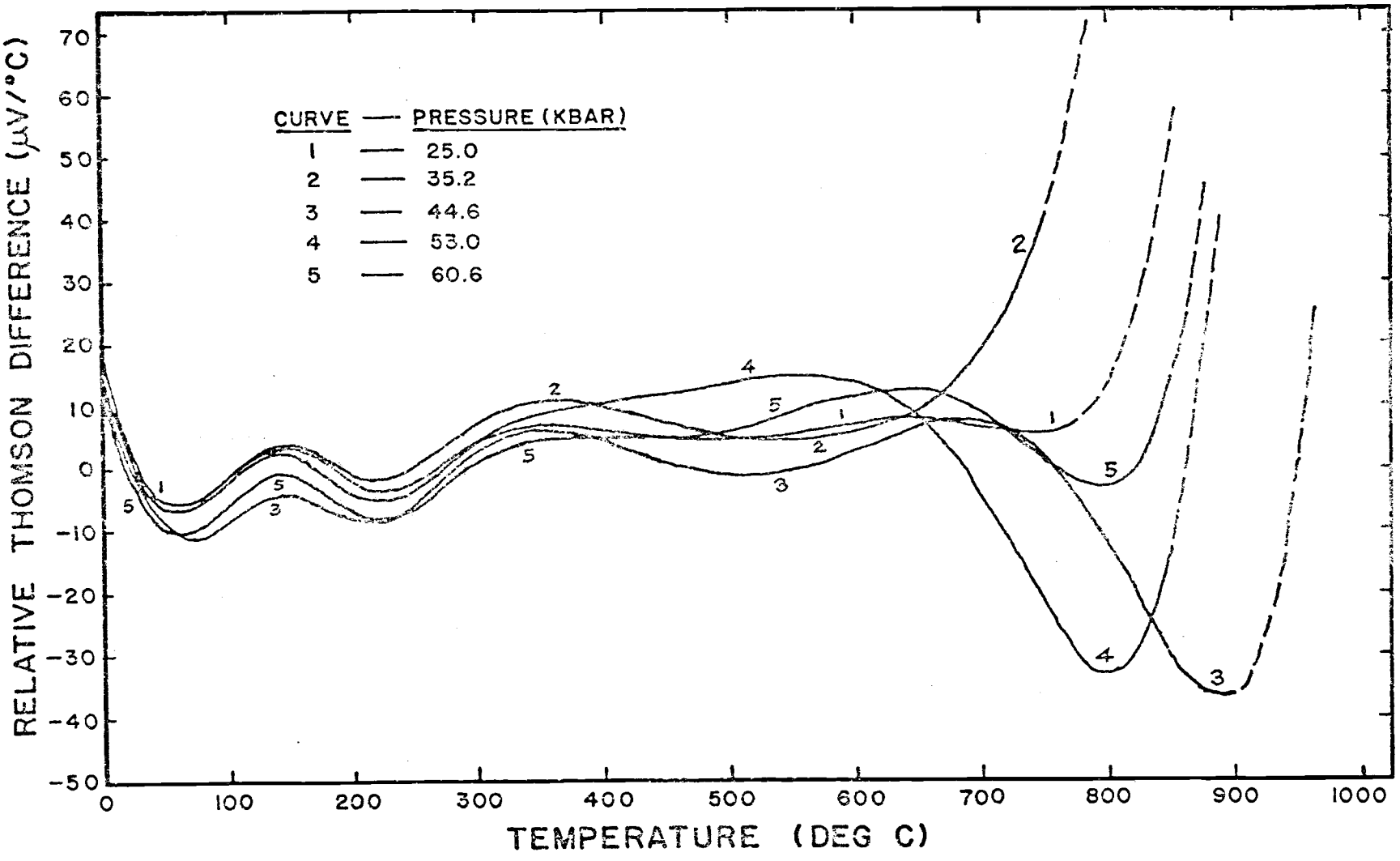


Figure 29. Effect of pressure on relative Thomson coefficient.

SUMMARY AND CONCLUSIONS

An indirect parametric method has been successfully used to determine the effect of ultra-high pressure on the thermal emf of a chromel/alumel thermocouple under pressures of 25.0 kbar, 35.2 kbar, 44.6 kbar, 53.0 kbar and 60.6 kbar, and temperatures up to approximately 900°C. A model is chosen which expresses the temperature of the pressurized thermocouple junction as a quadratic function of the electrical power delivered to the pressurized furnace, while the thermal emf of the pressurized junction is approximated using an eighth-degree polynomial power series function of the temperature. Combining the two functions to eliminate the unknown junction temperatures, the pressurized emf is given as a function of furnace power, which is nonlinear in its coefficients. Through the application of an iterative nonlinear least-squares algorithm, the coefficients are obtained. The nonlinear objective function (representing the sum of the squares of the residuals for the fit of the model to the emf-versus-power data) being minimized is found to possess multiple local minima, thus requiring carefully chosen initial values for the unknown parameters. The temperature corrections obtained using this method compare favorably with previous estimates obtained by other means, especially at the lower pressures studied.

Suggested further study of the method would include:

1. improved instrumentation allowing simultaneous digital recording of furnace power and thermocouple emf,
2. application of the method to other types of thermocouples, in particular ones such as Pt10%Rh/Pt for which the emf-versus-temperature curve can be fitted with a simpler polynomial power series,
3. modification of the Marquardt algorithm (70) or use of recently-developed more efficient nonlinear least-squares algorithms (49), and
4. attempts to systematically identify and compare the solutions corresponding to the multiple minima of the objective function (14, 15).

BIBLIOGRAPHY

1. Adler, Philip and Harold Margolin. Calibration experiments with a tetrahedral-type pressure apparatus. In: High-Pressure Measurement, ed. by A. A. Giardini and Edward C. Lloyd, Washington, D. C., Butterworth Inc., 1963, p. 95-114.

2. Adler, Philip N. and Harold Margolin. The pressure-temperature diagram of solid thallium. Transactions of the Metallurgical Society of the American Institute of Mining, Metallurgical, and Petroleum Engineers. 230:1048-1052. 1964.

3. Aoki, Masanao. Introduction to Optimization Techniques. New York, Macmillan, 1971. 335 p.

4. Bard, Yonathan. Nonlinear Parameter Estimation. New York, Academic Press, 1974. 341 p.

5. Barnard, R. D. The temperature, pressure, and concentration coefficients of resistivity of metals and their relation to diffusion thermopower. Physica Status Solidi (b) 46:369-375. 1971.

6. Barnard, R. D. Thermoelectricity in Metals and Alloys. London, Taylor and Francis Ltd., 1972. 259 p.

7. Barnett, J. Dean, Roy B. Bennion and H. Tracy Hall. High pressure X-ray diffraction studies on barium. Science 141:534-535. 1963.

8. Bell, P. M., F. R. Boyd, Jr. and J. L. England. The effect of pressure on the thermal emf of the platinum/platinum 10 percent rhodium thermocouple. In: Accurate Characterization of the High-Pressure Environment, U. S. National Bureau of Standards Special Publication 326:63-65. 1971.

9. Bevington, Philip R. Data Reduction and Error Analysis for the Physical Sciences. New York, McGraw Hill, 1969. 336 p.

10. Birch, Francis. Thermoelectric measurement of high temperatures in pressure apparatus. The Review of Scientific Instruments 10:137-140. 1939.

11. Bloch, Daniel and Francis Chaissé. Effect of pressure on emf of thermocouples. Journal of Applied Physics 38:409. 1967.

12. Bourassa, R.R., D. Lazarus and D.A. Blackburn. Effect of high pressure on the thermoelectric power and electrical resistance of aluminum and gold. The Physical Review 165:853-864. 1968.

13. Boyd, F.R. and J.L. England. Apparatus for phase-equilibrium measurements at pressures up to 50 kilobars and temperatures up to 1750°C. Journal of Geophysical Research 65:741-748. 1960.

14. Branin, F.H., Jr. Widely convergent method for finding multiple solutions of simultaneous nonlinear equations. IBM Journal of Research and Development 16:504-522. 1972.

15. Branin, Franklin H., Jr. and Stanley K. Hoo. A method of finding multiple extrema of a function of n variables. In: Numerical Methods for Non-Linear Optimization, ed. by F. A. Lootsma, London, Academic Press, 1972, p. 231-237.

16. Bridgman, P.W. Thermo-electromotive force, Peltier heat, and Thomson heat under pressure. Proceedings of the American Academy of Arts and Sciences 53:269-386. 1918.

17. Bridgman, P.W. Polymorphism, principally of the elements, up to 50,000 kg/cm^2. The Physical Review 48:893-906. 1935.

18. Bridgman, P.W. The measurement of hydrostatic pressure to 30,000 kg/cm^2. Proceedings of the American Academy of Arts and Sciences 74:1-10. 1940.

19. Bridgman, P.W. Pressure-volume relations for seventeen elements to 100,000 kg/cm^2. Proceedings of the American Academy of Arts and Sciences 74:425-440. 1942.

20. Bridgman, P.W. The resistance of 72 elements, alloys and compounds to 100,000 kg/cm^2. Proceedings of the American Academy of Arts and Sciences 81:165-251. 1952.

21. Bundy, F.P. Effect of pressure on emf of thermocouples. Journal of Applied Physics 32:483-488. 1961.

22. Bundy, F.P. A review of resistance-jump phase changes useful for high-pressure calibration. In: Accurate Characterization of the High Pressure Environment, U.S. National Bureau of Standards Special Publication 326:263-271. 1971.

23. Cheng, V.M., P.C. Allen and D. Lazarus. Pressure coefficient of thermoelectric power of platinum/platinum-10 percent rhodium and chromel/alumel thermocouples. Applies Physics Letters 26:6-7. 1975.

24. Deaton, B.C. and R.B. Graf. Pressure distribution and hysteresis effects in a tetrahedral anvil device. The Review of Scientific Instruments 34:45-47. 1963.

25. Decker, Daniel L. Equation of state of NaCl and its use as a pressure gauge in high-pressure research. Journal of Applied Physics 36:157-161. 1965.

26. Decker, D.L. and H.B. Vanfleet. Melting and high-temperature electrical resistance of gold under pressure. The Physical Review A138:129-133. 1965.

27. Decker, D.L. Equation of state of sodium chloride. Journal of Applied Physics 37:5012-5014. 1966.

28. Decker, Daniel L. Associate Professor, Brigham Young University, Physics Department. Personal communication. Provo, Utah. May 10, 1967.

29. Decker, D.L., W.A. Bassett, L. Merrill, H.T. Hall and J.D. Barnett. High-pressure calibration: a critical review. Journal of Physical and Chemical Reference Data 1:773-835. 1972.

30. Diatschenko, V. and C.W. Chu. Small effect of hydrostatic pressure on the emf of the Chromel/Alumel thermocouple between 4.2 and 300 K. The Review of Scientific Instruments 46:1291-1292. 1975.

31. Draper, N.R. and H. Smith. Applied Regression Analysis. New York, Wiley, 1966. 407 p.

32. Freud, Paul J. and Phillip N. LaMori. Pressure dependence of the thermoelectric power of thermocouple materials. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:67-75. 1971.

33. Getting, Ivan C. and George C. Kennedy. The effect of pressure on the emf of thermocouples. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:77-80. 1971.

34. Getting I. C. and G. C. Kennedy. Effect of pressure on the emf of Chromel-Alumel and Platinum-Platinum 10 Percent Rhodium Thermocouples. Journal of Applied Physics 41:4552-4562. 1970.

35. Hall, H. Tracy. Some high-pressure, high-temperature apparatus design considerations: Equipment for use at 100,000 atmospheres and 3000° C. The Review of Scientific Instruments 29:267-275. 1958.

36. Hall, H. T., L. Merrill and J. D. Barnett. High-pressure polymorphism in cesium. Science 146:1297-1299. 1964.

37. Hall, H. T. Distinguished professor, Brigham Young University. Department of Chemistry. Personal communication. Provo, Utah. August 23, 1968.

38. Hall, H. Tracy. High-pressure scale as determined by X-ray diffraction techniques up to approximately 100 kbar. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:303-306. 1971.

39. Hanneman, R. E. and H. M. Strong. Pressure dependence of the emf of thermocouples to 1300° C and 50 kbar. Journal of Applied Physics 36:523-528. 1965.

40. Hanneman, R. E. and H. M. Strong. Pressure dependence of the emf of thermocouples. Journal of Applied Physics 37:612-614. 1966.

41. Hanneman, R. E., H. M. Strong and F. P. Bundy. A critical review of the effect of pressure on thermocouple emf's. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:53-62. 1971.

42. Haygarth, J. C., I. C. Getting and G. C. Kennedy. Determination of the pressure of the barium I-II transition with single-stage piston-cylinder apparatus. Journal of Applied Physics 38:4557-4564. 1967.

43. Heydemann, Peter L.M. The Bi I-II transition pressure measured with a dead-weight piston guage. Journal of Applied Physics 38:2640-2644. 1967.

44. Houck, James C. and Ulric O. Hutton. Correlation of factors influencing the pressures generated in multi-anvil devices. In: High-Pressure Measurement, ed. by A.A. Giardini and Edward C. Lloyd, Washington, D.C., Butterworth Inc., 1963 p. 221-245.

45. Huebener, R.P. Thermoelectricity in metals and alloys. In: Solid State Physics, Vol. 27, ed. by F. Seitz and D. Turnbull, New York, Academic Press, 1972. p. 63-134.

46. Jayaraman, A., W. Klement, Jr., R.C. Newton and G.C. Kennedy. Fusion curves and polymorphic transitions of the group III elements--aluminum, gallium, indium and thallium--at high-pressures. Journal of Physics and Chemistry of Solids 24:7-18. 1963.

47. Jeffery, R,N., J.D. Barnett, H.B. Vanfleet and H.T. Hall. Pressure calibration to 100 kbar based on the compression of NaCl. Journal of Applied Physics 37:3172-3180. 1966.

48. Johnson, J.B. Thermal agitation of electricity in conductors. The Physical Review 32:97-109. 1928.

49. Jones, A. Spiral--a new algorithm for non-linear parameter estimation using least squares. The Computer Journal 13:301-308. 1970.

50. Kennedy, G.C. and P.N. LaMori. Some fixed points on the high-pressure scale. In: Progress in Very High Pressure Research, ed. by F.P. Bundy, W.R. Hibbard, Jr., and H.M. Strong. New York, John Wiley & Sons, Inc., 1961. p. 304-313.

51. Kennedy, G.C. and P.N. LaMori. The pressures of some solid-solid transitions. Journal of Geophysical Research 67:851-856. 1962.

52. Kowalik, J. and M.R. Osborne. Methods for Unconstrained Optimization Problems. New York, American Elsevier, 1968. 148 p.

53. Lallemand, M., J. Brielles, D. Vidal and P. Malbrunot. Contribution à l'étude de l'effect de la pression sur le couple platine/platine-rhodié 10%. Journal of Physics D: Applied Physics 6:1052-1057. 1973.

54. LaMori, Phillip N. Calibration experiments in a piston-cylinder apparatus. In: High-Pressure Measurement, ed. by A.A. Giardini and Edward C. Lloyd, Washington, D.C., Butterworths, 1963. p. 321-338.

55. LaMori, Phillip N. The use of solid-solid transitions at high temperatures for high-pressure calibration. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:279-282. 1971.

56. Lazarus, D., R.N. Jeffery, and J.D. Weiss. Relative pressure dependence of Chromel/Alumel and platinum/platinum-10% rhodium thermocouples. Applied Physics Letters 19:371-373. 1971.

57. Lees, J. The design and performance of U.H.P. equipment. An interim report on the tetrahedral anvil apparatus. In: Advances in High-Pressure Research, Vol. 1, ed. by R.S. Bradley, London, Academic Press, 1966, p. 1-83.

58. Lees, J. and B.H.J. Williamson. Combined very high pressure/high temperature calibration of the tetrahedral anvil apparatus, fusion curves of zinc, aluminum, germanium and silicon to 60 kilobars. Nature 208:278-279. 1965.

59. Lees, J. and J.H McCartney. Single crystal measurements and stress difference in solid pressure-transmitting media. Journal of Scientific Instruments (Journal of Physics E) 1 (series 2): 911-914. 1968.

60. Levenberg, Kenneth. A method for the solution of certain non-linear problems in least squares. Quarterly of Applied Mathematics 2:164-168. 1944.

61. MacDonald, D.K.C. Thermoelectricity: an introduction to the principles. New York, John Wiley & Sons, Inc., 1962. 133 p.

62. Marquardt, Donald W. An algorithm for least-squares estimation of nonlinear parameters. Journal of the Society of Industrial and Applied Mathematics 11:431-441. 1963.

63. Meyer, R.R. Theoretical and computational aspects of nonlinear regression. In: Nonlinear Programming, ed. by J.B. Rosen, O.L. Mangasarian and K. Ritter. New York, Academic Press, 1970. p. 465-486.

64. Paquin, R.A. and E. Gregory. Modification and calibration of a tetrahedral anvil apparatus. In: High-Pressure Measurement, ed. by A.A. Giardini and Edward C. Lloyd, Washington, D.C., Butterworth Inc., 1963, p. 274-285.

65. Peters, E.T. and J.J. Ryan. Comment on the pressure dependence of the emf of thermocouples. Journal of Applied Physics 37:933. 1966.

66. Schamp, H.W., J.N. Mundy and E. Rapoport. Use of melting points for measuring pressure in high-pressure, high-temperature vessels. In: High-Pressure Measurement, ed. by A.A. Biardini and Edward C. Lloyd, Washington, D.C., Butterworth Inc., 1963, p. 355-364.

67. Sclar, C.B., L.C. Carrison and C.M. Schwartz. The calcite-aragonite transition and the calibration of a belt-type apparatus between 15 and 35 kb, 700 to 1400°C. In: High-Pressure Measurement, ed. by A.A. Giardini and Edward C. Lloyd, Washington, D.C., Butterworth Inc., 1963, p. 286-300.

68. Stokes, John Loyal. Calibration of a thermocouple at high pressures using the Mössbauer effect. Doctoral dissertation. Provo, Utah, Brigham Young University, 1972. 112 numb. leaves. (Microfilm)

69. Strong H.M. High temperature methods at high pressure. In: Modern Very High Pressure Techniques, ed. by R.H. Wentorf, Jr., Washington, D.C., Butterworth, Inc., 1962, p. 93-117.

70. Tabata, T. and R. Ito. Effective treatment of the interpolation factor in Marquardt's nonlinear least-squares fit algorithm. The Computer Journal 18:250-251. 1975.

71. U.S. Department of Commerce. Thermocouple Reference Tables Based on the IPTS-68. National Bureau of Standards Monograph 125, 1974. 401 p.

72. Vereshchagin, L.F., E.V. Zubova, I.P. Buimova and K.P. Burdina. Measurement of pressures up to 100 kbars by the free-piston method. Doklady Academii Nauk, SSSR 169:74-76. 1966. (English translation in Soviet Physics-Doklady 11:585-586. 1967.)

73. Waxman, M., J.R. Hastings and W.T. Chen. Nonlinear statistical analysis of Burnett PVT data. In: Proceedings of the Fifth Symposium on Thermophysical Properties, ed. by C.F. Bonilla. New York, American Society of Mechanical Engineers, 1970. p. 248-255.

74. Waxman, M. and J.R. Hastings. Proposed experiment to determine the effect of pressure on the emf of thermocouples. Journal of Applied Physics 43:2629-2632. 1972.

75. Wentorf R.H., Jr. Temperature measurement by thermal noise at high pressures. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:81-89. 1971.

76. Zeto, R.J. and H.B. Vanfleet. Pressure calibration to 60 kbar based on the resistance change of a manganin coil under hydrostatic pressure. Journal of Applied Physics 40:2227-2231. 1969.

77. Zeto, R.J., H.B. Vanfleet, E. Hryckowian and C.D. Bosco. Characterization of the bismuth I-II and barium I-II points under hydrostatic pressure. In: Accurate Characterization of the High-Pressure Environment, U.S. National Bureau of Standards Special Publication 326:25-34. 1971.

78. Ziman, J.M. Electrons and Phonons. London, Oxford University Press, 1960. 554 p.

79. Zwart, Philip B. Non-linear programming: a quadratic analysis of ridge paralysis. Journal of Optimization Theory and Applications 6:331-339. 1970.

APPENDICES

APPENDIX A

Computer Program and

Subroutines

```
                                MAR04 SRC                              PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      PROGRAM MAR04   FORTRAN IV (POP 19.30)     S. A. EIDE    14 SEP 76
C
C      PURPOSE
C        PERFORMS A LEAST-SQUARES FIT TO DATA WITH A SPECIFIED
C        FUNCTION WHICH MAY BE NON-LINEAR IN ITS PARAMETERS.
C          UTILIZES AN ITERATIVE NON-LINEAR REGRESSION ALGORITHM OF
C          MARQUARDT.  (SEE J. SIAM, VOL 11, PP 431-441.  1963)
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        MAR04A
C          INITIALIZES PARAMETERS USED IN NON-LINEAR REGRESSION
C          ANALYSIS
C        MAR04B
C          HANDLES NON-LINEAR REGRESSION SUBROUTINES AND CLOCKS
C          THE CPU TIME REQUIRED FOR ANALYSIS
C        MAR04C
C          MONITORS CONVERGENCE, TERMINATES ITERATIONS AND CONTROLS
C          PRINT-OUT OF RESULTS
C        MAR04D
C          PROVIDES OUTPUT OPTIONS INCLUDING ANALYSIS OF RESIDUALS,
C          RESIDUAL HISTOGRAM, PRESSURE EFFECT ON EMF, SEEBECK,
C          PELTIER AND THOMSON COEFFICIENTS AS A FUNCTION OF
C          TEMPERATURE.  ALSO CONTROLS RESTART OPTIONS.
C        FUNCTN (X, I, A, K, L, MD)
C          EVALUATES FITTING FUNCTION FOR NON-LINEAR LEAST-SQUARES FIT
C        DERIV (X, I, A, K, L, MD, DERIV)
C          EVALUATES THE DERIVATIVES OF THE FITTING FUNCTION FOR
C          THE ITH TERM WITH RESPECT TO EACH PARAMETER
C        SUMSQR (Y, SIGMAY, NDREE, YFIT)
C          EVALUATES REDUCED CHI SQUARE FOR FIT TO DATA
C        MTXINV (ARRAY, DET)
C          INVERTS A SYMMETRIC TWO-DIMENSIONAL MATRIX AND CALCULATES
C          ITS DETERMINANT
C        MARQRT
C          PERFORMS A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTION
C          USING MARQUARDT'S ALGORITHM
C        PAGE (LINE, NPG, LUN, LADD)
C          COUNTS LINES AND NUMBERS PAGES OF PRINT-OUT
C        TTYPLT (X, Y, NPTS, LUN)
C          PRINTS A LINEAR PLOT OF ARRAYS X VS Y ON TELETYPE LUN
C        HISTG (X, NPTS, NINT, LUN)
C          PRODUCES SCALED HISTOGRAM OF NINT INTERVALS ON TTY LUN
C        TEMP (D, P, L, MD)
C          COMPUTES TEMPERATURE FOR IND VARIABLE P USING COEFFICIENTS A
C        EMF (D, T, K, L, ND)
C          COMPUTES EMF (FOR ND=0), FIRST PARTIAL DERIVATIVE OF EMF WITH
C          RESPECT TO TEMPERATURE (ND=1), OR SECOND PARTIAL (ND=2) FOR
C          TEMPERATURE T USING COEFFICIENT ARRAY A (CODE K,L)
C
C      COMMENTS
C        DIMENSION STATEMENT VALID FOR UP TO 100 DATA POINTS AND
C        UP TO 20 PARAMETERS (COEFFICIENTS) IN FITTING FUNCTION
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

```
                                MARQM SRC                          PAGE  2


C       PROGRAM MAR04
        DOUBLE PRECISION A, AGNK, AIN, COEF
        DIMENSION X(100),Y(100),SIGNAV(100),YFIT(100),A(20),COEF(12)
        DIMENSION SIGMAA(20),DERIV(20),FILEN(2),AGNK(20),AIN(20)
        DIMENSION E(100),DE(100),ITC(100),VX(100),C(100),NTC(100)
        COMMON NPTS,NTERMS,MODE,A,AGNK,AIN,KKK,IPRESS,A0,WTEMP,NIV
        COMMON X,Y,SIGNAV,YFIT,SIGMAA,DERIV,NF,JCODC,NSAV,L,K
        COMMON E,DE,ITC,V,C,NA,NC,L2,K2,L3,K3,FLAGDA,JOKIT,NTC
        COMMON PARTOL,CHITOL,ITMAX,ITER,JM,JS,JS10,NPR,LINE,NPG
        COMMON JSAV,NFREE,CHISQR,JPASS,CHISAV,IM,IS,IS10,SEC
        COMMON SECTOT,NSET,FILEN,SNUM,SET,KSAV,NTH,NTOT,COEF,JLAM,NQ
        CALL INIT(8,1)
        CALL BEGIN (2400)
    5   CALL ERASE
        NPTS = 0
C
C         NEXT 6 STATEMENTS ALLOW USER TO SELECT INPUT DEVICE
C
        WRITE(8,10)
   10   FORMAT(//5X,'DEPRESS DIGIT KEY INDICATING THE FORM OF',
         1 ' YOUR INPUT DATA.  '/10X,'1.  PAPER TAPE'/10X,
         2 '2.  DECTAPE (DT4)'/10X,'3.  TELETYPE KEYBOARD'/)
        CALL CHIN (J)
        IF (J - 50) 15,25,55
C
C         NEXT 6 STATEMENTS PREPARE FOR PAPER TAPE INPUT
C
   15   WRITE (8,20)
   20   FORMAT(//5X,'LOAD PAPER TAPE READER.  DEPRESS ANY CHARACTER',
         1 ' KEY TO CONTINUE.')
        KKK = 6
        CALL TPRUSE
        GO TO 70
C
C         NEXT 16 STATEMENTS OPEN INPUT FILE ON MAGNETIC TAPE (DECTAPE)
C
   25   WRITE(8,30)
   30   FORMAT(//5X,'ENTER DATA FILE NAME AND EXTENSION IN COLS 1-9',
         1 ' BELOW.'/5X,'THE FILE NAME MUST BEGIN IN COL 1 '/5X,
         2 'THE EXTENSION SRC MUST OCCUPY COLS 7-9.'/1X,'123456789')
   34   READ(8,35) FILEN
   35   FORMAT(A5,A4)
        CALL FSTAT (4, FILEN, LF)
        IF (LF .NE. 0) GO TO 45
        WRITE(8,40)
   40   FORMAT(/5X,'DATA FILE NOT FOUND.  TRY AGAIN.'/)
        GO TO 34
   45   WRITE(8,50)
   50   FORMAT(/5X,'DATA FILE FOUND.')
        CALL SEEK (1, FILEN)
        KKK = 1
        GO TO 70
C
C         NEXT 43 STATEMENTS ALLOW INPUT DATA FROM TELETYPE
C
   55   KKK = 8
```

```
                                MAIN SRC                          PAGE  3


      CALL ERASE
      WRITE(8,56)
   56 FORMAT(///' ENTER DATA FILE NAME (9 ALPHANUMERIC MAX)')
      READ(8,57) FILEN
   57 FORMAT(A5,A4)
      WRITE(8,58)
   58 FORMAT('0ENTER SAMPLE NUMBER (A4)')
      READ(8,59) SNUM
   59 FORMAT(A4)
      WRITE(8,60)
   60 FORMAT('0ENTER DATA SET NUMBER OR LETTER (A1)')
      READ(8,61) SET
   61 FORMAT(A1)
      WRITE(8,62)
   62 FORMAT('0ENTER HYDRAULIC PRESSURE IN PSI (I5)')
      READ(8,63) IPRESS
   63 FORMAT(I5)
      WRITE(8,64)
   64 FORMAT('0ENTER AMBIENT TEMPERATURE IN DEGREES CELSIUS (F4.1)')
      READ(8,65) A0
   65 FORMAT(F4.1)
      WRITE(8,66)
   66 FORMAT('0ENTER COOLING WATER TEMPERATURE (F4.1)')
      READ(8,65) WTEMP
      CALL ERASE
      WRITE(8,67)
   67 FORMAT(///' ENTER DATA IN FOLLOWING FORMAT.'/
     1 /5X,'COLS 1-7 = INDEPENDENT VARIABLE (F7.4)'/5X,
     2 'COL  9    = THERMOCOUPLE IDENTIFIER (AB=1,AC=2,BC=3,BC=4)'/5X,
     3 'COLS 11-17 = PRESSURIZED THERMOCOUPLE EMF (MILLIVOLTS) (F7.4)'
     4 /5X,'COLS 19-25 = STANDARD DEVIATION OF EMF (MILLIVOLTS) (F7.4)'
     5 //'0NEGATIVE VALUE OF INDEPENDENT VARIABLE TERMINATES INPUT.'/
     6 ' IND.VAR I **EMF** SIGMA**')
   68 READ(8,69) XIN, J, EMF, DEMF
   69 FORMAT(F7.4,1X,I1,1X,F7.4,1X,F7.4)
      IF (XIN .LT. 0.0) GO TO 85
      NPTS = NPTS + 1
      V(NPTS) = XIN
      NTC(NPTS) = J
      E(NPTS) = EMF
      DE(NPTS) = DEMF
      GO TO 68
C
C       NEXT 12 STATEMENTS READ INPUT DATA FROM PAPER TAPE OR DECTAPE
C
   70 CALL ERASE
      READ(KK,72) SNUM, SET
   72 FORMAT(7X,A4,1X,A1)
      READ(KK,74) IPRESS, A0, WTEMP
   74 FORMAT(I5,1X,F4.1,1X,F4.1)
      DO 78 J=1,100
      READ(KK,76) E(J),DE(J),NTC(J),V(J),C(J)
   76 FORMAT(F7.4,1X,F6.4,1X,I1,1X,F7.4,6X,F7.3)
      IF (E(J) .EQ. 0.0) GO TO 79
   78 NPTS = NPTS + 1
   79 IF (KK .EQ. 1) CALL CLOSE (1)
```

```
                                MAB04 SRC                          PAGE  4


   80 IF (KKK .EQ. 8) GO TO 100
C
C       NEXT 7 STATEMENTS ALLOW USER TO SELECT INDEPENDENT VARIABLE
C
   85 CALL ERASE
      WRITE(8,88)
   88 FORMAT(///5X,'DEPRESS DIGIT INDICATING INDEPENDENT VARIABLE'/
     1 10X,'1.  FURNACE POWER'/10X,'2.  FURNACE VOLTAGE'/10X,
     2 '3.  FURNACE CURRENT')
      CALL CHIN (JJ)
      NIV = JJ - 48
C
C       NEXT 30 STATEMENTS ALLOW CHOICE OF THERMOCOUPLE(S) TO BE
C       INCLUDED IN ANALYSIS.
C
  100 NP = 0
      JCODE = 0
  120 CALL ERASE
      IF (JCODE .GE. 15) GO TO 200
      WRITE(8,150)
  150 FORMAT(///5X,'DEPRESS DIGIT FOR DESIRED THERMOCOUPLE DATA'/
     1 10X,'0.  DATA ENTRY COMPLETED - BEGIN ANALYSIS'/
     2 10X,'1.  AB'/10X,'2.  AC'/10X,'3.  BB'/10X,'4.  DC'/
     X 10X,'5.  COMBINE 1,2,3,4 ABOVE AND BEGIN ANALYSIS')
      CALL CHIN (JJ)
      J = JJ - 48
      IF (J .EQ. 0) GO TO 200
      JCODE = JCODE + 2**(J-1)
      IF (J .EQ. 5) JCODE = 15
      DO 180 I=1,NPTS
      IF (J .EQ. 5) GO TO 160
      IF (NTC(I) .NE. J) GO TO 180
  160 NP = NP + 1
      ITC(NP) = NTC(I)
      IF (KKK .EQ. 8) GO TO 170
      IF (NIV - 2) 165, 170, 175
  165 X(NP) = V(I) * C(I)
      GO TO 178
  170 X(NP) = V(I)
      GO TO 178
  175 X(NP) = C(I)
  178 Y(NP) = E(I)
      SIGMAY(NP) = DE(I)
  180 CONTINUE
      IF (J .NE. 5) GO TO 120
C
C       NEXT 13 STATEMENTS CALL MAJOR SUBROUTINES AND PROVIDE
C       RESTART OPTIONS.
C
  200 NSAV = NPTS
      NPTS = NP
  210 CALL ERASE
      CALL MAB04A
  215 CALL MAB04B
      CALL MAB04C
      IF (IM .LT. 0) GO TO 215
```

```
CALL MM0040
IF (NSET .EQ. 1 .OR. NSET .EQ. 4) GO TO 210
NPTS = NSAV
IF (NSET .EQ. 2) GO TO 80
GO TO 5
END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MARQ4A   FORTRAN IV (PDP 15/30)    S. A. EIDE
C
C      PURPOSE
C        INITIALIZES PARAMETERS USED IN NON-LINEAR REGRESSION
C        ANALYSIS AND PRINTS FIRST PAGE OF PRINT-OUT
C
C      USAGE
C        CALL MARQ4A
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        PAGE (LINE, NPG, LUN, LADD)
C          COUNTS LINES AND NUMBERS PAGES OF PRINT-OUT
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE MARQ4A
      DOUBLE PRECISION A, ACHK, AIN, ATEST, COEF
      DIMENSION X(100),Y(100),SIGMAY(100),YFIT(100),A(20),TC(4)
      DIMENSION SIGMAA(20),DERIV(20),FILEN(2),ACHK(20),AIN(20),COEF(12)
      DIMENSION E(100),DE(100),ITC(100),V(100),C(100),NTC(100),FMARQ(2)
      COMMON NPTS,NTERMS,MODE,A,ACHK,AIN,KKK,IPRESS,AQ,NTEMP,NIV
      COMMON X,Y,SIGMAY,YFIT,SIGMAA,DERIV,NP,JCODE,NSAV,L,K
      COMMON E,DE,ITC,V,C,NA,NC,L2,K2,L3,K3,FLAMDA,JCRIT,NTC
      COMMON PARTOL,CHITOL,ITMAX,ITER,JN,JS,JS10,NPR,LINE,NPG
      COMMON JSAV,NFREE,CHISQR,JPASS,CHISAV,IN,IS,IS10,SEC
      COMMON SECTOT,NSET,FILEN,SNUM,SET,KSAV,NTH,NTOT,COEF,JLAM,MQ
      DATA BLANK/5H     /,AB/5HAB   /,AC/5HAC   /,DB/5HDB   /,
     1 DC/5HDC   /,FMARQ/5HMARQT,4H DAT/
      IF (NSET .EQ. 4) GO TO 297
C
C        NEXT 12 STATEMENTS ARE COEFFICIENTS USED IN FULL NBS TYPE K
C        THERMOCOUPLE EMF VS TEMPERATURE FUNCTION (NBS TYPE K TABLES
C        ARE GENERATED USING THESE COEFFICIENTS).
C
      COEF(1) =-1.85330633D-02
      COEF(2) = 3.89183446D-02
      COEF(3) = 1.66451544D-05
      COEF(4) =-7.87023744D-09
      COEF(5) = 2.28357856D-10
      COEF(6) =-3.57002313D-13
      COEF(7) = 2.99329091D-16
      COEF(8) =-1.28498488D-19
      COEF(9) = 2.22399743D-23
      COEF(10) = 0.125D0
      COEF(11) = 127.0D0
      COEF(12) = 65.0D0
C
C        NEXT 7 STATEMENTS ALLOW USER TO SELECT WEIGHTING MODE TO BE
C        USED IN FITTING DATA.
C
      WRITE(8,220)
  220 FORMAT(//// DEPRESS DIGIT TO INDICATE WEIGHTING MODE'/5X,
     1 '1. INSTRUMENTAL...WEIGHT(I) = 1./(SIGMAY(I)**2'/5X,
     2 '2. NO WEIGHTING.. WEIGHT(I) = 1.'/5X,
     3 '3. STATISTICAL....WEIGHT(I) = 1./Y(I)')
```

```
                                    MARQ4ASRC                                PAGE  2


      CALL CHIN (KK)
      MODE = 50 - KK
C
C       NEXT 6 STATEMENTS ALLOW CHOICE OF MODEL TEMPERATURE FUNCTION
C       THROUGH PARAMETER L.  ABSOLUTE VALUE OF L GIVES
C       DEGREE OF POLYNOMIAL (POWER SERIES).  ABS (L) .LE. 5
C
      WRITE(8,230)
  230 FORMAT(//' ENTER FUNCTION CODE FOR TEMPERATURE VS INDEPENDENT',
     1 ' VARIABLE (I2).')
      READ (8,235) L
  235 FORMAT(I2)
      IF (L .GE. 0) GO TO 239
C
C       NEXT 9 STATEMENTS ALLOW CONSTANT TERM IN TEMPERATURE FUNCTION
C       TO BE FIXED FOR L .LT. 0
C
      WRITE(8,236) A0
  236 FORMAT(' CURRENT VALUE OF A0 (FIXED AMBIENT TEMPERATURE) = ',
     1 F6.3,' DEG C'//'  TO CHANGE, TYPE 1; OTHERWISE, 2')
      CALL CHIN (IA0)
      IF (IA0 .NE. 49) GO TO 239
      WRITE(8,237)
  237 FORMAT(' ENTER NEW VALUE OF A0 FOR THIS ANALYSIS ONLY (F10.7)')
      READ(8,238) A0
  238 FORMAT(F10.7)
C
C       NEXT 14 STATEMENTS ALLOW CHOICE OF MODEL EMF FUNCTION THROUGH
C       PARAMETER K.  K MUST BE .LE. 11.  FOR K .LE. 10, K IS THE
C       DEGREE OF THE POLYNOMIAL (POWER SERIES) IN TEMPERATURE.
C       FOR K = 11 THE MODEL IS THE FULL NBS TYPE K FUNCTION WHICH
C       CONSISTS OF AN EIGHTH-DEGREE POLYNOMIAL (POWER SERIES) PLUS
C       A GAUSSIAN EXPONENTIAL TERM.
C
  239 CALL ERASE
      WRITE(8,240)
  240 FORMAT(//' ENTER FUNCTION CODE FOR THERMOCOUPLE EMF VS',
     1 ' TEMPERATURE (I2)')
      READ(8,235) K
      IF (L .GT. 0) GO TO 242
      NA = -1.
      GO TO 243
  242 NA = L + 1
  243 IF (K .LT. 11) GO TO 246
      NC = K + 1
      GO TO 247
  246 NC = K
  247 NTERMS = NA + NC
C
C       NEXT 9 STATEMENTS ALLOW OPTIONAL OUTPUT FILE TO BE CREATED
C       ON MAGNETIC TAPE (DECTAPE).  PARAMETER VALUES AND SUM OF
C       SQUARES OF RESIDUALS ARE RECORDED FOR EACH ITERATION.
C
      CALL ERASE
      WRITE(8,248)
  248 FORMAT(//' TYPE 1 TO CREATE DATA FILE MARQT DAT LISTING',
```

```
                                MAIN.MNSRC                          PAGE  3

     1 ' PARAMETER VALUES'/' AND CHI-SQUARE FOR EACH ITERATION ON',
     2 ' DECTAPE (.DAT SLOT 2), '/' OTHERWISE TYPE 2')
      CALL CHIN(MQ)
      MQ = MQ - 48
      IF (MQ .NE. 1) GO TO 249
      CALL ENTER (2, FMIN8)
C
C       NEXT 63 STATEMENTS CONTROL INPUT OF INITIAL ESTIMATES OF
C       MODEL PARAMETERS.
C
  249 CALL ERASE
      L2 = 0
      IF (L .LE. 0) L2 = 1
      K2 = 0
      IF (K .NE. 11) K2 = 1
      K3 = K2
      L3 = L2
      WRITE(8,250)
  250 FORMAT(//' TYPE 1 TO ENTER INITIAL ESTIMATES OF PARAMETERS,',
     1 ' OTHERWISE 2.')
      CALL CHIN (JJ)
      IF (JJ .NE. 49) GO TO 289
      CALL ERASE
      IF (L .EQ. 0) GO TO 267
      WRITE(8,252)
  252 FORMAT(//' ENTER INITIAL ESTIMATES OF PARAMETERS FOR TEMPERATURE',
     1 ' VERSUS')
      IF (NIV - 2) 253, 255, 257
  253 WRITE(8,254)
  254 FORMAT(5X,'FURNACE POWER FUNCTION IN COLS 1-15 BELOW (D15.8)')
      GO TO 259
  255 WRITE(8,256)
  256 FORMAT(5X,'FURNACE VOLTAGE FUNCTION IN COLS 1-15 BELOW (D15.8)')
      GO TO 259
  257 WRITE(8,258)
  258 FORMAT(5X,'FURNACE CURRENT FUNCTION IN COLS 1-15 BELOW (D15.8)')
  259 WRITE(8,260)
  260 FORMAT(/' **.********D+***')
      DO 265 LL=1, NA
      WRITE(8,262) L3
  262 FORMAT(' * A(',I2,') =  ****')
      READ(8,264) ATEST
  264 FORMAT(D15.8)
      IF (ATEST .EQ. 0.0) GO TO 265
      AIN(LL) = ATEST
  265 L3 = L3 + 1
      CALL ERASE
      IF (K .NE. 11) GO TO 267
      WRITE(8,268)
  268 FORMAT(//' IF YOU WISH TO USE NBS TYPE K TEMP VS EMF COEFFICIENTS',
     1', TYPE 1'/' OTHERWISE TYPE 2.')
      CALL CHIN (JJ)
      IF (JJ .NE. 49) GO TO 267
      DO 266 KK=1,NC
      AIN(NA+KK) = COEF(KK)
  266 CONTINUE
```

```
                                NAMQ4ASRC                          PAGE  4

      GO TO 280
  267 WRITE(8,270)
  270 FORMAT(///' ENTER INITIAL ESTIMATES OF PARAMETERS FOR PRESSURIZED',
     1 ' THERMOCOUPLE'/5X,'EMF VERSUS TEMPERATURE FUNCTION IN COLS',
     2 ' 1-15 BELOW (D15.8/')
      WRITE(8,200)
      DO 275 KK=1,NC
      WRITE(8,272) K3
  272 FORMAT(' * C(',I2,') =  ****')
      READ(8,264) ATEST
      IF (ATEST .EQ. 0.0) GO TO 275
      AIN(NA+KK) = ATEST
  275 K3 = K< + 1
  280 DO 285 J=1, NTERMS
      ACHK(J) = AIN(J)
  285 A(J) = AIN(J)
      CHISAV = 0.0
C
C       NEXT 4 STATEMENTS SET INITIAL VALUE OF DAMPING PARAMETER
C       LAMBDA.
C
      WRITE(8,290)
  290 FORMAT(///' ENTER INITIAL LAMBDA (TYPICALLY 0.001) (E9.2)')
      READ(8,295) FLAMDA
  295 FORMAT(E9.2)
C
C       NEXT 20 STATEMENTS ALLOW CHOICE OF CONVERGENCE CRITERION
C       AND ESTABLISH CONVERGENCE LIMIT.
C
  297 CALL ERASE
      WRITE(8,300)
  300 FORMAT(//5X,'CHOOSE CONVERGENCE CRITERION FOR TERMINATING',
     1 ' ITERATIONS'/10X,'1. FRACTIONAL CHANGE IN CHI SQUARE'/10X,
     2 '2. FRACTIONAL CHANGE IN ALL COEFFICIENTS')
      CALL CHIN(J)
      JCRIT = J - 48
      IF (JCRIT .EQ. 1) GO TO 304
      WRITE(8,301)
  301 FORMAT(///' ENTER LIMITING FRACTIONAL CHANGE FOR ALL COEFFICIENTS',
     1 ' (E9.2)')
      READ(8,302) PARTOL
  302 FORMAT(E9.2)
      DO 303 J=1, NTERMS
  303 ACHK(J) = A(J)
      GO TO 307
  304 WRITE(8,305)
  305 FORMAT(///' ENTER LIMITING FRACTIONAL CHANGE FOR CHI SQUARE',
     1 ' (E9.2)')
      READ(8,302) CHITOL
C
C       NEXT 14 STATEMENTS SET UPPER LIMIT ON TOTAL NUMBER OF
C       ITERATIONS (MAY BE INCREASED LATER).
C
  307 IF (NSET .NE. 4) GO TO 311
      WRITE(8,306)
  306 FORMAT(///' ENTER NUMBER OF ADDITIONAL ITERATIONS DESIRED. (I4)')
```

```
                                MARQNASRC                              PAGE  5


      READ(8,309) IT
      ITMAX = ITER + IT
      GO TO 313
  311 WRITE(8,308)
  308 FORMAT(///' ENTER MAXIMUM NUMBER OF ITERATIONS (I4)')
      READ(8,309) ITMAX
  309 FORMAT(I4)
      ITER = 0
      JM = 0
      JS = 0
      JS10 = 0
C
C       NEXT 20 STATEMENTS ALLOW CHOICE OF EXTENT AND FREQUENCY OF
C       PRINT-OUT (HARD COPY) FOLLOWING ITERATIONS.
C
  313 CALL ERASE
      WRITE(8,310)
  310 FORMAT(///' DEPRESS DIGIT INDICATING EXTENT OF PRINT-OUT',
     1 ' DESIRED'//10X,'1.  COMPLETE PRINT-OUT OF DATA AND RESULTS'/
     2 10X,'2.  SUMMARY OF NON-LINEAR REGRESSION ANALYSIS ONLY')
      CALL CHIN (NPR)
      NPR = NPR - 48
      KSAV = NTH = NTOT = 1
      WRITE(8,312)
  312 FORMAT(///' CHOOSE DESIRED PRINT-OUT OF CURRENT PARAMETER VALUES'/
     1 10X,'1.  HARD COPY FOR ALL ITERATIONS.'/
     2 10X,'2.  HARD COPY FOR EVERY NTH ITERATION ONLY.')
      CALL CHIN (KSAV)
      KSAV = KSAV - 48
      IF (KSAV .NE. 2) GO TO 318
      WRITE(8,314)
  314 FORMAT(///' ENTER DESIRED VALUE FOR NTH (I2).')
      READ(8,316) NTH
  316 FORMAT(I2)
      NTOT = NTH + ITER
C
C       NEXT 95 STATEMENTS CONTROL PRINT-OUT OF INITIAL VALUES
C
  318 LINE = 60
      IF (NSET .NE. 4) NPG = 1
      CALL PAGE (LINE, NPG, 3, 0)
      WRITE(3,320) IPRESS,FILEN,SO,SNUM,WTEMP,SET
  320 FORMAT(' BAROMETRIC PRESSURE = ',I5,' PSI',21X,'DATA FILE ',A5,A4//
     1 ' ANBIENT TEMPERATURE = ',F7.4,' DEG CELSIUS',10X,'SAMPLE',
     2 ' NUMBER ',A4//' WATER TEMPERATURE = ',F4.1,' DEG CELSIUS',15X,
     3 'DATA SET ',A1)
      GO TO (332, 334, 336), NIV
  332 WRITE(3,333)
  333 FORMAT(' INDEPENDENT VARIABLE, X = FURNACE POWER IN WATTS')
      GO TO 340
  334 WRITE(3,335)
  335 FORMAT(' INDEPENDENT VARIABLE, X = FURNACE VOLTAGE IN VOLTS')
      GO TO 340
  336 WRITE(3,337)
  337 FORMAT(' INDEPENDENT VARIABLE, X = FURNACE CURRENT IN AMPERES')
  340 WRITE(3,342)
```

```
MAIN04.SRC                                    PAGE  6

342 FORMAT(' DEPENDENT VARIABLE, Y = PRESSURIZED THERMOCOUPLE EMF',
   1 ' IN MILLIVOLTS')
    JSAV = JCODE
    DO 343 I=1,4
343 TC(I) = BLANK
    III = 0
    IF (JCODE / 8 .NE. 1) GO TO 344
    JCODE = JCODE - 8
    III = III + 1
    TC(III) = DC
344 IF (JCODE / 4 .NE. 1) GO TO 345
    JCODE = JCODE - 4
    III = III + 1
    TC(III) = DB
345 IF (JCODE / 2 .NE. 1) GO TO 346
    JCODE = JCODE - 2
    III = III + 1
    TC(III) = AC
346 IF (JCODE .NE. 1) GO TO 347
    III = III + 1
    TC(III) = AB
347 WRITE(3,348) (TC(I), I=III,1,-1)
348 FORMAT(' THERMOCOUPLE DATA INCLUDED = ',4A5)
    WRITE(3,354) NPTS
354 FORMAT(' NUMBER OF PAIRS OF DATA POINTS = ',I3)
    JCODE = JSAV
    WRITE(3,356) K, L
356 FORMAT(' FITTING FUNCTION CODE, K = ',I2,', L = ',I2)
    WRITE(3,358) NTERMS
358 FORMAT(' NUMBER OF PARAMETERS = ',I2)
    NFREE = NPTS - NTERMS
    WRITE(3,360) NFREE
360 FORMAT(' NUMBER OF DEGREES OF FREEDOM = ',I2)
    IF (MODE) 364, 366, 368
364 WRITE(3,365)
365 FORMAT(' METHOD OF WEIGHTING LEAST-SQUARES FIT, WEIGHT(I) = ',
   1 '1./Y(I)')
    GO TO 370
366 WRITE(3,367)
367 FORMAT(' METHOD OF WEIGHTING LEAST-SQUARES FIT, WEIGHT(I) = ',
   1 '1.')
    GO TO 370
368 WRITE(3,369)
369 FORMAT(' METHOD OF WEIGHTING LEAST-SQUARES FIT, WEIGHT(I) = ',
   1 '1./SIGMAY(I)**2')
370 WRITE(3,374)
374 FORMAT(' ITERATION TERMINATED WHEN FRACTIONAL CHANGE IN ')
    IF (JCRIT .NE. 1) GO TO 378
    WRITE(3,376) CHITOL
376 FORMAT(5X,'CHI-SQUARE LESS THAN ',1PE9.2)
    GO TO 380
378 WRITE(3,379) PARTOL
379 FORMAT(5X,'ALL PARAMETERS LESS THAN ',1PE9.2)
380 WRITE(3,382) FLAMDA
382 FORMAT(' INITIAL VALUE OF LAMBDA = ',1PE9.2)
    WRITE(3,384)
```

```
384 FORMAT(/5X,'INITIAL ESTIMATES OF PARAMETERS')
    LINE = 22
    L3 = L2
    K3 = K2
    DO 390 LL=1, NA
    CALL PAGE (LINE, NPG, 3, 0)
    WRITE(3,386) L3, A(LL)
386 FORMAT(8X,'A(',I2,') = ',1PD15.8)
390 L3 = L3 + 1
    WRITE(3,392)
392 FORMAT(' ')
    LINE = LINE + 1
    DO 400 KK=1, NC
    CALL PAGE (LINE, NPG, 3, 0)
    WRITE(3,396) K3, A(KK+NA)
396 FORMAT(8X,'C(',I2,') = ',1PD15.8)
400 K3 = K3 + 1
    WRITE(3,410)
410 FORMAT(' ')
    RETURN
    END
```

```
                                MAR04.USRC                              PAGE  1


CCCCCC,CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MAR04B   FORTRAN IV (PDP 15/30)   S. A. EIDE
C
C      PURPOSE
C        CONTROLS NON-LINEAR REGRESSION SUBROUTINES AND CLOCK CPU
C        TIME FOR ANALYSIS.
C
C      USAGE
C        CALL MAR04B
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        MARQRT
C          PERFORMS A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTION
C          USING MARQUARDT'S ALGORITHM.
C        FUNCTN (X, I, A, K, L, A0)
C          EVALUATES FITTING FUNCTION FOR NON-LINEAR LEAST-SQUARES FIT
C        DERIV1 (X, I, A, K, L, A0, DERIV)
C          EVALUATES FIRST PARTIAL DERIVATIVES OF FITTING FUNCTION WITH
C          RESPECT TO EACH PARAMETER AT ITH POINT.
C        MTXINV (ARRAY, DET)
C          INVERTS A SYMMETRIC TWO-DIMENSIONAL ARRAY AND CALCULATES
C          ITS DETERMINANT.
C        SUMSQR (Y, SIGMAY, NFREE, YFIT)
C          EVALUATES REDUCED CHI SQUARED FOR FIT TO DATA.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE MAR04B
      DOUBLE PRECISION A, ACHK, AIN
      DIMENSION X(100),Y(100),SIGMAY(100),YFIT(100),A(20)
      DIMENSION SIGMAA(20),DERIV(20),FILEN(2),ACHK(20),AIN(20)
      DIMENSION E(100),DE(100),ITC(100),V(100),C(100),NTC(100)
      COMMON NPTS,NTERMS,MODE,A,ACHK,AIN,KXK,IPRESS,A0,WTEMP,NIV
      COMMON X,Y,SIGMAY,YFIT,SIGMAA,DERIV,NP,JCODE,NSAV,L,K
      COMMON E,DE,ITC,V,C,NR,NC,L2,K2,L3,K3,FLAMDA,JCRIT,NTC
      COMMON PARTOL,CHITOL,ITMAX,ITER,JM,JS,JS10,NPP,LINE,NPG
      COMMON JSAV,NFREE,CHISQR,JPASS,CHISAV,IM,IS,IS10,SEC
      COMMON SECTOT,NSET,FILEN,SNUM,SET
  420 CALL TIME10 (IM, IS, IS10, IOFF)
      CALL MARQRT
      IOFF = 1
      RETURN
      END
```

```
                                    MAR04CSRC                                  PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MAR04C    FORTRAN IV (F0P 15/30)     S. A. EIDE
C
C      PURPOSE
C        MONITORS CONVERGENCE, TERMINATES ITERATIONS AND CONTROLS
C        PRINT-OUT OF RESULTS.
C
C      USAGE
C        CALL MAR04C
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        PAGE (LINE, NPG, LUN, LADD)
C          COUNTS LINES AND NUMBERS PAGES OF PRINT-OUT
C        EMF (A, T, K, L, ND)
C          COMPUTES EMF (FOR ND=0), FIRST PARTIAL DERIVATIVE OF EMF
C          WITH RESPECT TO TEMPERATURE (ND=1), OR SECOND PARTIAL (ND=2)
C          FOR TEMPERATURE T USING COEFFICIENTS IN ARRAY A (CODE K, L)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE MAR04C
      DOUBLE PRECISION A, ACHK, AIN, AJ, ACJ, DABS, COEF
      DIMENSION X(100),Y(100),SIGMAY(100),YFIT(100),A(20),NORD(100)
      DIMENSION SIGMAA(20),DERIV(20),FILEN(2),ACHK(20),AIN(20)
      DIMENSION E(102),DE(100),ITC(100),V(100),C(100),NTC(100)
      DIMENSION AT(4), BT(5), COEF(12), ECOR(5)
      COMMON NPTS,NTERMS,NODE,A,ACHK,AIN,KK,IPRESS,A0,NTEMP,NIV
      COMMON X,Y,SIGMAY,YFIT,SIGMAA,DERIV,NP,JCODE,NSAV,L,K
      COMMON E,DE,ITC,V,C,NA,NC,L2,K2,L3,K3,FLAMDA,JCRIT,NTC
      COMMON PCTTOL,CHITOL,ITMAX,ITER,JM,JS,JS10,NPG,LINE,NPG
      COMMON JSAV,NFREE,CHISQR,JPASS,CHISAV,IM,IS,IS10,SEC
      COMMON SECTOT,NSET,FILEN,SNUM,SET,KSAV,NTH,NTOT,COEF,JLAM,MQ
      DATA AT(1),AT(2)/2.4383248 E-02,9.7838851 E-09/
      DATA AT(3),AT(4)/3.6276955 E-12,-2.5756138 E-16/
      DATA BT(1),BT(2),BT(3)/6.2386571,2.4955174 E-02,-7.8739333 E-06/
      DATA BT(4),BT(5)/1.3250743 E-10,1.0580541 E-18/
      DATA BLANK,CONV/5H      ,5HCONVG/
      JM = JM + IM
      JS = JS + IS
      JS10 = JS10 + IS10
      ITER = ITER + 1
C
C        NEXT 3 STATEMENTS WRITE CURRENT PARAMETER VALUES AND SUM OF
C        SQUARES OF RESIDUALS ON DECTAPE (OPTIONAL).
C
      IF (MQ .NE. 1) GO TO 445
      WRITE(2,440) ITER,CHISQR, (A(I),I=1,NTERMS)
  440 FORMAT(1X,I4,30(1X,1PE12.5))
C
C        NEXT 16 STATEMENTS TEST FOR CONVERGENCE
C
  445 LUN = 8
      IF (KSAV .NE. 2 .OR. ITER .EQ. NTOT) LUN = 3
      IF (JCRIT .EQ. 1) GO TO 460
      JPASS = 0
      DO 450 J=1, NTERMS
```

```
                                MAR3040SRC                              PAGE  2


      AI = A(J)
      ACJ = ACHK(J)
      TEST = DABS((ACJ - AJ)/ACJ)
      IF (TEST .LT. PARTOL) JPASS = JPASS + 1
  450 CONTINUE
  460 TEST = (CHISQR - CHISAV)/CHISAV
      CTEST = ABS (TEST)
      PCTEST = 100.*TEST
  465 LT = 11 + NTERMS
      IF (KSAV.NE.2.OR.ITER.EQ.NTOT) CALL PAGE (LINE,NPG,LUN,LT)
      CALL ERASE
C
C       NEXT 15 STATEMENTS COMPUTE CPU TIME PER ITERATION AND
C       CUMULATIVE CPU TIME.
C
      SEC = FLOAT(IS) + FLOAT(IS10)/10.
  467 IF (SEC .LT. 60.) GO TO 468
      SEC = SEC - 60.
      IN = IN + 1
      GO TO 467
  468 IF (JS10 .LT. 10) GO TO 469
      JS10 = JS10 - 10
      JS = JS + 1
      GO TO 468
  469 SECTOT = FLOAT(JS) + FLOAT(JS10)/10.
  470 IF (SECTOT .LT. 60.) GO TO 472
      SECTOT = SECTOT - 60.
      JS = JS - 60
      JM = JM + 1
      GO TO 470
C
C       NEXT 78 STATEMENTS PRODUCE PRINT-OUT (HARD COPY OPTIONAL)
C       OF SUMMARY FOLLOWING EACH ITERATION.
C
  472 WRITE(LUN,473) ITER, CHISQR, PCTEST
  473 FORMAT(' ITERATION NUMBER ',I4,' REDUCED CHI-SQUARE = ',1PE13.6,3X,
     1 '(',0PF10.3,' % CHANGE)')
      WRITE(LUN,474) IN, SEC
  474 FORMAT(' CPU TIME FOR THIS ITERATION = ',I3,' MIN, ',F4.1,' SEC')
      WRITE(LUN,475) ITER, JM, SECTOT
  475 FORMAT(' TOTAL CPU TIME FOR ',I4,' ITERATIONS = ',I3,' MIN, ',
     1 F4.1,' SEC')
      WRITE(LUN,476) FLAMDA
  476 FORMAT(' CURRENT VALUE OF LAMBDA = ',1PE10.3)
      IF (JCRIT .EQ. 1) GO TO 1477
      IF (KSAV.NE.2.OR.ITER.EQ.NTOT) LINE=LINE+1
      WRITE(LUN,477) JPASS, NTERMS
  477 FORMAT(' PARAMETERS SATISFYING CONVERGENCE CRITERION = ',I2,
     1 ' OF ',I2)
 1477 DYMAX = 0.0
      DO 478 I=1, NPTS
      YTEST = ABS(Y(I) - YF(I))
      IF (YTEST .LE. DYMAX) GO TO 478
      DYMAX = YTEST
      IMAX = I
  478 CONTINUE
```

```
      DYNAX = Y(IMAX) - YSET(IMAX)
      PCDIF = 100. * DYNAX / Y(IMAX)
      XSET = X(IMAX)
      YSET = Y(IMAX)
      WRITE(LUN,479) DYNAX,PCDIF,XSET,YSET,JLAM
  479 FORMAT(' MAXIMUM RESIDUAL = ',1PE10.3,' = ',1PE8.1,' % AT X =',
     1 0PF8.2,' , Y =',0PF8.4,' CYCLES THIS ITERATION = ',I4,
     2,', CURRENT ENF PRESSURE CORRECTIONS (MV) ARE')
      DO 1479 I=1,5
      T = 200.0 * FLOAT(I)
      ECOR(I) = ENF (COEF,1,11,0,0) - ENF (A,T,K,L,0)
 1479 CONTINUE
      WRITE(LUN,1480) (ECOR(I),I=1,5)
 1480 FORMAT(1X,F7.3,'(200),  ',F7.3,'(400),  ',F7.3,'(600),  ',F7.3,
     1 '(800),  ',F7.3,'(1000 C)')
  480 WRITE(LUN,481)
  481 FORMAT(/5X,'CURRENT VALUE OF PARAMETERS',5X,'PERCENT CHANGE')
      K3 = K2
      L3 = L2
      DO 485 LL=1, NA
      AJ = A(LL)
      ACJ = ACHK(LL)
      PC = (AJ - ACJ)/ACJ
      PCC = 100. * PC
      PASS = BLANK
      IF (JCRIT .EQ. 1) GO TO 482
      IF (ABS(PC) .LT. PARTOL) PASS = CONV
  482 WRITE(LUN,483) L3, A(LL), PCC, PASS
  483 FORMAT(8X,'A(',I2,') = ',1PD15.8,7X,'(',0PF10.3,')',3X,A5)
  485 L3 = L3 + 1
      WRITE(LUN,487)
  487 FORMAT(' ')
      DO 490 KK=1, NC
      AJ = A(KK + NA)
      ACJ = ACHK(KK+NA)
      PC = (AJ - ACJ)/ACJ
      PCC = 100. * PC
      PASS = BLANK
      IF (JCRIT .EQ. 1) GO TO 488
      IF (ABS(PC) .LT. PARTOL) PASS = CONV
  488 WRITE(LUN,489) K3, A(KK+NA), PCC, PASS
  489 FORMAT(8X,'C(',I2,') = ',1PD15.8,7X,'(',0PF10.3,')',3X,A5)
  490 K3 = K3 + 1
      WRITE(LUN,491)
  491 FORMAT(' ')
      DO 492 J=1, NTERMS
  492 ACHK(J) = A(J)
      IF (ITER .EQ. NTOT) NTOT = NTOT + NTH
      CHISAV = CHISQR
      IF (ITER .EQ. 1) GO TO 498
      IF (JCRIT .EQ. 1) GO TO 495
      IF (JPASS .EQ. NTERMS) GO TO 520
      GO TO 498
  495 IF (CTEST .LT. CHITOL) GO TO 520
  498 IF (ITER .LT. ITMAX) GO TO 517
      CALL CHOUT (7)
```

```
                                MAIN04CSRC                              PAGE  4


C
C       NEXT 28 STATEMENTS CONTROL OPTIONS WHEN ITERATION LIMIT
C       IS REACHED.
C
  499 CALL ERASE
      WRITE(8,500)
  500 FORMAT(//5X,'MAXIMUM ITERATION NUMBER COMPLETED.'//5X,
     1 'SELECT DESIRED PROCEDURE BELOW.'//10X,'1.  INCREASE MAXIMUM',
     2 ' ITERATION NUMBER AND CONTINUE'/10X,'2.  PRODUCE FINAL',
     3 ' PRINT-OUT USING CURRENT PARAMETERS'/10X,'3.  DISPLAY',
     4 ' RESTART OPTIONS'/10X,'4.  ENTER NEW LAMBDA'/10X,
     5 '5.  ENTER NEW A(0)')
      CALL CHIN (JJ)
      JJ = JJ - 48
      GO TO (510, 520, 925, 502, 505), JJ
  502 WRITE(8,503)
  503 FORMAT(//' ENTER NEW VALUE FOR LAMBDA (E10.3)')
      READ(8,504) FLAMDA
  504 FORMAT(E10.3)
      GO TO 499
  505 WRITE(8,506) A0
  506 FORMAT(//' A(0) IS NOW = ',F8.4,'  ENTER NEW A(0) (F8.4)')
      READ(8,507) A0
  507 FORMAT(F8.4)
      GO TO 499
  510 WRITE(8,512)
  512 FORMAT(//5X,'ENTER NUMBER OF ADDITIONAL ITERATIONS DESIRED (I4)')
      READ(8,515) IT
  515 FORMAT(I4)
      ITMAX = ITMAX + IT
  517 IN = -10
      GO TO 925
C
C       REMINDER OF SUBROUTINE CONTROLS PRINT-OUT OF FINAL VALUES
C
  520 LINE = 61
      CALL PAGE (LINE, NPG, 3, 0)
      WRITE(3,540)
  540 FORMAT(/16X,'SUMMARY OF NON-LINEAR REGRESSION ANALYSIS'//
     1 13X,'FINAL VALUE',14X,'STD ERROR',2X,'STD ERROR'/13X,
     2 'OF PARAMETER',30X,'(PERCENT)')
      SECTOT = FLOAT(JS) + FLOAT(JS10)/10.
  550 IF (SECTOT  LT.  60. ) GO TO 560
      SECTOT = SECTOT - 60.
      JM = JM + 1
      GO TO 550
  560 K3 = K2
      L3 = L2
      DO 580 LL=1, NO
      PCU = ABS(SIGMAA(LL)/A(LL)) * 100.
      WRITE(3,570) L3, A(LL), SIGMAA(LL), PCU
  570 FORMAT(9X,'A(',I2,') = ',1PD15.8,3X,1PE15.8,4X,1PE10.3)
  580 L3 = L3 + 1
      WRITE(3,590)
  590 FORMAT(' ')
      LINE = LINE + 1
```

```
MAIN40SRC                                                    PAGE  9


      DO 620 KK=1, NC
      PCU = ABS(SIGMA(K3+NA)/A(K+NA)) * 100.
      WRITE(3,610) K3, A(K+NA), SIGMA(K+NA), PCU
  610 FORMAT(9X,'C(',I2,') = ',1PD15.8,3X,1PE15.8,4X,1PE10.3)
  620 K3 = K3 + 1
      WRITE(3,622) ITER, CHISQR
  622 FORMAT('0',9X,'TOTAL ITERATIONS = ',I4/9X,'REDUCED CHI-SQUARE = ',
     1 1PE13.6)
      WRITE(3,623) FLAMDA
  623 FORMAT(9X,'FINAL VALUE OF LAMBDA = ',1PE10.3)
      WRITE(3,624) JN, SECTOT
  624 FORMAT(9X,'TOTAL CPU TIME REQUIRED = ',I3,' MIN, ',F4.1,' SEC')
      WRITE(3,625) DYMAX, PCDIF
  625 FORMAT(9X,'MAXIMUM DEVIATION OF FITTING FUNCTION = ',1PE10.3,
     1 ' = ',1PE8.1,' %')
      WRITE(3,626) XSET, YSET
  626 FORMAT(1H0,9X,'AT X = ',F10.5,',  Y = ',F7.4)
      IF (NPR .NE. 1) GO TO 925
      LINE = 61
      CALL PAGE (LINE, NPG, 3, 5)
      WRITE(3,630)
  630 FORMAT(20X,'COMPARISON OF DATA AND RESULTS'//8X,'OBSERVED',2X,
     1 'OBSERVED',3X,'FITTED',3X,'STD DEV',3X,'RESIDUAL',2X,'RESIDUAL'/
     2 11X,'X',9X,'W',9X,'Y',9X,'Y',16X,'(% YOBS)')
      DO 640 I=1, NPTS
  640 XORD(I) = X(I)
      DO 850 II=1, NPTS
      XMIN = 9999.9
      DO 660 JJ=1, NPTS
      IF (XORD(JJ) .GE. XMIN) GO TO 660
      XMIN = XORD(JJ)
      JMIN = JJ
  660 CONTINUE
      DIFF = Y(JMIN) - YFIT(JMIN)
      PCDIF = 100.* DIFF / Y(JMIN)
      LINE = LINE + 1
      GO TO (700, 750, 800), NIV
  700 WRITE(3,710) X(JMIN),Y(JMIN),YFIT(JMIN),SIGMAY(JMIN),DIFF,PCDIF
  710 FORMAT(8X,F8.3,2X,F7.4,2X,F7.4,3X,F7.4,2X,F9.5,2X,F8.3)
      GO TO 850
  750 WRITE(3,770) X(JMIN),Y(JMIN),YFIT(JMIN),SIGMAY(JMIN),DIFF,PCDIF
  770 FORMAT(8X,F8.6,2X,F7.4,3X,F7.4,3X,F7.4,2X,F9.5,2X,F8.3)
      GO TO 850
  800 WRITE(3,820) X(JMIN),Y(JMIN),YFIT(JMIN),SIGMAY(JMIN),DIFF,PCDIF
  820 FORMAT(8X,F8.4,2X,F7.4,3X,F7.4,2X,F7.4,2X,F9.5,2X,F8.3)
      IF (LINE .LE. 58) GO TO 850
      CALL PAGE (LINE,NPG,3,5)
      WRITE(3,830)
  850 XORD(JMIN) = 9999.9
      LINE = 60
      CALL PAGE (LINE,NPG,3,4)
      WRITE(3,852)
  852 FORMAT(1X,T3,'NOS',T11,'PRESSURE  PRESSURE  PRESSURE'/
     1 T7,'OBSERVED  OBSERVED ITC  UNCORR.',T43,'CORR.',53,'CORR.',
     2 57,'CORR.'/1X,T4,'X',T20,'Y',T31,'IFNF(C)',T41,'TSHF(C)',
     3 T51,'(DEG C)',T61,'(% NBS)')
```

```
      DO 905 I=1,NPTS
      TM = 0.0
      L4 = 1
      IF (L .GE. 0) GO TO 860
      L4 = 0
      TM = TM + A0
  860 DO 870 J=1,NA
      TM = TM + A(J) * X(I)**(J-L4)
  870 CONTINUE
      EI = E(I) * 1000.0
      TNBS = 0.0
      IF(EI .GT. 16395.4) GO TO 875
      DO 872 I1=1,4
      TNBS = TNBS + BT(I1) * EI**I1
  872 CONTINUE
      GO TO 890
  875 DO 877 I1=1,5
      TNBS = TNBS + BT(I1) * EI**(I1-1)
  877 CONTINUE
  890 CORR = TM - TNBS
      PCOR = 100.* CORR/TNBS
      LINE = LINE + 1
      WRITE(3,900)X(I),E(I),ITC(I),TNBS,TM,CORR,PCOR
  900 FORMAT(6X,F8.3,2X,F7.4,3X,I1,3X,F7.2,3X,F7.2,3X,F7.2,2X,F8.3)
      IF (LINE .LE. 58) GO TO 905
      CALL PAGE (LINE,NPG,3,4)
      WRITE(3,852)
  905 CONTINUE
      JPASS = 0
  925 RETURN
      END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE MAR04D     FORTRAN IV (PDP 15/30)     S. A. EIDE
C
C     PURPOSE
C       PROVIDES OUTPUT OPTIONS INCLUDING ANALYSIS OF RESIDUALS,
C       RESIDUAL HISTOGRAM, PRESSURE EFFECT ON EMF, SEEBECK,
C       PELTIER AND THOMSON COEFFICIENTS AS A FUNCTION OF TEMPERATURE.
C       ALSO CONTROLS RESTART OPTIONS.
C
C     USAGE
C       CALL MAR04D
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C       TTYPLT (X, Y, NPTS, LUN)
C         PRINTS A LINEAR PLOT OF ARRAYS X VS Y ON TELETYPE LUN
C       HISTO (X, NPTS, NINT, LUN)
C         PRODUCES SCALED HISTOGRAM OF NINT INTERVALS ON TELETYPE LUN
C       PAGE (LINE, NPG, LUN, LADD)
C         COUNTS LINES AND NUMBERS PAGES OF PRINT-OUT
C       EMF (A, T, K, L, ND)
C         COMPUTES EMF (FOR ND=0), FIRST PARTIAL DERIVATIVE OF EMF WITH
C         RESPECT TO TEMPERATURE (ND=1), OR SECOND PARTIAL DERIVATIVE
C         (ND=2) FOR TEMPERATURE T USING COEFFICIENT ARRAY A (CODE K,L).
C       TEMP (A, P, L, A0)
C         COMPUTES TEMPERATURE FOR INDEPENDENT VARIABLE P USING
C         COEFFICIENTS IN ARRAY A.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE MAR04D
      DOUBLE PRECISION A, ACHK, AIN, COEF
      DIMENSION XPLT(60),YPLT(60),RES(100),XORD(100),COEF(12)
      DIMENSION X(100),Y(100),SIGMAY(100),YFIT(100),A(20)
      DIMENSION SIGMAA(20),DERIV(20),FILEN(2),ACHK(20),AIN(20)
      DIMENSION E(100),DE(100),ITC(100),V(100),C(100),NTC(100)
      COMMON NPTS,NTERMS,MODE,A,ACHK,AIN,KCK,IPRESS,A0,NTEMP,NIV
      COMMON X,Y,SIGMAY,YFIT,SIGMAA,DERIV,NP,JCODE,NSAV,L,K
      COMMON E,DE,ITC,V,C,NA,NC,L2,K2,L3,K3,FLAMDA,JCRIT,NTC
      COMMON PARTOL,CHITOL,ITMAX,ITER,JM,JS,JS10,NFR,LINE,NPG
      COMMON JSAV,NFREE,CHISQR,JPASS,CHISAV,IN,IS,IS10,SEC
      COMMON SECTOT,NSET,FILEN,SNUM,SET,KSAV,NTH,NTOT,COEF,JLAM,MQ
      RABS = 0.0
      RSUM = 0.0
      N4 = 53
      TMAX = 1350.0
C
C       NEXT 15 STATEMENTS PERFORM PRELIMINARY ANALYSIS OF RESIDUALS
C
      YMAX = Y(1)
      DO 1010 I=1, NPTS
      IF (Y(I) .GT. YMAX) YMAX = Y(I)
      RES(I) = Y(I) - YFIT(I)
      RSUM = RSUM + RES(I)
      RABS = RABS + ABS(RES(I))
 1010 CONTINUE
      RABS = RABS / FLOAT(NPTS)
```

```
                                MAIN.SRC                                PAGE  2


      XMEAN = RSUM / FLOAT(NPTS)
      RSUM = 0.0
      DO 1020 I=1, NPTS
      RSUM = RSUM + (RES(I) - XMEAN)**2
 1020 CONTINUE
      RVAR = RSUM / FLOAT(NPTS - NTERMS)
      RSIG = SQRT (RVAR)
C
C       NEXT 18 STATEMENTS ALLOW USER TO CHOOSE ONE OF NINE
C       OUTPUT OPTIONS.
C
 1025 CALL ERASE
      WRITE(8,1030)
 1030 FORMAT(//' CHOOSE DESIRED OUTPUT OPTION BELOW'//5X,'1.  ANALYSIS OF
     1 RESIDUALS W/PLOT'/5X,'2.  PRESSURE CORRECTIONS FOR EMF AND TEMP W/
     2PLOTS(2)'/5X,'3.  PRESSURE EFFECT ON SEEBECK, PELTIER AND THOMSON
     3COEFFICIENTS'/5X,'4.  PLOT TEMP VS PRESSURIZED SEEBECK COEFFICIENT'
     4/5X,'5.  PLOT TEMP VS PRESSURIZED PELTIER COEFFICIENT'/5X,'6.  PLOT
     5TEMP VS PRESSURIZED THOMSON COEFFICIENT'/5X,'7.  PLOT FITTED EMF V
     6S OBSERVED EMF'/5X,'8.  PLOT INDEPENDENT VARIABLE VS RESIDUAL EMF'/
     75X,'9.  DISPLAY RESTART OPTIONS')
      CALL CHIN (IOPT)
      IOPT = IOPT - 48
      IF (IOPT .GE. 9) GO TO 1700
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1), SET
 1040 FORMAT(1X,'INPUT DATA FILE ',A5,A1/)
      GO TO (1050,1130,1300,1500,1550,1600,1650,1680), IOPT
C
C       NEXT 45 STATEMENTS COMPLETE ANALYSIS OF RESIDUALS AND PRINT
C       RESULTS INCLUDING TELETYPE PLOT OF FITTED EMF VS RESIDUAL EMF.
C
 1050 WRITE(7,1060) XMEAN,RVAR,RSIG,PABS
 1060 FORMAT(1X,T25,'ANALYSIS OF RESIDUALS'//1X,T12,'RESIDUAL MEAN',5X,
     1'= ',F10.6/1X,T12,'RESIDUAL VARIANCE = ',F10.6/1X,T12,'RESIDUAL',
     2' STD DEV  = ',F10.6/1X,T12,'RESIDUAL ABS MEAN = ',F10.6//
     31X,T27,'RESIDUAL HISTOGRAM'/)
      CALL HISTO (RES, NPTS, 30, 3)
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1), SET
      WRITE(3,1070)
 1070 FORMAT(1X,T25,'ANALYSIS OF RESIDUALS'//1X,T12,'CUMULATIVE FREQUENCY
     1 *** UNIT NORMAL DEVIATE PLOT'//1X,T33,'UNIT NORMAL',T49,'CUMULATI
     2VE'/1X,T13,'RANK    RESIDUAL    DEVIATE FORM    FREQUENCY')
      LINE = 10
      DO 1090 I=1,NPTS
      RTEST = RES(I)
      DO 1080 J=1,I
      IF (J .EQ. I) GO TO 1075
      IF (RTEST .GE. XORD(J)) GO TO 1080
      DUMMY = XORD(J)
      XORD(J) = RTEST
      RTEST = DUMMY
      GO TO 1080
```

```
                                MAB040:SRC                          PAGE  3


 1075 XORD(J) = RTEST
 1080 CONTINUE
 1090 CONTINUE
      DO 1110 I=1,NPTS
      UNIT = (XORD(I) - XMIN)/RES+0
      CUMFQ = (FLOAT(I) - 0.5)/ FLOAT(NPTS)
      WRITE(3,1100) I, XORD(I), UNIT, CUMFQ
 1100 FORMAT(1X,T12,I2,T20,F9.3,T33,F8.3,T49,F7.4)
      LINE = LINE + 1
      IF (LINE .LE. 59) GO TO 1110
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1), SET
      WRITE(3,1070)
      LINE = 10
 1110 CONTINUE
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1), SET
      WRITE(3,1120)
 1120 FORMAT(1X,T13,'X = FITTED EMF (MV) VS Y = RESIDUAL EMF (MV)')
      CALL TTYPLT (YFIT, RES, NPTS, 3)
      GO TO 1025
C
C       NEXT 73 STATEMENTS COMPUTE, PRINT AND PLOT TEMPERATURE AND
C       EMF CORRECTIONS.
C
 1130 WRITE(3,1135)
 1135 FORMAT(1X,T5,'NBS      FITTED     TEMP',T35,'NBS',T44,'FITTED',T55,
     1'EMF',T63,'FURNACE'/1X,T5,'TEMP',T14,'TEMP',T23,'DIFF',T33,'EMF',
     2T45,'EMF',T55,'DIFF',T64,'POWER'/1X,T4,'(DEG C)  (DEG C)  (DEG C)'
     3,T35,'(MV)',T45,'(MV)',T55,'(MV)',T62,'(WATTS)')
      T = TFIT = 0.0
      P = 10.0
      DO 1200 I=1,53
      IF (I .EQ. 1) GO TO 1175
      T = 25.0 + FLOAT (I-1)
      DP = 10.0
 1140 TEST = T - TEMP (AIN,P,L,A0)
      IF (ABS(TEST) .LE. 0.001) GO TO 1170
      NS = NS + 1
      IF (NS .GT. 150) GO TO 1210
      IF (TEST .LT. 0.0) GO TO 1150
      P = P + DP
      GO TO 1140
 1150 DP = -ABS(DP/2.)
 1160 P = P + DP
      TEST = T - TEMP (AIN,P,L,A0)
      IF (ABS(TEST) .LE. 0.001) GO TO 1170
      NS = NS + 1
      IF (NS .GT. 150) GO TO 1210
      IF (TEST .LT. 0.0) GO TO 1150
      DP = ABS(DP/2.)
      GO TO 1160
 1170 EFIT = EMF (A,T,P,L,0)
      NS = 0
      DT = 100.0
```

```
                                    MAP04.OSRC                          PAGE  4


      TFIT = 0.0
1174  TFIT = TFIT + DT
      TEST = EFIT - EMF (COEF,TFIT,11,0,0)
      IF (ABS(TEST) .LE. 0.0002) GO TO 1175
      DT = ABS(DT)
      IF (TEST .LT. 0.0) DT = -DT/2.0
      N5 = N5 + 1
      IF (N5 .GT. 500) GO TO 1210
      GO TO 1174
1175  YP = T - TFIT
      EFIT = EMF (A,T,K,L,0)
      ENBS = EMF (COEF,T,11,0,0)
      XO = ENBS - EFIT
      IF (I .EQ. 1) P = 9.989
      N5 = 0
      WRITE(3,1180) T,TFIT,YP,ENBS,EFIT,XO,P
1180  FORMAT(3X,F7.2,2X,F7.2,2X,F7.2,3X,F8.4,2X,F8.4,2X,F8.4,3X,F6.1)
      IF (I .EQ. 1) P = 10.0
      IF (ENBS .GT. YMAX) GO TO 1200
      N4 = I
      YPLT(I) = YP
      XPLT(I) = T
      XORD(I) = XO
      TMAX = T
1200  CONTINUE
1210  I = N4
1215  LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1), SET
      WRITE(3,1220)
1220  FORMAT(1X,T19,'X = UNCORRECTED TEMPERATURE (DEG C)'/1X,T35,'VS')
      WRITE(3,1230)
1230  FORMAT(1X,T12,'Y = TEMPERATURE CORRECTION (DEG C) DUE TO',
     1' PRESSURE')
      CALL TTYPLT (XPLT, YPLT, I, 3)
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1),SET
      WRITE(3,1220)
      WRITE(3,1240)
1240  FORMAT(1X,T17,'Y = EMF CORRECTION (MV) DUE TO PRESSURE')
      CALL TTYPLT (XPLT,XORD, I, 3)
      GO TO 1025
C
C       NEXT 67 STATEMENTS COMPUTE, PRINT AND PLOT CORRECTIONS FOR
C       SEEBECK, PELTIER AND THOMSON COEFFICIENTS.
C
1300  WRITE(3,1320)
1320  FORMAT(1X,T17,'NBS',T24,'FITTED   SEEBECK',T46,'NBS',T54,
     1'FITTED   DS/DT'/1X,T5,'TEMP',T15,'SEEBECK   SEEBECK   DIFF',T45,
     2'DS/DT    DS/DT    DIFF'/1X,T4,'(DEG C)',T16,'(UV/C)   (UV/C)   (U
     3V/C)    (MV/C2)  (MV/C2)  (MV/C2)')
      DO 1350 I=1,50
      T = 25.0 + FLOAT(I-1)
      SBFIT = 1000.0 * EMF (A,T,K,L,1)
      SBNBS = 1000.0 * EMF (COEF,T,11,0,1)
```

```
      YP = SBFIT - SBNBS
      DSFIT = 1.026 * EMF (A,T,K,L,2)
      DSNBS = 1.026 * EMF (CUEF,T,11,0,2)
      XO = DSFIT - DSNBS
      WRITE(3,1340) T,SBNBS,SBFIT,YP,DSNBS,DSFIT,XO
1340 FORMAT(4X,F6.1,2X,3(1X,F8.3),2X,3(1X,F8.2))
      IF (T .GT. TMAX) GO TO 1350
      XPLT(I) = T
      YPLT(I) = YP
      XORD(I) = XO
      N4 = I
1350 CONTINUE
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1),SET
      WRITE(3,1360)
1360 FORMAT(1X,T22,'X = TEMPERATURE (DEG C)'/1X,T34,'VS')
      WRITE(3,1370)
1370 FORMAT(1X,T10,'Y = SEEBECK PRESSURE CORRECTION (MICROVOLTS/DEG',
     1' C)')
      CALL TTYPLT (XPLT,YPLT,N4,3)
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1),SET
      WRITE(3,1400)
1400 FORMAT(1X,T17,'NBS    FITTED   PELTIER',T46,'NBS',T54,
     1'FITTED  THOMSON  THOMSON    DIFF'/1X,T6,'TEMP',T15,'PELTIER  PELTIER   DIFF',T44,
     2'THOMSON  THOMSON    DIFF'/1X,T4,'(DEG C)',T17,'(MV)',T26,'(MV)',
     3T34,'(MV)',T45,'(UV/C)   (UV/C)   (UV/C)')
      DO 1420 I=1,53
      T = 20.0 + FLOAT(I-1)
      PIFIT = (T + 273.15) * EMF (A,T,K,L,1)
      PINBS = (T + 273.15) * EMF (CUEF,T,11,0,1)
      YP = PIFIT - PINBS
      THFIT = 1000.0 * (T + 273.15) * EMF (A,T,K,L,2)
      THNBS = 1000.0 * (T + 273.15) * EMF (CUEF,T,11,0,2)
      XO = THFIT - THNBS
      WRITE(3,1340) T,PINBS,PIFIT,YP,THNBS,THFIT,XO
      IF (T .GT. TMAX) GO TO 1429
      YPLT(I) = YP
      XORD(I) = XO
1420 CONTINUE
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1),SET
      WRITE(3,1430)
      WRITE(3,1470)
1430 FORMAT(1X,T10,'Y = PELTIER PRESSURE CORRECTION (MILLIVOLTS)')
      CALL TTYPLT (XPLT,YPLT,N4,3)
      LINE = 60
      CALL PAGE (LINE,NPG,3,0)
      WRITE(3,1040) FILEN(1),SET
      WRITE(3,1440)
      WRITE(3,1480)
1440 FORMAT(1X,T10,'Y = THOMSON PRESSURE CORRECTION (MICROVOLTS/',
     1'DEG C)')
```

```
                                    MAIN.NOSRC                          PAGE  6

      CALL TTYPLT (XPLT,XOPS,N4,3)
      GO TO 1025
C
C       NEXT 11 STATEMENTS COMPUTE AND PLOT PRESSURIZED SEEBECK
C       COEFFICIENT VS TEMPERATURE.
C
 1500 WRITE(3,1360)
      WRITE(3,1510)
 1510 FORMAT(1X,T8,'Y = PRESSURIZED SEEBECK COEFFICIENT (MICROVOLTS/',
     1'DEG C)')
      DO 1540 I=1,N4
      T = 25.0 * FLOAT(I-1)
      XPLT(I) = T
      YPLT(I) = 1000.0 * EMF (A,T,K,L,1)
 1540 CONTINUE
      CALL TTYPLT (XPLT,YPLT,N4,3)
      GO TO 1025
C
C       NEXT 10 STATEMENTS COMPUTE AND PLOT PRESSURIZED PELTIER
C       COEFFICIENT VS TEMPERATURE.
C
 1550 WRITE(3,1360)
      WRITE(3,1560)
 1560 FORMAT(1X,T11,'Y = PRESSURIZED PELTIER COEFFICIENT (MILLIVOLTS)')
      DO 1580 I=1,N4
      T = 25.0 * FLOAT(I-1)
      XPLT(I) = T
      YPLT(I) = (T + 273.15) * EMF (A,T,K,L,1)
 1580 CONTINUE
      CALL TTYPLT (XPLT,YPLT,N4,3)
      GO TO 1025
C
C       NEXT 11 STATEMENTS COMPUTE AND PLOT PRESSURIZED THOMSON
C       COEFFICIENT VS TEMPERATURE.
C
 1600 WRITE(3,1360)
      WRITE(3,1610)
 1610 FORMAT(1X,T8,'Y = PRESSURIZED THOMSON COEFFICIENT (MICROVOLTS/',
     1'DEG C)')
      DO 1620 I=1,N4
      T = 25.0 * FLOAT(I-1)
      XPLT(I) = T
      YPLT(I) = 1000.0 * (T + 273.15) * EMF (A,T,K,L,2)
 1620 CONTINUE
      CALL TTYPLT (XPLT,YPLT,N4,3)
      GO TO 1025
C
C       NEXT 4 STATEMENTS PLOT OBSERVED EMF VS FITTED EMF
C
 1650 WRITE(3,1660)
 1660 FORMAT(1X,T12,'X = FITTED EMF (MV) VS Y = OBSERVED EMF (MV)')
      CALL TTYPLT (YFIT,Y,NPTS,3)
      GO TO 1025
C
C       NEXT 4 STATEMENTS PLOT RESIDUAL EMF VS INDEPENDENT VARIABLE
C
```

```
 1680 WRITE(3,1690)
 1690 FORMAT(1X,T14,'X = IND VARIABLE VS Y = RESIDUAL ENF (NV)')
      CALL TTYPLT (2,RES,NP(3,3)
      GO TO 1025
C
C       REMAINDER OF SUBROUTINE CONTROLS RESTART OPTIONS.
C
 1700 CALL ERASE
      WRITE(3,1710)
 1710 FORMAT(///' SELECT DESIRED RESTART OPTION'//5X,
     1'1. SAME DATA SET, NEW FITTING FUNCTION'/5X,
     2'2. NEW DATA SET, SAME DATA FILE'/5X,
     3'3. NEW DATA FILE (RESTART PROGRAM)'/5X,
     4'4. CONTINUE ITERATIONS WITH NEW CONVERGENCE CRITERION'/5X,
     5'5. ENTER NEW LAMBDA'/5X,
     6'6. CLOSE OUTPUT FILE MAROT.DAT ON UNIT 2.')
      CALL CHIN (NSET)
      NSET = NSET - 48
      IF (NSET .NE. 6) GO TO 1715
      CALL CLOSE(2)
 1715 CONTINUE
      IF (NSET .NE. 5) GO TO 1740
      WRITE(3,1720)
 1720 FORMAT(///' ENTER NEW VALUE OF LAMBDA (E10.3)')
      READ(3,1730) FLAMDA
 1730 FORMAT(E10.3)
      GO TO 1700
 1740 RETURN
      END
```

```
                                FUNCTN$SRC                              PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      FUNCTION FUNCTN      FORTRAN IV (F/OP 15/30)      S. A. EIDE
C
C      PURPOSE
C        EVALUATE FITTING FUNCTION FOR NON-LINEAR LEAST SQUARES FIT
C
C      USAGE
C        RESULT = FUNCTN (X, I, A, K, L, A0)
C
C      DESCRIPTION OF PARAMETERS
C        X  = ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C        I  = INDEX OF DATA POINTS
C        A  = ARRAY OF FUNCTION PARAMETERS
C        K  = FUNCTION CODE FOR EMF VS TEMPERATURE
C        L  = FUNCTION CODE FOR TEMPERATURE VS POWER (A0 FIXED IF L<0)
C        A0 = AMBIENT TEMPERATURE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      FUNCTION FUNCTN (X, I, A, K, L, A0)
      DOUBLE PRECISION A, E, DEXP
      DIMENSION X(1), A(1)
      L2 = L
      L1 = 1
C
C       NEXT 18 STATEMENTS COMPUTE TEMPERATURE ACCORDING TO MODEL
C       FUNCTION CODE L.   ABS(L) .LE. 5.
C
      IF (L) 5, 3, 10
    3 T = X(I)
      L1 = 0
      GO TO 20
    5 L2 = -L
      L1 = 0
   10 T = 0.0
      XI = X(I)
      GO TO (15, 14, 13, 12, 11), L2
   11 T = A(L1+5) * XI**5
   12 T = T + A(L1+4) * XI**4
   13 T = T + A(L1+3) * XI**3
   14 T = T + A(L1+2) * XI**2
   15 T = T + A(L1+1) * XI
      IF (L1 .EQ. 1) GO TO 19
      T = T + A0
      GO TO 20
   19 T = T + A(1)
C
C       NEXT 23 STATEMENTS COMPUTE EMF ACCORDING TO MODEL FUNCTION
C       CODE K .LE. 11  (K = 11 IS FULL NBS TYPE K MODEL).
C
   20 F = 0.0
      IF (K .NE. 11) GO TO 205
      K1 = L1 + L2 + 1
      GO TO 23
  205 K1 = L1 + L2
      IF (K .GT. 7) GO TO 207
```

```
      GO TO (30, 29, 28, 27, 26, 25, 24), K
  200 K2 = K - 7
      GO TO (23, 22, 21, 20), K2
   21 F = A(K1+10) * T**10
   22 F = F + A(K1+9) * T**9
   23 F = F + A(K1+8) * T**8
   24 F = F + A(K1+7) * T**7
   25 F = F + A(K1+6) * T**6
   26 F = F + A(K1+5) * T**5
   27 F = F + A(K1+4) * T**4
   28 F = F + A(K1+3) * T**3
   29 F = F + A(K1+2) * T**2
   30 F = F + A(K1+1) * T
      IF (K .NE. 11) GO TO 40
      E = -0.5 * ((T - A(K1+10))/ A(K1+11))**2
      F = F + A(K1) + A(K1+9) * DEXP(E)
   40 FUNCTN = F
      RETURN
      END
```

```
                                DERIV1.SRC                          PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE DERIV1    FORTRAN IV (PDP 15/30)     S.A.EIDE
C
C     PURPOSE
C       EVALUATES FIRST PARTIAL DERIVATIVES OF FITTING FUNCTION FOR
C       NON-LINEAR LEAST-SQUARES SEARCH (MARQUARDT ALGORITHM)
C
C     USAGE
C       CALL DERIV1 (X, I, A, K, L, A0, DERIV)
C
C     DESCRIPTION OF PARAMETERS
C       X      = ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C       I      = INDEX OF DATA POINT
C       A      = ARRAY OF FITTING FUNCTION PARAMETERS
C       K      = FUNCTION CODE FOR EMF VS TEMPERATURE
C       L      = FUNCTION CODE FOR TEMPERATURE VS POWER (A0 FIXED IF L<0)
C       A0     = AMBIENT TEMPERATURE
C       DERIV = ARRAY OF FIRST PARTIAL DERIVATIVES OF FITTING FUNCTION
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE DERIV1 (X, I, A, K, L, A0, DERIV)
      DOUBLE PRECISION A, EX, DEXP
      DIMENSION X(1), A(1), DERIV(20)
      XI = X(I)
      L1 = 1
      L2 = L
C
C       NEXT 17 STATEMENTS COMPUTE TEMPERATURE ACCORDING TO MODEL
C       FUNCTION CODE L.
C
      IF (L) 10, 5, 20
    5 T = XI
      L1 = 0
      GO TO 90
   10 L2 = -L
      L1 = 0
   20 T = 0.0
      GO TO (25,24,23,22,21), L2
   21 T = A(L1+5) * XI**5
   22 T = T + A(L1+4) * XI**4
   23 T = T + A(L1+3) * XI**3
   24 T = T + A(L1+2) * XI**2
   25 T = T + A(L1+1) * XI
      IF (L1 .EQ. 1) GO TO 30
      T = T + A0
      GO TO 90
   30 T = T + A(1)
   90 IF (K .EQ. 11) GO TO 130
C
C       NEXT 14 STATEMENTS COMPUTE FIRST DERIVATIVES OF EMF FUNCTION
C       USING POWER SERIES MODEL.
C
      SUMK = 0.0
      DO 100 N=1, K
      SUMK = SUMK + FLOAT(N) * A(L2+L1+N) * T**(N-1)
```

```
  100 CONTINUE
      JMAX = L2 + L1
      IF (L .EQ. 0) GO TO 112
      DO 110 J=1, JMAX
  110 DERIV(J) = SUMK * XI**(J-LL)
  112 K1 = L2 + L1 + 1
      K2 = K1 + K - 1
      DO 120 J=K1,K2
      JJ= J - JMAX
  120 DERIV(J) = T**JJ
      GO TO 200
C
C       NEXT 20 STATEMENTS COMPUTE FIRST DERIVATIVES OF ENF FUNCTION
C       USING FULL NBS TYPE K MODEL.
C
  130 K1 = L2 + L1 + 1
      SUM11 = 0.0
      DO 140 M=1, 8
  140 SUM11 = SUM11 + FLOAT(M) * A(K1+M) * T**(M-1)
      PROD = (T - A(K1+10)) / A(K1+11)
      EX = -0.5 * PROD**2
      SUM11 = SUM11 - A(K1+9) * PROD * DEXP(EX) / A(K1+11)
      IF (L .EQ. 0) GO TO 152
      JMAX = L2 + L1
      DO 150 J=1, JMAX
  150 DERIV(J) = SUM11 * XI**(J-L1)
  152 DERIV(K1) = 1.0
      K2 = K1 + 1
      K3 = K1 + 8
      DO 160 J=K2, K3
      JJ = J - K1
  160 DERIV(J) = T**JJ
      DERIV(K1+9) = DEXP(EX)
      DERIV(K1+10) = DERIV(K1+9) * A(K1+9) * PROD / A(K1+11)
      DERIV(K1+11) = DERIV(K1+10) * PROD
  200 RETURN
      END
```

```
                                SUMSQRSRC                                PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      FUNCTION SUMSQR    FORTRAN IV (P&P 135/30)     S. A. EIDE
C
C      PURPOSE
C        EVALUATE REDUCED CHI SQUARE FOR FIT TO DATA
C           SUMSQR = SUM ((Y - YFIT)**2 / SIGMA**2) /NFREE
C
C      USAGE
C        RESULT = SUMSQR (Y, SIGMAY, NFREE, YFIT)
C
C      DESCRIPTION OF PARAMETERS
C        Y       = ARRAY OF DATA POINTS
C        SIGMAY  = ARRAY OF STANDARD DEVIATIONS FOR DATA POINTS
C        NPTS    = NUMBER OF DATA POINTS
C        NFREE   = NUMBER OF DEGREES OF FREEDOM
C        MODE    = DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT
C                  +1 (INSTRUMENTAL ) WEIGHT(I) = 1./SIGMAY(I)**2
C                   0 (NO WEIGHTING)  WEIGHT(I) = 1.
C                  -1 (STATISTICAL)   WEIGHT(I) = 1./Y(I)
C        YFIT    = ARRAY OF CALCULATED VALUES OF Y
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      FUNCTION SUMSQR (Y, SIGMAY, NFREE, YFIT)
      DOUBLE PRECISION CHISQ, WEIGHT
      DIMENSION Y(1), SIGMAY(1), YFIT(1)
      COMMON NPTS, NTERMS, MODE
      CHISQ = 0.0
      IF (NFREE .GT. 0) GO TO 10
      SUMSQR = 0.0
      RETURN
C
C       NEXT 11 STATEMENTS ACCUMULATE THE SUM OF THE SQUARES
C
   10 DO 30 I=1, NPTS
      IF (MODE) 12, 20, 25
   12 IF (Y(I)) 16, 20, 14
   14 WEIGHT = 1. / Y(I)
      GO TO 30
   16 WEIGHT = 1. / (-Y(I))
      GO TO 30
   20 WEIGHT = 1.
      GO TO 30
   25 WEIGHT = 1. / SIGMAY(I)**2
   30 CHISQ = CHISQ + WEIGHT * (Y(I) - YFIT(I))**2
C
C       COMPUTE REDUCED CHI SQUARED AND RETURN
C
      SUMSQR = CHISQ / FLOAT (NFREE)
      RETURN
      END
```

```
                                MTXINV/SRC                              PAGE  1

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       SUBROUTINE MTXINV     FORTRAN IV (PDP 15/30)     S. A. EIDE
C
C       PURPOSE
C         INVERT A SYMMETRIC MATRIX USING GAUSS-JORDAN ELIMINATION
C         METHOD AND CALCULATE THE DETERMINANT.
C
C       USAGE
C         CALL MTXINV (ARRAY, DET)
C
C       DESCRIPTION OF PARAMETERS
C         ARRAY  = INPUT MATRIX WHICH IS REPLACED BY ITS INVERSE
C         NORDER = DEGREE OF MATRIX (ORDER OF DETERMINANT)
C         DET    = DETERMINANT OF INPUT MATRIX
C
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C         NONE
C
C       COMMENTS
C         DIMENSION STATEMENT VALID FOR NORDER UP TO 20
C         INVERSE MATRIX OVERLAYS ORIGINAL MATRIX.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE MTXINV (ARRAY, DET)
      DOUBLE PRECISION ARRAY, AMAX, SAVE, DABS
      DIMENSION ARRAY(20,20), IK(20), JK(20)
      COMMON NPTS, NORDER, NODE
      DET = 1.0
      DO 100 K=1, NORDER
C
C       NEXT 8 STATEMENTS LOCATE THE LARGEST ELEMENT IN REMAINDER
C       OF MATRIX.
C
      AMAX = 0.0
   20 DO 30 I=K, NORDER
      DO 30 J=K, NORDER
      IF (DABS(AMAX) - DABS(ARRAY(I,J)) .GT. 0.0) GO TO 30
      AMAX = ARRAY(I,J)
      IK(K) = I
      JK(K) = J
   30 CONTINUE
C
C       NEXT 15 STATEMENTS INTERCHANGE ROWS AND COLUMNS IF NECESSARY
C       TO PLACE LARGEST ELEMENT ON DIAGONAL FOR GREATER PRECISION.
C
      IF (AMAX .NE. 0.0) GO TO 40
      DET = 0.0
      RETURN
   40 I = IK(K)
      IF (I - K) 20, 51, 45
   45 DO 50 J=1, NORDER
      SAVE = ARRAY(K,J)
      ARRAY(K,J) = ARRAY(I,J)
   50 ARRAY(I,J) = -SAVE
   51 J = JK(K)
```

```
      IF (J - K) 20, 65, 55
   55 DO 60 I=1, NORDER
      SAVE = ARRAY(I,K)
      ARRAY(I,K) = ARRAY(I,J)
   60 ARRAY(I,J) = -SAVE
C
C        NEXT 15 STATEMENTS COMPUTE ELEMENTS OF INVERSE MATRIX
C        AND DETERMINANT.
C
   65 DO 70 I=1, NORDER
      IF (I .EQ. K) GO TO 70
      ARRAY(I,K) = -ARRAY(I,K) / AMAX
   70 CONTINUE
      DO 80 I=1, NORDER
      DO 80 J=1, NORDER
      IF (I .EQ. K .OR. J .EQ. K) GO TO 80
      ARRAY(I,J) = ARRAY(I,J) + ARRAY(I,K) * ARRAY(K,J)
   80 CONTINUE
      DO 90 J=1, NORDER
      IF (J .EQ. K) GO TO 90
      ARRAY(K,J) = ARRAY(K,J) / AMAX
   90 CONTINUE
      ARRAY(K,K) = 1. / AMAX
  100 DET = DET * AMAX
C
C        NEXT 35 STATEMENTS RESTORE INVERSE MATRIX TO ITS ORIGINAL
C        ORDERING OF ROWS AND COLUMNS.
C
      DO 130 L=1, NORDER
      K = NORDER - L + 1
      J = IK(K)
      IF (J .LE. K) GO TO 115
      DO 110 I=1  NORDER
      SAVE = ARRAY(I,K)
      ARRAY(I,K) = -ARRAY(I,J)
  110 ARRAY(I,J) = SAVE
  115 I = JK(K)
      IF (I .LE. K) GO TO 130
      DO 120 J = 1, NORDER
      SAVE = ARRAY(K,J)
      ARRAY(K,J) = -ARRAY(I,J)
  120 ARRAY(I,J) = SAVE
  130 CONTINUE
      RETURN
      END
```

```
                                    MARQRTSRC                                PAGE  1

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C       SUBROUTINE MARQRT    FORTRAN IV (PGP 15/30)    S. A. EIDE
C
C       PURPOSE
C         MAKE A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTION COMBINING A
C         GRADIENT SEARCH WITH A LINEARIZATION OF THE FITTING FUNCTION
C         UTILIZING MARQUARDT'S ALGORITHM (J. SIAM, VOL 11, PP. 431-441.
C         1963. )
C
C       USAGE
C         CALL MARQRT
C
C       DESCRIPTION OF PARAMETERS
C         X       = ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C         Y       = ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE
C         SIGMAY  = ARRAY OF STANDARD DEVIATIONS FOR Y DATA POINTS
C         NPTS    = NUMBER OF PAIRS OF DATA POINTS
C         NTERMS  = NUMBER OF PARAMETERS
C         MODE     = DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT
C                     +1 (INSTRUMENTAL) WEIGHT(I) = 1./SIGMAY(I)**2
C                      0 (NO WEIGHTING) WEIGHT(I) = 1.
C                     -1 (STATISTICAL)  WEIGHT(I) = 1./Y(I)
C         A       = ARRAY OF PARAMETERS
C         SIGMAA  = ARRAY OF STANDARD DEVIATIONS FOR PARAMETERS A
C         PLAMDA  = PROPORTION OF GRADIENT SEARCH INCLUDED
C         YFIT    = ARRAY OF CALCULATED VALUES OF Y
C         CHISQR  = REDUCED CHI SQUARE FOR FIT
C
C       SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C         FUNCTN (X, I, A, K, L, F0)
C            EVALUATES THE FITTING FUNCTION FOR THE ITH TERM
C         SUMSQR (Y, SIGMAY, NFREE, YFIT)
C            EVALUATES REDUCED CHI SQUARE FOR FIT TO DATA
C         DERIV1 (X, I, A, K, L, F0, DERIV)
C            EVALUATES THE DERIVATIVES OF THE FITTING FUNCTION
C            FOR THE ITH TERM WITH RESPECT TO EACH PARAMETER
C         MTXINV (ARRAY, DET)
C            INVERTS A SYMMETRIC TWO-DIMENSIONAL MATRIX OF DEGREE
C            NTERMS AND CALCULATES ITS DETERMINANT
C
C       COMMENTS
C         DIMENSION STATEMENT VALID FOR UP TO 20 PARAMETERS (NTERMS)
C         PLAMDA GENERALLY SET = 0.001 AT BEGINNING OF SEARCH
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE MARQRT
      DOUBLE PRECISION A, ACHK, AIN, ARRAY, B, ALPHA, DSQRT, COEF
      DIMENSION X(100),Y(100),SIGMAY(100),YFIT(100),A(20),B(20),COEF(12)
      DIMENSION SIGMAA(20),DERIV(20),FLCN(2),ACHK(20),AIN(20)
      DIMENSION E(190),DE(100),IIC(100),V(100),C(100),NTC(100)
      DIMENSION WEIGHT(100),ALPHA(20,20),BETA(20),ARRAY(20,20)
      COMMON NPTS,NTERMS,MODE,NFREE,FLD,KEC,IFREES,ND,NTEMP,NIV
      COMMON X,Y,SIGMAY,YFIT,SIGMAA,DERIV,NP,ICODE,NSMV,LL,MK
      COMMON E,DE,IIC,V,C,NAC,NC,LC,KP,KC,KS,PLAMDA,JCFIT,NIC
      COMMON PARTOL,CHITOL,ITMAX,ITER,JN,JC,JS10,NPR,LINE,NPG
```

```
                                NAPSOR1.SRC                          PAGE  2

      COMMON JSAV,NFREE,CHISQR,JPASS,CHISQV,IM,IS,IS10,SEC
      COMMON SECTOT,NSET,FILEN,SAVE,SET,ISAV,NTH,NTOT,COEF,JLAM
      FNU = 10.0
      NFREE = NPTS - NTERMS
      JLAM = 0
      IF (NFREE .GT. 0) GO TO 10
      CHISQR = 0.0
      RETURN
C
C       NEXT 11 STATEMENTS COMPUTE AND STORE WEIGHTING FACTORS TO BE
C       USED IN LEAST-SQUARES FIT.
C
   10 DO 30 I=1, NPTS
      IF (MODE) 12, 20, 25
   12 IF (Y(I)) 18, 20, 16
   16 WEIGHT(I) = 1./Y(I)
      GO TO 30
   18 WEIGHT(I) = 1./(-Y(I))
      GO TO 30
   20 WEIGHT(I) = 1.
      GO TO 30
   25 WEIGHT(I) = 1./SIGNAY(I)**2
   30 CONTINUE
C
C       NEXT 15 STATEMENTS COMPUTE SYMMETRIC CURVATURE MATRIX (ALPHA)
C       AND MATRIX BETA.
C
      DO 40 J=1, NTERMS
      BETA(J) = 0.0
      DO 40 K=1, J
   40 ALPHA(J,K) = 0.0
      DO 50 I=1, NPTS
      CALL DERIV1(X, I, A, KK, LL, A0, DERIV)
      DO 45 J=1, NTERMS
      BETA(J) = BETA(J) + WEIGHT(I)*(Y(I)-FUNCTN(X,I,A,KK,LL,A0))
     1  * DERIV(J)
      DO 45 K=1, J
   45 ALPHA(J,K) = ALPHA(J,K) + WEIGHT(I)*DERIV(J)*DERIV(K)
   50 CONTINUE
      DO 55 J=1, NTERMS
      DO 55 K=J, J
   55 ALPHA(K,J) = ALPHA(J,K)
C
C       NEXT 3 STATEMENTS COMPUTE INITIAL SUM OF SQUARES
C
      DO 60 I=1, NPTS
   60 YFIT(I) = FUNCTN(X, I, A, KK, LL, A0)
      CHISQ1 = SUMSQR (Y, SIGNAY, NFREE, YFIT)
C
C       NEXT 4 STATEMENTS SCALE CURVATURE MATRIX AND MODIFY
C       DIAGONAL ELEMENTS.
C
   65 DO 75 J=1, NTERMS
      DO 70 K=1, NTERMS
   70 ARRAY(J,K) = ALPHA(J,K) / DSQRT (ALPHA(J,J) * ALPHA(K,K))
   75 ARRAY(J,J) = 1. + ALAMDA
```

```
C
C       NEXT 2 STATEMENTS INVERT MODIFIED CURVATURE MATRIX AND
C       INCREMENT INVERSION COUNTER.
C
      JLAM = JLAM + 1
      CALL MTXINV (ARRAY, DET)
C
C       NEXT 4 STATEMENTS COMPUTE NEW PARAMETER VALUES
C
      DO 80 J=1, NTERMS
      B(J) = R(J)
      DO 80 K=1, NTERMS
   80 B(J) = B(J) + BETA(K)*ARRAY(J,K)/DSQRT(ALPHA(J,J)*ALPHA(K,K))
C
C       NEXT 6 STATEMENTS COMPUTE NEW SUM OF SQUARES.  IF GREATER
C       THAN INITIAL SUM OF SQUARES, FLAMDA IS MULTIPLIED BY FACTOR
C       FNU AND NEW PARAMETERS COMPUTED.  PROCESS REPEATED UNTIL
C       SUM OF SQUARES DECREASES.
C
      DO 90 I=1, NPTS
   90 YFIT(I) = FUNCTN (X, I, B, KK, LL, A0)
      CHISQR = SUMSQR (Y, SIGMAY, NFREE, YFIT)
      IF (CHISQR .LT. CHISQ1) GO TO 100
      FLAMDA = FNU * FLAMDA
      GO TO 65
C
C       NEXT 5 STATEMENTS REPLACE OLD PARAMETERS WITH NEW AND COMPUTE
C       PARAMETER UNCERTAINTIES.  FLAMDA IS DIVIDED BY FNU BEFORE
C       RETURNING CONTROL TO CALLING PROGRAM.
C
  100 DO 110 J=1, NTERMS
      R(J) = B(J)
      IF (ARRAY(J,J) .LT. 0.0) ARRAY(J,J) = -ARRAY(J,J)
  110 SIGMA(J) = DSQRT (ARRAY(J,J) / ALPHA(J,J))
      FLAMDA = FLAMDA / FNU
      RETURN
      END
```

```
                                PAGE  SRC                              PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE PAGE      FORTRAN IV (PDP 15/20)      S. A. EIDE
C
C      PURPOSE
C        COUNTS LINES OF PRINT-OUT, EJECTS AFTER 58 LINES, PRINTS
C        PAGE NUMBER IN UPPER RIGHT-HAND CORNER OF PAGE
C
C      USAGE
C        CALL PAGE (LINE, NPG, LUN, LADD)
C
C      DESCRIPTION OF PARAMETERS
C        LINE = LINE NUMBER (EJECTS WHEN LINE EXCEEDS 57)
C        NPG  = PAGE NUMBER (USED FOLLOWING PAGE EJECT ONLY)
C        LUN  = NUMBER OF PRINT-OUT UNIT
C        LADD = NUMBER OF LINES FOR TEST OF REMAINING SPACE ON PAGE
C                  (WILL ADVANCE TO NEXT PAGE AND SET LINE = LT IF
C                   LT LINES WILL NOT FIT ON CURRENT PAGE)
C
C      COMMENTS
C        PRIOR TO FIRST CALL SET LINE = 60 AND NPG = 1
C        SUBROUTINE CALLED IMMEDIATELY BEFORE EACH PRINT-OUT LINE
C        TO PRINT BLOCK OF N LINES ALL ON SAME PAGE, SET LT = N
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE PAGE (LINE, NPG, LUN, LT)
      LINE = LINE + LT
      IF (LINE .LE. 58) GO TO 20
      WRITE (LUN, 10) NPG
   10 FORMAT(1H1,62X,4HPAGE,I3 /)
      NPG = NPG + 1
      LINE = LT
   20 LINE = LINE + 1
      RETURN
      END
```

```
                                TTYPLTSRC                              PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE TTYPLT      FORTRAN IV (H-OP 15/30)      S. A. EIDE
C
C      PURPOSE
C        PRINTS A ONE-PAGE LINEAR PLOT OF X VS Y ON TELETYPE LUN
C
C      USAGE
C        CALL TTYPLT (X,Y,NPTS,LUN)
C
C      DESCRIPTION OF PARAMETERS
C        X      = ARRAY OF DATA TO BE PLOTTED ON HORIZONTAL AXIS
C        Y      = ARRAY OF DATA TO BE PLOTTED ON VERTICAL AXIS
C        NPTS   = NUMBER OF PAIRS OF DATA POINTS TO BE PLOTTED
C        LUN    = LOGICAL UNIT NUMBER OF OUTPUT TELETYPE
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C      COMMENTS
C        PLOT REQUIRES 53 LINES INCLUDING X-AXIS LABEL
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE TTYPLT (X,Y,NPTS,LUN)
      DIMENSION X(1),Y(1),CHAR(10),A(60)
      DATA CHAR/1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,1H*/
      DATA BLANK/1H /
C
C       NEXT 10 STATEMENTS COMPUTE SCALE FACTORS FOR X AND Y AXES
C
      XMAX = XMIN = X(1)
      YMAX = YMIN = Y(1)
      DO 10 I=2,NPTS
      IF (X(I) .GT. XMAX) XMAX = X(I)
      IF (X(I) .LT. XMIN) XMIN = X(I)
      IF (Y(I) .GT. YMAX) YMAX = Y(I)
      IF (Y(I) .LT. YMIN) YMIN = Y(I)
   10 CONTINUE
      XINC = (XMAX - XMIN)/60.0
      YINC = (YMAX - YMIN)/50.0
C
C       NEXT 40 STATEMENTS SCAN DATA IN X-DIRECTION STARTING WITH
C       MAXIMUM Y, PRINTING Y-LABELS AND APPROPRIATE CHARACTER IN
C       50 LINES OF 60 CHARACTERS EACH (3000 ADDRESSABLE REGIONS).
C
      IF = 1
      YHI = YMAX + YINC
      DO 500 JY=1,50
      YHI = YHI - YINC
      YLO = YHI - YINC
      DO 30 K=1,60
   30 A(K) = 0.0
      DO 200 I=1,NPTS
      IF (JY .EQ. 1 .AND. Y(I) .GT. YLO) GO TO 100
      IF (JY .EQ. 50 .AND. Y(I) .LE. YHI) GO TO 100
      IF (Y(I) .LE. YHI .AND. Y(I) .GT. YLO) GO TO 100
```

```
      GO TO 200
  100 XLO = XMIN - XINC
      DO 200 JX=1,60
      XLO = XLO + XINC
      XHI = XLO + XINC
      IF (JX .EQ. 1 .AND. X(I) .LT. XHI) GO TO 150
      IF (JX .EQ. 60 .AND. X(I) .GE. XLO) GO TO 150
      IF (X(I) .GE. XLO .AND. X(I) .LT. XHI) GO TO 150
      GO TO 200
  150 A(JX) = A(JX) + 1.0
  200 CONTINUE
  300 CONTINUE
      DO 450 K=1,60
      IF (A(K) .EQ. 0.0) GO TO 400
      IF (A(K) .GT. 9.0) A(K) = 10.0
      IK = IFIX (A(K))
      A(K) = CHAR (IK)
      GO TO 450
  400 A(K) = BLANK
  450 CONTINUE
      IF (IP .EQ. 2) GO TO 480
      WRITE(LUN,470) YHI, (A(JX),JX=1,60)
  470 FORMAT(1X,1PE10.3,1X,'+',60A1)
      IP = 2
      GO TO 500
  480 WRITE(LUN,490) (A(JX),JX=1,60)
  490 FORMAT(12X,'.',60A1)
      IP = 1
  500 CONTINUE
C
C       NEXT 11 STATEMENTS PRINT AND LABEL X-AXIS.
C
      WRITE(LUN,510) YMIN
  510 FORMAT(1X,1PE10.3,1X,'+',6(' . . . . +'))
      X10 = 10.0 * XINC
      X1 = XMIN + X10
      X2 = X1 + X10
      X3 = X2 + X10
      X4 = X3 + X10
      X5 = X4 + X10
      WRITE(LUN,520) X1,X3,X5,XMIN,X2,X4,XMAX
  520 FORMAT(1X,1PE10.3,2(10X,1PE10.3),/7X,1PE10.3,2(10X,1PE10.3),
     1 6X,1PE10.3)
      RETURN
      END
```

```
                                HISTO SRC                          PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     SUBROUTINE HISTO    FORTRAN IV (PDP 15/30)     S. A. EIDE.
C
C     PURPOSE
C       PLOTS A SCALED HISTOGRAM ON TELETYPE LUN
C
C     USAGE
C       CALL HISTO (Y, NPTS, NINT, LUN)
C
C     DESCRIPTION OF PARAMETERS
C       Y      = ARRAY OF DATA POINTS TO BE PLOTTED
C       NPTS   = NUMBER OF DATA POINTS TO BE PLOTTED
C       NINT   = NUMBER OF INTERVALS IN HISTOGRAM (MAX = 55)
C       LUN    = LOGICAL UNIT NUMBER OF OUTPUT TELETYPE
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C       NONE
C
C     COMMENTS
C       PRINT-OUT REQUIRES NINT + 2 LINES
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE HISTO (Y, NPTS, NINT, LUN)
      DIMENSION Y(1), INT(56), ASTER(45)
      DATA ASTER/45*1H*/
C
C       NEXT 10 STATEMENTS COMPUTE SCALED HISTOGRAM FOR GIVEN
C       NUMBER OF INTERVALS UP TO 55.
C
      IF (NINT .GT. 55) NINT = 55
      YMAX = ABS(Y(1))
      DO 100 I=2, NPTS
      IF (ABS(Y(I)) .GT. YMAX) YMAX = ABS(Y(I))
  100 CONTINUE
      YINC = 2. * YMAX / FLOAT(NINT)
      DO 200 J=1,NINT
  200 INT(J) = 0
      INT(NINT+1) = 0
      DO 300 I=1,NPTS
      J = IFIX ((Y(I) + YMAX)/YINC) + 1
      INT(J) = INT(J) + 1
  300 CONTINUE
      INT(NINT) = INT(NINT) + INT(NINT+1)
      IMAX = INT(1)
      DO 400 J=2,NINT
      IF (INT(J) .GT. IMAX) IMAX = INT(J)
  400 CONTINUE
C
C       NEXT 13 STATENENTS PRINT SCALED HISTOGRAM ON OUTPUT TELETYPE
C
      WRITE(LUN,500)
  500 FORMAT(/,' INTERVAL',9X,'NO.',11X,'SCALED HISTOGRAM'/)
      YNI = YMAX
      AMAX = FLOAT(IMAX)
      DO 600 J=1,NINT
```

```
      JJ = NINT - J + 1
      YLO = YHI - YINC
      RINT = FLOAT(INT(JJ))
      RNUM = RINT * 45./RMAX
      NUM = IFIX (RNUM)
      WRITE(IUN,550) YLO,YHI,INT(JJ),(MSTER(K),K=1,NUM)
  550 FORMAT(1X,1PE10.3,1X,1PE10.3,1X,I3,1X,45A1)
  600 YHI = YLO
      RETURN
      END
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     FUNCTION TEMP      FORTRAN IV      S. A. EIDE      26 APR 76
C
C     PURPOSE
C       EVALUATES TEMPERATURE IN DEGREES CELSIUS FOR GIVEN SET OF
C       COEFFICIENTS A(J) AND INDEPENDENT VARIABLE X
C
C     USAGE
C       RESULT = TEMP (A, X, L, A0)
C
C     DESCRIPTION OF PARAMETERS
C       A  = ARRAY OF COEFFICIENTS (SEE FUNCTN)
C       X  = VALUE OF INDEPENDENT VARIABLE
C       L  = CODE FOR INDEPENDENT VARIABLE VS TEMPERATURE FUNCTION
C              (SEE FUNCTN)
C       A0 = CONSTANT TERM (USED ONLY WHEN L<0
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C       NONE
C
C     COMMENTS
C       ORDER OF COEFFICIENTS A(J) IS IDENTICAL TO THAT USED BY
C       SUBROUTINES FUNCTN AND DERIV1 OF THE MARQ4 SYSTEM
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      FUNCTION TEMP(A, X, L, A0)
      DOUBLE PRECISION A
      DIMENSION A(1)
      L1 = IABS(L)
      T = A(1)
      IF (L .LE. 0) T = A0
      L2 = 1
      IF (L .LT. 0) L2 = 0
      IF (L .EQ. 0) GO TO 20
      DO 10 I=1,L1
      T = T + A(I+L2) * X**I
   10 CONTINUE
   20 TEMP = T
      RETURN
      END
```

```
                                EMF    SRC                              PAGE  1


CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      FUNCTION EMF      FORTRAN IV      S.A.RIDE     24 APR 76
C
C      PURPOSE
C        FOR A GIVEN TEMPERATURE T (DEG C) AND SET OF COEFFICIENTS A(J)
C        THIS FUNCTION COMPUTES EITHER THE EMF(MV), THE FIRST
C        PARTIAL DERIVATIVE OF EMF WITH RESPECT TO T, OR THE SECOND
C        PARTIAL DERIVATIVE OF EMF WITH RESPECT TO T AS PARAMETER
C        ND = 0, 1, OR 2 RESPECTIVELY.
C
C      USAGE
C        RESULT = EMF (A, T, K, L, ND)
C
C      DESCRIPTION OF PARAMETERS
C        A    = ARRAY OF COEFFICIENTS FOR EMF FUNCTION (SEE FUNCTN)
C        T    = TEMPERATURE IN DEGREES CELSIUS
C        K    = CODE FOR TEMPERATURE VS EMF FUNCTION (SEE FUNCTN)
C        L    = CODE FOR POWER VS TEMPERATURE FUNCTION (SEE FUNCTN)
C        ND   = CODE FOR ORDER OF EMF DERIVATIVE DESIRED
C             = 0; EMF = EMF (MV)
C             = 1; EMF = FIRST PARTIAL OF EMF (MV/DEG)
C             = 2; EMF = SECOND PARTIAL OF EMF (MV/DEG**2)
C
C      SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        NONE
C
C      COMMENTS
C        ORDER OF COEFFICIENTS A(J) AND CODES K AND L ARE IDENTICAL
C        TO THOSE USED BY SUBROUTINES FUNCTN AND DERIV1 OF THE
C        MARQ4 SYSTEM.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      FUNCTION EMF (A,T,K,L,ND)
      DOUBLE PRECISION A
      DIMENSION A(1)
      NN = ND + 1
      L1 = L + 1
      IF (L .LE. 0) L1 = IABS(L)
      OUT = 0.0
      IF (K .EQ. 11) GO TO 100
C
C       NEXT 13 STATEMENTS COMPUTE EMF FUNCTION OR APPROPRIATE
C       DERIVATIVE WITH RESPECT TO TEMPERATURE FOR POWER SERIES
C       MODEL ACCORDING TO CODE K, L.
C
      GO TO (10,30,50),NN
   10 DO 20 N=1,K
      OUT = OUT + A(L1+N) * T**N
   20 CONTINUE
      GO TO 500
   30 DO 40 N=1,K
      OUT = OUT + FLOAT(N) * A(L1+N) * T**(N-1)
   40 CONTINUE
      GO TO 500
   50 DO 60 N=2,K
```

```
      OUT = OUT + FLOAT(N*(N-1)) * A(L1+N) * T**(N-2)
   60 CONTINUE
      GO TO 500
C
C       NEXT 10 STATEMENTS COMPUTE EMF FUNCTION OR APPROPRIATE
C       DERIVATIVE FOR FULL N2S TYPE K MODEL.
C
  100 EX = ((T - A(L1+11))/A(L1+12))**2
      EXX = A(L1+10) * EXP (-0.5 * EX)
      GO TO (110,130,150),NN
  110 DO 120 N=1,9
      OUT = OUT + A(L1+N) * T**(N-1)
  120 CONTINUE
      OUT = OUT + EXX
      GO TO 500
  130 DO 140 N=1,8
      OUT = OUT + A(L1+N+1) * FLOAT(N) * T**(N-1)
  140 CONTINUE
      OUT = OUT - (T - A(L1+11)) * EXX /A(L1+12)**2
      GO TO 500
  150 DO 160 N=2,8
      OUT = OUT + A(L1+N+1) * FLOAT(N*(N-1)) * T**(N-2)
  160 CONTINUE
      OUT = OUT + (EX - 1.0) * EXX / A(L1+12)**2
  500 EMF = OUT
      RETURN
      END
```

APPENDIX B

Sample Computer Output

```
                                                                    PAGE  1

HYDRAULIC PRESSURE = 10000 PSI                          DATA FILE R2017B3RC
AMBIENT TEMPERATURE = 11.1[illegible] DEG CELSIUS       SAMPLE NUMBER 2017
WATER TEMPERATURE =  9.2 DEG CELSIUS                    DATA SET A
INDEPENDENT VARIABLE, X = FURNACE POWER IN WATTS
DEPENDENT VARIABLE, Y = PRESSURIZED THERMOCOUPLE EMF IN MILLIVOLTS
THERMOCOUPLE DATA INCLUDED = AB
NUMBER OF PAIRS OF DATA POINTS =  21
FITTING FUNCTION CODE, K =  8, L = -2
NUMBER OF PARAMETERS = 10
NUMBER OF DEGREES OF FREEDOM = 11
METHOD OF WEIGHTING LEAST-SQUARES FIT, WEIGHT(I) = 1.
ITERATION TERMINATED WHEN FRACTIONAL CHANGE IN
    ALL PARAMETERS LESS THAN  1.00E-07
INITIAL VALUE OF LAMBDA =  1.00E-03

     INITIAL ESTIMATES OF PARAMETERS
        A( 1) =  1.388227350+00
        A( 2) =  7.592046660-04

        C( 1) =  3.893861000-02
        C( 2) =  5.117805000-05
        C( 3) = -4.755624950-07
        C( 4) =  2.042506000-09
        C( 5) = -4.625686060-12
        C( 6) =  5.730822050-15
        C( 7) = -3.784051000-18
        C( 8) =  1.011255060-21

ITERATION NUMBER     5
REDUCED CHI-SQUARE =  2.233037E-03    (    -21.309 % CHANGE)
CPU TIME FOR THIS ITERATION =    0 MIN, 11.0 SEC
TOTAL CPU TIME FOR    5 ITERATIONS =    0 MIN, 51.9 SEC
CURRENT VALUE OF LAMBDA =  1.000E-04
PARAMETERS SATISFYING CONVERGENCE CRITERION =  0 OF 10
MAXIMUM RESIDUAL =  7.445E-02 =  2.4E+01 % AT X =  445.23 , Y = 30.6030
CYCLES THIS ITERATION =    2, CURRENT EMF PRESSURE CORRECTIONS (MV) ARE
  0.245(200),   0.678(400),   0.722(600),   0.273(800),   -0.983(1000 C)

     CURRENT VALUE OF PARAMETERS      PERCENT CHANGE
        A( 1) =  1.333183920+00        (     1.014)
        A( 2) =  7.106696590-04        (     2.663)

        C( 1) =  3.807412240-02        (    -0.726)
        C( 2) =  4.730684770-05        (    -1.308)
        C( 3) = -4.732314090-07        (    -0.023)
        C( 4) =  2.047825510-09        (     0.015)
        C( 5) = -4.622673870-12        (    -0.003)
        C( 6) =  5.720774410-15        (    -0.002)
        C( 7) = -3.786711130-18        (     0.005)
        C( 8) =  1.010736780-21        (     0.013)
```

```
ITERATION NUMBER =  10
REDUCED CHI-SQUARE =  7.977139E-04    (     -0.203 % CHANGE)
CPU TIME FOR THIS ITERATION =    9 MIN,  0.3 SEC
TOTAL CPU TIME FOR  10 ITERATIONS =    1 MIN, 35.7 SEC
CURRENT VALUE OF LAMBDA =  1.000E-03
PARAMETERS SATISFYING CONVERGENCE CRITERION =  0 OF 10
MAXIMUM RESIDUAL = -4.074E-02 = -4.0E-01 % AT X =  173.40 , Y = 10.2821
CYCLES THIS ITERATION =    1,  CURRENT ENF PRESSURE CORRECTIONS (MV) ARE
  0.228(200),   0.648(400),   0.635(600),   0.231(800),  -0.311(1000 C)

    CURRENT VALUE OF PARAMETERS      PERCENT CHANGE
       A( 1) =  1.325700620+00        (     -0.483)
       A( 2) =  7.349929300-04        (     -2.739)

       C( 1) =  3.878528550-02        (     -0.009)
       C( 2) =  4.631950290-05        (      5.478)
       C( 3) = -4.810523160-07        (      1.575)
       C( 4) =  2.063190960-09        (      0.359)
       C( 5) = -4.615034650-12        (     -0.134)
       C( 6) =  5.764401390-15        (     -0.115)
       C( 7) = -3.807283420-18        (      0.307)
       C( 8) =  1.032244540-21        (      1.012)

ITERATION NUMBER =  15
REDUCED CHI-SQUARE =  7.779373E-04    (     -0.095 % CHANGE)
CPU TIME FOR THIS ITERATION =    0 MIN, 11.0 SEC
TOTAL CPU TIME FOR  15 ITERATIONS =    2 MIN, 30.2 SEC
CURRENT VALUE OF LAMBDA =  1.000E-03
PARAMETERS SATISFYING CONVERGENCE CRITERION =  0 OF 10
MAXIMUM RESIDUAL = -4.290E-02 = -4.2E-01 % AT X =  173.40 , Y = 10.2821
CYCLES THIS ITERATION =    2,  CURRENT ENF PRESSURE CORRECTIONS (MV) ARE
  0.198(200),   0.624(400),   0.637(600),   0.287(800),  -0.154(1000 C)

    CURRENT VALUE OF PARAMETERS      PERCENT CHANGE
       A( 1) =  1.321704800+00        (      0.027)
       A( 2) =  7.596045930-04        (     -0.376)

       C( 1) =  3.883486740-02        (     -0.001)
       C( 2) =  4.261083390-05        (     -0.248)
       C( 3) = -4.949976190-07        (     -0.219)
       C( 4) =  2.091101680-09        (     -0.143)
       C( 5) = -4.621834390-12        (     -0.066)
       C( 6) =  5.713136870-15        (      0.020)
       C( 7) = -3.749149010-18        (      0.113)
       C( 8) =  1.006639700-21        (      0.208)
```

```
ITERATION NUMBER    20
REDUCED CHI-SQUARE =  7.7473942E-04    (     -0.046 % CHANGE)
CPU TIME FOR THIS ITERATION =    0 MIN, 11.0 SEC
TOTAL CPU TIME FOR   20 ITERATIONS =    3 MIN, 24.7 SEC
CURRENT VALUE OF LAMBDA =  1.000E-08
PARAMETERS SATISFYING CONVERGENCE CRITERION =  0 OF 10
MAXIMUM RESIDUAL = -4.306E-02 = -4.2E-01 % AT X =  173.40 , Y = 10.2821
CYCLES THIS ITERATION =    2, CURRENT EMF PRESSURE CORRECTIONS (MV) ARE
  0.198(200),    0.607(400),    0.582(600),    0.201(800),   -0.224(1000 C)

     CURRENT VALUE OF PARAMETERS      PERCENT CHANGE
        A( 1) =  1.31381000D+00          (     0.027)
        A( 2) =  7.46033020D-04          (    -0.372)

        C( 1) =  3.88212357D-02          (    -0.006)
        C( 2) =  4.80464918D-05          (    -0.190)
        C( 3) = -4.89979497D-07          (    -0.190)
        C( 4) =  2.87743653D-09          (    -0.128)
        C( 5) = -4.69791294D-12          (    -0.061)
        C( 6) =  5.71861039D-15          (     0.017)
        C( 7) = -3.75275952D-18          (     0.105)
        C( 8) =  1.01622765D-21          (     0.196)

ITERATION NUMBER    25
REDUCED CHI-SQUARE =  7.6554836E-04    (     -0.046 % CHANGE)
CPU TIME FOR THIS ITERATION =    0 MIN, 13.6 SEC
TOTAL CPU TIME FOR   25 ITERATIONS =    4 MIN, 19.2 SEC
CURRENT VALUE OF LAMBDA =  1.000E-08
PARAMETERS SATISFYING CONVERGENCE CRITERION =  0 OF 10
MAXIMUM RESIDUAL = -4.357E-02 = -4.2E-01 % AT X =  173.40 , Y = 10.2821
CYCLES THIS ITERATION =    3, CURRENT EMF PRESSURE CORRECTIONS (MV) ARE
  0.207(200),    0.575(400),    0.472(600),   -0.011(800),   -0.805(1000 C)

     CURRENT VALUE OF PARAMETERS      PERCENT CHANGE
        A( 1) =  1.32497854D+00          (    -0.046)
        A( 2) =  7.10554060D-04          (     0.521)

        C( 1) =  3.88034206D-02          (     0.108)
        C( 2) =  4.55671579D-05          (    -0.903)
        C( 3) = -4.67728186D-07          (    -0.328)
        C( 4) =  2.69277934D-09          (    -0.131)
        C( 5) = -4.49343634D-12          (    -0.025)
        C( 6) =  5.62265581D-15          (     0.027)
        C( 7) = -3.74009763D-18          (     0.038)
        C( 8) =  1.02316968D-21          (     0.022)
```

```
ITERATION NUMBER   30
REDUCED CHI-SQUARE =   7.6015260D-04    (     -0.016 % CHANGE)
CPU TIME FOR THIS ITERATION =    3 MIN, 29.5 SEC
TOTAL CPU TIME FOR   30 ITERATIONS =    5 MIN, 21.6 SEC
CURRENT VALUE OF LAMBDA =  1.0000D-05
PARAMETERS SATISFYING CONVERGENCE CRITERION =  2 OF 10
MAXIMUM RESIDUAL = -4.3825E-02 = -4.3E-01 % AT X =  173.40 , Y = 10.6201
CYCLES THIS ITERATION =    9, CURRENT END PRESSURE CORRECTIONS (PSF) ARE
  0.207(200),    0.508(400),    0.278(600),   -0.345(800),   -1.592(1000 C)

     CURRENT VALUE OF PARAMETERS      PERCENT CHANGE
        A( 1) =  1.33120810D+00        (     -0.000)
        A( 2) =  6.630124030-04        (     -0.000)

        C( 1) =  3.820416880-02        (      0.000)
        C( 2) =  4.377894520-05        (      0.001)
        C( 3) = -4.515859630-07        (     -0.000)
        C( 4) =  1.962530570-09        (     -0.000)
        C( 5) = -4.457023550-12        (     -0.000)    CONVG
        C( 6) =  5.678940450-15        (      0.000)    CONVG
        C( 7) = -3.841080720-18        (      0.000)
        C( 8) =  1.068597250-21        (      0.000)
```

PAGE 5

SUMMARY OF NON-LINEAR REGRESSION ANALYSIS

	FINAL VALUE OF PARAMETER	STD ERROR	STD ERROR (PERCENT)
A(1) =	1.331209810D+00	5.202141285E-04	3.945E-02
A(2) =	6.030124111D-04	1.182452237E-06	1.783E-01
C(1) =	1.980416480D-02	1.374736778E-05	3.543E-02
C(2) =	4.177804520D-05	1.825968316E-08	4.171E-02
C(3) =	-4.316852630D-07	2.302631144E-11	4.876E-03
C(4) =	1.962530570D-09	2.507109332E-14	1.303E-03
C(5) =	-4.457062360D-12	2.910411480E-17	6.530E-04
C(6) =	5.670040450D-15	3.271963518E-20	5.762E-04
C(7) =	-3.941080720D-18	3.646660010E-23	9.494E-04
C(8) =	1.268597350D-21	4.037225825E-26	3.778E-03

TOTAL ITERATIONS = 31
REDUCED CHI-SQUARE = 7.681590E-04
FINAL VALUE OF LAMBDA = 1.000E+02
TOTAL CPU TIME REQUIRED = 5 MIN. 51.1 SEC
MAXIMUM DEVIATION OF FITTING FUNCTION = -4.386E-02 = -4.3E-01 %
AT X = 173.39030. Y = 10.2821

COMPARISON OF DATA AND RESULTS

OBSERVED X	OBSERVED Y	FITTED Y	STD DEV Y	RESIDUAL	RESIDUAL (% YOBS)
0.000	0.4437	0.4353	0.0083	0.00839	1.216
30.296	2.0922	2.0900	0.0011	0.00224	0.107
47.358	3.0354	3.0469	0.0010	-0.01138	-0.375
67.910	4.2059	4.2082	0.0021	-0.00232	-0.055
84.149	5.1292	5.1230	0.0026	0.00622	0.121
100.650	6.0502	6.0376	0.0064	0.01258	0.207
119.893	7.1541	7.1695	0.0114	-0.01536	-0.215
136.263	8.1446	8.1172	0.0026	0.02736	0.336
173.398	10.2821	10.3200	0.0222	-0.04386	-0.427
204.354	12.2605	12.2547	0.0101	0.00582	0.047
235.827	14.2481	14.3166	0.0070	-0.03151	0.220
264.743	16.3082	16.3084	0.0350	-0.00016	-0.001
292.117	18.2519	18.2823	0.0141	-0.03043	-0.167
319.848	20.4020	20.3708	0.0280	0.03121	0.153
349.068	22.5400	22.6683	0.0226	-0.02831	-0.125
372.202	24.5669	24.5556	0.0240	0.01037	0.042
445.233	30.8010	30.7891	0.0680	0.01388	0.045
478.471	33.5900	33.6173	0.0242	-0.02733	-0.081
496.241	35.1050	35.0874	0.0815	0.01760	0.050
526.335	37.5483	37.5496	0.0664	-0.00164	-0.004
546.421	39.3100	39.3101	0.0120	-0.00010	-0.000

OBSERVED X	OBSERVED Y	ITC	NBS UNCORR. TEMP(C)	PRESSURE CORR. TEMP(C)	PRESSURE CORR. (DEG C)	PRESSURE CORR. (% NBS)
0.000	0.4437	1	10.82	11.17	0.35	-3.224
30.293	2.0922	1	51.09	52.11	1.03	2.007
47.358	3.0354	1	74.12	75.70	1.52	2.045
67.910	4.2859	1	102.92	104.63	1.71	1.665
84.149	5.1332	1	125.78	127.88	2.10	1.671
100.650	6.0292	1	149.08	151.87	2.79	1.873
119.893	7.1541	1	175.59	180.30	4.71	2.681
136.263	8.1446	1	200.07	204.87	4.81	2.403
173.398	10.2821	1	252.81	261.93	9.12	3.609
204.454	12.2605	1	301.29	310.90	9.61	3.189
235.827	14.3481	1	351.67	361.98	10.31	2.932
264.743	16.3082	1	397.76	410.07	12.30	3.093
292.117	18.2519	1	443.71	456.61	12.91	2.909
319.849	20.4928	1	494.11	504.78	10.67	2.159
349.068	22.5400	1	546.64	556.64	10.00	1.829
372.202	24.5600	1	591.98	598.50	6.52	1.102
445.223	30.8030	1	749.36	735.30	-5.06	-0.684
478.471	33.5980	1	807.86	799.90	-7.96	-0.985
496.241	35.1058	1	844.97	835.04	-9.93	-1.175
526.335	37.5489	1	905.52	895.51	-10.01	-1.106
546.421	39.3100	1	949.80	936.53	-13.27	-1.398

PAGE 8

INPUT DATA FILE R2017A

ANALYSIS OF RESIDUALS

RESIDUAL MEAN = 0.000156
RESIDUAL VARIANCE = 0.000769
RESIDUAL STD DEV = 0.027720
RESIDUAL ABS MEAN = 0.015479

RESIDUAL HISTOGRAM

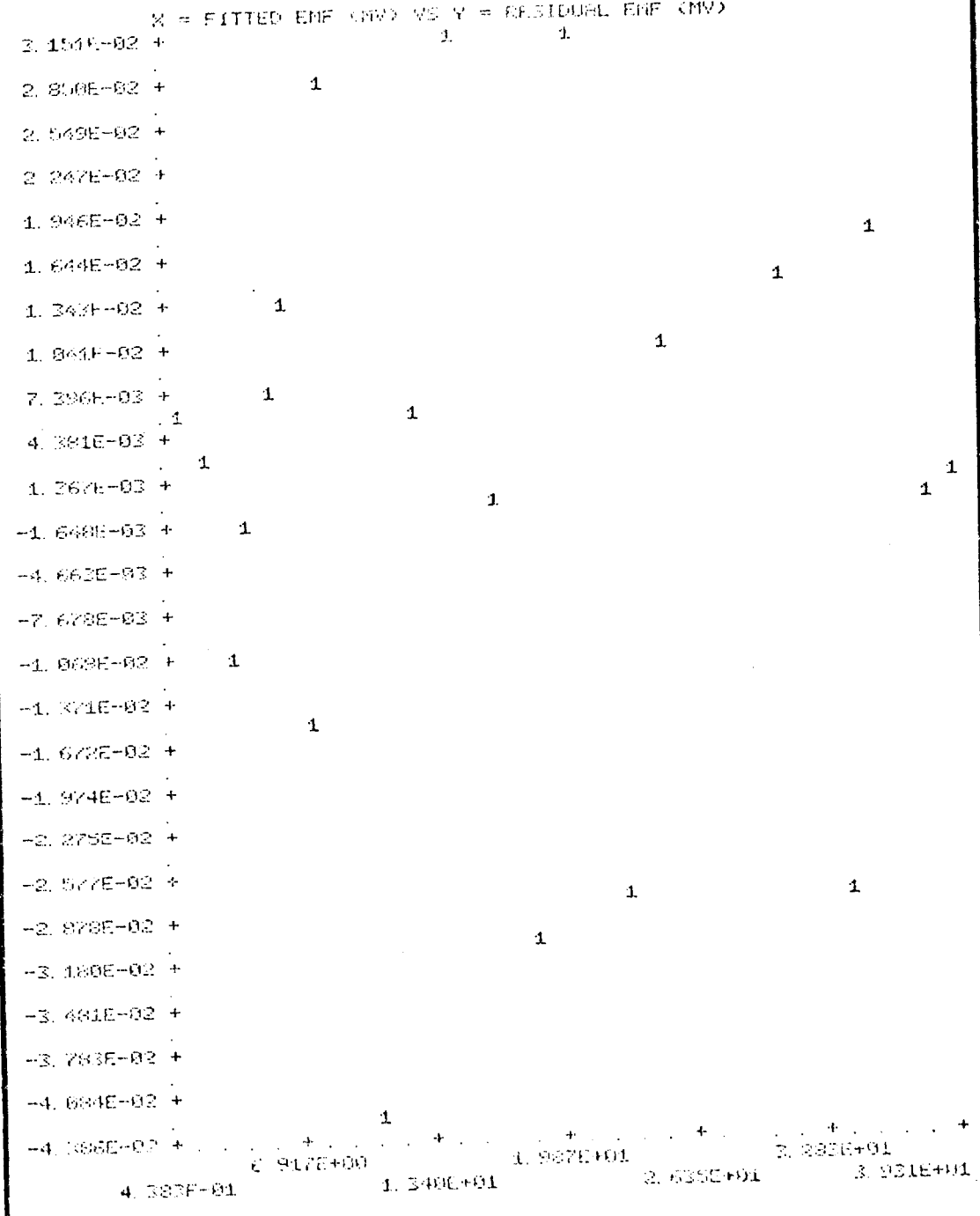
INTERVAL		NO.	SCALED HISTOGRAM
4.093E-02	4.386E-02	0	
3.801E-02	4.093E-02	0	
3.508E-02	3.801E-02	0	
3.216E-02	3.508E-02	0	
2.924E-02	3.216E-02	2	**********
2.631E-02	2.924E-02	1	**********
2.339E-02	2.631E-02	0	
2.047E-02	2.339E-02	0	
1.754E-02	2.047E-02	1	**********
1.462E-02	1.754E-02	0	
1.169E-02	1.462E-02	2	**********
8.771E-03	1.169E-02	1	**********
5.847E-03	8.771E-03	1	**********
2.924E-03	5.847E-03	2	**********
-5.585E-19	2.924E-03	1	**********
-2.924E-03	-5.585E-19	4	**********
-5.847E-03	-2.924E-03	0	
-8.771E-03	-5.847E-03	0	
-1.169E-02	-8.771E-03	1	**********
-1.462E-02	-1.169E-02	0	
-1.754E-02	-1.462E-02	1	**********
-2.047E-02	-1.754E-02	0	
-2.339E-02	-2.047E-02	0	
-2.631E-02	-2.339E-02	2	**********
-2.924E-02	-2.631E-02	1	**********
-3.216E-02	-2.924E-02	0	
-3.508E-02	-3.216E-02	0	
-3.801E-02	-3.508E-02	0	
-4.093E-02	-3.801E-02	1	**********

INPUT DATA FILE R2017A

ANALYSIS OF RESIDUALS
CUMULATIVE FREQUENCY *** UNIT NORMAL DEVIATE FORM ***

RANK	RESIDUAL	UNIT NORMAL DEVIATE FORM	CUMULATIVE FREQUENCY
1	-0.044	-1.596	0.0238
2	-0.030	-1.110	0.0714
3	-0.028	-1.033	0.1190
4	-0.027	-0.997	0.1667
5	-0.015	-0.563	0.2143
6	-0.011	-0.418	0.2619
7	-0.002	-0.090	0.3095
8	-0.002	-0.065	0.3571
9	-0.000	-0.012	0.4048
10	-0.000	-0.009	0.4524
11	0.002	0.076	0.5000
12	0.005	0.190	0.5476
13	0.006	0.205	0.5952
14	0.006	0.220	0.6429
15	0.010	0.370	0.6905
16	0.013	0.451	0.7381
17	0.014	0.498	0.7857
18	0.018	0.633	0.8333
19	0.027	0.987	0.8810
20	0.031	1.126	0.9286
21	0.032	1.137	0.9762

INPUT PATH FILE R2017A



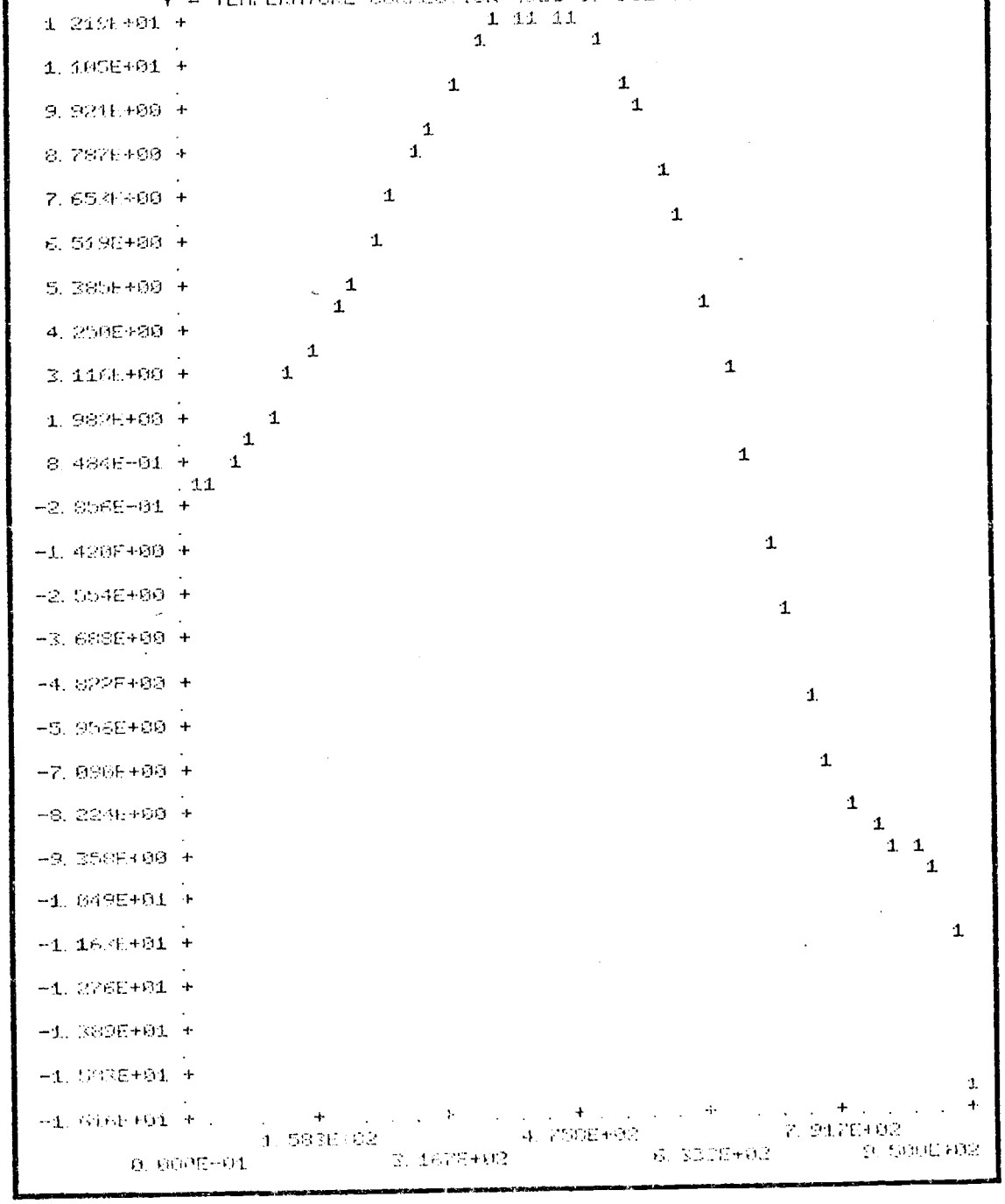
PAGE 11

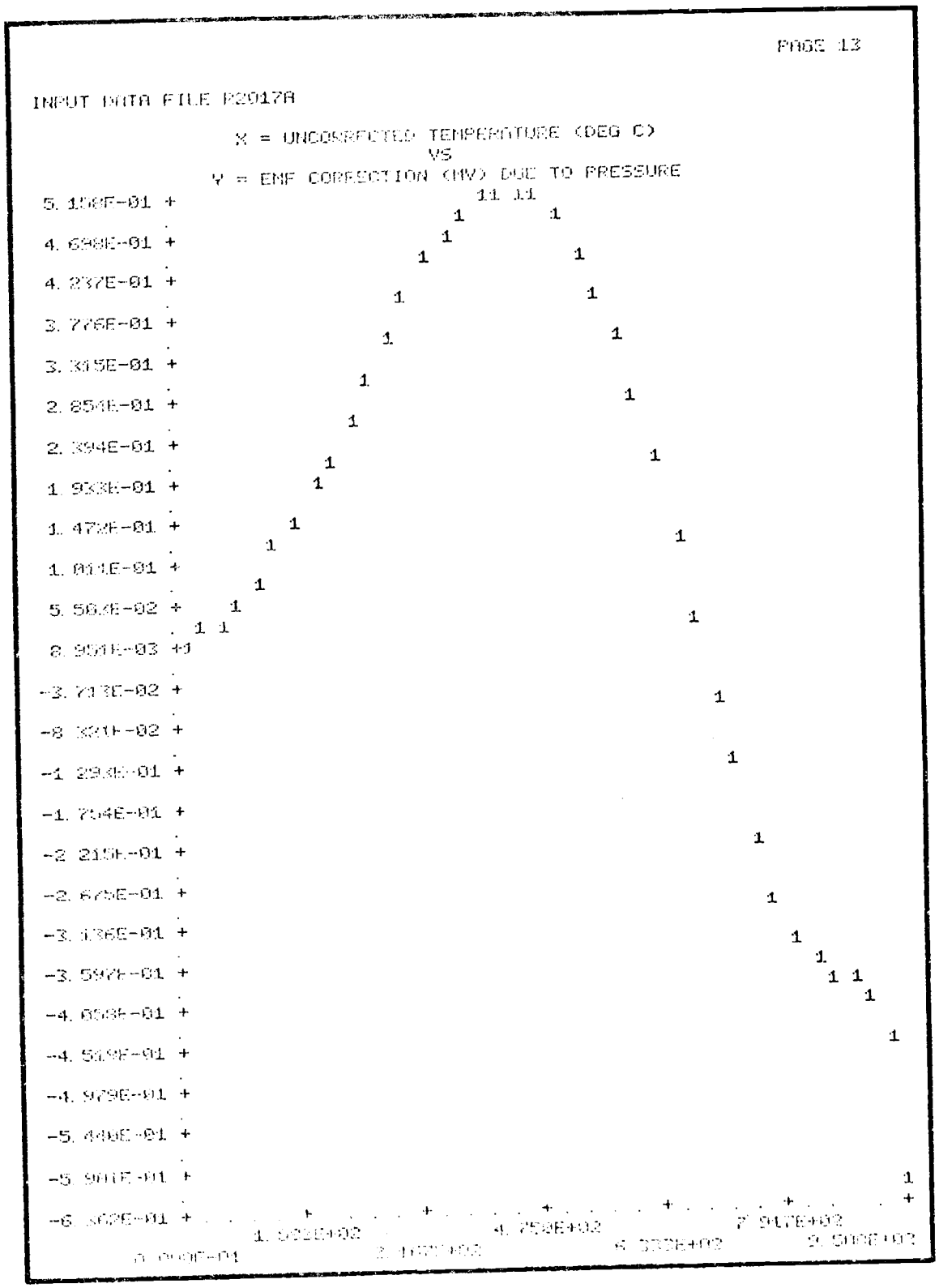
INPUT DATA FILE R3017A

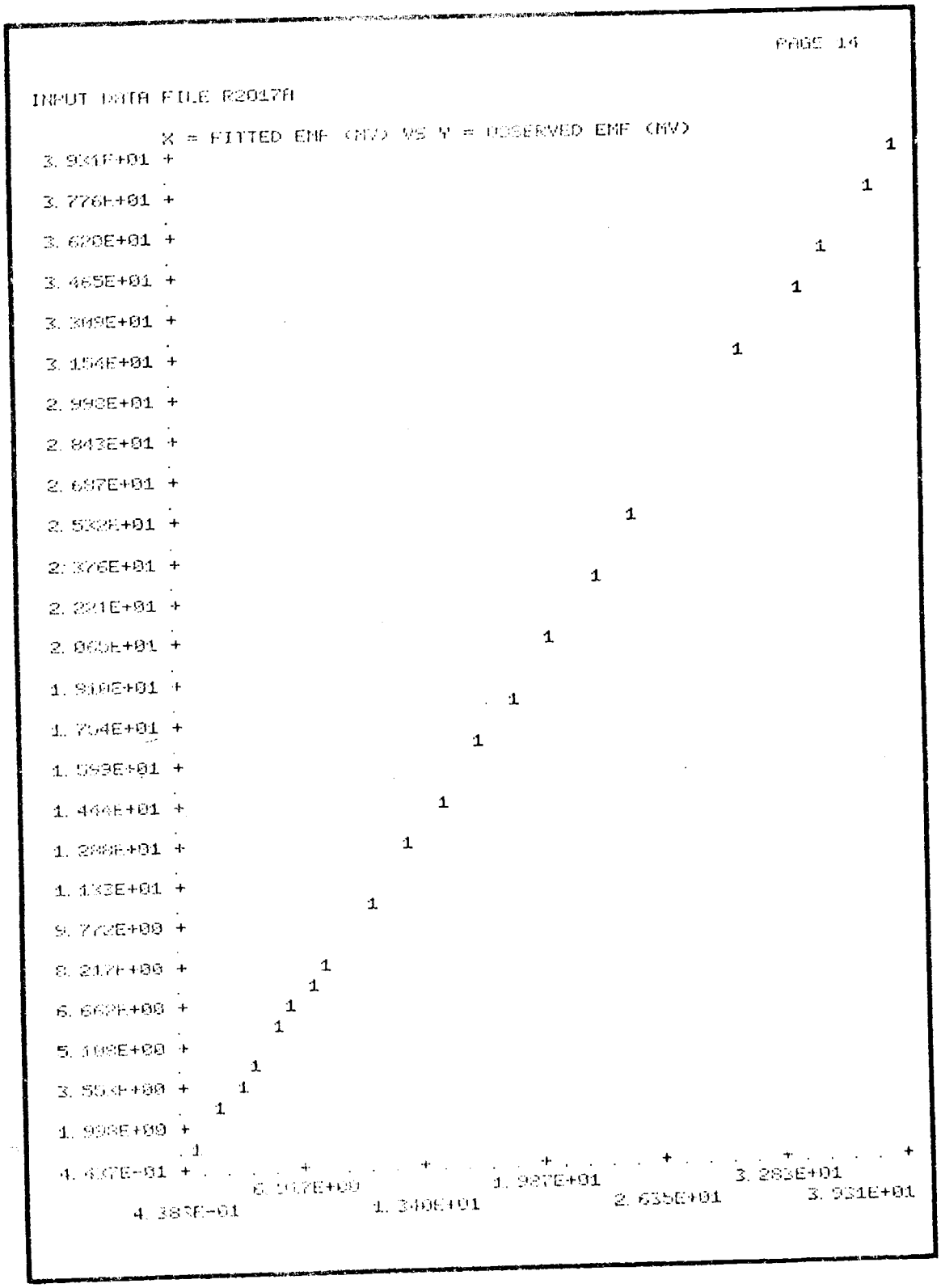
NBS TEMP (DEG C)	FITTED TEMP (DEG C)	TEMP DIFF (DEG C)	NBS EMF (MV)	FITTED EMF (MV)	EMF DIFF (MV)	FURNACE POWER (WATTS)
0.00	0.00	0.00	0.0000	0.0000	0.0000	****.*
25.00	24.78	0.22	1.0002	0.9911	0.0090	10.7
50.00	49.56	0.44	2.0224	2.0042	0.0183	29.6
75.00	74.05	0.95	3.0580	3.0185	0.0395	48.2
100.00	98.27	1.73	4.0653	4.0235	0.0718	66.4
125.00	122.35	2.65	5.1235	5.0154	0.1081	84.2
150.00	146.46	3.54	6.1372	5.9947	0.1425	101.7
175.00	170.64	4.36	7.1389	6.9646	0.1743	118.9
200.00	194.81	5.19	8.1366	7.9293	0.2072	135.7
225.00	218.90	6.10	9.1390	8.8936	0.2454	152.3
250.00	242.87	7.13	10.1515	9.8615	0.2899	168.6
275.00	266.77	8.23	11.1748	10.8367	0.3381	184.7
300.00	290.69	9.31	12.2074	11.8218	0.3857	200.5
325.00	314.71	10.29	13.2471	12.8186	0.4285	216.1
350.00	338.92	11.08	14.2922	13.8282	0.4641	231.5
375.00	362.32	11.68	15.3419	14.8510	0.4908	246.6
400.00	387.95	12.05	16.3954	15.8873	0.5082	261.5
425.00	412.81	12.19	17.4526	16.9367	0.5158	276.3
450.00	437.90	12.10	18.5128	17.9991	0.5137	290.8
475.00	463.21	11.79	19.5756	19.0741	0.5014	305.2
500.00	488.76	11.24	20.6402	20.1614	0.4787	319.4
525.00	514.56	10.44	21.7058	21.2607	0.4452	333.4
550.00	540.61	9.39	22.7719	22.3715	0.4005	347.2
575.00	566.91	8.09	23.8375	23.4929	0.3445	360.9
600.00	593.47	6.53	24.9016	24.6238	0.2778	374.5
625.00	620.26	4.74	25.9635	25.7624	0.2011	387.8
650.00	647.24	2.76	27.0224	26.9059	0.1166	401.1
675.00	674.37	0.63	28.0776	28.0389	0.0388	414.2
700.00	701.53	-1.53	29.1283	29.1925	-0.0642	427.2
725.00	728.64	-3.64	30.1740	30.3260	-0.1519	440.0
750.00	755.58	-5.58	31.2143	31.4454	-0.2312	452.7
775.00	782.28	-7.28	32.2485	32.5454	-0.2968	465.3
800.00	808.42	-8.42	33.2768	33.6216	-0.3448	477.8
825.00	834.18	-9.18	34.2988	34.6722	-0.3736	490.2
850.00	859.55	-9.55	35.3138	35.7069	-0.3931	502.4
875.00	884.75	-9.75	36.3225	36.7143	-0.3918	514.5
900.00	910.38	-10.38	37.3247	37.7347	-0.4100	526.6
925.00	936.96	-11.96	38.3204	38.7946	-0.4742	538.5
950.00	966.16	-16.16	39.3096	39.9457	-0.6362	550.3
975.00	999.91	-24.91	40.2923	41.2653	-0.9730	562.0
1000.00	1041.13	-41.13	41.2687	42.8687	-1.6000	573.7
1025.00	1093.98	-68.98	42.2386	44.8803	-2.6416	585.2
1050.00	1164.42	-114.42	43.2020	47.5202	-4.3182	596.6
1075.00	1261.38	-186.38	44.1586	51.0385	-6.8799	608.0
1100.00	1393.25	-293.25	45.1083	55.7654	-10.6571	619.2
1125.00	1572.44	-447.44	46.0505	62.1191	-16.0686	630.4
1150.00	1711.80	-561.80	46.9849	70.6224	-23.6375	641.5
1175.00	1804.93	-629.93	47.9109	81.0214	-34.0104	652.5
1200.00	1875.98	-675.98	48.8280	96.0563	-47.2782	662.4
1225.00	1936.93	-711.93	49.7357	113.2358	-63.5000	674.3
1250.00	1989.86	-739.86	50.6339	141.2420	-90.7081	685.1
1275.00	2039.04	-764.04	51.5210	173.5420	***.****	695.8
1300.00	2087.74	-787.74	52.3963	214.4754	***.****	706.4

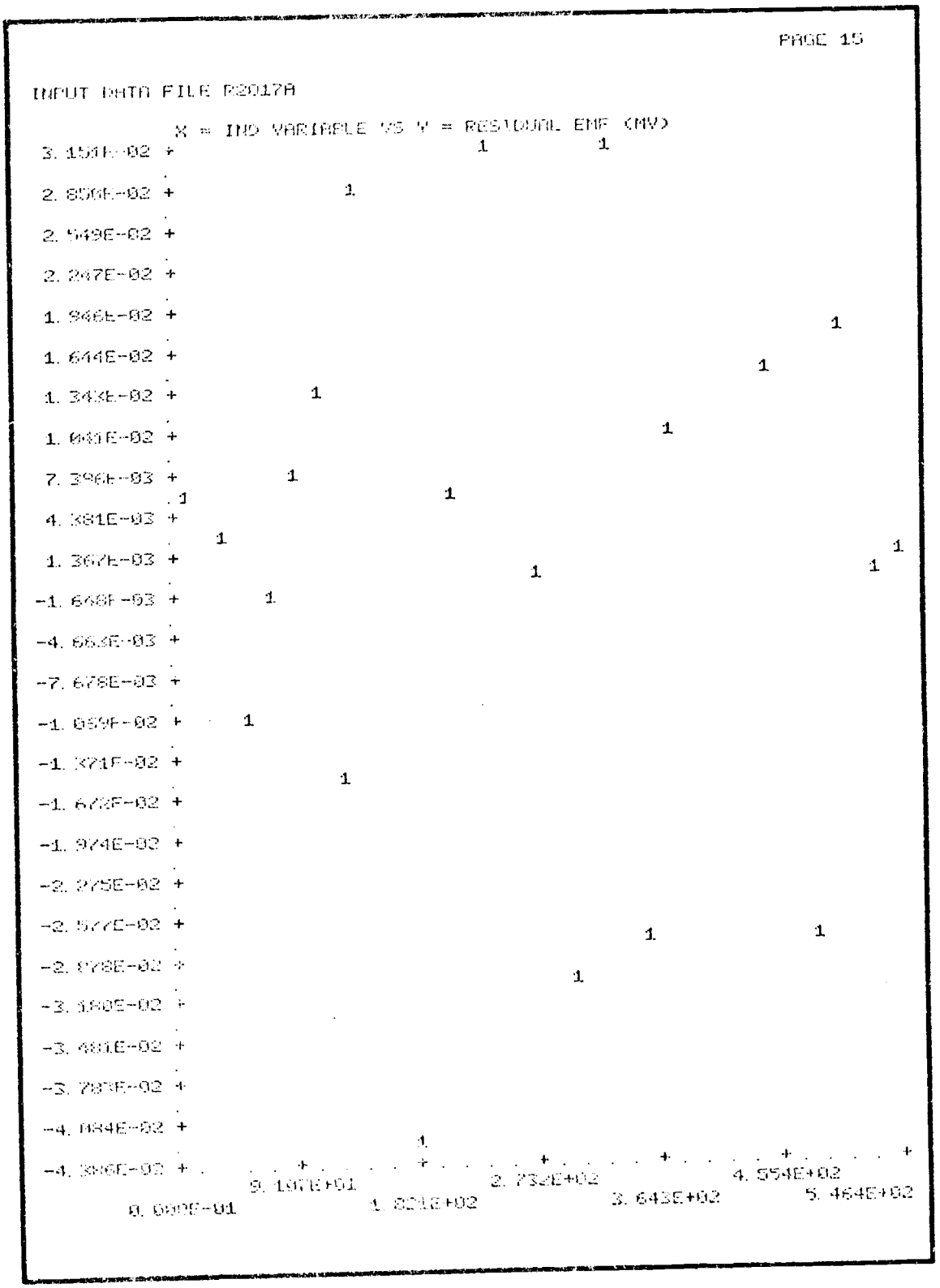
INPUT DATA FILE R2017A

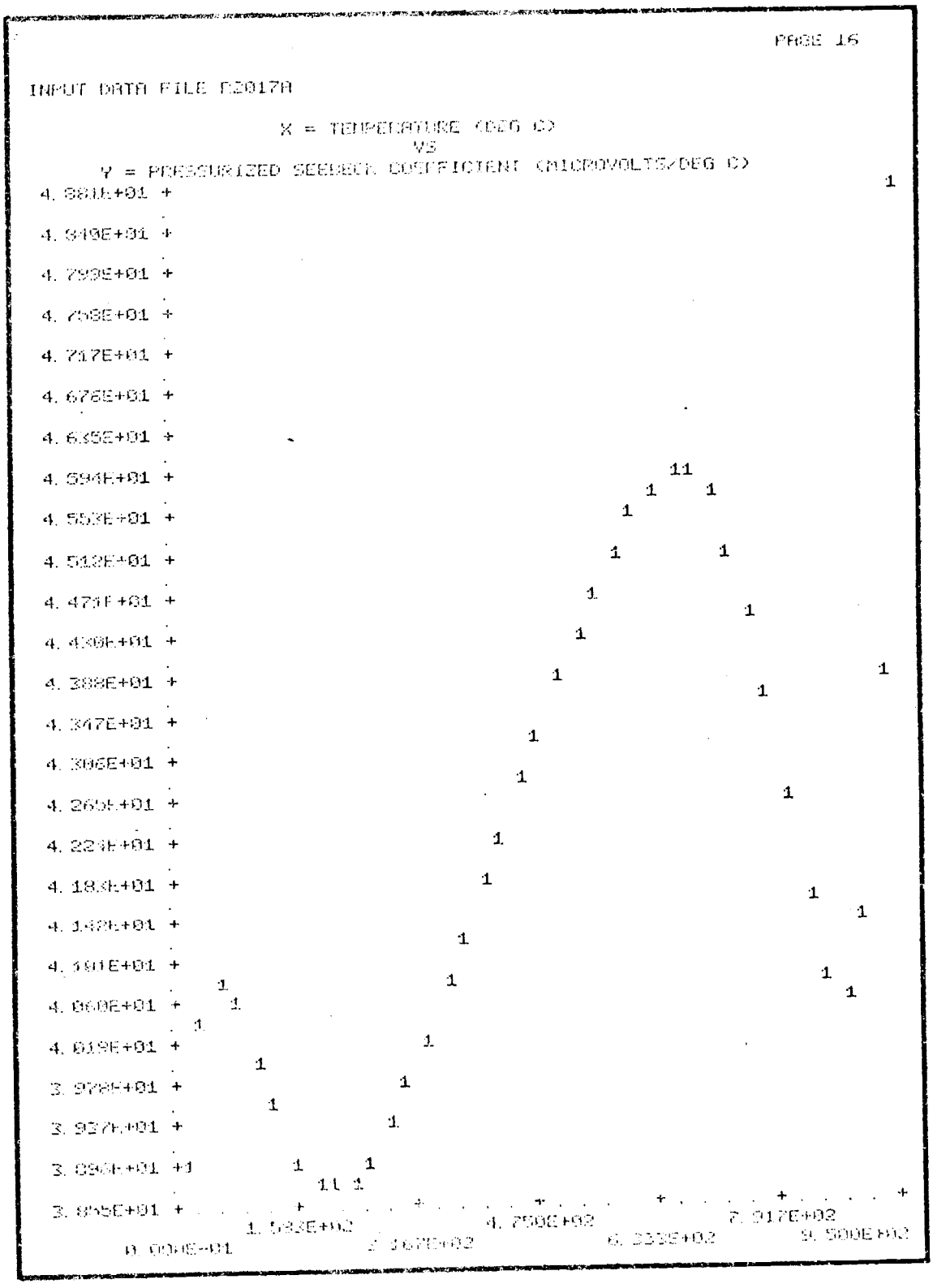
X = UNCORRECTED TEMPERATURE (DEG C)
VS
Y = TEMPERATURE CORRECTION (DEG C) DUE TO PRESSURE

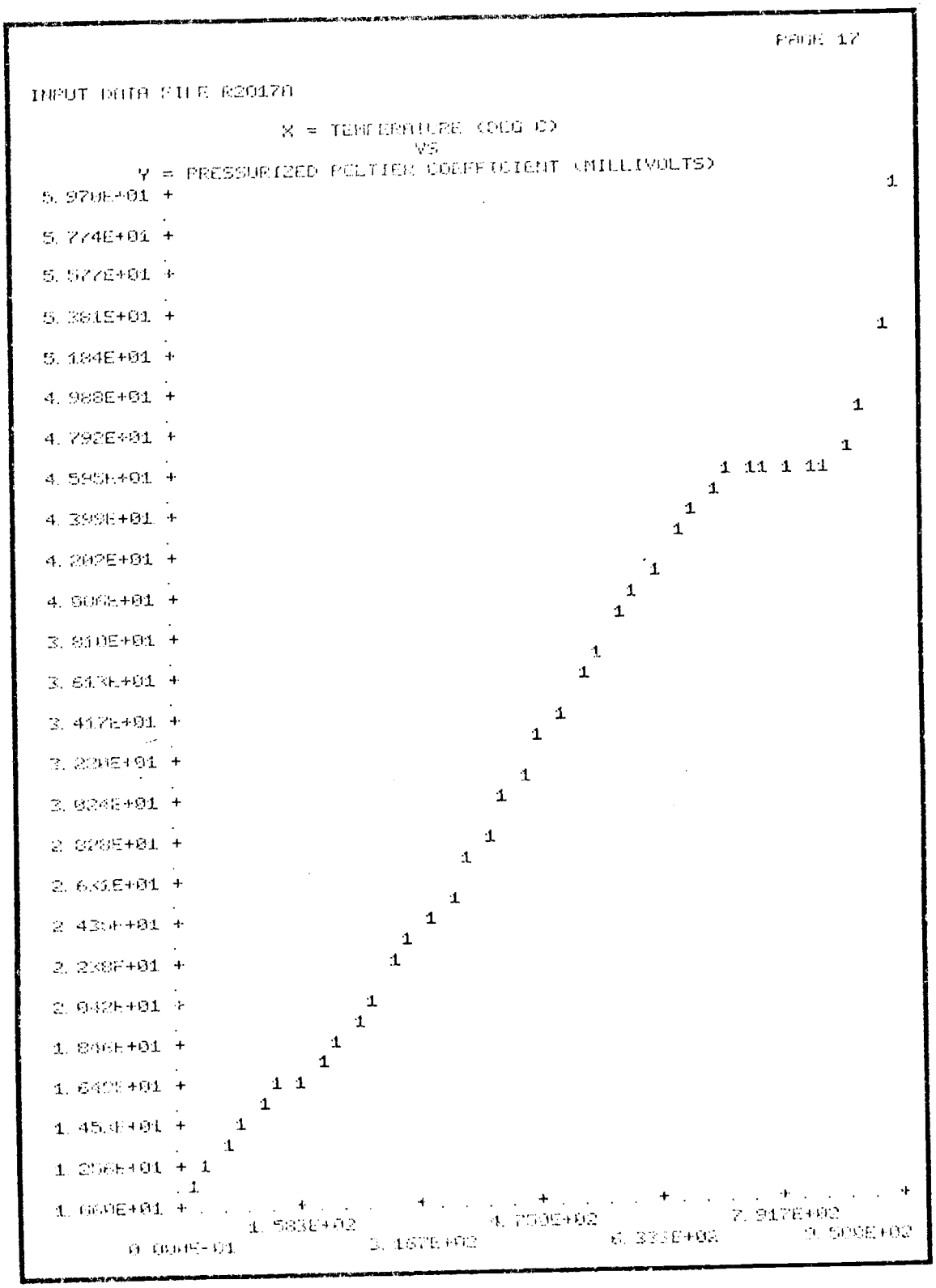



PAGE 13
INPUT DATA FILE P2017A
X = UNCORRECTED TEMPERATURE (DEG C)
VS
Y = ENF CORRECTION (MV) DUE TO PRESSURE
5.156E-01
4.698E-01
4.237E-01
3.776E-01
3.315E-01
2.854E-01
2.394E-01
1.933E-01
1.472E-01
1.011E-01
5.504E-02
8.901E-03
-3.717E-02
-8.321E-02
-1.293E-01
-1.754E-01
-2.215E-01
-2.675E-01
-3.136E-01
-3.597E-01
-4.058E-01
-4.519E-01
-4.979E-01
-5.440E-01
-5.901E-01
-6.362E-01
1.502E+02
4.750E+02
7.997E+02
9.000E+02


PAGE 16
INPUT DATA FILE R2017A
X = FITTED EMF (MV) VS Y = OBSERVED EMF (MV)
3.931E+01
3.776E+01
3.620E+01
3.465E+01
3.309E+01
3.154E+01
2.998E+01
2.843E+01
2.687E+01
2.532E+01
2.376E+01
2.221E+01
2.065E+01
1.910E+01
1.754E+01
1.599E+01
1.443E+01
1.288E+01
1.133E+01
9.770E+00
8.217E+00
6.662E+00
5.108E+00
3.553E+00
1.998E+00
4.437E-01
4.387E-01
1.340E+01
2.635E+01
3.931E+01

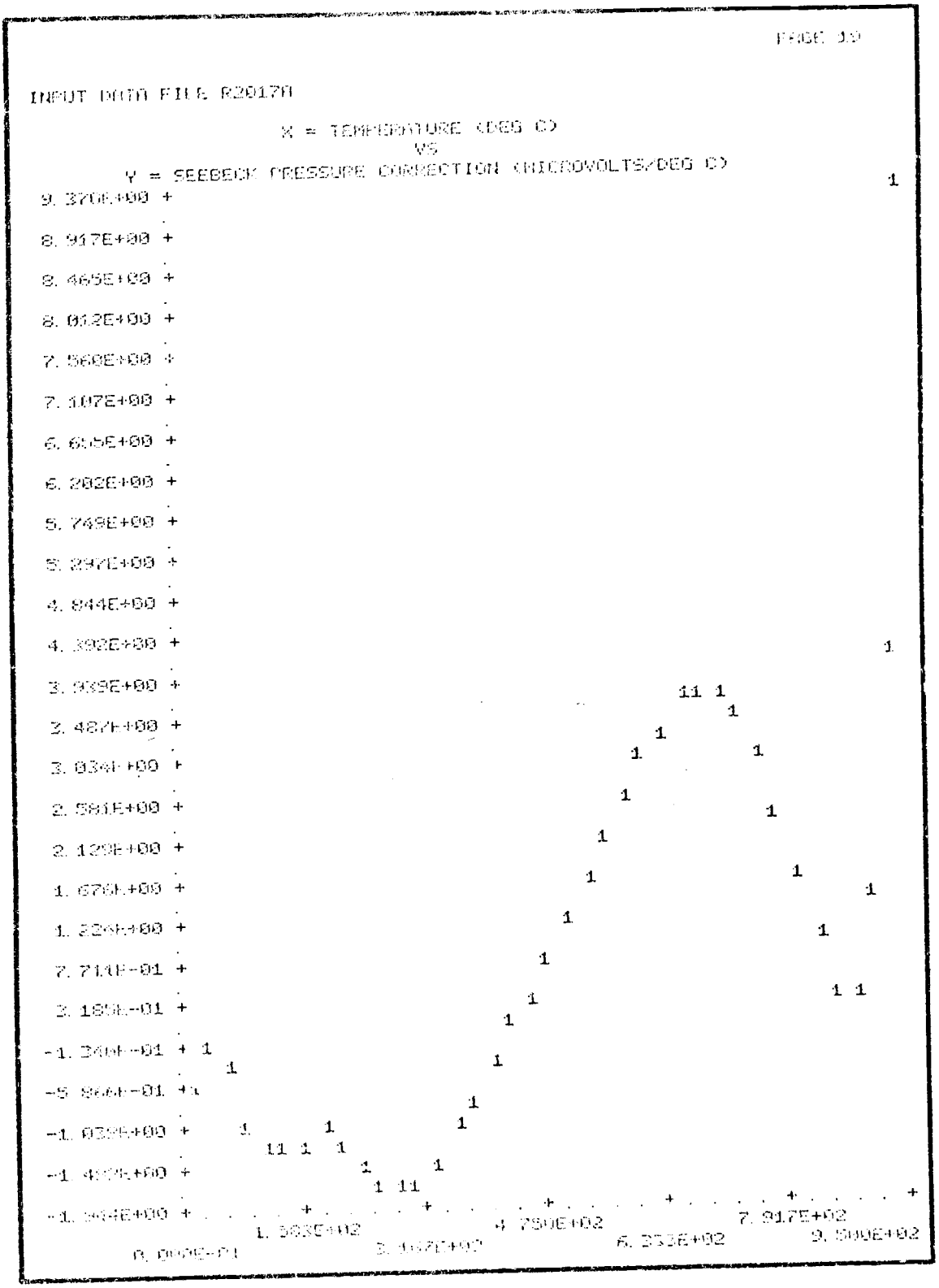

PAGE 15
INPUT DATA FILE R2017A
X = IND VARIABLE VS Y = RESIDUAL ENF (MV)
3.151E-02
2.850E-02
2.549E-02
2.247E-02
1.946E-02
1.644E-02
1.343E-02
1.041E-02
7.396E-03
4.381E-03
1.367E-03
-1.648E-03
-4.664E-03
-7.678E-03
-1.069E-02
-1.371E-02
-1.672E-02
-1.974E-02
-2.275E-02
-2.577E-02
-2.878E-02
-3.180E-02
-3.481E-02
-3.783E-02
-4.084E-02
-4.386E-02
0.000E-01
9.197E+01
1.821E+02
2.734E+02
3.643E+02
4.554E+02
5.464E+02


PAGE 16
INPUT DATA FILE C:2017A
X = TEMPERATURE (DEG C)
VS
Y = PRESSURIZED SEEBECK COEFFICIENT (MICROVOLTS/DEG C)
4.881E+01
4.640E+01
4.398E+01
4.158E+01
3.917E+01
3.676E+01
3.435E+01
3.194E+01
2.953E+01
2.712E+01
2.471E+01
2.230E+01
1.989E+01
1.748E+01
1.507E+01
1.266E+01
1.025E+01
7.839E+00
5.430E+00
3.021E+00
1.583E+02
4.750E+02
7.917E+02


PAGE 17
INPUT DATA FILE R2017A
X = TEMPERATURE (DEG C)
VS
Y = PRESSURIZED MELTING COEFFICIENT (MILLIVOLTS)
5.970E+01
5.774E+01
5.577E+01
5.381E+01
5.184E+01
4.988E+01
4.792E+01
4.595E+01
4.399E+01
4.202E+01
4.006E+01
3.810E+01
3.613E+01
3.417E+01
3.220E+01
3.024E+01
2.828E+01
2.631E+01
2.435E+01
2.238E+01
2.042E+01
1.846E+01
1.649E+01
1.453E+01
1.256E+01
1.060E+01
1.583E+02
4.750E+02
7.917E+02
3.167E+02
6.333E+02
9.500E+02

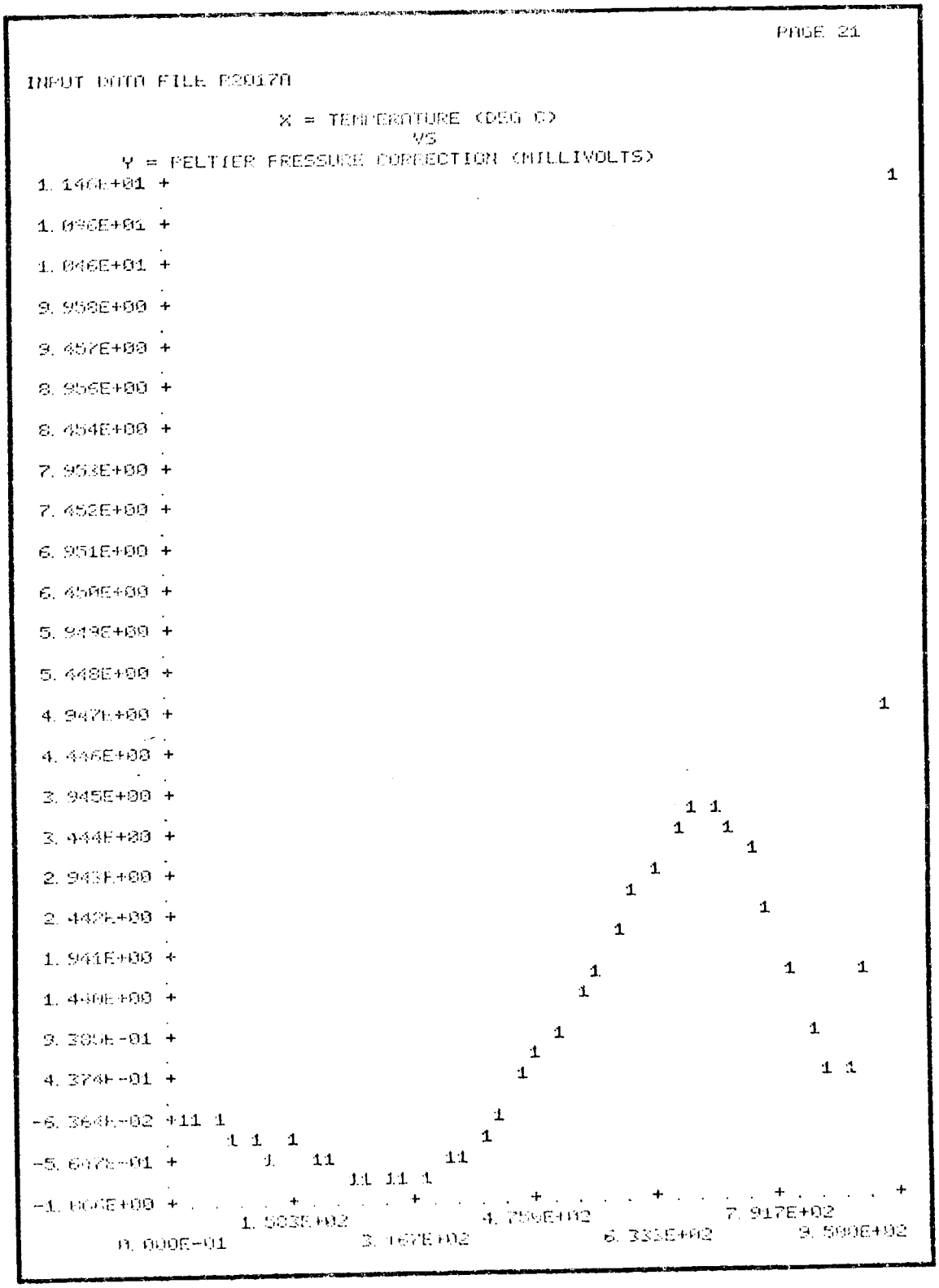
INPUT DATA FILE R2017A

TEMP (DEG C)	NBS SEEBECK (UV/C)	FITTED SEEBECK (UV/C)	SEEBECK DIFF (UV/C)	NBS DS/DT (NV/C2)	FITTED DS/DT (NV/C2)	DS/DT DIFF (NV/C2)
0.0	39.475	38.804	-0.671	45.65	87.56	41.91
25.0	40.498	40.260	-0.237	35.72	33.20	-2.52
50.0	41.226	40.647	-0.579	21.61	0.80	-20.81
75.0	41.537	40.432	-1.105	2.81	-15.82	-18.63
100.0	41.371	39.946	-1.425	-15.28	-21.61	-6.33
125.0	40.849	39.409	-1.440	-24.38	-20.44	3.94
150.0	40.266	38.957	-1.309	-20.14	-15.25	4.90
175.0	39.922	38.662	-1.261	-6.36	-8.19	-1.83
200.0	39.953	38.550	-1.403	8.17	-0.78	-8.95
225.0	40.279	38.618	-1.661	16.59	6.02	-10.57
250.0	40.722	38.842	-1.880	17.80	11.67	-6.12
275.0	41.134	39.190	-1.944	14.85	15.94	1.09
300.0	41.459	39.628	-1.831	11.21	18.85	7.64
325.0	41.704	40.123	-1.582	8.61	20.56	11.95
350.0	41.899	40.648	-1.252	7.16	21.32	14.16
375.0	42.067	41.183	-0.884	6.34	21.43	15.09
400.0	42.217	41.716	-0.502	5.68	21.14	15.46
425.0	42.351	42.239	-0.112	4.95	20.69	15.74
450.0	42.464	42.750	0.286	4.05	20.19	16.14
475.0	42.552	43.249	0.697	2.99	19.70	16.71
500.0	42.602	43.734	1.122	1.80	19.15	17.35
525.0	42.641	44.204	1.563	0.51	18.23	17.88
550.0	42.637	44.659	2.013	-0.84	17.10	18.02
575.0	42.589	45.057	2.459	-2.21	15.25	17.46
600.0	42.527	45.404	2.878	-3.55	12.30	15.85
625.0	42.422	45.662	3.240	-4.83	8.05	12.88
650.0	42.286	45.795	3.509	-6.02	2.34	8.36
675.0	42.122	45.766	3.644	-7.09	-4.85	2.24
700.0	41.933	45.542	3.609	-8.02	-13.29	-5.27
725.0	41.722	45.096	3.374	-8.81	-22.44	-13.63
750.0	41.494	44.422	2.928	-9.43	-31.30	-21.87
775.0	41.252	43.546	2.294	-9.90	-38.36	-28.46
800.0	41.000	42.537	1.537	-10.22	-41.43	-31.21
825.0	40.742	41.532	0.790	-10.41	-37.55	-27.13
850.0	40.480	40.750	0.270	-10.49	-22.79	-12.29
875.0	40.218	40.524	0.307	-10.49	7.84	18.33
900.0	39.956	41.327	1.370	-10.42	60.59	71.02
925.0	39.697	43.802	4.105	-10.34	143.14	153.48
950.0	39.439	48.809	9.370	-10.27	264.76	275.03
975.0	39.183	57.457	18.274	-10.24	436.55	446.79
1000.0	38.926	71.163	32.237	-10.30	671.60	681.90
1025.0	38.667	91.691	53.024	-10.47	985.24	995.71
1050.0	38.402	121.227	82.825	-10.77	1395.24	1406.01
1075.0	38.127	162.426	124.298	-11.21	1922.06	1933.28
1100.0	37.840	218.498	180.658	-11.81	2589.12	2600.93
1125.0	37.536	293.271	255.735	-12.54	3422.99	3435.53
1150.0	37.212	391.286	354.074	-13.37	4453.75	4467.12
1175.0	36.867	517.880	481.013	-14.26	5715.18	5728.44
1200.0	36.499	677.781	642.782	-15.12	7245.11	7260.26
1225.0	36.111	880.725	844.613	-15.85	9083.76	9101.62
1250.0	35.706	1136.548	1100.840	-16.33	11282.87	11299.19
1275.0	35.289	1454.327	1419.038	-16.39	13894.22	13910.57
1300.0	34.867	1843.995	1809.128	-15.71	16964.80	16980.50


PAGE 10
INPUT DATA FILE R20170
X = TEMPERATURE (DEG C)
VS
Y = SEEBECK PRESSURE CORRECTION (MICROVOLTS/DEG C)
9.370E+00
8.917E+00
8.465E+00
8.012E+00
7.560E+00
7.107E+00
6.655E+00
6.202E+00
5.749E+00
5.297E+00
4.844E+00
4.392E+00
3.939E+00
3.487E+00
2.034E+00
2.581E+00
2.129E+00
1.676E+00
1.224E+00
7.719E-01
3.195E-01
-1.329E-01
-5.853E-01
-1.038E+00
-1.492E+00
-1.945E+00
1.362E+02
4.750E+02
7.917E+02
9.500E+02
6.333E+02
3.167E+02
0.000E-01

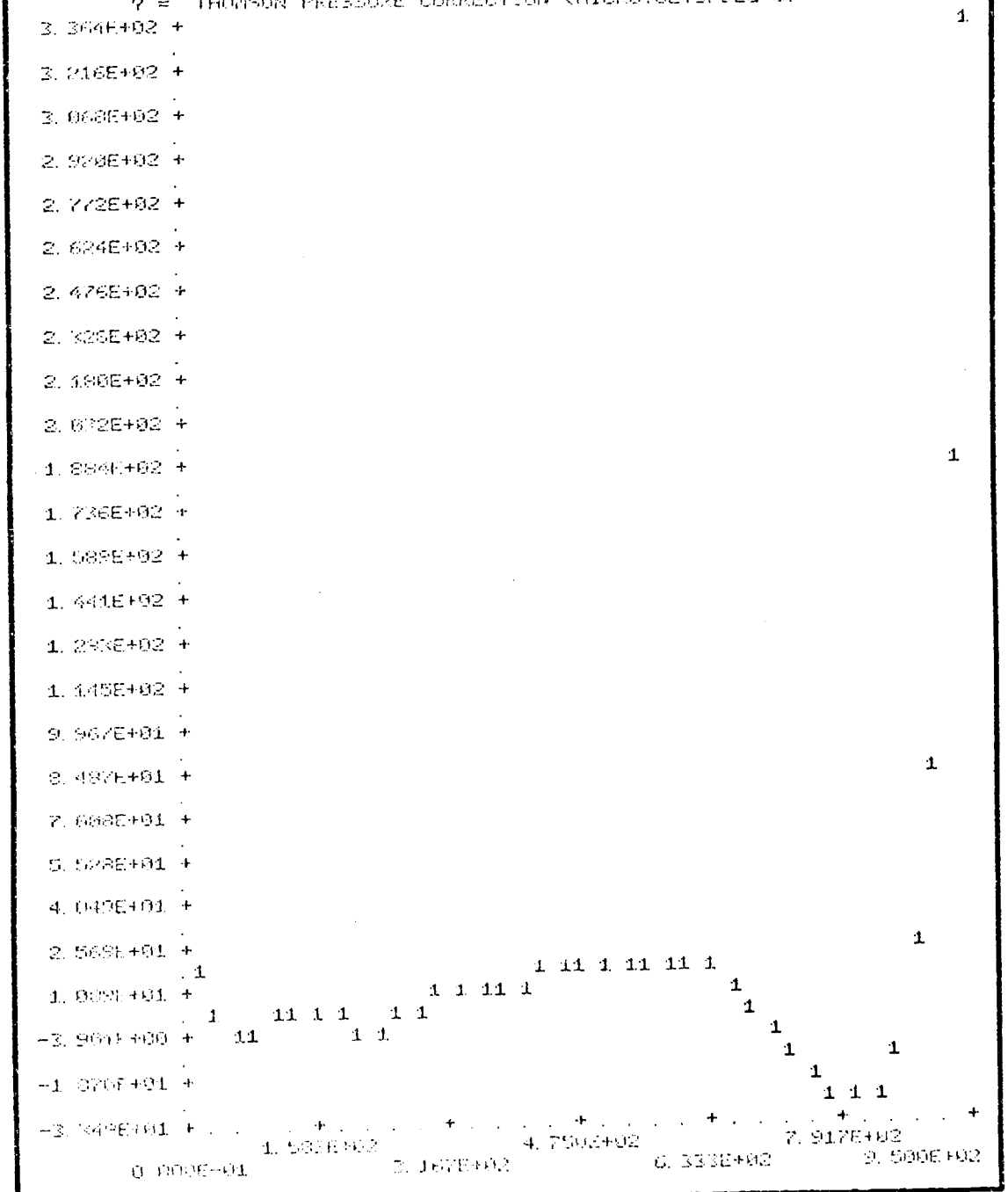
INPUT DATA FILE R3017A

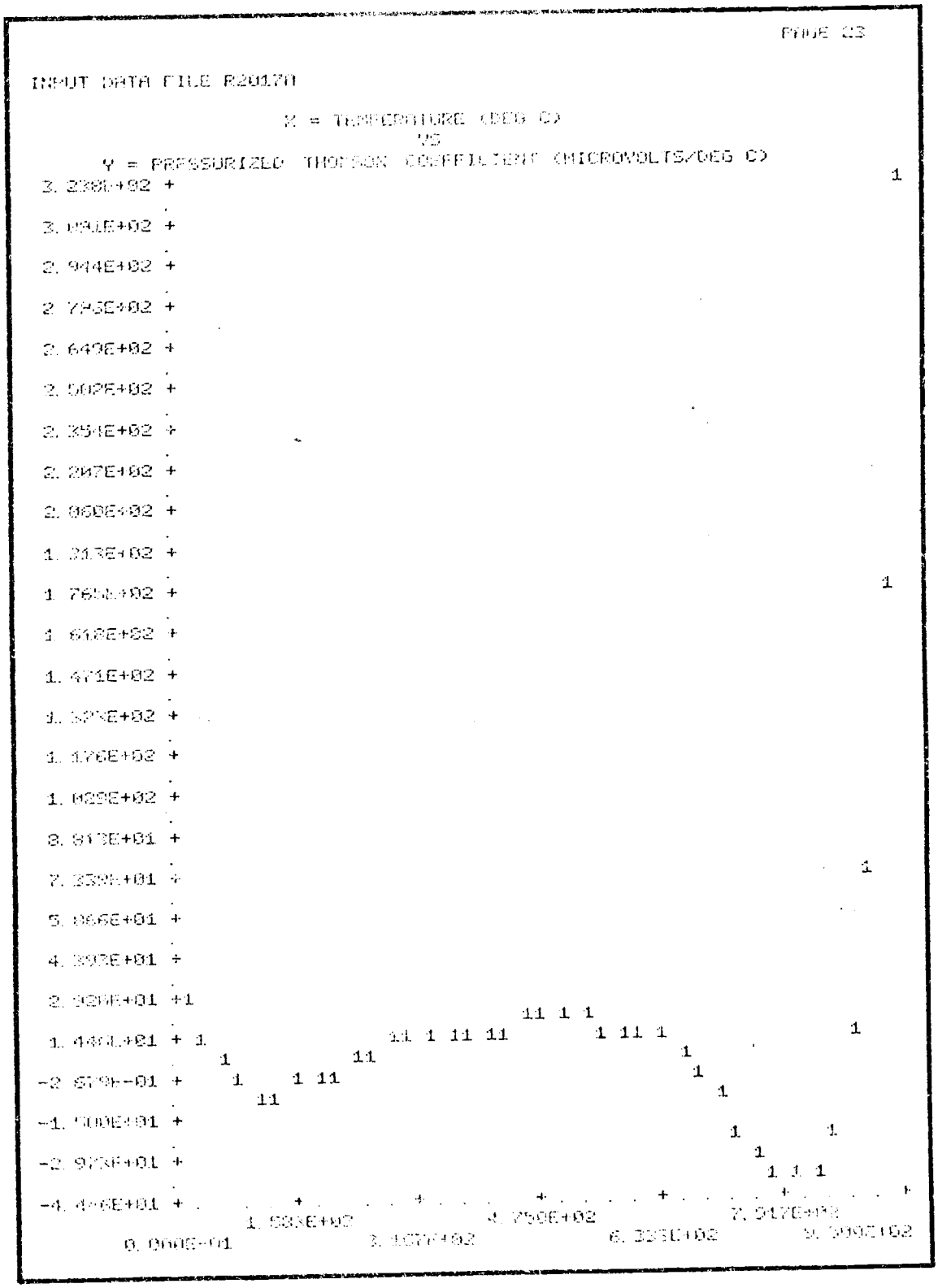
TEMP (DEG C)	NBS PELTIER (MV)	FITTED PELTIER (MV)	PELTIER DIFF (MV)	NBS THOMSON (UV/C)	FITTED THOMSON (UV/C)	THOMSON DIFF (UV/C)
0.0	10.783	10.539	-0.183	12.47	22.92	11.45
25.0	12.074	12.004	-0.071	10.65	9.90	-0.75
50.0	13.322	13.135	-0.187	6.98	0.26	-6.72
75.0	14.461	14.076	-0.385	0.38	-5.51	-6.49
100.0	15.438	14.906	-0.532	-5.70	-8.06	-2.36
125.0	16.264	15.691	-0.573	-9.71	-8.14	1.57
150.0	17.039	16.485	-0.554	-8.52	-6.45	2.07
175.0	17.892	17.326	-0.565	-2.85	-3.67	-0.82
200.0	18.904	18.240	-0.664	3.87	-0.37	-4.24
225.0	20.065	19.238	-0.828	8.27	3.00	-5.26
250.0	21.304	20.320	-0.983	9.31	6.11	-3.20
275.0	22.548	21.482	-1.066	8.14	8.74	0.60
300.0	23.762	22.713	-1.050	6.43	10.80	4.38
325.0	24.945	23.999	-0.946	5.15	12.30	7.15
350.0	26.110	25.330	-0.780	4.46	13.29	8.83
375.0	27.266	26.693	-0.573	4.11	13.89	9.78
400.0	28.419	28.081	-0.338	3.83	14.23	10.41
425.0	29.567	29.489	-0.078	3.46	14.44	10.99
450.0	30.707	30.915	0.207	2.93	14.60	11.67
475.0	31.835	32.356	0.521	2.24	14.74	12.50
500.0	32.946	33.813	0.868	1.39	14.81	13.41
525.0	34.024	35.282	1.258	0.40	14.68	14.27
550.0	35.047	36.754	1.657	-0.69	14.15	14.84
575.0	36.130	38.215	2.085	-1.87	12.94	14.81
600.0	37.132	39.645	2.513	-3.10	10.74	13.84
625.0	38.101	41.011	2.910	-4.34	7.23	11.57
650.0	39.036	42.275	3.239	-5.56	2.16	7.72
675.0	39.938	43.393	3.455	-6.72	-4.60	2.12
700.0	40.807	44.319	3.512	-7.81	-12.94	-5.13
725.0	41.645	45.012	3.367	-8.79	-22.40	-13.61
750.0	42.454	45.459	3.006	-9.65	-32.02	-22.37
775.0	43.238	45.642	2.404	-10.38	-40.21	-29.83
800.0	43.999	45.649	1.650	-10.97	-44.46	-33.49
825.0	44.740	45.608	0.868	-11.44	-41.23	-29.79
850.0	45.465	45.769	0.303	-11.79	-25.59	-13.81
875.0	46.176	46.528	0.352	-12.04	9.01	21.05
900.0	46.875	48.482	1.608	-12.23	71.09	83.31
925.0	47.562	52.481	4.919	-12.39	171.50	183.89
950.0	48.240	59.701	11.461	-12.56	323.84	336.40
975.0	48.906	71.715	22.809	-12.79	544.88	557.67
1000.0	49.559	90.601	41.042	-13.11	855.04	868.16
1025.0	50.195	119.020	68.825	-13.59	1278.99	1292.58
1050.0	50.811	159.402	108.591	-14.25	1846.11	1860.36
1075.0	51.401	218.074	167.673	-15.12	2591.23	2606.35
1100.0	51.960	300.008	248.048	-16.22	3565.25	3581.46
1125.0	52.481	410.457	357.977	-17.53	4785.86	4803.39
1150.0	52.959	556.859	503.901	-19.01	6338.26	6357.27
1175.0	53.392	749.998	696.606	-20.65	8276.44	8297.10
1200.0	53.769	1000.682	946.913	-22.39	10672.17	10694.56
1225.0	54.100	1324.454	1270.354	-24.26	13611.84	13636.09
1250.0	54.389	1731.124	1676.735	-26.27	17187.62	17214.89
1275.0	54.648	2245.[illegible]	2190.[illegible]	-28.51	21506.70	21535.21
1300.0	54.898	2895.[illegible]	2840.[illegible]	-31.12	26698.32	26729.44


PAGE 21
INPUT DATA FILE P2017A
X = TEMPERATURE (DEG C)
VS
Y = PELTIER PRESSURE CORRECTION (MILLIVOLTS)
1.140E+01
1.086E+01
1.046E+01
9.958E+00
9.457E+00
8.956E+00
8.454E+00
7.953E+00
7.452E+00
6.951E+00
6.450E+00
5.949E+00
5.448E+00
4.947E+00
4.446E+00
3.945E+00
3.444E+00
2.943E+00
2.442E+00
1.941E+00
1.430E+00
9.385E-01
4.374E-01
-6.364E-02
-5.647E-01
-1.080E+00
0.000E-01
1.583E+02
3.167E+02
4.750E+02
6.333E+02
7.917E+02
9.500E+02

INPUT DATA FILE R2017A

X = TEMPERATURE (DEG C)
VS
Y = THOMSON PRESSURE CORRECTION (MICROVOLTS/DEG C)




PAGE 03
INPUT DATA FILE R20170
X = TEMPERATURE (DEG C)
VS
Y = PRESSURIZED THOMSON COEFFICIENT (MICROVOLTS/DEG C)
3.238E+02
3.091E+02
2.944E+02
2.796E+02
2.649E+02
2.502E+02
2.354E+02
2.207E+02
2.060E+02
1.913E+02
1.765E+02
1.618E+02
1.471E+02
1.324E+02
1.176E+02
1.029E+02
8.817E+01
7.339E+01
5.866E+01
4.393E+01
2.920E+01
1.447E+01
-2.617E-01
-1.500E+01
-2.973E+01
-4.446E+01
0.000E+01
1.583E+02
3.167E+02
4.750E+02
6.333E+02
7.917E+02
9.500E+02