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Hot-Pressing Study on Mixed Uranium-Plutonium Nitride for Advanced Reactor Fuel

Ji Young Chang

OAK RIDGE NATIONAL LABORATORY

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**HOT-PRESSING STUDY ON MIXED URANIUM-PLUTONIUM
NITRIDE FOR ADVANCED REACTOR FUEL**

J. Young Chang

**Based on a Dissertation Presented to the Graduate Council
of the Inha University in Partial Fulfillment of the
Requirements for the Degree of Doctor of Philosophy
in Metallurgical Engineering**

NOVEMBER 1975

**OAK RIDGE NATIONAL LABORATORY
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CONTENTS

ABSTRACT	1
INTRODUCTION	1
EXPERIMENTAL APPARATUS AND PROCEDURE	6
Hot Press Design	6
Continuous Densification Measurement	6
System Checkup with Uranium Nitride	8
UN-207 PuN Hot-Pressing	8
Analog Computer Simulation of Hot-Pressing	10
Digital Computer Program to Predict Densification of UN-207 PuN at Various Pressures and Temperatures	11
TEST RESULTS AND DISCUSSION	12
Densification of Mixed (U,Pu)N and UN	12
Analog Computer Simulation of Hot-Pressing	18
Digital Computer Simulation of Hot-Pressing	18
CONCLUSIONS AND RECOMMENDATIONS	20
ACKNOWLEDGMENTS	21
APPENDIX A. DESCRIPTION OF HOT PRESS USED IN GLOVE BOX AND RECOMMENDED DESIGN POINTS	25
APPENDIX B. NUMERICAL SOLUTION OF EQ. (11) FOR COMPUTER SIMULATION	29
APPENDIX C. PROGRAM FOR DIGITAL COMPUTER SIMULATION OF HOT PRESSING	33
APPENDIX D. VARIABLES AVAILABLE FOR HOT PRESS DIGITAL COMPUTER PROGRAM	59

HOT-PRESSING STUDY ON MIXED URANIUM-PLUTONIUM NITRIDE FOR ADVANCED REACTOR FUEL

Ji Young Chang¹

ABSTRACT

The hot-pressing characteristics of mixed (U,Pu)N for advanced reactor fuel were studied in order to provide a better insight into the densification process and thus improve fuel fabrication technique.

A detailed experimental procedure for continuous measurement of densification and an analog computer circuit to simulate hot-pressing are presented.

Mixed (U,Pu)N of 99% density was fabricated at 4000 psi (28 MPa) and 1450°C, and 94% density was obtained with 3000 psi (21 MPa) at 1450°C. A digital computer program for the densification process was also written to analyze and predict the density of the pellet at any given time or at different applied pressures than those actually tested.

The time dependence of the temperature in the proposed equation to simulate the experimental heating period of the die was first introduced to improve the interpretation of experimental data in order to correlate with the equation:

$$\frac{d\rho}{dt} = f(\rho, \rho_0) \equiv \frac{A}{\tau(\rho)} (1 - \rho) \left[\frac{1}{1 - (1 - \rho)^{2/3}} + B \ln(1 - \rho) \right].$$

The best values of the hot-pressing coefficients, defined as $A = 30 \ln 2 \rho_0^2 / \tau \rho^2$ and $B = \sqrt{2} \tau_0 / \tau$, were determined by curve fitting of the equation with experimental data. The values are $A = 1.296$ and $B = 0.352$ for mixed (U,Pu)N that had been fabricated with a starting density of 63% and a hot-pressing pressure of 3000 psi (21 MPa) at 1450 ± 10°C.

INTRODUCTION

Hot-pressing has been actively considered for fabrication of high-temperature ceramics in recent years with its potential density control

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and microstructure improvement. A densification study of mixed uranium-plutonium nitride using this hot-pressing technique was therefore undertaken.

The mixed nitride of uranium and plutonium has high potential for use as fuel in fast breeder reactors. Plutonium nitrides possess some significant advantages over their oxides and carbides, such as higher values of fissile density, thermal conductivity, and melting point. Mixed nitride fuel will provide further advantages by stabilizing the high decomposition pressure of PuN and dilution of fissionable atoms to remove heat effectively, breed additional fuel, provide greater irradiation stability, and offer fewer compatibility problems.

In the past, many scientists have investigated the densification mechanism in the hope of obtaining a simple functional description of densification as a function of time, pressure, and temperature. Hot-pressing theory has been reviewed by Thümler and Thomas² and by Ramqvist.³ Densification during hot pressing can be described by three general mechanisms: (a) plastic flow,⁴⁻¹⁰ (b) particle rearrangement,

²F. Thümler and W. Thoma, "The Sintering Process," *Met. Rev.* 12: 69-108 (1967).

³L. Ramqvist, "Theories of Hot Pressing," *Powder Met.* 9(17): 1-25 (1966).

⁴J. K. Mackenzie and R. Shuttleworth, "A Phenomenological Theory of Sintering," *Proc. Phys. Soc., London*, 62: 833-52 (1949).

⁵P. Murray, E. P. Rodgers, and A. E. Williams, *Practical and Theoretical Aspects of the Hot Pressing of Refractory Oxides*, AERE-M/R-893 (July 30, 1952).

⁶J. D. McClelland, "Kinetics of Hot Pressing," pp. 157-71 in *Powder Met. Proc. Int. Conf., New York, 1960*, ed. by W. LeSzynski, Wiley, New York, 1961.

⁷M. S. Kovalchenko and G. V. Samsonov, "Application of Viscous Flow Theory to Densification of Powders by Hot Pressing," *Porosh. Met.*, 1961 (2): 3-13.

⁸S. Scholz and B. Lersmacher, "The Densification Rate During Hot Pressing," *Arch. Eisenhüttenw.*, 41: 98-108 (1964).

⁹S. Scholz, "Some New Views on the Hot Pressing of Refractory Compounds," *Sov. Powder Met. Metal Ceram. (English Transl.)* 1963(3): 170-75.

¹⁰G. E. Mangsen, W. A. Lambertson, and B. Best, "Hot Pressing of Aluminum Oxide," *J. Amer. Ceram. Soc.* 43: 55-58 (1960).

sliding, and fragmentation;^{11,12} and (c) stress-enhanced diffusion.¹³⁻¹⁶
 The more important equations that may be used to fit the experimental data of mixed nitride fuels are listed below.

Mackenzie and Shuttleworth⁴ sintering mechanism:

$$\left(\frac{\dot{\rho}}{\dot{\rho}_s}\right) = \frac{3}{2} \left(\frac{4\pi}{3}\right)^{1/3} \frac{Y \tau_c^{1/3}}{\tau_\infty} (1 - \rho)^{2/3} \rho^{1/3} \left[1 - z \left(\frac{1}{z} - 1 \right)^{1/3} \ln \frac{1}{1 - z} \right], \quad (1)$$

where

$$z = \sqrt{2} \left(\frac{3}{4\pi} \right)^{1/3} \frac{\tau_c}{2Y \tau_c^{1/3}}.$$

Murray, Rodgers, and Williams⁵ modification of Eq. (1) for hot-pressing:

$$\frac{\dot{\rho}}{\dot{\rho}_s} = \left(\frac{\dot{\rho}}{\dot{\rho}_s} \right)_s + \frac{3\tau}{4\pi} (1 - \rho). \quad (2)$$

Pressure correction by McClelland⁶ from Eq. (2):

$$\frac{\dot{\rho}}{\dot{\rho}_s} = \frac{3\tau}{4\pi} (1 - \rho) \left[\frac{1}{1 - (1 - \rho)^{2/3}} + \frac{\sqrt{2} \tau_c}{P} \rho^{1/3} (1 - \rho) \right]. \quad (3)$$

¹¹E. J. Felton, "Hot-Pressing of Alumina Powders at Low Temperature," *J. Amer. Ceram. Soc.*, 44: 381-85 (1961).

¹²R. Chang and C. G. Rhodes, "High-Pressure Hot-Pressing of Uranium Carbide Powders and Mechanism of Sintering of Refractory Bodies," *J. Amer. Ceram. Soc.*, 45: 379-82 (1962).

¹³R. L. Coble and J. S. Ellis, "Hot-Pressing Alumina - Mechanisms of Material Transport," *J. Amer. Ceram. Soc.*, 46: 438-41 (1963).

¹⁴T. Vasilos and R. M. Spriggs, "Pressure Sintering: Mechanisms and Microstructures for Alumina and Magnesia," *J. Amer. Ceram. Soc.*, 46: 493-96 (1963).

¹⁵R. C. Rossi and R. M. Fulrath, "Final Stage Densification in Vacuum Hot-Pressing," *J. Amer. Ceram. Soc.*, 48: 558-64 (1965).

¹⁶G. M. Fryer, "Hot Pressing of Alumina, a New Treatment of Final Densification," *Trans. Brit. Ceram. Soc.*, 66: 127-34 (1967).

Viscosity correction as a function of porosity and grain growth [Eq. (4)] by Kovalichenko and Samsonov⁷ from Eq. (2), using the diffusional creep models of Nabarro¹⁷ and Herring:¹⁸

$$\frac{\dot{\epsilon}}{\dot{\epsilon}_0} = \frac{P(1-\rho)(2+b)}{4\eta_0(1+bt)(2-1)} \quad (4)$$

New viscosity correction as a function of porosity by Scholz and Lersmacher⁹ using Eq. (4):

$$\frac{\dot{\epsilon}}{\dot{\epsilon}_0} = \frac{3P}{4\eta_0} \frac{(1-\rho)}{(1+bt)} \quad (5)$$

Empirical formula established by Carlson and Westerman;¹⁹ $\log(1-\rho)$ is linear in $\log \dot{\epsilon}$. Then

$$\frac{\dot{\epsilon}}{\dot{\epsilon}_0} = \frac{K}{\dot{\epsilon}}(1-\rho) \quad (6)$$

where

$$K = f(\sigma, \dot{\epsilon}).$$

Empirical equation by Scholz:⁹

$$\rho = 1 - (1 - \rho_0)(1 + bt)^{-n} \quad (7)$$

where

$$n = \frac{15\Omega}{2kR_0^2} \frac{PD}{bt}.$$

¹⁷R.F.N. Nabarro, "Deformation of Crystals by the Motions of Single Ions," pp. 75-90 in *Report of a Conference on Strength of Solids, Held at the H. H. Wills Physical Laboratory, University of Bristol on 7-9 July 1947*, Physical Society of London, 1948.

¹⁸C. Herring, "Diffusional Viscosity of a Polycrystalline Solid," *J. Appl. Phys.* 21: 437-45 (1950).

¹⁹R. G. Carlson and F. E. Westerman, "Hot Pressing of Lead Spheres," *Platzseeber. Pulvermet.* 10: 15-23 (1962); *Trans. Met. Soc. AIME* 221: 649-50 (1961).

Rossi and Fulrath^{1,5} stress-enhanced diffusion:

$$\frac{d\rho}{dt} = \frac{10^{10}}{Z} D (1 - \rho) \quad Z \approx 3 \text{ to } 4. \quad (8)$$

Fryer^{1,6} vacancy diffusion:

$$\frac{1}{\rho} \frac{d\rho}{dt} = -\frac{Z}{kT} \frac{\gamma}{r} \left(\frac{r}{r_0}\right)^{5/3}. \quad (9)$$

The symbols used in these and subsequent equations are listed below.

- k = constant
- D = diffusion coefficient, cm^2/sec
- k_B = Boltzmann constant, 1.38×10^{-6} erg/K
- $\bar{r}$ = mean pore separation, cm
- N_v = number of voids/ cm^3
- P = pressure, dynes/ cm^2
- r = grain radius, cm
- r_0 = original grain radius, cm
- t = time, sec
- T = temperature, K
- V_c = volume of compact, cm^3
- V_s = volume of solid material, cm^3
- C = numerical constant depending mainly on the pore geometry
- $\left(\frac{d\rho}{dt}\right)_0$ = densification rate in the absence of pressure (normal sintering)
- γ = constant
- γ_s = surface tension, dynes/cm
- η = viscosity, dynes sec cm^{-2}
- η_∞ = viscosity in infinite shear rate, dynes sec cm^{-2}
- η_0 = viscosity before grain growth, dynes sec cm^{-2}
- V_v = vacancy volume, cm^3
- ρ = density, fraction of theoretical
- ρ_0 = density before hot pressing, fraction of theoretical
- τ_c = critical shear stress, dynes/ cm^2

It is postulated on the basis of all the experimental work that either the above-mentioned mechanisms are operating simultaneously or predominantly one mechanism operates, depending upon the hot-pressing conditions and the material. The theory of hot-pressing requires further development to resolve the discrepancies among the existing equations and also to better interrelate the competing mechanisms to describe their relative importance under varying hot-pressing conditions.

At present, even though the assumptions and mechanisms proposed are not perfectly applicable to all cases, each of these theoretical or phenomenological equations has in many cases proved very useful for practical prediction and analysis of hot-pressing.

It is not very economical to run many hot-pressing experiments to obtain the appropriate pressure and temperature necessary to give a desired densification in a specified time for uranium-plutonium nitride reactor fuel. Therefore, computer simulation of densification for hot-pressing was developed. The empirical model of hot-pressing with computer calculation can be used to predict the density of mixed uranium-plutonium nitride fuel pellets obtained at a given pressure, temperature, and time.

EXPERIMENTAL APPARATUS AND PROCEDURE

Hot Press Design

A high-frequency induction hot press was designed as described in Appendix A, to fit a small glove box 32 by 43 by 32 in. (0.8 by 1.1 by 0.8 m), with emphasis on a number of aspects, such as safety and compactness. Figure 1 shows a schematic drawing of the design. The advantage of this hot press compared with conventional design is that a sample can be removed by remote control (i.e., from outside the glove box) without disassembling the furnace after each operation. This feature is necessary to avoid the difficulties inherent in handling the sample through the gloves. The hot-pressing capability was 10,000 psi (70 MPa) in 1/2-in. (13-mm) die size at 1600°C. However, a 3/8-in.-diam. (9.5-mm) die was used for all tests.

The temperature of the hot press die was measured with an optical pyrometer and a platinum vs platinum-rhodium thermocouple. Calibration of the optical pyrometer included absorption of rays by the prism and the glove box window.

The pellets were fabricated by use of a tungsten die in an argon atmosphere. With the size of the die used for all tests we were able to produce 0.372-in.-diam by 0.25 to 0.39-in.-high (9.45-by 6.4-9.9-mm) pellets.

Continuous Densification Measurement

The height of the pellet during pressing was measured continuously by a linear transducer attached near the loading shaft and a recorder located outside the glove box. Figure 2 represents a typical recorder chart of the transducer readout for loading shaft movements. Since the diameter was assumed to be constant; the height increases linearly with the instantaneous density. Analytical methods to describe the continuous density increase of the test specimen in the hot press were developed on the basis of this chart and the conventionally measured final density. Referring to Fig. 2, at A the sample expands as the temperature of die increases. At B densification of the sample starts. At C the sample plastically deforms when pressure is applied to it. At D the same point is shown with different recorder scales, and at E the system shows deformation. Finally F, G, and H represent the shrinkage of the system resulting from cooling.

Fig. 1. Induction Hot Press Designed for Glove Box.

Fig. 2. Typical Transducer Chart Used for Measuring Continuous Densification of Test Specimen in Hot Press. A, start heating die; B, start densification; C, increase pressure and plastic deformation of test sample; D, recorder scale change; E, deformation of LAVITE; F, start cooling die; G, lower pressure, and H, check position at room temperature.

System Checkup with Uranium Nitride

The system was checked with 20%-enriched uranium nitride, fabricated by the hydride-dehydride-nitride process. The powder used in this initial experiment had 5000 ppm O_2 contamination, and the average particle size was less than 3 μm . The material was first cold-pressed at 35,000 psi without binder to a green density of 48.4%. It was then hot-pressed in argon at 6400 psi (44 MPa) and 1415°C for 90 min. Figure 3 shows the densification history of the UN pellet.

The final density (end point density) of the sample was 99%, and the impurity can be detected as second-phase UO_2 in the microstructure, as shown in Fig. 4. The grain size of the product was extremely small compared with material cold-pressed and sintered at 2150°C.

The uranium nitride was etched with 90 ml lactic acid, 30 ml HNO_3 , 3 ml HF for 45 to 50 sec to reveal the general microstructure. After completion of system checkup with a few more test samples with different pressing conditions, UN-20% PuN hot pressing was initiated.

UN-20% PuN Hot-Pressing

Plutonium nitride was prepared by hydriding the plutonium metal at 170°C and then reacting with nitrogen at 1000°C by evacuating the furnace and refilling with nitrogen. The use of high-purity hydrogen generated by decomposition of UH_3 also improved the quality of hydride, thus producing low-oxygen PuN. Since no techniques were available at that time to evaluate plutonium powder with electron microscopy, new powder replication techniques and hot-stage microscopy to evaluate the synthesis

Fig. 3. Densification of UN with 5000 ppm O_2 (Test CH-1).

Fig. 4. UN Hot-Pressed at 6400 psi (44 MPa) at 1400°C for 90 min. Second phase is UO_2 from 5000 ppm impurity oxygen (Test CH-1). Etched with 90 volumes lactic acid, 30 volumes HNO_3 , 3 volumes HF for 45 sec.

process were also initiated. However, these techniques were not perfected before the termination of the project.

Uranium nitride powder was prepared by passing undiluted hydrogen over the uranium metal in the tube furnace at 220°C. Excess hydrogen was vented to the box atmosphere, and the flow of argon through the box was adjusted to dilute the hydrogen at least to 4 vol %. The resulting hydride, UH_3 , was decomposed to activated uranium powder by heating in a vacuum at 450°C and then converted to the nitride by slowly introducing nitrogen at a pressure of 3 in. Hg (76 torr or 10 kPa). Then the temperature of the furnace was raised in steps to 200°C and the nitrogen pressure to 1 atm (0.1 MPa) for 7 hr. The resulting nitride, U_2N_3 , was reduced to a nominal composition of UN by heating to 1350°C in a vacuum. The particles as produced are agglomerated; however, many of the ultimate particles are estimated to be smaller than 3 μm in diameter.

The high-temperature reaction furnace, built by the Richard D. Brew Company, was capable of producing temperatures to 2200°C in argon and 2400°C in nitrogen, each at 1 atm pressure, or to 3000°C in vacuum. The furnace was placed in the glove box and used to synthesize nitride powders from metal chips.

The oxygen content in the glove box atmosphere was held to less than 10 ppm and moisture to less than 20 ppm at argon flow rates that produce complete atmosphere exchange in the box 5 times per hour. The supply argon contained, on the average, 5 ppm O_2 and 10 ppm moisture by volume.

Uranium nitride powder was mixed with 20% plutonium nitride and was cold-pressed at 50,000 psi (345 MPa) to a green density of 63%. The pellet was then hot-pressed at 3000 psi (21 MPa) at $1450 \pm 10^\circ\text{C}$. The density and temperature increase of the die were recorded simultaneously. The resulting densification curve was used for the computer simulation of the UN-20% PuN hot pressing, which is described in the following sections in detail.

Analog Computer Simulation of Hot-Pressing

For simulation, Eq. (3) was rearranged and appropriate units were added as follows:

$$\frac{d\rho}{dt} = \frac{5.40}{\beta} \frac{P}{\eta} \left[\frac{1 - \rho}{1 - (1 - \rho)^{2/3}} \right] + \frac{2.198}{\beta} \frac{\tau_c}{\eta} (1 - \rho) \left[0.40 \log(1 - \rho) \right] \quad (10)$$

Figure 5 shows the analog simulation circuit for hot-pressing.

Since an analog computer normally does not allow more than three variables, a digital computer program was written to handle the variables required to simulate the actual hot-press conditions.

Fig. 5. Analog Simulation Circuit for Hot-Pressing.

Digital Computer Program to Predict Densification of UN-20Z PuN at Various Pressures and Temperatures

Systematic analysis of densification during hot-pressing would reduce operational costs of fuel fabrication since a minimal number of experiments would be required to establish the desired fabrication conditions for the various batches of starting material.

The author suggests fitting the model described in Eq. (11) below to the densification data obtained from a hot-pressing experiment and then implementing the model with calculated constants to predict densification characteristics at different pressures. The possibility of predicting the densification for a new temperature profile was also considered.

For hot-pressing mixed (U,Pu)N, the main portion of densification is assumed to be due to the plastic flow mechanism. We define ρ , the densification function, to be the ratio of the density of the compact to the theoretical density. During the period of densification the densification function, ρ , satisfies approximately the differential equation

$$\frac{d\rho}{dt} = f(t, \rho) \equiv \frac{A}{T(t)}(1 - \rho) \left[\frac{1}{1 - (1 - \rho)^{2/3}} + B \ln(1 - \rho) \right], \quad (11)$$

where

$$A = 30D\Omega_0 P/kR^2,$$

$$B = \sqrt{2}\tau_c/P,$$

and

- T = temperature, K,
- D = diffusion coefficient, cm^2/sec ,
- Ω_0 = original vacancy volume, cm^3 ,
- P = pressure, dynes/cm^2 ,
- k = Boltzman constant, 1.38×10^{-16} erg/K,
- R = grain radius, cm, or powder particle radius, cm,
- τ_c = critical shear stress, dyne/cm^2 ,
- t = time, sec.

The time dependence of the temperature is introduced in Eq. (11) to simulate the experimental heating period of the die in the hot press while the

temperature is raised to the desired level. Equation (11) is based on the work of McClelland,²⁰ Murray et al.,²¹ and MacKenzie and Shuttleworth.²²

Appendix B describes the method of numerical solution of Eq. (11). The computer program developed for this purpose is given in Appendix C, and the handling of variables for the calculation is described in Appendix D.

TEST RESULTS AND DISCUSSION

Densification of Mixed (U,Pu)N and UN

Hot-pressing test conditions and the end-point density of UN and mixed (U,Pu)N are shown in Table 1. Referring to tests Pu-1 and Pu-2, the difference in the density is considered due to the hot-pressing pressures of 3.0 and 4.0 ksi (21 and 28 MPa); densification is quite sensitive to pressure at this temperature (1450°C). However, even though pressure is further increased to 5.0 ksi (34 MPa) for test Pu-3, the pellet density does not increase because the temperature is lower (1200°C). Introducing a slightly higher temperature (1300°C) and higher pressure [6.7 ksi (46 MPa)] results in a 98% dense pellet in test Pu-4. This combination of test conditions resulted in an end-point density nearly the same as in test Pu-2, which involved 4.0 ksi (28 MPa) and 1450°C. In this case, the fabrication conditions of test Pu-2 are considered to be better because the life of the hot-pressing die is longer.

To find the effect of pressure in detail, the pellet of test Pu-5 was hot pressed at 3.0 ksi (21 MPa), as shown in Table 1, while the remaining conditions were the same as in test Pu-2, except that the green density was 3% lower. An end-point density of 94% was obtained. The result indicated that at 1450°C one can achieve and control end-point densities between 95 and 99% by suitably increasing the hot-pressing pressures from 3.0 to 4.0 ksi (21 to 28 MPa) with starting green densities between 62% and 66%. As can be ascertained from Table 1, tests Pu-1 and Pu-5 involved nearly identical test conditions except for the higher plutonium nitride content in test Pu-1, and yet the same density resulted. Also, as shown in Fig. 6, the reproducibility of the test method was good. The densification history of these two materials as shown in Figs. 7 and 8 indicates that even though the loading history and the rate of density increase are different, the density of both mixed nitrides reached almost the same point (93%) after 75 min from the initiation of significant deformation. This suggested that the study of temperature-pressure combinations could lead to production of the soundest pellets.

²⁰J. D. McClelland, "Kinetics of Hot Pressing," pp. 157-71 in *Powder Met. Proc. Int. Conf.*, New York, 1960, ed. by W. LeSzyński, Wiley, New York, 1961.

²¹P. Murray, E. P. Rodgers, and A. E. Williams, *Practical and Theoretical Aspects of the Hot Pressing of Refractory Oxides*, AERE-M/R-893 (July 30, 1952).

²²J. K. MacKenzie and R. Shuttleworth, "A Phenomenological Theory of Sintering," *Proc. Phys. Soc., London*, 62: 833-52 (1949).

Table 1. Hot-Pressing Test Conditions and the Results of UN and Mixed (U,Pu)N

Test	Material	Cold Press			Hot Press					
		Pressure		Green Density (%)	Pressure ^a		Temperature (°C)	Time (min)	Pellet Density (%)	Figures Showing Results
		(ksi)	(MPa)		(ksi) ^a	(MPa)				
CH-1	UN	35	241	48	6.4	44	1400 ± 10	90	99+	3, 4, 6
UT-1	UN	40	276	50	2.4	17	1425	90	86	6, 9
UN-1	UN	40	276	60	6.3	43	1400	120	97	6, 11
UN-2	UN	28	193	56	3.1	21	1600	90	81	6, 10
Pu-1	UN-45% PuN	40	276	62	3.0	21	1450	90	94	6, 7
Pu-2	UN-20% PuN	40	276	66	4.0	28	1450	90	99	6, 12
Pu-3	UN-20% PuN	40	276	52	5.0	34	1200	60	80	6
Pu-4	UN-20% PuN	60	414	67	6.7	46	1330	60	98	6
Pu-5	UN-20% PuN	50	345	63	3.0	21	1450	120	94	6, 8

^aAlthough pressures could be controlled to ±20 psi (0.15 MPa) values here are rounded off to 0.1 ksi because of insensitivity of the densification to smaller pressure differences.

Fig. 6. End-Point Density of UN and Mixed (U,Pu)N. Open circles are calculated values.

Fig. 7. Densification of UN-45% PuN, Hot Pressed at 3010 psi (20.8 MPa) at 1450°C (Test Pu-1).

Fig. 8. Densification of UN-20% PuN, Hot Pressed at 3000 psi and $1450 \pm 10^\circ\text{C}$ (Test Pu-5).

Open circles in Fig. 6 indicate an end point density calculated with Eq. (3) based on Pu-5 for the upper curve and Pu-3 for the lower curve. As can be seen, the UN in test UT-1 had a very low hot-pressing pressure of 2.4 ksi (17 MPa) at 1425°C (detailed densification history of this sample is shown in Fig. 9), while test UN-2 shows very low density because of the low hot-pressing pressure of 3.1 ksi (21 MPa) even though the temperature was 1600°C . From this result, it was again suggested that the optimal temperature-pressure combination be found to fabricate the best pellets. Figure 10 shows the microstructure of that sample. It shows the large grain size and pores, which made this pellet extremely friable. Thus, higher pressures and lower temperatures were recommended to control the pellet microstructure.

To prove this point, test UN-1 was hot-pressed at 6.3 ksi (43 MPa) and 1400°C , resulting in an end-point density of 97%. The microstructure of this sample is shown in Fig. 11. The grain size was about half that of the earlier sample, and the pores were smaller and more evenly distributed. Also, this pellet was much stronger than those of test UT-1.

Finally, a high-density mixed (U,Pu)N fuel pellet was fabricated by use of reasonable combinations of conditions in test Pu-2. The pellet was formed in a 0.371-in. (9.42-mm) die at 40 ksi (276 MPa) and a green density of 66% was obtained. The detailed pressure and temperature rise during the hot pressing is shown in Fig. 12. The green pellet was compressed at a lower pressure of 1400 psi (9.6 ksi) to prevent cracking at room temperature. Then the furnace was heated at the rate of $5^\circ\text{C}/\text{min}$. At $940 \pm 10^\circ\text{C}$ densification began, and when the temperature reached 1245°C the density of the pellets had increased from 66 to 72%; at this point, the pressure was raised gradually to 4000 psi (28 MPa). The temperature

ORNL-DWG 75-3478

Fig. 9. Densification of UN Hot-Pressed at 2400 psi (17 MPa) and 1425°C for 100 min (Test UT-1).

Fig. 10. Microstructure of UN Hot-Pressed at 3080 psi and 1600°C (Test UN-2). Density 81%. Etched with 90 volumes lactic acid, 30 volumes HNO₃, 3 volumes HF for 45 sec.

Fig. 11. Microstructure of UN Hot-Pressed at 6300 psi (43 MPa) and 1400°C for 1.5 hr (Test UN-1). Second phase is UO_2 . Density 97%. Etched with 90 volumes lactic acid, 30 volumes HNO_3 , 3 volumes HF for 45 sec.

Fig. 12. Densification of UN-20% PuN Hot-Pressed at 4000 psi (28 MPa) and 1450°C.

continued to increase during this period of time. A smooth density increase was thus accomplished, thereby avoiding gas trapping in the pellets. After 90 min hot-pressing, 99%-dense pellets were obtained.

Analog Computer Simulation of Hot-Pressing

Figure 13 shows the simulation of hot-pressing using the values $\eta = 30 \times 10^{10}$ poise, $P = 3000$ psi, $\tau_c = 1500$ psi, and multiples of these values as listed in Table 2. Referring to Fig. 13, curves B and A are preferable for practical fabrication because of the short period of hot-pressing to obtain maximum density. The limiting factor beyond the B line is the capability of the hot-pressing equipment. According to the results of the simulator we could observe the following:

1. The densification is very sensitive to pressure for the high-viscosity material (D and G) but not for the low-viscosity case (A and E).
2. High pressure with low viscosity will result in maximum density (B), and low pressure with high viscosity will show minimum density (G), as expected.
3. The higher the shear stress the lower is the density (F and H).
4. Limited densities can be obtained after 4 hr of hot-pressing time (C, D, F, H, and G). Thus if we want to obtain 100% of theoretical density within favorable time — such as for B, A, and E — we could estimate from preliminary data and Fig. 13 the minimum pressure and temperature needed.
5. One could predict the minimum pressure required to get high density in reasonable hot-pressing time (compare B and E). Application of unnecessarily high pressure could be avoided to extend die life.
6. The final density is very sensitive to viscosity at high pressures (A and C). Thus, raising the pressing temperature may be more effective than raising the additional pressure for this case.

Digital Computer Simulation of Hot-Pressing

A family of computer-derived densification curves for hot-pressing mixed (U,Pu)N is shown in Fig. 14. Superimposed is a dashed curve of data taken from a hot-pressing experiment on mixed nitride run at 3000 psi (21 MPa) with a steady-state temperature of 1450°C beginning at 65 min. The curve using the model of Eq. (11) that best approximates the experimental curve was obtained with the hot-pressing coefficients $A = 1.296$ and $B = 0.352$. The values of A and B were obtained by trial and error. The remaining curves were obtained by use of the model of Eq. (11) with the same values of A and B but with the pressure varied to predict the densification behavior at different conditions. The curves have been traced from a Calcomp plot of the computer output.

ORNL-DWG 65-1424

Fig. 13. Calculated Densification with Various Numerical Values Simulating Hot-Pressing with Analog Computer.

Table 2. Numerical Values Used for Analog Computer Simulation of Hot-Pressing

Curve ^a	Pressure (psi)	Viscosity (poise)	Shear Stress (psi)
A	3000	3×10^{10}	1500
B	6000	3	1500
C	3000	30	1500
D	3000	300	1500
E	1500	3	1500
F	1500	30	1500
G	1500	300	1500
H	1500	30	3000

^aValues shown are for curves in Fig. 13.

Fig. 14. Calculated Densification of UN-20% PuN Fuel Pellets with Various Hot-Pressing Pressures and Times at 1450°C, Simulated by Digital Computer, Compared with Experimental Data at 3000 psi (21 MPa).

CONCLUSIONS AND RECOMMENDATIONS

1. A green density of 60 to 65% is preferable for fabricating high-density pellets. A density of 99% for mixed (U,Pu)N was obtained at 4000 psi (28 MPa) and 1450°C; a 94% pellet density was obtained at 3000 psi (21 MPa) and 1450°C.

2. As shown in test CH-1, increasing the pressure is a very effective means of increasing the densification of pellets at a given temperature; however, when the temperature is low and the viscosity of the material is high, the pressure is not as effective as the temperature, as shown in test Pu-4. Thus, increasing the temperature of the pellets with low pressure [1400 psi (9.6 MPa)] and then applying higher pressure after the temperature of the pellets exceeds 1250°C for mixed (U,Pu)N is highly recommended. Such an example is shown in Fig. 12.

3. An Analog computer provides an excellent means to check roughly with minimum cost and time how the densification takes place for various materials at elevated temperature and pressure.

4. A computer program was written to simulate hot-pressing. It can be used to predict densification for any high-temperature ceramic materials that follow plastic densification mechanisms. The constants that characterize a given ceramic material must be determined experimentally.

5. Measuring and analyzing techniques developed for continuous densification by hot-pressing proved to be very useful both for the determination of the best fabrication conditions and the evaluation of the fuel pellets. They were used to determine the hot-pressing coefficients,

$$A = 3000P/kP^2 \text{ and } B = \sqrt{2}\tau_c/P.$$

For mixed uranium-plutonium nitride at 1450°C and 3000 psi (21 MPa) the values are $A = 1.296$ and $B = 0.352$. However, care must be exercised in the application of the results. Additional experimental data are required to obtain more reliable A and B values for each hot-pressing temperature and especially for the different starting materials and the different testing conditions, such as powder characteristics, green density of starting material, or heating rate of hot press die and loading sequence during hot-pressing.

6. On the basis of all the experimental work, the three mechanisms: (a) plastic flow; (b) particle rearrangement, sliding, and fragmentation; and (c) stress-enhanced diffusion appear to operate simultaneously or one mechanism operates predominantly, depending upon the hot-pressing conditions and the stage of the densification process. The theory of hot-pressing requires further development to better interrelate the competing mechanisms to describe their relative importance under varying hot-pressing conditions.

At present, even though the assumptions and mechanisms proposed are not perfectly applicable to mixed (U,Pu)N, it appears that mixed (U,Pu)N follows very closely the plastic flow mechanism above 85% of theoretical density under the conditions described for test Pu-5. The utilization of computer programs together with the experimental technique developed in this report is just beginning to serve its useful purpose of prediction and fabrication of advanced reactor fuel and other high-temperature ceramic materials for the future.

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APPENDIX A
DESCRIPTION OF HOT PRESS USED IN GLOVE BOX
AND RECOMMENDED DESIGN POINTS

**Description of Hot Press Used in Glove Box
and Recommended Design Points**

1. Design Data of Hot Press for Glove Box Use

Available space in glove box, in. (m)	30 × 30 × 30 (0.78)
Diameter of die (ATJ or POCO graphite with tungsten die inserts), in. (mm)	
ID of tungsten inserts	0.370 to 0.375 (9.40-9.52)
OD of graphite	2 to 4 (50-100)
Fracture strength of ATJ die, psi (MPa)	3000 to 4000 (21-28)
Maximum pressure applicable to the ATJ punch, psi (MPa)	3000 to 20,000 (21-138)
Induction coil dimensions, in. (m)	
Diameter	5 to 7 (0.13-0.18)
Height	6 to 7 (0.5-0.18)
Coupling efficiency, % (induction coil to die)	94
Power required to heat to 1850°C, kW	12 to 25
A schematic drawing of the design is shown in Fig. 1, p. 7.	

2. Points of Emphasis for a Hot Press Designed for Use in a Glove Box

1. Elimination of the need for disassembling the furnace body after each hot-pressing cycle,
2. reproducibility of the operation, such as automatic sample positioning in the center of the furnace,
3. enough distance between the induction coil and the structural frame to eliminate coupling,
4. no greater voltage across the induction coil than needed,
5. elimination of sharp corners and provision of enough working space to permit the safe handling of plutonium with gloves,
6. prevention of argon leakage from the area where parts are attached to the glove box, and
7. furnace design that eliminates the difficulty of repair and maintenance in a small glove box.

APPENDIX B

NUMERICAL SOLUTION OF EQ. (11) FOR COMPUTER SIMULATION

Numerical Solution of Eq. (11) for Computer Simulation

D. E. Arnurius, V. A. Singletary, and J. Y. Chang studied how to solve numerically the initial value problem:

$$y' = f(t, y), \quad (1)$$

$$y(\hat{t}) = \varepsilon(0, \eta), \quad (2)$$

on the interval $I = [t_0, t_1]$, where (1) t is a piecewise-continuous, non-decreasing, linear polynomial on I , (2) $\hat{t} \in I$, and (3) η is the unique zero ($B > 0$) of f in $(0, 1)$ when f is regarded as a function of its second argument. Let $I = UI_\alpha$ where I_α is a closed interval and ' T ' is constant on the interior of I_α . Let J be the interior of any of the I_α . If y_1 is a solution of (2), then on J y_1 has derivatives of all orders and $y_1 > 0$, $y_1' > 0$, $y_1'' < 0$, and $y_1''' > 0$. Let y_2 be a solution of (2) and suppose that $y_1(\tilde{t}) - y_2(\tilde{t}) > 0$ for some $\tilde{t} \in I$. Then the function $e_1 = y_1 - y_2$ satisfies $e_1 > 0$, $e_1' < 0$, and $e_1'' > 0$ on J . Thus the solutions of distinct initial-value problems of the type described in (2) have an inherent tendency to approach one another as t increases. Thus an error introduced at $t = x$ by a numerical approximation to a solution of (2) is diminished naturally if the approximation is determined in the direction of increasing t . Of course an error at $t = x$ is magnified if the approximation is determined in the direction of decreasing t . For this reason, if $\hat{t} \in (t_0, t_1)$, a shooting procedure is employed to approximate the solution on $(t_0, \hat{t})$.

Let ρ be the solution of an initial-value problem (2) that we want to approximate numerically. Let $\varepsilon > 0$ ($\varepsilon \approx 10^{-3}, 10^{-4}$) be given. Then the computer program determines a numerical approximation, ρ_α , that satisfies

$$|\rho(\tilde{t}) - \rho_\alpha(\tilde{t})| \leq \varepsilon$$

for all discrete points $\tilde{t}$ at which ρ_α is determined.

The program used the Taylor expansion method of order 3 to determine ρ_α at successively higher values of t . In particular, suppose

$$|\rho(x) - \rho_\alpha(x)| \leq \varepsilon \quad (3)$$

for some $x \in J$. Let y_1 and $\tilde{\rho}_\alpha$ satisfy the initial-value problems (2) with $y_1(x) = \rho_\alpha(x) + \varepsilon$ and $\tilde{\rho}_\alpha(x) = \rho_\alpha(x)$, respectively. Let $e_1 = y_1 - \tilde{\rho}_\alpha$. It turns out that if

$$y_1(x+h) - \rho_\alpha(x+h) \leq e_1(x) = \varepsilon, \quad (4)$$

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then (3) is satisfied with $x = x + h$. Using Taylor's formula

$$\begin{aligned} e_1(x+h) - \rho_a(x+h) &= [e_1(x+h) - \tilde{\rho}_a(x+h)] + [\tilde{\rho}_a(x+h) - \rho_a(x+h)] \\ &= e_1(x+h) + \frac{h^3}{3!} \tilde{\rho}_a'''(x+\theta h) \\ &= e_1(x) + h e_1'(x) + \frac{h^2}{2!} e_1''(x+\hat{\theta}h) + \frac{h^3}{3!} \tilde{\rho}_a'''(x+\theta h) \end{aligned}$$

with $\theta = \theta(h)$, $\hat{\theta} = \hat{\theta}(h) \in (0, 1)$. Thus (4) is equivalent to

$$e_1'(x) + \frac{h}{2!} e_1''(x+\hat{\theta}h) + \frac{h^2}{3!} \tilde{\rho}_a'''(x+\theta h) \leq 0 \quad (5)$$

with $\theta, \hat{\theta} \in (0, 1)$. The coefficients of h and h^2 are positive, and $e_1'(x) < 0$. Upper bounds for e_1'' and $\tilde{\rho}_a'''$ valid on $[x, x+v]$ are calculable. From these an $H > 0$ is determined so that (5) holds for all $h \in [0, H]$. Thus, except for machine rounding errors,

$$\rho_a(x+h) = \tilde{\rho}_a(x) + h \tilde{\rho}_a'(x) + \frac{h^2}{2!} \tilde{\rho}_a''(x)$$

for $h \in [0, H]$. Since (4) is satisfied with strict inequality for all $h \in [0, H]$, it is believed that the inequality (3) is not vitiated by machine rounding errors.

APPENDIX C

PROGRAM FOR DIGITAL COMPUTER SIMULATION OF HOT PRESSING

PROGRAM TEST (INPUT, OUTPUT, TAPES0, TAPES=INPUT, TAPES=OUTPUT)

NOT PRESSING STUDY ON THE MIXED URANIUM, PLUTONIUM NITRIDE
FOR ADVANCED REACTOR FUEL

BY JI YOUNG CHANG

DIMENSION T(2000), Y(2000)
COMMON/DHA/RHOF, TOP, TO, TOSS, YPB, TONCPR, YTFM, YMSER, YLCEB, TOSAV,
1 TGB, TLIN, TIMST, DA, XEXP(100), YEXP(100), TEMP2C(100), TTT(50), TMP(50),
2 PSIS, TPTVAR,
3 NPK, NPRS, NPLOT, NPLOTS, NAB, NABS, NSERCH, NSRCHP, NSTEAD, NPHOFL, NFXPDY,
4 INPUT, NOXEXP
COMMON XL, ZL, XM, ZM, A, B, TEMP, TB, TF, YB, EMX, TINCPR, RHOFCS, N
COMMON/DEA/T, Y

WE WANT TO SOLVE THE INITIAL VALUE PROBLEM
$$Y' = (A/TMP(T)) (1-Y) (1/(1-(1-Y)^{(2/3)})) + B(LN(1-Y))$$

Y(TSP)=YB
WHERE A AND B ARE CONSTANTS WITH A.GT.0, B.GE.0
AND WHERE TMP(T) IS A CONTINUOUS FUNCTION OF TIME IN SECONDS.
Y.GT.0 AND IF YF IS THE UNIQUE ZERO OF
$$1/(1-(1-Y)^{(2/3)}) + B(LN(1-Y))$$
 IN (0,1) (B.GT.0), THEN MUST HAVE
YB.LT.YF
THEN Y(T).LT.YF FOR T.GE.TOP. BETWEEN NODES OF TEMP. PROFILE,
Y HAS DERIVATIVES OF ALL ORDERS. HENCE IT HAS A TAYLOR SERIES EXP
THERE. IN THESE INTERVALS WE APPROX. SOL. BY USING THE TAYLOR
APPROX THRU THE QUADRATIC TERM. I.E., $Y(T+H) = Y(T) + H*Y'(T) + H^2*Y''(T)$.
TWO ERRORS ARE INVOLVED IN OUR CASE. (1) THE TRUNCATION
ERROR ASSOCIATED WITH OUR TAYLOR APPROX. AND (2) THE ERROR IN OUR
APPROXIMATION TO THE TRUE SOLUTION AT T.

CURRENT TEMP. PROFILE IS A PIECEWISE CONTINUOUS LINEAR POLY. WITH
TEMP. VALUES AT THE NODE POINTS GIVEN IN THE ARRAY TMP.
TMP(1) CORRESPONDS TO TIME TGB (THIS IS BASE TIME FOR PROFILE
INTERNALLY TIME IS RECORDED IN SECONDS), TMP(2) TO TIME TGB+TLIN.

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```

45      C      THE LAST DEFINED ELEMENT IN ARRAY TMP CORRESPONDS TO TIME TPTVAR.
      C      THE TEMP. IS ASSUMED CONSTANT FOR TIME .GE. TPTVAR. THE SLOPE OF
      C      TEMP. PROFILE (TS IN PROG.) ON INTERVAL DETERMINED BY THE M-TM
      C      , (M+1)-TM NODES IS (TMP(M+1)-TMP(M))/TLIN.
50      C      CONSTANT TEMPERATURE CASE IS HANDLED IN SUB. TMPCON
      C
      C      IF DA .GT. 0 THEN CYCLE THRU PROG. TWICE WITH TEMP. PROFILES
      C      TMP=DA AND TMP=DA RESPECTIVELY. SINCE DON'T KNOW TRUE TEMP.
55      C      PROFILE, WE MAY WANT TO BOUND TRUE PROFILE BETWEEN 2 PROFILES
      C      DEFINED IN ABOVE MANNER. WITH TEMP. OF ORDER 1300 SOL. SEEMS
      C      INSENSITIVE TO SMALL CHANGES (9 DEGREES) IN PROFILE. VARIABLE TPIC
      C      IS USED IN THIS CONNECTION. IF DA.EQ.0, RUN WITH STORED TEMP.
      C      PROFILE.
60      C      TODAY=DATE(DUMMY)
      C      MLOW=.100
      C      MLOW IS MIN. STEP SIZE ALLOWED IN REG. SIVL.LE.VI.
      C      TLIN = TIME INCREMENT IN SECONDS BETWEEN TWO CONSECUTIVE
      C      TEMPERATURES IN ARRAY TMP.
65      C      NSTEAD POINTS TO LAST ELEMENT IN TMP ARRAY.
      C      TMP(NSTEAD)=STEADY STATE TEMPERATURE.
      C      TIMST=BEGINNING TIME OF STEADY STATE (TEMPERATURE).
      C      O3=1.00/3.00
      C      T3=2.00/3.00
70      C      T9=2.00/9.00
      C      Q=-3.00
      C      SET NPROFL=1 AND NEXPOT=1 INITIALLY TO READ TEMP. PROFILE AND
      C      EXPERIMENTAL DATA.
      C      NPROFL=1
75      C      NEXPOT=1
      C      NSEARCH=0
      C      777 CONTINUE
      C      IPSK=0
      C      ISKIP=0
80      C
      C      EITHER PROGRAM IS SEARCHING FOR AN INITIAL Y AT THE INITIAL TIME.
      C      TOP, SO AS TO MATCH WITH A GIVEN Y,VTFM, AT TIME TO OR ELSE IT IS
      C      RUNNING A NORMAL CASE.
85      C      IF (NSEARCH.EQ.0) GO TO 4250
      C      RHOF=8.00
      C      NSEARCH=NSEARCH+1
      C      IF (N.GT.1) GO TO 4251

```

PROGRAM TEST 7600 OPT=1 FTN NO.1 LEVEL 71 07/15/75 08.20.55

```

90      PRINT 4252
        4252 FORMAT('IN=1 IN SEARCH')
        GO TO 791
C      KNOW T(N).LE.TP EST. Y(TF) BY LIN. INTERPOLATION
C      TF AND T ARRAY ARE BOTH IN TERMS OF SECONDS WHEN ARRIVE AT 4251.
C      IMPORTANT THING IS THAT THEY HAVE THE SAME UNITS OF TIME.
95      4251 YTF=Y(N-1)+(Y(N)-Y(N-1))*(TF-T(N-1))/(T(N)-T(N-1))
        IF (ABS(YTF-YTFM).LE.EMX) GO TO 4253
        IF (YTF.LT.YTFM) GO TO 4254
        YMSER=Y8DOON
        GO TO 4255
100     4253 Y8=Y8DOON
        4250 NSRCHP=NSRCHP-NSERCH
        NSRCH=0
        TO=TOSS
        NP=NPQS
        NPLOT=NPLOTS
        NAB=NABS
        GO TO 4271
        4254 YLSER=Y8DOON
110     4255 Y8=.500*(YLSER+YMSER)
        IF (NSRCH.EQ.0) GO TO 4256
        GO TO 4271
        4250 CALL INDATA
        PSIC=PSIS
        4271 CONTINUE
C
115     IF (Y8.GT.0.00) GO TO 3000
        CAL. Y8 FROM STORED EXP. CURVE.
        IF (TOP.CE.XEXP(1)) GO TO 3001
        3003 INPUT=1
        GO TO 709
120     3001 IF (TOP.CE.XEXP(NOXEXP)) GO TO 3003
        XEXP(1).LE.TOP.LY.XEXP(NOXEXP)
        3002 DO 3004 I=2,NOXEXP
        IF (TOP.CE.XEXP(I)) GO TO 3004
        Y8=YEXP(I-1)+(TOP-XEXP(I-1))*(YEXP(I)-XEXP(I-
        1))
        GO TO 3000
125     3004 CONTINUE
        3000 CONTINUE
        Y(1)=Y8
        Y8DOON=Y8
C      CONVERT TIME IN MIN TO SEC
130

```

```

      TBP=60.00*TOP
      TF=60.00*TD
135      TINCPR=60.00*TONGPR
      TF1=AMIN1(TF,TF1VAR)
      MEMX=.500*EMX
      TPIC=-DA
      T(1)=TOP
140      IF(TBP.LT.TF1VAR) GO TO 4130
      TINC=0.00
      TB=TBP
      GO TO 4131
4130      W1=TBP-TGB
145      IF(W1.LT.0.00) GO TO 711
      JG=W1/TLIN
      TB=TGB+JG*TLIN
      TINC=TBP-TB
4131      TINGS=TINC
150      TGS=TB
      INPUT=0
      IF(RHOF.LE.0.00) GO TO 5011
      IF(RHOF.LT.1.00) GO TO 5012
      INPUT=1
155      GO TO 705
C      CAL. B
5012      RHOFB=1.00-RHOF
      B=-1.00/(ALOG(RHOFB)*(1.00-RHOFB**TJ))
      GO TO 5003
160      C      SUPPOSE B IS GIVEN. FIND RHO FINAL. NEED TO THREE FIGURES ONLY.
C      USE BISECTION IN OPEN UNIT INTERVAL. IF B=0, THEN RHO FINAL = 1.
5011      IF(B.GT.0.00) GO TO 5000
      IF(B.EQ.0.00) GO TO 5010
C      B.LT.0
165      INPUT=1
      GO TO 705
5010      RHOF=1.00
      GO TO 5003
5000      TL=0.00
170      TM=1.00
      DO 5001 I=1,10
      TM=.500*(TL+TM)
      TMC=1.00-TM
      GV=1.00/(1.00-TMC**TJ)+B*ALOG(TMC)
175      IF(GV.GT.0.00) GO TO 5002
      TM=TM

```

```

PROGRAM TEST          7800      OPT=1          PTM 4.1 LEVEL 71      07/15/75      08.20.56

      GO TO 5001
5002 TL=TM
5001 CONTINUE
      WOP=.500*(TL+TM)
5003 CONTINUE
      XL=0.00
      XM=1.00
      AT27=2.700*B
      DO 10 I=1,8
      X=.500*(XL+XM)
      CAL M(B,X)^(1/5)
      M1X04=((16.400-X)*X-1.00)*X-AT27*(1.00-X)*X
      IF(M1X05.GT.0.00) GO TO 11
      XL=X
      XM=X
      GO TO 10
11 XM=X
10 CONTINUE
      ZL=XL*.1.5
      ZM=XM*.1.5
      FV1V=(19*(5.00-XL)/( SORT(XL)*(1.00-XL)*.11)+0/2L)
      FV1M=(19*(5.00-XM)/( SORT(XM)*(1.00-XM)*.11)+0/2M)
      U02=AMAX1(FV1V,FV1M)
      IF(18.LT.FV1V) GO TO 5133
      IM=CONST. TEMP. ZONE
      T00=TMP(MSTEAD)+TPIC
      GO TO 5136
5133 T00=TMP(JG+1)+TPIC+TINC*(TMP(JG+2)-TMP(JG+1))/TLIM)
5136 Y0=1.00-Y11
      IF(A.GT.0.00) GO TO 5200
      IF(VPM.GT.0.00) GO TO 5100
      CAL Y*(18) USING EXP. DATA CURVE
      C ASSUME ARRAY XEXP IS INCREASING
      C BINARY SEARCH MORE EFF. BUT DONE ONLY ONCE.
      IF(TOP.GE.XEXP(1)) GO TO 5101
      C CANNOT CAL. DER. FROM EXP. DATA CURVE.
      GO TO 5102
5101 IF(TOP.LT.XEXP(NOXP)) GO TO 5103
      C CANNOT CAL. DER. FROM EXP. DATA CURVE.
5102 PRINT 5104
5104 FORMAT(1)CANNOT CAL. Y*(17 INIT.) FROM DATA CURVE.*/))
      INPUT=1
      GO TO 705
5101 DO 5105 I=2,NOXP
      IF(TOP.GE.XEXP(I)) GO TO 5104
220

```


PROGRAM TEST 7600 CONT=1 FTM 4.1 LEVEL 71 07/15/75 08.20.55

```

C      XEXP(I-1),LE.TOP,LT,XEXP(I), I.GY.1
5106 VPA=(VEXP(I)-VEXP(I-1))/(60.00*(XEXP(I)-XEXP(I-1)))
C      IF (TOP.LT..500*(XEXP(I)+XEXP(I-1)))GO TO 5107
C      VPA IS HIGH EST.
C      VPA=.98500*VPA
C      GO TO 5108
5107 VPA=1.01500*VPA
5108 VPB=VPA
C      GO TO 5100
5105 CONTINUE
5100 CONTINUE
A=(VPB*TOON)/(YBC*(1.00/(1.00-YBC**T3)+R*ALOG(Y3C)))
C      GO TO 5677
5200 VPB=A*YBC*(1.00/(1.00-YBC**T3)+B*ALOG(YAC))/TOON
5677 CONTINUE
IF (ISKIP.GT.0) GO TO 6999
ASAVE=A
BSAVE=B
ISKIP=1
C      CHECK INITIAL VALUE AGAINST RHOF
6999 IF (VP.LT.RHOF) GO TO 705
INPUT=1
705 CONTINUE
RHOFCS=1.00-RHOF
IF (NSRCH.NE.0) GO TO 4270
PRINT 1151,YB,TOP,TO,TONCPR,A,B,EMX,DA,RHOF,VPB,PSIC
1151 FORMAT(1Y9,1PE11.4,1X INITIAL TIME(MIN)=0PF9.2/
1X FINAL TIME(MIN)=0F9.2,1X TIME INCREMENT FOR PLOT AND LIST(MIN)=0F
28.3,1X A=1PE11.4/
3X B=1PE11.4,1X MAX. ERROR IN NUMERICAL APPROX.=1PE11.4/
4X TEMP. SHIFT PARA.=1PE11.4/
5X RHO FINAL =0E11.4,1X Y=0F11.4,1X E11.4/
6X PRESSURE(PSI)=0PF8.1/)
PRINT 1989,TMP(NSSTEAD),TIMST
1989 FORMAT(1X STEADY STATE TEMP.=0F7.1,1X BEGIN STEADY STATE =0F7.2/)
PRINT 1152,NPR,NPLOT,NAB,TODAY
1152 FORMAT(1X NPR =12.3X,NPLOT =12.3X,NAB =12.10X,DATE = A8)
IF (NSRCH.NE.0) PRINT 4291,TOSAV,YTFM,NSRCHP
NSRCHP=0
4291 FORMAT(1X MATCH TIME =0F6.2,5X MATCH VALUE =0F7.5,5X NO. ITER.=13
1)
PRINT 2,PSIS
2 FORMAT(1X EXPERIMENTAL DATA=10X,PRESSURE (PSI)=0F8.1//
16X TIME=6X,RHO=6X,TEMP(UNSHIFTED)=/)

```

PROGRAM TEST

7600 OPT=1

FTN 4.1 LEVEL 71 07/15/75 08.20.45

```

265      PRINT 160,(XEXP(I),YEXP(I),TEMPZC(I),I=1,NOXEXP)
      160 FORMAT(F11.2,F10.5,F9.1)
      4270 CONTINUE
      IF (INPUT.EQ.0) GO TO 5050
      PRINT 5057
270      5057 FORMAT(// * TROUBLE WITH PARAMETERS.*/)
      GO TO 791
      5050 CONTINUE
      IF (NPLOT.NE.0) GO TO 715
      IF (IPSY.GT.0) GO TO 715
275      IPSK=1
      CALL GRAPH(XEXP,YEXP,NOXEXP,1,CMOF,YB,YPB,A,R,TOP,ENH,PSIC,
      1TMP(INSTEAD),TIMST)
      715 CONTINUE
      152 CONTINUE
280      TINC=TINGS
      TB=TBS
      YB=Y(1)
      YH=1.00-ZH
      YL=1.00-ZL
285      YBC=1.00-YB
      YINC=0.00
      N=1
      M=JG
      H=150.00
290      C MAY USE PRINT FACILITIES OF REG. 3 WHEN CROSS REG. 2. H MAY BE
      C SMALL. NSJ USED TO SET H TO 150.00 FIRST TIME IN REG. 3.
      NSJ=1
      IF (TB.LT.TFTVAR) GO TO 2002
      C IF HERE TEMPERATURE IS CONSTANT.
295      TEMP=TMP(INSTEAD)+TPIC
      GO TO 2001
      2002 IF (YB.GE.YH) GO TO 2003
      C NS1=0 IN REGION 1. I.E., Y.LE.YH
      NS1=0
300      GO TO 200
      2003 IF (YB.GE.YL) GO TO 2004
      C NS1=1 IN REGION 2. I.E., YH.LE.Y.LE.YL.
      NS1=1
      YH=YL
305      200 M=M+1
      YPR=TINGPR+TINC
      TA=TMP(M)+TPIC
      TS=(TMP(M+1)-TMP(M))/TLIN

```

```

310      TSM3=Q*TS
          TS2T2=2.00*TS*TS
901      YC=YBC-YINC
          TT=TA+TS*TING
          YC23=YC**T3
          ADT=A/TT
315      C=B*ALOG(YC)
          D=1.00-YC23
          F=ADT*(YC*(1.00/D+C))
          FY=-ADT*(C+B*(1.00-03*YC23)/(D*D))
          YMC=YC-EMX
320      IF(YMC.LE.RHOFCS) GO TO 700
          FM=ADT*YMC*(1.00/(1.00-YMC**T3)+B*ALOG(YMC))
          IF(FM.LT.0.00) GO TO 400
          IF(INS1.EQ.J) GO TO 971
          FYY=ADT*BOV2
325      GO TO 972
          971 CONTINUE
          FYY=ADT*(T3*(5.00-YC23)/(SQRT(YC23)*D*D*D)+B/YC)
          972 FYYF=F*FYY
          OYP=FY-TS/TT
330      C    P0 IS (3-ND DERIVATIVE OF Y EVALUATED AT X)/6
          P0=(FYYF+FY*(FY+TSM3/TT)+TS2T2/(TT*TT))*F/6.00
          C0=(FM-F)/P0
          C1=MEMX*(FYYF+FY*OYP)/P0
          ZNEG=(-C1-SQRT(C1*C1-4.*C0))*0.5
335      H=.9500*C0/ZNEG
          IF(H*(H+C1)+C0.GE.0.00) GO TO 500
          C    WORK IN INTERVALS DETERMINED BY SUCCESSIVE NODES. CAL. H MAY
          C    BE SO LARGE THAT WE WOULD LEAVE CURRENT INTERVAL.
          IF(TINC+H.LE.TLIN) GO TO 902
          H=TLIN-TINC
340      C    TINC+H.GE.TLIN BY ROUNDING ON IBM 360 LINE.
          902 DYPL=.500*OYP
          DY=H*F*(1.00+H*DYPL)
          IF(YB+(YINC+DY).GE.YM) GO TO 600
345      977 CONTINUE
          IF(TINC+H.LT.TPR) GO TO 303
          HC=TPR-TINC
          TBL=TB+TINC
          950 OYC=HC*F*(1.00+HC*DYPL)
350      TPR=TPR+TINCPR
          TBLHC=TBL+HC
          IF(TBLHC.GT.TF) GO TO 700

```

FTN 4.1 LEVEL 71 07/15/75 08.20.55

PROGRAM TEST 7600 OPT=1

```

355      N=N+1
          T(N)=TBLMC
          Y(N)=YB+(YINC+OYC)
          MC=MC+TINCP
          951 IF (MC.LE.M) GO TO 950
          903 YINC=YINC+Y
              TINC=TINC+H
          IF (TINC.L.TLIN) GO TO 901
          C      MUST GO TO NEXT TIME PERIOD
              TB=TB+TLIN
              YB=YB+YINC
              YBC=1.00-Y3
              YINC=0.00
              YINC=0.00
          IF (YB.LY.TF1) GO TO 203
          IF (TB.GE.TF) GO TO 156
              TEMP=TA+TS*TLIN
          2001 CALL TMCPCN
          156 CONTINUE
          700 IF (NSECH.GT.0) GO TO 777
          713 DO 713 I=2,N
              713 T(I)=T(1)/60.00
              IF (MPR.NE.1) GO TO 731
                  MP=N/4
              IF (N-4*MP.EQ.0) GO TO 3300
                  T(N+1)=0.00
                  T(N+2)=0.00
                  T(N+3)=0.00
                  Y(N+1)=0.00
                  Y(N+2)=0.00
                  Y(N+3)=0.00
                  MP=MP+1
          9300 NROW=0
              II=1
          9102 NROW=NROW+50
              IF (MP.GT.NROW) GO TO 9100
                  MP=MP-NROW+50
                  NCOL2=MPR
                  NCOL3=MPR+MPR
                  NCOL4=MPR+NCOL3
                  NSTOP=1
                  IT=II+MPR-1
                  GO TO 9750
          9100 NCOL2=50

```

PROGRAM TEST 7600 OPT=1 FTN 4.1 LEVEL 71 07/13/75 08.20.55

```

C      IT=I+49
    Y(I)=Y8
9750 PRINT 9010,RHOF,Y(1),YPB,A,B,TOP,EMX,PSIC,TODAY
9010 FORMAT(*1RHOF=F6.3,X*Y8=F6.3,X*YPB=*F6.3,X*A=*FP6.3,X*B*=
    F7.3,X*TOP=F7.3,X*EMX=*F6.3,X*PSI=*FP6.3,X*DATE =A8//
    26*X*TIME*5X*RHO*8X*TIME*5X*RHO*8X*TIME*5X*RHO*)
9103 PRINT 9020,(TK),Y(K),T(K*NCOL2),Y(K*NCOL3),Y(K*NCOL4)
    T(K*NCOL4),Y(K*NCOL4),K=II,IY
9020 FORMAT(4(F11.2,F9.5))
    II=II+200
    IF(NSTOP.EQ.0) GO TO 9102
701 IF(MPLOT.NE.0) GO TO 702
    CALL GRAPH(T,Y,N-2,RHOF,Y8,YPB,A,B,TOP,EMX,PSIC,TMP(NSTEAD),
        TIMST)
702 IF(IDA.EQ.0.00) GO TO 703
    TPIC=TPIC+DA*OA
    IF(TPIC.LE.OA) GO TO 152
703 CONTINUE
704 IF(INAB.EQ.0) GO TO 777
    NAB=NAB-I
    READ(S,150) PSIC
    IF(Eof(S)) STOP,69
150 FORMAT(E9.3)
    69 A=ASAVE*(PSIC/PSIS)
    B=BSAVE*(PSIS/PSIC)
    RHOF=0.DD
    Y8=Y(1)
    GO TO 3000
400 GO TO 700
500 PRINT 599
599 FORMAT(*1QUADRATIC INEQUALITY NOT SATISFIED BY M*)
    GO TO 700
600 IF(NS1.NE.0) GO TO 603
    C   IF HERE, Y(X) IN REG. 1
    C   CHECK TO SEE IF CAL. H ACCEPTABLE THRUOR INTO) REG. 2
    C   IF NOT, OOM-T TRY TO MODIFY CAL. H TO GET ACCEPTABLE VALUE THAT
    C   WE CAN USE TO COME INTO REG. 2. JUST CAL. H SO THAT
    C   VIX(H)=YM. PROG. RUNS TOO FAST TO WORRY ABOUT THIS INEFFICIENCY.
    B0=P*AO7+B0VZ
    Q0=(BO+F)*Y*(F+(TSM3/TI)+TS2T2/(TI*T))*F/B.OO
    CC0=(FH-F)/QQ

```

PROGRAM TEST

7600

OPT=1

FTN 4.1 LEVEL 71

07/15/75

08.20.55

```

      CC1=MEHX*(80+FY*DYP)/Q0
      IF (H*(H+CC1)+CC0.GE.0.00) GO TO 602
C     CAN CAL. Y INTO REG. 2 FROM OUR CURRENT TIME VALUE.
      IF (YB+(YINC+DY).GE.YL) GO TO 603
445 C     OUR Y(X+H) IN REGION 2. SETUP LOOP FOR REGION 2.
      604 NS1=1
      YH=YL
      GO TO 977
C     IF COME TO 602, CAN'T CAL. INTO REG. 2 FROM CURRENT PT. MUST
450 C     DETERMINE H SO THAT Y(X+H)=YH. H SATISFIES YB+YINC+(H*(1+H*DYPL)
C     )=YH
      602 E1=1.00/DYPL
      E0=(YINC-(YH-YB))/(F*DYPL)
      ZP=(-E1+DSQRT(E1**2-4.00*E0))*0.500
455 H=E0/ZP
      DY=(YH-YB)-YINC
      GO TO 604
C     IF AT 603 Y CAN BE CAL. THRU WHOLE OF REG. 2   CAL. H SO THAT
C     Y(X+H)=YL
460 603 E0=(YINC-(YL-YB))/(F*DYPL)
      E1=1.00/DYPL
      ZP=(-E1+DSQRT(E1**2-4.00*E0))*0.500
      H=E0/ZP
C     GO TO REGION 3
465 GO TO 360
      711 PRINT 712
      712 FORMAT(*1 TIME IS TOO SMALL FOR TEMP. PROFILE.*)
      791 IF (NAB.EQ.0) GO TO 777
      DO 792 I=1,NAB
470 READ(5,150) ABH
      IF (EOF(5)) 2000,69
      792 CONTINUE
      GO TO 777
C     REGION 3 FOLLOWS. YL.LE.Y.
475 2004 H=150.00
      300 M=M+1
      TPR=TINCPR+TINC
      TA=TMP(M)+TPIC
      TS=(TMP(M+1)-TMP(M))/TLIN
480 TSM3=Q*TS
      TS2T2=2.00*TS*TS
      301 YC=YBC-YINC
C     MAY USE PRINT FACILITIES OF REG. 3 WHEN CROSS REG. 2. H MAY BE
C     SMALL. NS3 USED TO SET H TO 150.00 FIRST TIME IN REG. 3.

```

PROGRAM TEST

7600

OPT=1

FTN 4.1 LEVEL 71

07/15/76 08.20.55

```

485      IF(NS3.EQ.0) GO TO 4728
        M=150.00
        NS3=C
4728     CONTINUE
        TT=TA+TS*TING
490      YC2J=YC**TJ
        ADT=A/TT
        C=B*ALOG(YC)
        D=1.00-YC2J
        F=ADT*(YC*(1.00/D+C))
495      FY=-ADT*(C+B*(1.00-03*YC2J)/(D*D))
        YHC=YC-EMX
        IF(YHC.LE.RHOFCS) GO TO 700
        FH=ADT*YHC*(1.00/(1.00-YHC**TJ)+B*ALOG(YHC))
        IF(FH.LT.0.00) GO TO 400
500      OYP=FY-TS/TT
        DYPL=.500*OYP
        P2=FH-F
        HOLD=FY*OYP
        HOLD1=FY*(FY+TSM3/TT)+TS2T2/(TT*TT)
505      JI=0
        JD=0
        GO TO 305
303     IF(JD.GT.0) GO TO 320
        JI=1
510      305     MS=M
        M=1.500*M
        UVS=DY
302     DY=M*F*(1.00+M*DYPL)
        YCRJ=YC-DY
515      YCRJ2J=YCRJ**TJ
        FYYJ=AOT*(T9*(5.00-YCRJ2J)/( SORT(YCRJ2J)*(1.00-YCRJ2J)**3)+B/YCRJ
        1)
        FYYF=FYYJ*F
        P0=(FYYF+HOLD1)*F/6.00
520      P1=(HOLD+FYYF)*HEMX
        IF((M*P0+P1)*M+P2.LT.0.00) GO TO 303
        IF(JI.GT.0) GO TO 304
        JD=1
        M=TJ*M
525      IF(M.GT.HLOW) GO TO 302
        PRINT 1003,M,HLOW
1003     FORMAT(*1M= *E11.4,5X*LESS THAN HLOW= *F11.4)
        GO TO 700

```

PROGRAM TEST

7600

OPT=1

FTN 4.1 LEVEL 71

07/15/75

00.20.55

```
530      304 H=HS
C      C WORK IN INTERVALS DETERMINED BY SUCCESSIVE NODES. CAL. H MAY
C      BE SO LARGE THAT WE WOULD LEAVE CURRENT INTERVAL.
      320 IF(TINC+H.LE.TLIN) GO TO 360
      H=TLIN-TINC
535      360 DY=H*F*(1.00+H*DYPL)
      IF(TINC+H.LT.TPR) GO TO 323
      MC=TPR-TINC
      YBL=YB+TINC
      350 DYC=MC*F*(1.00+MC*DYPL)
      TPR=TPR+TINCPR
540      YBLMC=YBL+MC
      IF(YBLMC.GT.TF) GO TO 700
      N=N+1
      T(N)=YBLMC
      Y(N)=YB+(YINC+DYC)
545      351 MC=MC+TINCPR
      IF(MC.LE.H) GO TO 350
      323 YINC=YINC+DY
      YINC=YINC+H
      IF(TINC.LT.TLIN) GO TO 301
550      TB=TB+TLIN
      YB=YB+YINC
      YBC=1.00-YB
      YINC=0.00
      YINC=0.00
555      IF(TB.LT.TF1) GO TO 300
      IF(TB.GE.TF) GO TO 700
      TEMP=TA+TS*TLIN
      GO TO 2001
560      2000 IF(NPLOT.EQ.0) CALL PLOT3
      STOP
      END
```



```

      SUBROUTINE THPCON
      C THIS SUBROUTINE APPLIES WHEN TEMPERATURE IS CONSTANT.
      COMMON XL,ZL,XM,ZM,A,B,TEMP,TB,TF,YB,EHX,TINCPR,HMOFGS,N
      COMMON/DEA/T,Y
5      DIMENSION Y(2000),Y(2000)
      C SOLVE DIFF EQ.  $Y' = F(X,Y) = A/T(X) \cdot (1-Y) \cdot (1/(1-(1-Y)^2/3) + B \cdot \log(1-Y))$ 
      C WHERE T(X) IS NOW CONSTANT AND AN INITIAL VALUE, YB, IS GN. WITH
      C ERROR +OR- EHX (1.001 OR SO FOR EHX). THEORETICALLY THE ERROR
      C DIMINISHES WITH INCREASING X. CODED IN HOPE THAT THE ERROR IN
10      C OUR NUMERICAL APPROX. IS +OR- EHX AT MOST.
      C USE TAYLOR APPROX THRU QUAD. TERM. THUS ERROR OF ORDER  $H^3$ 
      C WHERE H IS THE STEP SIZE. OUR APPROX VALUE IS LOW. H IS COMPUTED
      C AT EACH STEP TO INSURE COMPLETE ERROR CONTROL.
      C ISOLATE THE ZERO OF  $H(B,X)$  THAT LIES IN THE INTERVAL (0,1) BY
15      C BISECTION, WHERE  $H(B,X) = -5X + 34X^2 - 5X^3 - 13.5B \cdot (1-X)^4$ 
      C AND  $X = U^2 = (1-Y)^2/3$ , Y IN (0,1). LET (UL,UH) BE THE DETERMINED
      C INTERVAL AND LET  $UL = (1-YL)^2/3$ ,  $UH = (1-YH)^2/3$ . THEN  $YH, LT, YL$ 
      C ESSENTIALLY 3 REGIONS FOR DIFF. EQ., (0,YH), (YH,YL), (YL,1)
      C IN REGION 1, (0,YH) FYY IS MONO. DECREASING.
20      C IN REGION 2, (YH,YL) FYY LE. MAX(FYY(YH), FYY(YL))
      C IN REGION 3, (YL,1) FYY IS MONO. INCREASING
      YH = 1.00 - ZH
      YL = 1.00 - ZL
      HLOW = .00100
25      T3 = 2.00/3.00
      O3 = 1.00/3.00
      T9 = 2.00/9.00
      TEMX = 3.00 * EHX
      ADT = A/TEMP
      ADTM = -ADT
      T3S = TB
      YBS = YB
      FYYL = ADT * (T9 * (5.00 - XL) / (SQRT(XL) * (1.00 - XL)**3) + B/ZL)
      FYYH = ADT * (T9 * (5.00 - XM) / (SQRT(XM) * (1.00 - XM)**3) + B/ZM)
35      BOREG2 = AMAX1(FYYL, FYYH)
      YBC = 1.00 - YB
      YCK = YH - YB
      RG2Y = YH - YB
      RG3Y = YL - YB
40      YINC = 0.00
      TINC = 0.00
      IF (RG2Y.GT.0.00) GO TO 100
      IF (RG3Y.GT.0.00) GO TO 200
      H = .500

```

SUBROUTINE TMPCON

7600

OPT=1

FTN 4.1 LEVEL 71

07/15/75 00.21.07

```

45      GO TO 301
      200 NSW=1
          YH=VL
          YCK=VL-YB
          GO TO 101
50      100 NSW=0
      101 VC=YBC-YINC
          VC23=VC**T3
          C=.9*ALOG(VC)
          Q=1.00-VC23
55      F=ADT*VC*(1.00/D+C)
          FY=ADTM*(C+B*(1.00-Q3*VC23)/(D*D))
          YMC=VC-EMX
          IF(YMC.LE.RHOFCS) GO TO 300
          FH=ADT*YMC*(1.00/(1.00-YMC**T3)+B*ALOG(YMC))
60      IF(FH.LT.0.00) GO TO 400
          C1=TEHX/F
          IF(NSW.EQ.0) GO TO 104
          C0=6.00*(FH-F)/(F*(BDREG2*F+FY**2))
          GO TO 105
65      104 CONTINUE
          FYY=ADT*(T3*(5.00-VC23)/(SQRT(VC23)*D*D)+B/YC)
          C0=6.00*(FH-F)/(F*(FYY*F+FY**2))
      C   CALCULATE NEG. ROOT ,THEN POS
      105 CONTINUE
          ZNEG=(-C1-SQRT(C1*C1-4.*C0))*.5
          H=.9500*C0/ZNEG
      C   CHECK ON H
          IF(H*(H+C1)+C0.GE.0.00) GO TO 500
          DY=H*F*(1.00+.500*H*FY)
75      YINC=YINC+DY
      C   IF GO TO 600 CALCULATED Y NOT IN REGION 1
          IF(YINC.GT.YCK) GO TO 600
      106 CONTINUE
          TINC=TINC+H
          IF(TINC.LT.TINCPR) GO TO 102
          FY02=.900*FY
          YT=YB+(YINC-DY)
          TCP=TINCPR
          HC=H-TINC
85      590 HC=HC+TINCPR
          DYC=HC*F*(1.00+HC*FY02)
          TBTCP=TB+TCP
          IF(TBTCP.GT.TF) GO TO 300

```

```

      M=N+1
      Y(N)=YT+DYC
      Y(N)=YB+YCP
      TCP=TCP+TINCPR
      IF (TCP.LE.TINC) GO TO 550
      TINC=TINC-(TCP-TINCPR)
      YINC=(YB-Y(N))+YINC
      YB=Y(N)
      TB=T(N)
      YBC=1.00-YB
      YCK=YH-YB
100      102 IF (YB+YINC.LT.YF) GO TO 101
      GO TO 300
      400 GO TO 700
      500 PRINT 2001
      2001 FORMAT('1QUAD. INEQ. NOT SAT. IN SUB TMPCON.'//)
      GO TO 700
105      C ARRIVE AT 500 WHEN CAL. Y(X+H) IS NOT IN REGION 1 AND Y(X) IS.
      600 IF (YB+YINC.GT.YL) GO TO 601
      C ARRIVE HERE IF CAL. Y(X+H) LIES IN REGION 2.
      IF (H*(H+C1)+6.00*(FH-F)/(F*(BDREG2*F+FY**2)).LT.0.00) GO TO 502
110      C IF HERE, CAL Y(X+H) MAY HAVE TOO MUCH ERROR ASSOCIATED WITH IT.
      C CHOOSE NEW H SO THAT Y(X+H)=YH(1)SAVED IN YHS). THIS H IS ACCEPTABLE
      C AND SATISFIES YH-(YB+YINC-CY)=F*H+.5*FY*H**2. WE SOLVE
      C  $H**2+(2*F/FY)*H-(2/FY)*(YH-(YB+YINC-DY))=0$ 
      C FOR THE SMALLER POS. ZERO.
115      627 CONTINUE
      D1=(F+F)/FY
      D0=2.00*(YJ+(YINC-DY)-YH)/FY
      ZP=(-D1+SQRT(D1*D1-4.*D0))*.5
      C ZP IS LARGER ZERO
120      H=D0/ZP
      C H IS SMALLER ZERO.
      YINC=YH-YB
      602 YCK=YL-YB
      YH=YL
      NSH=1
      GO TO 106
      601 YC=YBC-YINC
      C Y(X+H).GT.YL MUST CHECK THAT H SATISFIES INEQ. WITH VALUE OF FYY
      C APPROPRIATE FOR REGION 3.
      YC23=YC**T3
130      FYY=AOT*(T3*(5.00-YC23)/(SQRT(YC23)*(1.00-YC23)**3)+B/YC)
      IF (H*(H+C1)+6.00*(FH-F)/(F*(FYY*F+FY**2)).LT.0.00) GO TO 650

```

SUBROUTINE TMPCON

7600 OPT=1

FTM 4.1 LEVEL 71 07/19/79 00.21.02

```

C      SEE IF INEQ. PERTINENT TO REGION 2 IS SATISFIED.
C      IF (H*(H+C1)+6.00*(FH-F)/(F*(BREG2*F+FY**2)).GE.0.00) GO TO 427
135  C      Y(X+H) IS NOT ACCEPTABLE. NOW CHOOSE H SO THAT Y(X+H)=YL. THIS H
C      IS ACCEPTABLE AND SATISFIES  $YL-(YB+YINC-DY)=F*H+.5*FY*H**2$ . WE
C      SOLVE  $H**2+(2F/FY)*H+(2/FY)*(YB+YINC-DY-YL)=0$ 
C      FOR SMALLER ZERO.
C      E1=(F+F)/FY
140  C      E0=2.00*(YB+(YINC-DY)-YL)/FY
      MP=(1-E1+SQRT(E1**2-4.*E0))*.5
C      MP IS LARGER ZERO
      H=E0/MP
C      H IS SMALLER ZERO
145  C      YINC=YL-YB
      YINC=YINC+H
      FYD2=.500*FY
      GO TO 651
301  YC=YBC-YINC
150  C      YC23=YC**Y3
      C=B*ALOG(YC)
      D=1.00-YC23
      F=ADT*YC*(1.00/D+C)
      FY=ADTM*(C+B*(1.00-03*YC23)/(D*D))
155  C      YHC=YC-EMX
      IF (YHC.LE.0.00) GO TO 300
      FH=ADT*YHC*(1.00/(1.00-YHC**Y3))+B*ALOG(YHC)
      IF (FH.LT.0.00) GO TO 400
      C1=TEMX/F
      SFHMF=6.00*(FH-F)
      FY2=FY*FY
      FYD2=.500*FY
      JI=0
      JD=0
165  C      GO TO 305
303  IF (JD.GT.0) GO TO 320
      JI=JI+1
305  MS=M
      M=1.500*M
      DYS=0Y
170  C      302 DY=M*F*(1.00+M*FYD2)
      YCR3=YC-DY
      YCR323=YCR3**Y3
      FYY3=ADT*(Y9*(5.00-YCR323)/(SQRT(YCR323)*(1.00-YCR323)**3))+B/YCR3
175  C      1)
      IF (H*(H+C1)+SFHMF/(F*(FYY3*F+FY2)).LT.0.00) GO TO 303

```

SUBROUTINE TMPCON

7600

OPT=1

FTN 4.1 LEVEL 71

07/15/79

08.71.02

```
      IF(JI.GT.0) GO TO 304
      JD=JD+1
      M=TJ*M
180      IF(M.GT.HLOW) GO TO 302
      PRINT 1003,M,HLOW
1003  FORMAT(*1H= *E11.4,5X,*LESS THAN HLOW= *E11.4)
      GO TO 700
304  M=MS
185  DY=DYS
320  YINC=YINC+DY
      TINC=TINC+M
651  CONTINUE
      IF(TINC.LT.TINCPR) GO TO 310
190  YT=YB+(YINC-DY)
      TCP=TINCPR
      HC=M-TINC
450  MC=MC+TINCPR
      DYC=MC*F*(1.00+MC*FYD2)
195  TBTCP=TB+TCP
      IF(TBTCP.GT.TF) GO TO 300
      N=N+1
      Y(N)=YT+DYC
      T(N)=TBTCP
      TCP=TCP+TINCPR
200  IF(TCP.LE.TINC) GO TO 450
      TINC=TINC-(TCP-TINCPR)
      YINC=(YB-Y(N))+YINC
      YB=Y(N)
205  TB=T(N)
      YBC=1.00-YB
310  IF(TB+TINC.LT.TF) GO TO 301
300  RETURN
650  TINC=TINC+M
210  FYD2=FY*.500
      GO TO 651
700  GO TO 300
      END
```

SUBROUTINE INDATA 7600 OPT=1

FTN 1.1 LEVEL 71 07/15/75 00.21.07

```

SUBROUTINE INDATA
COMMON XL,ZL,XH,ZH,A,B,TEMP,TB,TF,YB,EMX,TINCPR,RHOFCS,W
COMMON/BHA/RHOF, TOP, TO, TOSS, YPB, TONCPR, YTFM, YHSE, YLSER, TOSAV,
5 1TGB, TLIN, TIMST, OA, XEXP(100), YEXP(100), TEMPZC(100), TTT(40), TMP(10),
2PSIS, TFTVAR,
3NPR, NPRS, NPLOT, NPLOTS, NAB, NABS, NSERCH, NSRCHP, NSTEAD, NPROFL, NEXPOT,
4INPUT, NOEXP
DATA ISW/0/
IF(IABS(NPROFL)+IABS(NEXPOT).EQ.0) GO TO 1
10 C OA=0 MEANS TEMP. PROFILE IS UNSHIFTED.
OA=0.00
CALL INEXPT
1 CONTINUE
READ(5,150) RHOF, TOP, A, B, TO, TOSS, YTFM, EMX, YB, YPB, TONCPR,
15 1TCONST, NSRCHP, NPROFL, NEXPOT, NPR, NPLOT, NAB
IF(EOF(5)) 2000,69
150 FORMAT(12E6.1,I2,4I1,I2)
65 IF(TONCPR.LE.0.00) TONCPR=.500
IF(TO.LE.0.00) TO=120.00
20 IF(TOSS.LE.0.00) TOSS=120.00
NSERCH=NSRCHP
IF(1TCONST.LE.0.00) GO TO 20
DO 200 I=1,NSTEAD
200 TMP(I)=TTT(I)*(1TCONST/TTT(NSTEAD))
GO TO 202
25 20 GO 201 I=1,NSTEAD
201 TMP(I)=TTT(I)
202 TOSAV=TO
IF(NPLOT.EQ.0) ISW=1
IF(NSERCH.EQ.0) GO TO 100
YLSER=0.00
YHSE=1.00
NPRS=NPR
NPLOTS=NPLOT
35 NABS=NAB
NPR=1
NPLOT=1
NAB=0
IF(EMX.LE.0.00) EMX=.000100
40 GO TO 101
100 IF(EMX.LE.0.00) EMX=.00100
101 RETURN
2000 IF(ISW.NE.0) CALL PLOT3
STOP

```

51

SUBROUTINE INDATA 7500 OPT=1

FTN 4.1 LEVEL 71 07/15/75 04.01.07

45

END

SUBROUTINE INEXPT 7600 OPT=1

FTN 4.1 LEVEL 71 07/15/75 08.21.10

```

SUBROUTINE INEXPT
COMMON/BMA/RHOF,TOP,TO,TOSS,YPB,TONCPR,YTFH,YMSER,YLSER,TOSAV,
1TGB,TLIN,TIMST,DA,XEXP(100),YEXP(100),TEMPZC(100),TTT(50),TMP(50),
2PSIS,TFTVAR,
5 3NPR,NPRS,NPLOT,NPLOTS,NAB,NABS,NSERCH,NSRCHP,NSTEAD,NPROFL,NEXPOT,
  4INPUT,NOXEXP
  IF(NPROFL.NE.1) GO TO 10
C  READ IN NEW TEMPERATURE PROFILE.
  READ 11,TGB,TLIN,NSTEAD
10 11 FORMAT(2E10.2,I6)
  TGBL=TGB
  TLINL=TLIN
  TIMST=TGB*(NSTEAD-1)*TLIN
  TFTVAR=60.00*TIMST
15  TGB=60.00*TGB
  TLIN=60.00*TLIN
  IF(NSTEAD.GE.1) GO TO 2
  5 PRINT 3,NSTEAD
  3 FORMAT(*1NSTEAD=*I6,2X*IS OUT OF RANGE.*)
20  4 STOP
  2 IF(NSTEAD.GT.50) GO TO 5
  6 FORMAT(8E10.2)
  READ 6,(TTT(I),I=1,NSTEAD)
25  10 IF(INEXPOT.NE.1) GO TO 100
C  READ IN NEW EXPERIMENTAL DATA AND ASSOCIATED PRESSURE.
  READ 1,NOXEXP,PSIS,(XEXP(I),YEXP(I),I=1,NOXEXP)
  1 FORMAT(I10,E10.0/I8E10.0)
  IF(NOXEXP.LE.100) GO TO 4901
  4902 PRINT 4900,NOXEXP
30  4900 FORMAT(*1NOXEXP=*I10,2X*IS OUT OF RANGE.*)
  4903 STOP
  4901 IF(NOXEXP.LT.1) GO TO 4902
  IF(NOXEXP.EQ.1) GO TO 4906
  DO 4904 I=2,NOXEXP
35  IF(XEXP(I).GT.XEXP(I-1)) GO TO 4904
  PRINT 4905
  4905 FORMAT(*1EXPERIMENTAL DATA TIMES ARE NOT STRICTLY MONOTONE INCREAS
    1ING.*)
  GO TO 4903
40  4904 CONTINUE
C
C  CALCULATE TEMPERATURE ASSOCIATED WITH THE TIME OF THE EXPERIMENTAL
C  DATA
C

```


SUBROUTINE INEXPT 7600 OPT=1

FTN 4.1 LEVEL 71 07/15/75 08.21.10

```
45      4906 CONTINUE
        100 DO 4510 I=1,N0XEXP
            IF(XEXP(I).GE.TIMST) GO TO 4501
            IF(XEXP(I).LE.TGBL) GO TO 4500
            NTI=(XEXP(I)-TGBL)/TLINL
            TLOW=TGBL+TLINL*NTI
            NTI=NTI+1
            TEMP2C(I)=TTT(NTI)+(XEXP(I)-TLOW)*(TTT(NTI+1)-TTT(NTI))/TLINL
            GO TO 4510
50      4500 TEMP2C(I)=0.00
            GO TO 4510
55      4501 TEMP2C(I)=TTT(INSTEAD)
        4510 CONTINUE
            RETURN
            END
```

SUBROUTINE GRAPH

7600

OPT=1

FTN 4.1 LEVEL 71

07/15/75

06.21.13

```

      SUBROUTINE GRAPH(X,Y,N,IG,RHOF,YC,YPB,A,B,TOP,EHX,P,SSTEMP,
1SSTIME)
      DIMENSION X(1),Y(1),XTIT(5),YTIT(5),GTIT(7),SCR(3)
      DATA XTIT/50HTIME (MINUTES)
      DATA YTIT/50HNORMALIZED DENSITY
      DATA GTIT/70H
1
      SIZE=.06
      XMIN=X(1)
10      XMAX=X(1)
      YMIN=Y(1)
      YMAX=Y(1)
      DO 1 I=1,N
      XMAX=AMAX1(XMAX,X(I))
15      XMIN=AMIN1(XMIN,X(I))
      YMAX=AMAX1(YMAX,Y(I))
      YMIN=AMIN1(YMIN,Y(I))
1
      CONTINUE
      CALL PDVICE(4)
20      CALL AICRT4(10,0,X,Y,-N,1,2,1,1,GTIT,XTIT,YTIT,1,1
      1,16.,16.,2,XMIN,XMAX,2,YMIN,YMAX,1,1,1,0)
10
      FORMAT(20HSTEADY STATE TEMP. =,F7.1)
      ENCODE(27,10,SCR) SSTEMP
      XINCH=.1*(XMAX-XMIN)
25      YINCH=.1*(YMAX-YMIN)
      X0=XMIN+.375*XINCH
      Y0=YMIN+.7*YINCH
      CALL MXLABL(X0,Y0,0.,SIZE,27,SCR)
20
      FORMAT(20HBEGIN STEADY STATE =,F7.2)
      ENCODE(27,20,SCR) SSTIME
      X0=XMIN+.375*XINCH
      Y0=YMIN+.5*YINCH
30      CALL MXLABL(X0,Y0,0.,SIZE,27,SCR)
30
      FORMAT(6HTOP =,F8.3)
      ENCODE(14,30,SCR) TOP
      X0=XMIN+.65*XINCH
      Y0=YMIN+.5*YINCH
35      CALL MXLABL(X0,Y0,0.,SIZE,14,SCR)
40
      FORMAT(6HYPB =,1PE8.2)
      ENCODE(14,40,SCR) YPB
      X0=XMIN+.82*XINCH
      Y0=YMIN+.5*YINCH
40
      CALL MXLABL(X0,Y0,0.,SIZE,14,SCR)
50
      FORMAT(6HB =,F8.3)

```

```
45      ENCODE(14,50,SCR) B
      XD=XMIN+6.5*XINCH
      YD=YMIN+.7*YINCH
      CALL MXLABL(XD,YD,0.,SIZE,14,SCR)
60      FORMAT(6HEHX = ,1PE8.2)
50      ENCODE(14,60,SCR) EMX
      XD=XMIN+8.2*XINCH
      YD=YMIN+.7*YINCH
      CALL MXLABL(XD,YD,0.,SIZE,14,SCR)
69      FORMAT(6HXA = ,F8.3)
55      ENCODE(14,69,SCR) A
      XD=XMIN+6.5*XINCH
      YD=YMIN+.9*YINCH
      CALL MXLABL(XD,YD,0.,SIZE,14,SCR)
70      FORMAT(6HRHOF = ,F8.3)
60      ENCODE(14,70,SCR) RHOF
      XD=XMIN+8.2*XINCH
      YD=YMIN+.9*YINCH
      CALL MXLABL(XD,YD,0.,SIZE,14,SCR)
80      FORMAT(6HPSI = ,F8.3)
65      ENCODE(14,80,SCR) P
      XD=XMIN+6.5*XINCH
      YD=YMIN+1.1*YINCH
      CALL MXLABL(XD,YD,0.,SIZE,14,SCR)
90      FORMAT(6HY3 = ,F8.3)
70      ENCODE(14,90,SCR) YC
      XD=XMIN+8.2*XINCH
      YD=YMIN+1.1*YINCH
      CALL MXLABL(XD,YD,0.,SIZE,14,SCR)
      CALL PLOT3
75      RETURN
      END
```

APPENDIX D
VARIABLES AVAILABLE FOR HOT PRESS DIGITAL COMPUTER PROGRAM

Variables Available for Hot Press Digital Computer Program

Description of Input Variables

Many of the defining parameters of the problem may be given by explicit values on the data card or may be calculated from other values on the input card.

RHOF If $RHOF > 0$, then this is the value to use for $RHOF$.
This case will be skipped if $RHOF > 1$

If $RHOF > 0$, then the value of B on the data card is not used
and B is calculated in the program to be

$$B = \frac{-1}{[\log(1 - RHOF)][1 - (1 - RHOF)^{2/3}]}$$

If $RHOF = 0$, then the value of $RHOF$ is calculated, and the value of B on the data card is the value of B used by program. If B (value on data card) < 0 , this case is skipped. If $B = 0$, then $RHOF = 1$. If $B > 0$, then the calculated $RHOF$ is within 2^{-11} of the unique zero (this zero is the limiting density as time increases) of the function

h defined by

$$h(y) = \frac{1}{1 - (1 - y)^{2/3}} + B \ln(1 - y),$$

which lies in the unit interval $[0, 1]$.

TOP Initial time (in minutes) of the time interval on which we want to approximate the solution of the differential equation.

A If A (value on data card) > 0 , then this is the value used for A .

If $A \leq 0$, then A is determined by the equation

$$YPB = Y'(TOP) = \frac{A}{T(TOP)} (1 - YB) \left[\frac{1}{1 - (1 - YB)^{2/3}} + B \log(1 - YB) \right]$$

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where YPB and YB are defined below and where $T(TOP)$ is the temperature at time TOP.

B If input RHOF > 0, then value of B on data card is not used and the value of B used by program is determined by

$$B = \frac{-1}{\log(1 - RHOF) * 1 - (1 - RHOF)^{2/3}}$$

If input RHOF ≤ 0, then input value of B (if B < 0, case skipped) is used.

T0 If NSRCHP = 0, then T0 is final time (in minutes) of the time interval on which we want to approximate the solution of the differential equation.

If NSRCHP > 0, then T0 is the matching time. Look at YTFM.

If T0 < 0, then program sets T0 = 120

T0SS If NSRCHP = 0, then T0SS is not used.

If NSRCHP > 0, then when we have satisfied the matching criterion (see EHX below) or when we have performed NSRCHP iterations the density curve is calculated from TOP to time T0SS (in minutes).

If T0SS ≤ 0, then program sets T0SS = 120.

YTFM If NSRCHP = 0, then value of YTFM is not used.

If NSRCHP > 0, then YTFM = desired density at the matching time T0. See EHX below.

EHX If EHX (input value) ≤ 0 and NSRCHP = 0, then program sets EHX = 0.001.

If EHX (input value) ≤ 0 and NSRCHP > 0, then program sets EHX = 0.0001.

The value of EHX is an upper bound for the magnitude of the absolute error in our calculated density curve.

If NSRCHP > 0, then EHX is also used in the matching criterion:

$$|YTFM - Y(N)| < EHX \text{ implies acceptance}$$

of calculated $\bar{Y}$ (density curve), where $Y(N)$ is the calculated density at time T_0 . The method of bisection is used to obtain a matching curve. We begin with the interval $[YLSER, YHSER] = [0, 1]$. We are assuming that if $YB = 0$ (actually mean if YB is extremely close to 0), then calculated value at matching time will be low. Also YB near 1 will give a calculated value at matching time that will be too high. On the initial trial YB is defined as in YB below. On successive trials $YB = (1/2) [YLSER + YHSER]$. If the acceptance inequality: $|YTFM - Y(N)| \leq EMX$ is not satisfied, then set $YLSER = YB$ if $Y(N) < YTFM$ and set $YHSER = YB$ if $Y(N) > YTFM$. This process is repeated no more than NSRCHP times.

YB If input value of YB is positive, then this value is used as the value of the density function at the initial time T_0 .

If input value of $YB \leq 0$, then the initial density value is calculated from the experimental curve that has already been read into machine. If T_0 lies outside the time interval covered by the experimental curve in the machine, then the case is skipped.

Also if $YB > RHOF$ (where YB and $RHOF$ are either the input values or the appropriate calculated values), then the case is skipped.

YPB If input values of $A > 0$, then input value of YPB is not used.

Suppose $A \leq 0$, then:

- (1) If input value of $YPB > 0$, then it is used as the value of the first derivative of the density function with respect to time (in seconds) at time T_0 . This value is used in the equation under A (above) to determine the value of A .
- (2) If input value of $YPB \leq 0$, then the first derivative is approximated by calculating the derivative of the experimental curve stored in the machine. If T_0 lies outside time interval covered by experimental curve in the machine, then the case is skipped.

TONCPR If input value of TONCPR ≤ 0 , then program sets

$$\text{TONCPR} = 0.5$$

TONCPR is the numerical value of the time step used in tabulating the approximate solution of the differential equation.

TCNST If input value of TCNST ≤ 0 , then temperature profile stored currently in the computer will be used as is.

If input value of TCNST > 0 , then the current temperature profile stored in the computer is multiplied by a constant to give the temperature profile to be used by the program for this case. The constant is chosen so that the steady state temperature of the new profile is equal to the value of TCNST. The old temperature profile is not altered by this process.

NSRCHP If NSRCHP = 0, then matching is not requested. If NSRCHP > 0 , then matching will be done as described under EHX.

NPROFL If NPROFL = 1, then a new temperature profile will be read in for the next case (not this one).

If NPROFL $\neq 1$, then current profile will be used for the next case.

Note well. Before your first case you must have the necessary data for a temperature profile followed by the experimental data that is to be used with your first case. (NPROFL is initially set to 1 by the program).

NEXPDT If NPROFL = 1, then new experimental data (and associated pressure) will be read in for the next case (not this one).

If NPROFL $\neq 1$, then current experimental data will be used for the next case.

See note well under NPROFL. (NEXPDT = 1 initially)

NPR If NPR = 0, then tabulated density curve is printed.
If NPR $\neq 0$, then tabulated density curve is not printed.

NPL~~OT~~ If **NPL~~OT~~** = 0, then the tabulated density curve is plotted.

 If **NPL~~OT~~** $\neq$ 0, then the tabulated density curve is not plotted.

NAB If **NAB** = 0, then we do not want a family of curves.

 If **NAB** > 0, then we do want a family of curves with exactly **NAB** members. Each member is determined by a pressure value read in from a card with format E9.3. Thus, if **NAB** = 7, then 7 cards (each card of format E9.3) should follow the data card that contains the value of **NAB**. Actually the family will have (**NAB** + 1) members, since the pressure corresponding to the experimental curve will automatically be used.

Format of Input Temperature Profile Data

First Card **FORMAT** (2E10.2, 16)

TGB Column 1-10	Initial time (minutes) of temperature profile
TLIN Column 11-20	Time step (minutes) between successive temperature recordings
NSTEAD Column 21-26	Number of temperature recordings to read into array. The last element read in is taken as the steady state temperature
	$1 \leq \text{NSTEAD} \leq 50$

Second Card **FORMAT** (8E10.2)

Column 1-10	Temperature at time TGB
Column 11-20	Temperature at time TGB + TLIN
Column 21-30	Temperature at time TGB + 2 * TLIN

Use as many cards as are needed for temperature profile. All are to have the same format as card 2.

Format of Input for Experimental Data

Card 1 FORMAT (I10, E10.0)

N~~0~~XEXP Column 1-10

Number of experimental data

 $1 \leq N_{XEXP} \leq 100$

PSIS Column 11-20

Pressure associated with experimental data

Card 2 FORMAT (8E10.0)

Column 1-10

Time (minutes) of first experimental point

Column 11-20

Experimental density of first point

Column 21-30

Time of second point

Column 31-40

Density of second point

Column 41-50

Time of third point

Column 51-60

Density of third point

Column 61-70

Time of fourth point

Column 71-80

Density of fourth point

Use as many cards as are needed for experimental data. All are to have the same format as card 2.

Format of Input for Calculation and Plot

Card 1 FORMAT (I2E6.1, I2, 4I1, I2)

RH~~0~~F Column 1-6T~~0~~P Column 7-12

A Column 13-18

B Column 19-24

T~~0~~ Column 25-30T~~0~~SS Column 31-36

YTFM Column 37-42
EHX Column 43-48
YB Column 49-54
YPB Column 55-60
T~~O~~NCPR Column 61-66
T~~O~~NST Column 67-72
NSRCHP Column 73-74
NPR~~O~~FL Column 75
NEXPOT Column 76
NPR Column 77
NPLOT Column 78
NAB Column 79-80