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TEMPERATURE PROFILES WITHIN CYLINDERS CONTAINING INTERNAL HEAT SOURCES AND MATERIALS OF TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITIES. DESCRIPTION OF FAST COMPUTER PROGRAMS AS APPLIED TO SOLIDIFIED RADIOACTIVE WASTES

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CHEMICAL TECHNOLOGY DIVISION

Chemical Development Section B

TEMPERATURE PROFILES WITHIN CYLINDERS CONTAINING INTERNAL HEAT SOURCES AND MATERIALS OF TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITIES. DESCRIPTION OF FAST COMPUTER PROGRAMS AS APPLIED TO SOLIDIFIED RADIOACTIVE WASTES

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OAK RIDGE NATIONAL LABORATORY Oak Ridge, Tennessee operated by UNION CARBIDE CORPORATION for the U. S. ATOMIC ENERGY COMMISSION



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ABSTRACT

The safety and economic aspects of producing and storing radioactive wastes as solids, usually in vessels having a cylindrical geometry, require that we know the maximum internal temperatures to be expected as a result of decay heat. Such information is mandatory for materials that have variable thermal conductivities under different storage conditions.

This report presents a computer program (STORE), which was written to permit more rapid calculation of temperature profiles within cylinders containing homogeneously distributed heat sources and materials whose thermal conductivities can be expressed as a tabular function of temperature. A simplified version of this program was prepared for the cases in which the thermal conductivity is constant or is a linear function of temperature. Both of these programs have short execution times, typically from a few to 20 seconds on the IBM/360-75 as compared with the five or more minutes required for the more accurate finite-difference method. They are based on the assumption that the material density and, therefore, the power density of the heat source are independent of temperature; this assumption is, of course, contrary to physical reality. However, in a test example involving a hypothetical vessel of glass containing a large internal (fission product) heat source with a specific power density of 0.2 cal sec⁻¹ cm⁻³ (i.e., 80,910 Btu hr^{-1} ft⁻³), the temperature difference between the wall and the center of a 6-in.-diam by 6.25-ft-long cylinder was overestimated by 36°C (an error of only about 10%, as compared with the "exact" value that is obtained by solving finite-difference equations and compensating for the reduction in the heat-source strength as the density decreases with increasing temperature). Within the uncertainties inherent in thermal conductivity, density, and heat capacity measurements of systems of interest in the storage of solidified radioactive process wastes, the method and the program presented in this report offer adequate accuracy and a large time savings as compared with the more exact calculations. Also, they are applicable to cylinders with any specified length/diameter ratio.

1. INTRODUCTION

On the basis of safety and economic studies, it appears rather probable that high- $^{1-4}$ and intermediate-level⁵ radioactive wastes which accumulate from the processing of nuclear reactor fuels will be converted to solids for permanent storage at some time – from 30 days to 30 years – after removal of the fuel from the reactor. Essentially all of the beta energy, and more than half of the gamma energy, from the fission products will usually be absorbed by the solid within which they are contained; therefore, the temperature in the interior will be raised to a level higher than that of the surface. The extent of this temperature elevation depends on the thermal conductivity of the solid, the diameter of the storage vessel (which is usually considered to be a right circular cylinder), and the specific fission product power density. In calculations it is assumed that the radioactive materials are distributed isotropically throughout the cylinder; then, at steady state, the temperature, T(r, z), at any point (r, z) is given by the equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left[Kr\frac{\partial T}{\partial r}\right] + \frac{\partial}{\partial z}\left[K\frac{\partial T}{\partial z}\right] + A = 0, \qquad (1)$$

where

K = temperature-dependent thermal conductivity, cal cm⁻¹ sec⁻¹ °C⁻¹,

T = temperature, °C,

r = radial variable, cm,

z = vertical variable, cm,

A = sum of (fission product) power densities (i.e., absorbed power density), cal sec -1 cm -3.

The quantity A is actually a function of temperature; that is, it decreases as the temperature of the solid increases because the material specific volume increases (the density decreases). However, the definition of A (above) points out that it is the absorbed energy that is important. The fraction of the total gamma-ray energy that is absorbed is a function of the dimensions of the cylinder.⁶ Because of the temperature dependence of A, an "exact" solution of Eq. (1) can be obtained only by use of finite-difference methods. However, in practical cases the thermal conductivity is affected much more strongly by temperature than the density is. For example, the effect of temperature on the thermal conductivity of materials of interest is on the order of $(50 \text{ to } 200) \times 10^{-6} \text{ eC}^{-1}$, while the coefficient of volume expansion is in the range $(1 \text{ to } 5) \times 10^{-6} \text{ eC}^{-1}$. Thus, to a first approximation, the quantity A may be assumed to be independent of temperature.

This report presents a computer program (STORE) which was written to provide approximate solutions of Eq. (1) in terms of temperature as a function of spatial location within a cylinder of arbitrary length/diameter ratio. Such a program can be very useful for evaluating the advantages, with respect to safety and economics, of storing radioactive waste materials because it can be executed much faster than a program based on the more exact finite-difference method.

Additional reports, which are now being written, will illustrate the application of this program, and the simpler programs derived from it, to the calculation of internal temperatures in cylinders containing intermediate-level waste solids that are dispersed in an organic matrix (such as asphalt, polyethylene, or other plastics) or high-level waste, existing as calcine or as solids that are dissolved, or dispersed, in an inorganic matrix (such as a glass or a microcrystalline solid).

2. METHODS OF SOLUTION

It is convenient to express Eq. (1) in terms of a dimensionless temperature, v, defined as

$$v \equiv (T - T_{o})/T_{o} , \qquad (2)$$

where T_{o} is a convenient reference temperature. In this report, T_{o} was chosen as temperature of the surface of the cylinder. By combining Eqs. (1) and (2), we obtain

$$\frac{1}{r} \frac{\partial}{\partial r} \left[Kr \frac{\partial v}{\partial r} \right] + \frac{\partial}{\partial z} \left[K \frac{\partial v}{\partial z} \right] + \frac{A}{T_o} = 0 , \qquad (3)$$

with the boundary conditions

$$v = 0 \text{ at } z = 0, h \text{ for } 0 \le r \le a$$

$$v = 0 \text{ at } r = a \text{ for } 0 \le z \le h$$

$$(4)$$

where

a = radius of the cylinder, cm,

h = length of the cylinder, cm.

Using the notation of Carslaw and Jaeger,⁷ we define

$$\Theta(\mathbf{r}, \mathbf{z}) = \frac{1}{K_o} \int_0^{\mathbf{v}_s} K \, d\mathbf{v} , \qquad (5)$$

from which it follows that

$$\frac{\partial \Theta}{\partial r} = \frac{K}{K_o} \frac{\partial v}{\partial r}; \quad \frac{\partial \Theta}{\partial z} = \frac{K}{K_o} \frac{\partial v}{\partial z} \quad . \tag{6}$$

On substituting the quantities of Eq. (6) into Eq. (3), we obtain

$$\frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial \Theta}{\partial r} \right] + \frac{\partial}{\partial z} \left[\frac{\partial \Theta}{\partial z} \right] + \frac{A}{K_0 T_0} = 0 \quad . \tag{7}$$

Here, K_0 is the thermal conductivity of the material at temperature T_0 . The boundary conditions for Θ are as follows:

Further, it is convenient to define

$$x \equiv r/a, \quad Z \equiv z/a, \quad \ell \equiv h/a$$
 (9)

With these definitions, the solution of Eq. (7) is given by

$$U(x,Z) = \frac{Z(\ell-Z)}{2} - \frac{4\ell^2}{\pi^3} \sum_{m=1}^{\infty} \frac{I_o[(2m-1)\pi x/\ell] \sin[(2m-1)\pi Z/\ell]}{(2m-1)^3 I_o[(2m-1)\pi/\ell]}, \quad (10)$$

and

$$\Theta = A a^2 U/K_o T_o .$$
 (11)

After having calculated Θ , it is a straightforward process to calculate T. In particular we have, from Eqs. (2) and (5),

$$\Theta = \frac{1}{K_0 T_0} \int_{T_0}^{I} K \, dT \,.$$
(12)

For the case in which thermal conductivity can be expressed as a tabular function of temperature, we first determine Θ from Eqs. (10) and (11) and then evaluate v and T from Eqs. (5) and (12). To do this, we must perform the numerical integration indicated by Eq. (5) in order to calculate a table of Θ as a function of v. We then obtain v by quadratic interpolation in this table with the known value of Θ . Calculations are performed by program STORE.

There are two special cases of considerable importance in radioactive waste storage: the case in which thermal conductivity is a linear function of temperature and the case in which the thermal conductivity is constant.

When thermal conductivity is a linear function of temperature, we require two thermal conductivities at two temperatures, (T_1, K_1) and (T_2, K_2) , from which we obtain

$$K = K_{o} [1 + b(T - T_{o})], \qquad (13)$$

$$K_{o} = \frac{K_{1} (T_{2} - T_{o}) - K_{2} (T_{1} - T_{o})}{(T_{2} - T_{1})}, \qquad (13)$$

$$\Theta = \frac{1}{K_{o}} \int_{0}^{v} K \, dv = \int_{0}^{v} (1 + bT_{o}v) dv = v + \frac{bT_{o}v^{2}}{2} \quad .$$
(14)

In this case, the value of $\ensuremath{\mathbb{B}}$ is known and v and T - T can be calculated from the relationships

$$\mathbf{v} = \left[\sqrt{1 + 2bT_0 \Theta} - 1\right] / bT_0 \tag{15}$$

$$T - T_o = [\sqrt{1 + 2bT_o \Theta} - 1]/b$$
. (16)

By replacing v by $(T - T_o)/T_o$ and using the definition of K as a linear function of temperature to eliminate b from Eq. (14), we obtain

$$\Theta(x, Z) = \frac{(T - T_o)}{T_o K_o} \left(\frac{K + K_o}{2}\right) = \frac{\overline{K} \Delta T}{T_o K_o} , \qquad (17)$$

where the average thermal conductivity, \overline{K} , at the two temperatures is

$$\overline{K} = \frac{K + K_{o}}{2}$$
(18)

and we have defined

$$\Delta T = T - T_{O} . \tag{19}$$

On replacing $\Theta(x, Z)$ on the left-hand side of Eq. (17) by its value from Eq. (11), we obtain

$$A = \frac{\overline{K} \Delta T}{a^2 U} \qquad (20)$$

Equation (20) is quite similar to that for thermal diffusion in an infinite cylinder, namely,

$$A = \frac{4\overline{K} \ \Delta T}{a^2} \quad . \tag{21}$$

This equation may be derived in a manner analogous to that described, for example, by McAdams,⁸ except that K would be a linear function of temperature rather than a constant. Equation (21), while strictly applicable only to an infinite cylinder, is frequently used and yields a rather accurate estimate of the specific power, A, as a function of ΔT , providing that the cylinder is long (i.e., a cylinder with a length/ diameter ratio in excess of about 3 or 4).

Equations (20) and (21) imply that for an infinitely long cylinder we have

$$U = 1/4$$
. (22)

The quantity U, calculated in program STORE, has values of 0.201, 0.245, 0.249, and 0.250 for cylinders of length/diameter ratios of 1, 2, 2.5, and 5, respectively. Thus, as expected, Eq. (21) overestimates the ΔT for a given value of A, but to a significant extent only if the length/diameter ratio is less than 2. In connection with the mathematical reduction of Eq. (20) to Eq. (21), we note that, at the center of a cylinder, namely at x = 0 and Z = $\ell/2$, Eq. (10) reduces to

$$U(0, \ell/2) = \frac{\ell^2}{8} \left\{ 1 - \frac{32}{\pi^3} \sum_{m=1}^{\infty} \frac{\sin\left[(2m-1)\pi/2\right]}{(2m-1)^3 I_0 \left[(2m-1)\pi/\ell\right]} \right\}.$$
 (23)

It can be shown that

$$\lim_{\ell \to \infty} \left\{ \sum_{m=1}^{\infty} \frac{\sin\left[(2m-1)\pi/2\right]}{(2m-1)^{3} I_{o}\left[(2m-1)\pi \alpha/h\right]} \right\} = \frac{\pi^{3}}{32} \left[1 - \frac{2\alpha^{2}}{h^{2}}\right].$$
(24)
$$(\alpha/h \to \infty)$$

Thus, for $a/h \ll 1$, we would obtain Eq. (21) from Eq. (20).

The simplest calculations involve a constant thermal conductivity. In this case, we solve for $(T - T_0)$ by the procedure

$$\frac{T - T_o}{T_o} = \Theta = A a^2 U / K_o T_o .$$
(25)

3. INPUT STATEMENTS

While program STORE properly accounts for the variation of thermal conductivity with temperature, it does not describe the variation of A [see Eq. (1)] with temperature. The power density decreases as the specific volume increases, that is, as the density of the material decreases. Use of this program (or programs for the simpler relationships between thermal conductivity and temperature) is advantageous because the execution time is significantly shorter than that of a program based on the more accurate finite-difference equations.

The first three READ statements are:

READ 9001, NR, NZ, NOM READ 9011, (R(I), I = 1, NR) READ 9011, (Z(J), J = 1, NZ)

9001 FORMAT (1615)

9011 FORMAT (16 F5.3)

Here

- NR is the number of relative-radius units at which output data are to be printed. The program is set for NR = 17 and for the values described below.
- NZ is the number of vertical units at which output data are to be printed. A reasonable number is in the range 20 to 45.
- NOM is the number of terms to be used, instead of an infinite number, in evaluating U(x, Z), Eq. (10). We have used as many as 100 and as few as 5; in general, a value in the range 10 to 20 will be adequate.

- R(I) are the NR radial positions at which data are printed. Output formats carry headings of 0.0 (corresponding to the centerline of the cylinder), 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, and 1.0. Thus, the output tables will list temperatures, and other values, for the centerline and for distances of 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 60, 70, 80, 90, 95, and 100% of the distance from the centerline to the wall. If these 17 values are not used, then certain format statements will have to be changed.
- Z(J) are the distances, in radius units, from the top or the bottom of the cylinder. Convenient values are 0.0, 0.005, 0.01, 0.02, etc., corresponding to locations on the top (or bottom) surface followed by distances of 0.005 radius, 0.01 radius, etc., into the cylinder from the top (or bottom). The last value of Z(J), namely Z(NZ), is used as the cylinder height/radius ratio. Thus, if NZ = 25 and Z(25) = 25, then the length of the cylinder is 25 times that of the radius.

Most of the values of Z(J) should correspond to relative heights of less than one-half the cylinder height. About the fourth from the last value of Z(J) should be the half-cylinder height [i.e., 12.5 in the above example]. The subsequent two values should be on the order of 0.9 times Z(NZ) and 0.95 times Z(NZ), respectively. These values are used to check for passage beyond the midplane of the cylinder; their judicial choice minimizes unnecessary duplication in the calculation of temperatures beyond the midplane. In the example above, it would be appropriate to use 30 or even 40 horizontal spacings for Z(J) < 12.5 followed by the four values 12.5, 22.5, 24.0, and 25.0.

It should be noted that the above READ statements are entered only once, regardless of how many calculational cases are to be performed. Thus, whether the radius of the cylinder is subsequently set to 0.1, 5.0, 25.0, or 100.0 cm, all the calculations will be performed at the centerline and, for example, 5%, 10%, etc., out toward the surface.

Program STORE uses thermal conductivity as a tabular function of temperature. This table, which is read only once and is used for all cases to be calculated, is entered as follows:

READ 9021, TP(NT), TK(NT)

9021 FORMAT (8E 10.4)

One temperature, TP(NT), and its thermal conductivity, TK(NT), are punched on a card, at 50°C intervals as the program is now written. DIMENSION allows a maximum of 99 such pairs of values. At the end of the table, any negative floatingpoint number, such as -1.0, is entered in the TP(NT) field (columns 1 - 10) to indicate the end of the table. The temperature interval 50.0°C was chosen because it is appropriate for materials heated to temperatures in the range 0.0 to 3000°C or higher. This interval is specifically involved in the integration shown in Eq. (5) for evaluating Θ as a function of v. Since it occurs in only a few statements, the program could be modified fairly easily.

In addition to the READ statements already described, there is one READ statement required for each case to be calculated, namely,

READ 9021, A, RAD, TINT, TO

Here

- A is the internal (absorbed) power density in cal sec⁻¹ cm⁻³, as in Eq. (1). Values in the range 0.1 to 0.8 are significant in connection with highlevel radioactive wastes from nuclear fuel processing.
- RAD is the cylinder radius, cm.
- TINT is the temperature interval at which temperature profiles are desired. For example, if the temperature difference (T - T_o) is expected to be on the order of 100°C, then TINT might be assumed to be 5. or 10., corresponding to the radial and vertical locations of temperatures spaced 5 or 10°C apart.

TO is the surface temperature, °C or °K, whichever is convenient.

TK0 is the thermal conductivity of the material at T_{o} , cal cm⁻¹ sec⁻¹ °C⁻¹.

4. EXECUTION TIMES AND OUTPUT

Each of the three programs (see Appendix A), namely, STORE, TKLIN (when K is a linear function of T), and TKCON (when K is constant), has been executed many times on the IBM/360-75 at ORNL to calculate temperature profiles in cylinders containing high- or intermediate-level radioactive wastes generated by the processing of nuclear fuels. Typically, the programs require 30 to 40 sec for compilation. Depending primarily on the number of temperatures at which profile data are desired, TKCON and TKLIN require 1 to 10 sec per case. Program STORE has a longer execution time, again depending (but less strongly) on the number of temperatures at which profile values are required; it generally requires 5 to 30 sec per case. For comparison, a more accurate evaluation of Eq. (1), based on the use of finite-difference equations, a grid of 30 radial divisions, 120 vertical divisions, and the near-minimum of 500 iterations, requires on the order of 5 min with FORTRAN IV, level H execution under optimum timing. The time savings of TKCON, TKLIN, and STORE are thus rather significant, while the loss of accuracy is not very great, as described below.

Output from STORE includes a table (Table 1) of NZ times NR values of U [Eq. (10)], a table (Table 2) of temperatures above the surface temperature, $(T - T_o)$, and a table of Θ values. Output also includes a table (Table 3) of distances, in radius units, measured from the bottom or the top of the cylinder, where heating above the surface temperature occurs by multiples of the quantity TINT. Finally, each program outputs a table of the number of iterations required to obtain each multiple of TINT at each radial location. The maximum number of such iterations in the studies reported here was 20; usually, however, this number did not exceed 2. In addition to the tables just mentioned, program STORE outputs a table of values for T, K, Θ , XTA, XTB, and XTC [where T, K, and Θ have been defined previously and XTA, XTB, and XTC are the constants used to represent T as a quadratic function

Table 1. Example of Output of the Dimensionless Quantity U [Eq. (10)] at Grid Points

HEIGHT

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THE DIMENSIONLESS U(I,J) FROM WHICH WE CALCULATE THETA(I,J), V(I,J), AND T(I,J). 50 TERMS ARE USED IN THE BESSEL FUNCTION SUMMATION. Values of the relative distance (R/A) from the cylinder axis are given in the first row of this table

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0.0 0.00 0
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Table 2. Example of Output of Temperatures Above the Surface Temperature at Grid Points

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TEMPERATURES ABOVE THE SURFACE TEMPERATURE. THE CYLINDER DIAMETER IS 15.2 CM. THE STRENGTH DF THE INTERNAL HEAT SUURCE IS 2.00E-01 CALORIES/CM**3/SEC, 8.37E-01 WATTS/CM**3 SOURCE STRENGTH IN OTHER UNITS IS 80910.6 BTU/FT**3/HR AND 1.41E 02 MEV*CURIES/CM**3. THE THERMAL CONDUCTIVITY COEFFICIENT AT THE SURFACE TEMPERATURE OF 200. DEGREES C IS 5.63E-03 CAL/CM/SEC/DEG C. UNITS

VALUES OF THE RELATIVE DISTANCE (R/A) FROM THE CYLINDER AXIS ARE GIVEN IN THE FIRST RDW OF THIS TABLE

(Z/A)	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.60	0.70	0.80	0.90	0,95	1.00	
	•									,								
0.0	a a	0.0	0.0	0.0	0.0		0.0		~ ^	0.0	• •			• •	• •			
0.005	5.4	5.4	5.4	6.7	5 3	5.2	U.U	6.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
0.010	10.9	10.7	10.7	10.5	9.5	10 7	5+1	5.0	4.7	······································	4.5	4.1	3.3	2.00	1.0	1.1	0.0	
0.015	15.0	16.0	15 0	16.9	10.5	10.5	10+1	7.7	7.0	9.3	9.0	12.0	1.0	2.2	2+2	2.1	0.0	
0.020	21.2	21 1	21 0	20.0	19.0	20.2	20.0	14.1	14.5	13.7	13.3	12.0	13 7	10.0	2.2	5.1	0.0	
0.025	26 4	21+1	21.0	20.9	20.0	20+3	20.0	19.3	22 6	70.4	21 0	10.7	12+1	10.0	0.0	4.1	0.0	
0.027	20.3	20.2	20.1	20.9	22.0	27.2	24+5	24.2	23.5	22.0	21.9	17.1	20.2	15.4	0.4	5.0	0.0	
0.040	41 1	61 0	21.1	5015 6015	60.0	30.0	27.7	20.0	20.0	21+1	20.0	20.0	20.2	12.7	7.7	7.5	0.0	
0.050	41.1 20 5		40.0	40.9	40.0	57.4 60 E		21+0	2040	33.0	63.0	30.0	20.4	20.1	16.4	7.5	0.0	
0.040	50.5	50.5	50.2	47.0	47.7	40.07	41.0 54 3	40.0	47.2	4247	42.0	21.0	36.4	22.4	10.0	9.0	0.0	
0.030	2 701	39.0	2 2 2 2	20.3	20.2	21.3	20.2	24.9	22+4	50.3	47.0	44.1 51 3	10.2	29.0	10.5	10.4	0.0	
0.010	77 3	77 1	74 7	74 1	76.7	76 1	04.0 777	71 0	61.0	24.3	57.0	57 6	42.0	24+1	20.0	11.0	0.0	
0.000	11.C	96 4	10.1	10.1	12.2	14.1	12.1	79.7	74 5	72 0	70 0	21.0	47.2	20.2	23+1	16.0	0.0	
0.090	43.7	5J+4 03 E	32.0	74.3	02.4	80.0	00.9	94 1	10.9	13.7	77 4	40 7	50 4	46.0	27.4	14.02	0.0	
0.130	100 2	100.0	72.1	92.5	91.5	106 7	102 7	100.3	07 5	00.9	00 3	81 0	57.4	40.0	21+5	17.5	0.0	
0.140	132 9	124 4	122.0	122.0	120.4	110 7	114 4	112 7	110 6	106 6	102.3	01.6	77 9	50 7	26 2	10 6	0.0	
0.140	127.0	123.0	12 3 . 0	126.0	120.0	133 0	170.4	126 7	122 4	110.0	112.5	1.01 4	96 1	45 0	39.4	21 1	0.0	
0.190	157 - 1	157.4	140.9	149 6	144.0	144 5	161 6	120.3	122+0	120.7	124 1	110.9	03.0	71.5	41.7	22.7	0.0	
0.200	142 1	142 0	149.0	143.5	140.0	166 3	141.0	140 4	134.2	130 0	134 0	110.7	101 1	76.8	44.6	26.2	0.0	
0.250	103.1	102.0	102.0		196.7	193.0	170 1	174 0	145.0	157.7	154 5	120 4	117 2	88 6	50.9	27.6	0.0	
0.200	171+6	215 4	214 2	212 4	200.0	204 4	202 2	107 0	107.0	194 0	176 0	156.3	131.0	99.5	56.2	30.1	0.0	
0.350	213.0	212.4	21443	222 4	207.0	200.4	202.02	216 4	209 6	201 8	102 0	170 9	142.0	107.0	60.7	32.6	0.0	
0.600	251.44	255 9	255.6	252 2	249 0	244 8	239 5	233.3	225.9	217.3	207.5	183.6	153.1	114.2	64.5	34.4	0.0	
0.450	270.3	277.5	224.2	264 5	245.0	260 5	254.8	248.1	240.1	230.9	220.3	194.7	162.0	120.5	67.8	36.1	0.0	
0.400	21247	2971	245 5	200.7	279.1	274.3	269.3	261.1	252.6	242.8	231.5	204.3	169.6	126.0	70.7	37.6	0.0	
0.550	201.0	300 0	209 4	202.1	291.6	286.5	280.1	272.5	263.6	253.2	241.4	212.7	176.3	130.7	73.2	38.9	0.0	
0.500	312.0	211 4	273.4	306 7	302.6	297.2	290.5	292.6	273.2	262.3	250.0	220.0	182.2	134.8	75.4	40.0	0.0	
0.700	241 0	320.3	328.4	325.3	320.8	315.0	307.8	299.2	289.1	217.5	264.1	232.1	191.8	141-6	78.9	41.9	0.0	
0.100	345 4	345.1	343.1	339.7	335.0	328.8	321-2	312.1	301.5	289.2	275.1	241.4	199.2	146.8	81.7	43.3	0.0	
0.000	357.4	356.7	354.6	351.1	346.1	339.7	331.7	322.2	311.1	298.3	283.7	248.7	204.9	150.8	83.8	44.4	0.0	
1 000	365 5	3.5.7	363.6	359.9	354.8	348.1	339.9	330.1	318.6	305-4	290.4	254.3	209.4	154.0	85.5	45.2	0.0	
1 750	361 6	390 7	378 4	374.5	369.1	362.1	353.4	343.1	331.0	317-1	301.3	263.6	216.7	159.1	88.2	46.7	0.0	
1.6.00	20147	10011	386.4	392.4	376.9	369.6	360.7	350.1	337.7	323.4	307.2	268.6	220.6	161.9	89.7	47.4	0.0	
1.750	104 0	303.0	330.8	386.7	381.1	373.7	364.7	353.9	341.3	326.8	310.4	271.3	222.8	163.4	90.5	47.8	0.0	
2 000	204 2	105 5	323.1	399.0	344.3	375.9	366.8	355.9	343.2	328.6	312.1	272.7	223.9	164.1	90.9	48.1	0.0	
2.000	207 6	146 6	394.7	390.1	384.4	376.9	367.9	356-9	344.1	329.5	312.9	273.4	224.4	164.5	91.1	48.2	0.0	
2 600	277.44	30.0	304.5	390.4	344.7	377.2	368.1	357.2	344 4	329.8	313.2	273.6	224.6	164.6	91.2	48.2	0.0	
2.000	397.0	195.5	393.1	189.0	383.4	375.9	366.8	355.9	343.2	328.6	312.1	272.7	223.9	164.1	90.9	48.0	0.0	
5 0 70 6 0 00	346 5	365.7	363.6	359.9	354.8	348.1	339.9	330.1	318.6	305.4	290.4	254.3	209.4	154.0	85.5	45.2	0.0	
++UUUU	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
2.000	0.0	U • U			2.0					• -	· • -						. –	

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Table 3. Example of Temperature-Profile Table

TEMP DEG C. DISTANCES, IN RADIUS UNITS, MEASURED FROM THE BOTTOM OR TOP OF THE CYLINDER, AT WHICH OCCUR HEATING ABOVE The Surface temperature by amounts shown in the first Column.

VALUES OF THE RELATIVE DISTANCE (R/A) FROM THE CYLINDER AXIS ARE GIVEN IN THE FIRST ROW OF THIS TABLE

0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50 0.60 0.70 0.80 0.90 0.95 1.0D

50.	0.049 0	0.050	0.050	0.050	0.051	0.052	0.053	0.054	0.056	0.058	0.060	0.068	0.081	0.111	0.242
100.	9.108 6	0.108	0.109	0.110	0.111	0.113	0.116	0.120	0.124	0.129	0.136	0.157	0.197	0.308	
150.	0.179 (0.179	0.180	0.182	0.185	0.189	0.194	0.201	0.210	0.220	0.235	0.281	0.384	0.877	
200.	0.267 (0.268	0.270	0.273	0.279	0.286	0.295	0-307	0.323	0.345	0.374	0.477	0.812		
250.	0.383 .0	0.384	0.385	0.394	0.403	0.416	0.434	0.457	0.489	0.534	0.600	0.921			
300.	0.548 0	j.550	0.557	0.569	0.588	0.614	0.652	0.705	0.787	0.922	1.211				
350.	0.833 (3.539	0.857	0.889	0.942	1.026	1.171	1.494							

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of Θ after Eq. (5) is integrated to evaluate Θ as a function of T and K].

In one test example, the thermal conductivity of a hypothetical glass was assumed to be a linear function of temperature up to 1000°C (see Table 4). Other properties were as follows: power density, 0.2 cal sec⁻¹ cm⁻³; radius of the vessel, 7.6 cm (6 in. in diameter); and length/radius ratio, 25. Program TKLIN gave a maximum centerline temperature of 599.5°C for this example when the surface temperature was maintained at 200°C; execution time was 5.0 sec. For comparison, the maximum centerline temperature was also calculated by using a program based on finite-difference equations; in this program, the density-vs-temperature properties (Table 4) were those of an alkali borate glass.⁹ As the temperature increased from 200 to 550°C, the density decreased and the specific power density decreased by about 3.6%. With the latter program, the maximum centerline temperature was found to be 564.0°C after either 1500 or 2000 iterations. After 500 and 1000 iterations the maximum calculated temperatures were 557.4°C and 563.9°C, respectively. Each 500 iterations consumed approximately 5 min of execution time on the IBM/360-75.

As expected, TKLIN overestimates the temperature rise because it does not compensate for the reduction in fission product power density as the temperature increases. In the example described above the error is about 36°C out of a "true" temperature elevation of 364°C (i.e., a 10% overestimation of the temperature rise). This error is small enough to be neglected in most instances, where the existence of only very crude specific heat data plus uncertainties in densities and thermal conductivities easily lead to larger errors.

Temp (°C)	Thermal Conductivity (<u>cal</u> (cm•sec•°C)	Specific Heat (<u>cal</u> g.°C)	Density $\left(\frac{g}{cm^3}\right)$
50	0.00443	0.2	2.313
100	0.00483	0.2	2.305
150	0.00523	0.2	2.296
200	0.00563	0.2	2.288
250	0.00603	0.2	2.281
300	0.00643	0.2	2.275
350	0.00683	0.2	2.264
400	0.00723	0.2	2.253
450	0.00763	0.2	2.239
500	0.00803	0.2	2.225
550	0.00843	0.2	2.206
600	0.00883	0.2	2.188
650	0.00923	0.2	2.167
700	0.00963	0.2	2.146
750	0.01003	0.2	2.120
800	0.01043	0.2	2.095
850	0.01083	0.2 .	2.068
900	0.01123	0.2	2.042
950	- 0.01164	0.2	2.017
1000	0.01207	0.2	1.992
1050	0.01252	0.2	1.966
1100	0.01299	0.2	1.940
1150	0.01348	0.2	1.914
1200	0.01399	0.2	1.888
1250	0.01452	0.2	1.862
1300	0.01507	0.2	1.836

Table 4.	Physical and Thermal Properties of Hypothetical Glass Used to Obtain
Estim	ates of Errors in Program TKLIN Due to Decrease in Density with
	Increasing Temperature

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- G. W. Morey, <u>The Properties of Glass</u>, 2d ed., Reinhold, New York, 1954; see data for 10.6 wt % Li₂O/26.4 wt % Na₂O/34.4 wt % K₂O.

6. APPENDIX

This appendix contains listings of program STORE, subroutine THERMY, and the two functions XINT and BIZERO. The subroutine is used to calculate the coefficients A_i , B_i , and C_i , which will permit the determination of a dependent variable Y when the value of the independent variable X is known. Thus,

$$Y = A_{i} + B_{i}X + C_{i}X^{2}$$
 (A-1)

For example, by use of Eq. (12) we obtain Θ as a function of T. Since we wish to determine T as a function of Θ , we use Eq. (A-1) to solve for the coefficients in the equation

$$T = A_i + B_i \Theta + C_i \Theta^2$$

FUNCTION XINT(Y, L, H) is used to obtain the integral of Eq. (12), while FUNCTION BIZERO(X) is used to evaluate the terms I_0 of Eq. (10).

С *** ******** THIS IS PROGRAM STORE ********* С С * ** ** ** ** ** ** ** ** ** ** *** *** *** *** ** ** ** ** ** ** ** ** ** С THIS PROGRAM CALCULATES TEMPERATURE AS A FUNCTION OF POSITION WITHIN A CYLINDER OF GLASS CONTAINING AN INTERNAL HEAT SOURCE. С SUCH AS FISSION PRODUCTS. THE COEFFICIENT OF THERMAL CONDUCTIVITY С С IS A TABULAR FUNCTION OF TEMPERATURE. THE SURFACE TEMPERATURE IS A CONSTANT, TO. THIS TEMPERATURE IS A MAJOR FACTOR IN CONTROL OF С С THE INTERNAL TEMPERATURE. THE PROGRAM WILL HANDLE MORE THAN ONE CASE AT A TIME, BUT ALL HAVE. Ç C THE SAME VALUES OF NR, NZ, NOM, R(I), AND Z(J). THESE ARE C READ IN UNLY ONCE PER COMPUTER JOB. DIMENSION DZDT(20,50) DIMENSION IPRNT(50) DIMENSION LCOUNT(20,50) DIMENSION Q1(200),Q2(200),Q3(200),Q4(200),Q5(200),Q6(200) DIMENSION Q7(200,20),Q8(50) DIMENSION R(50) DIMENSION SAVEZ(35) DIMENSION T(20,50), TCALC(20,50), THETA(20,50), THETAC(20,50), TT(50) DIMENSION TK(100), TP(100), VT(100), THT(100) DIMENSION TN(100), TKN(100) DIMENSION U(20,50) DIMENSION V(20,50), VCALC(20,50) DIMENSION XT(100), XTA(100), XTB(100), XTC(100) DIMENSION Y(100) DIMENSION Z(50),ZCALC(20,50) TYPE DOUBLE Q3,Q4,Q5,Q6,Q7,ARG1,ARG2,PI,PI3,VI01,VI02,BIZERO DATA (PI=3.14159265359), (PI3=31.0062766803) С PI=3.1415927 PI**3=31.0062767 C 9001 FORMAT(1615) 9011 FORMAT(16F5.3) 9021 FORMAT(8E10.4) 9101 FORMAT(81H THE NUMBER OF RADIAL POSITIONS EXCEEDS THAT FOR WHICH **1THIS PROGRAM WAS WRITTEN.**) 9111 FORMAT(81H THE NUMBER OF HEIGHT POSITIONS EXCEEDS THAT FOR WHICH **ITHIS PROGRAM WAS WRITTEN.)** 9121 FORMAT(83H THE NUMBER OF TERMS IN THE BESSEL FUNCTION SUMMATION E IXCEEDS THE DIMENSION OF Q7.) 9131 FORMAT(46H THE TEMPERATURE INTERVAL HAS BEEN SET TO 0.0) 9141 FORMAT(74H THE NUMBER OF TEMPERATURE PROFILES REQUESTED IS TOO LA THE VALUE OF TINT SHOULD BE INCREASED.) 1RGE FOR DIMENSION./42H 9151 FORMAT(32H THE CALCULATED VALUE OF IPRNT(,12,59H) EXCEEDS 17, POS ISIBLY BECAUSE TINT HAS BEEN SET TOO SMALL.) 9201 FORMAT(83H1 HEIGHT TEMPERATURES ABOVE THE SURFACE TEMPERATU IRE. THE CYLINDER DIAMETER IS, F8.1, 4H CM./ 58H IN THE S 2TRENGTH OF THE INTERNAL HEAT SOURCE IS, 1PE9.2 , 20H CALORIES/CM**3 3/SEC,,E9.2 , 12H WATTS/CM**3/48H RADIUS SOURCE STRENGTH IN 40THER UNITS IS,0PF9.1,18H BTU/FT**3/HR AND,1PE9.2,18H MEV*CURIES/ 5CM**3./81H UNITS THE THERMAL CONDUCTIVITY COEFFICIENT AT T 6HE SURFACE TEMPERATURE OF, OPF6.0, 13H DEGREES C IS, 1PE9.2, 18H CAL 7/CM/SEC/DEG C./1HO) VALUES OF THE RELATIVE DISTANCE (R/A) FROM TH 9211 FORMAT(120H 1E CYLINDER AXIS ARE GIVEN IN THE FIRST ROW OF THIS TABLE 1 2130H0 (Z/A) 0.00 0.05 0.10 0.15 0.20 0.25 0.30 0. 0.45 0.50 0.60 0.70 0.80 0.90 0.95 1.00 335 0.40 4 /1HO) VALUES OF THE RELATIVE DISTANCE (R/A) FROM TH .9221 FOR MAT(120H

**FTN,E,G,L.

PROGRAM STORE

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1E CYLINDER AXIS ARE GIVEN IN THE FIRST ROW OF THIS TABLE
                 0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.
            ·^ 0.45
    2130H0
                        0.50 0.60 0.70 0.80 0.90 0.95 1.00
    335
         0.40
    4 /1HO)
9231 FORMAT(F7.3,17F7.1)
                                 DISTANCES, IN RADIUS UNITS, MEASURED FRO
9241 FORMAT(120H1 TEMP
    1M THE BOTTOM OR TOP OF THE CYLINDER, AT WHICH OCCUR HEATING ABOVE/
                         THE SURFACE TEMPERATURE BY AMOUNTS SHOWN IN THE
    2120H DEG C.
                                                                   11
    3 FIRST COLUMN.
9251 FORMAT(F6.0,3X,17F7.3)
9261 FORMAT(7X,17(15,2X))
9271 FORMAT(1H1)
9281 FORMAT(37HOTHE EXECUTION TIME FOR THIS CASE WAS, F7.1, 8H SECONDS)
9291 FORMAT(315,5E15.5)
                                 THETA, A FUNCTION OF RELATIVE TEMP V, WHE
9301 FORMAT( 91H1HEIGHT
                                                                      THE S
    IN THE SURFACE TEMPERATURE IS KEPT AT, F6.0/ 58H
                                                         IN
    2TRENGTH OF THE INTERNAL HEAT SOURCE IS, F8.5, 20H CALORIES/CM**3/SE
                                                   SOURCE STRENGTH IN OTH
    3C,,F8.5, 12H WATTS/CM##3/ 48H RADIUS
    4ER UNITS IS,F9.1, 18H BTU/FT**3/HR AND,F9.1, 18H MEV*CURIES/CM**3
5./ 54H UNITS THE THERMAL CONDUCTIVITY COEFFICIENT AT,F6.0,
    6 13H DEGREES C 15,F8.5, 18H CAL/CM/SEC/DEG C./1H0)
9311 FORMAT(F7.3,2X,17F7.3)
                                 THE DIMENSIONLESS U(I,J) FROM WHICH WE C
9321 FORMATE 95H1HEIGHT
     1ALCULATE THETA(I,J), V(I,J), AND T(I,J)./15H
                                                                    ,I3,49H
     2 TERMS ARE USED IN THE BESSEL FUNCTION SUMMATION.)
9331 FORMAT(8E15.8)
9341 FORMAT(24H1TO HAS BEEN SET TOO LOW)
9351 FORMAT(45H1TO HAS NOT BEEN SET TO AN INTEGER TIMES 50.0)
9361 FORMAT(F10.0,F10.6,F10.5,3E16.8)
 9371 FORMAT(7H1THETA(,I2,1H,,I2,2H)=,F6.3)
 9381 FORMAT(1H0)
 9391 FORMAT(15F6.0)
 9401 FORMAT(F7.3,17F7.2)
 9411 FORMAT(F7.3,17F7.3)
      READ 9001,NR,NZ,NOM
С
      R(I) IS THE RELATIVE RADIUS = RADIAL COORDINATE/RADIUS OF CYLINDER
С
      Z(J) IS THE RELATIVE HEIGHT = HEIGHT CODRDINATE/RADIUS OF CYLINDER
С
C
      IF(NR-17)21,21,11
   11 PRINT 9101
      GO TO 4001
   21 IF(NZ-50)41,41,31
   31 PRINT 9111
      GO TO 4001
   41 IF(NDM-200)61,61,51
   51 PRINT 9121
      GO TO 4001
   61 READ 9011, (R(I), I=1, NR)
      READ 9011, (Z(J), J=1, NZ)
      BQ=0.0
      DO 101 L=1,NOM
           3Q = 8Q + 1.0
           Q1(L) = 2.0 \times BQ - 1.0
           Q_2(L) = Q_1(L) * Q_1(L)
           Q3(L) = Q1(L) * Q2(L)
           Q4(L)=Q1(L) \neq PI/Z(NZ)
           Q5(L)=Q4(L) \neq R(NR)
           Q6(L) = BIZERO(Q5(L))
  101 CONTINUE
       00 111 J=1,NZ
           08(J) = Z(J) * (Z(NZ) - Z(J)) * 0.5
```

111 CONTINUE CON1=4.0*Z(NZ)*Z(NZ)/PI3 DO 121 I=1,NR U(I,1)=0.0 U(I, NZ) = 0.0**121 CONTINUE** NZ1=NZ-1 00 131 J=2,NZ1 U(NR, J) = 0.0**131 CONTINUE** NR1 = NR - 100 221 J=2,NZ1 00 211 I=1,NR1 SUM=0.0 DO 201 M=1,NOM ARG1=Q4(M)*R(I)ARG2=05(M) VI02=Q6(M) IF(ARG1)151,141,151 141 VI01=1.0 GO TO 181 151 IF(ARG1-ARG2)171,161,171 161 VI01=VI02 GO TO 181 171 Q7(M,I)=BIZERO(ARG1) VI01=Q7(M,I)181 SUM=SUM+VI01*SIN(Q4(M)*Z(J))/Q3(M)/VI02 201 CONTINUE $U(I_{J})=Q8(J)-CON1 \neq SUM$ 211 CONTINUE 221 CONTINUE PRINT 9321,NOM **PRINT 9211** 00 231 LK=1,NZ PRINT 9311, (Z(LK), (U(J,LK), J=1, NR)) 231 CONTINUE NT=0241 NT=NT+1 READ 9021, TP(NT), TK(NT) IF(TP(NT))251,241,241 251 NT=NT-1 NTEMP=NT-1 301 READ 9021, A, RAD, TINT, TO IF(A)4001,4001,311 311 INTIME=ICLOCKF(DUMMY) DIA=2.0*RAD A0=A/T0JN=0 341 JN=JN+1 IF(TO-TP(JN))361,401,341 361 IF(JN-1)371,371,381 371 PRINT 9341 GO TO 301 381 IF(JN-NT) 341, 341, 391 391 PRINT 9351 GO TO 301 401 J0=JN TKO = TK(JO)CON 2= AO *R AD *R AD / TKO HUNIT1=A*4.185 HUN IT 2= A* 2.8317*3.6*3.9685E04 HUNIT3=A*2611.6/3.7

JT=NT-JO+1JTEMP = JT - 1JR=JT-2 THT(1)=0.0THT(2)=25.0*(TK(J0)+TK(J0+1))/T0/TK0 Y(1) = TK(JQ)Y(2) = TK(J0+1)DO 411 II=3,JTEMP Y(II) = TK(II+JO-1)THT(II)=XINT(Y,11,50.0)/TO/TKO 411 CONTINUE DO 421 I=J0,NT JK=I-J0+1 TN(JK) = TP(I) - TOTKN(JK) = TK(1)421 CONTINUE CALL THERMY(THT,TN,XT,XTA,XTB,XTC,JT,JTEMP,1.0,1.0,100) **PRINT 9271** PRINT 9001, J0 DO 431 JK=1,JTEMP PRINT 9361, TN(JK), TKN(JK), THT(JK), XTA(JK), XTB(JK), XTC(JK) 431 CONTINUE DO 581 J=1,NZ DD 571 I=1,NR THETA(I,J)=A0*RAD**2*U(I,J)/TK0 MT=0 MT = MT + 1451 IF(THETA(I,J)-THT(MT))461,561,451 IF(MT-1)471,471,491 461 TEMP=THETA(I,J)-THT(MT) 471 IF(TEMP+0.003)481,561,561 PRINT 9371, I, J, TEMP 481 GO TO 301 IF(MT-JTEMP)501,571,571 491 NIT=MT-1 T(I,J) = XTA(NIT) + THETA(I,J) * (XTB(NIT) + THETA(I,J) * XTC(NIT))501 GO TO 571 T(I,J)=TN(MT)561 CONTINUE 571 581 CONTINUE **J=**0 TMAX=0.0601 J=J+1 IF(J-NZ)611,611,641 611 IF(TMAX-T(1,J))621,621,601 621 TMAX=T(1, J.) 631 GO TO 601 641 IF(TMAX-10.0)651,661,661 651 IFMT=3 GO TO 691 661 IF(TMAX-100.0)671,681,681 671 IFMT=2 -GO TO 691 681 IFMT=1 691 CONTINUE PRINT 9201, DIA, A, HUNIT1, HUNIT2, HUNIT3, TO, TKO **PRINT 9211** GO TO (701,721,741),IFMT 701 DO 711 LL=1,NZ PRINT 9231, (Z(LL), (T(J,LL), J=1, NR)) 711 CONTINUE GO TO 761

721 DO 731 LL=1.NZ PRINT 9401, (Z(LL), (T(J,LL), J=1,NR)) 731 CONTINUE GO TO 761 741 00 751 LL=1,NZ PRINT 9411, (Z(LL), (T(J,LL), J=1, NR)) 751 CONTINUE 761 CONTINUE PRINT 9301, TO, A, HUNIT1, HUNIT2, HUNIT3, TO, TKO PRINT 9211 00 811 LL=1,NZ PRINT 9311, (Z(LL), (THETA(J,LL), J=1, NR)) 811 CONTINUE IF(TINT)831,821,831 821 PRINT 9131 GO TO 4001 831 DO 851 J=1+NZ IF(T(1,J)/TINT-50.0)851,851,841 841 **PRINT 9141** GO TO 4001 851 CONTINUE DO 871 L=1,50 IPRNT(L)=000 861 IR=1,20 LCOUNT(IR,L)=0 CONTINUE 861 871 CONTINUE NL=0 00 2801 I=1,NR L=1 TCHECK=TINT **J**=0 1001 J=J+1IF(J-NZ+2)1011,1011,2801 1011 TEMP=T(I,J)-TCHECK IF(ABS(TEMP)-0.05)1021,1021,1031 1021 ZCALC(I,L)=Z(J)GU TO 1761 1031 IF(TEMP)1001,1001,1041 1041 K2=J K1=J-1 IF(T(1,K2)-T(1,K1))2801,2801,1051 1051 IF(T(I,K2+1)-T(I,K2))1071,1071,1061 1061 J1=K1 J2=K2 J3=K2+1 GO TO 1141 1071 J1=K1-1 J2=K1 J 3=K2 1141 TERM1=(T(I,J3)-T(I,J1))/(2(J3)-2(J1)) TERM2=(T(I,J2)-T(I,J1))/(Z(J2)-Z(J1)) CONB=(Z(J3)-Z(J2))/(TERM1-TERM2)CONA={Z(J3)+Z(J1)-CONB*TERM1)/2.0 CONC=T(I, J2)-(Z(J2)-CONA)*(Z(J2)-CONA)/CONB RUDT=SQRT(CONB*(TCHECK-CONC)) IF(CON8)1161,1151,1151 1151 DZDT(I,L)=CONB/2.0/ROOT Z T=CONA+ROOT GŨ TO 1171 1161 DZDT(I,L) =- CONB/2.0/ROOT ZT=CUNA-ROOT

1171	
	$\frac{1}{1} \left(\frac{1}{1} \right) = \frac{1}{1} \left(\frac{1}{1} \right) = \frac{1}{1} \left(\frac{1}{1} \right) = \frac{1}{1}$
1501	L(I) (N + (1 + 1) - 10) (15) (1 + 15) (1 + 15) (1 + 20) (1 + 15)
1511	
	DD = 1601 M=1, NUM
	$ARGI=U4(M) \times K(I)$
	ARG2=Q5(M)
	VIO2=Q6(M)
	IF(ARGI)1531,1521,1551
1521	VI:01=1.0
	GO TO 1561
1531	IF(ARG1-ARG2)1551,1541,1551
1541	$V_{1}O_{1} = V_{1}O_{2}$
	GO TO 1561
1551	V I = Q7(M, I)
1561	ARG3=Q4(M)*Z1
	IF (ABS(ARG3)-1.0E15)15/15/1901
1571	SUM=SUM+VI01#SINLARG37745(M777102
	SUMD=SUMD+VIOI#CUSTARGSI/Q2(HT) VIO2
1601	CONTINUE
	THE TAC(I,L)=CON2*(ZT*(Z(NZ)-ZT)+0.9-CONT.9000
	M T = 0
1651	MT=MT+1
-	IF(THETAC(I,L)-THT(MT))1661,1701,1851
1661	IF(MT-1)301,301,1681
1681	IF(MT-JTEMP)1691,1781,1781
1691	NIT=MT-1
	TCALC(I,L)=XTA(NIT)+THETAL(I,L)+(XTB(NIT)+THETAL)
1	XTC(NIT))
	GO TO 1711
1701	TCALC(I,L) = TN(MT)
1711	TEMP=TCALC(I,L)-TCHECK
	IF(ABS(TEMP)-0.05)1751,1751,1721
1721	ZT=ZT-TEMP*DZDT(I,L)
	KK=LCQUNT(I,L)
	SAVEZ(KK+1)=ZT
	GO TO 1501
1751	2CALC(I,L)=ZT
1761	TT(L) = L + TINT
	IPRNT(L) = IPRNT(L) + I
	IF(IPRNT(L)-17)1781,1781,1771
1771	PRINT 9151,L
	GO TO 4001
1781	TCHECK=TCHECK+TINT
	IF(L-NL)1801,1801,1791
1791	NL=L
1801	
	GO TO 1011
2001	ZMIN=Z(K1)
	ZMAX = Z(KZ)
2011	ZT=0.5*(ZMIN+ZMAX)
	SUM=0.0
	SUMD=Q.0
	DO 2101 M=1,NUM
	$ARG1=Q4(M) \neq R(1)$
	ARG2=Q5(M)
	VI02=Q6(M)
	IF(ARG1)2031,2021,2031
2021	V I = 1.0
	GO TU 2061

x

,

2031	IF (ARG1-ARG2) 2051, 2041, 2051
2041	VI01=VI02
	GO TO 2061
2051	V I:01 = Q7(M, I)
2061	$ARG3=Q4(M) \neq ZT$
	IF(ABS(ARG3)-1.0E15)2071,301,301
2071	SUM=SUM+VI01#SIN(ARG3)/Q3(M)/VI02
2101	CONTINUE
	THETAC(I,L)=CON2*(ZT*(Z(NZ)-ZT)*0.5-CON1*SUM)
	MT=0
2151	M T = MT + 1
	IF(THETAC(I,L)-THT(MT))2161,2201,2151
2161	IF(MT-1)301,301,2181
2181	IF(MT-JTEMP)2191,1781,1781
2191	N I T = M T - 1
	TCALC(I,L)=XTA(NIT)+THETAC(I,L)*(XTB(NIT)+THETAC(I,L)*
1	L XTC(NIT))
	GO TO 2211
2201	TCALC(I,L)=TN(MT)
2211	TEMP=TCALC(I,L)-TCHECK
	IF(ABS(TEMP)-0.05)1751,1751,2221
2221	IF(TEMP)2241,2231,2231
2231	Z MA X = Z T
	GO TO 2301
2241	Z MI N= ZT
2301	LCDUNT(I,L)=LCDUNT(I,L)+1
	IF(LCOUNT(I,L)-30)2011,2011,2801
2801	CONTINUE
	PRINT 9241
	PRINT 9221
	DO 3021 LL=1,NL
	NA=IPRNT(LL)
	PRINT 9251,(TT(LL),(ZCALC(J,LL),J=1,NA))
3021	CONTINUE
	PRINT 9271
	00 3031 LL=1,NL
	NA=IPRNT(LL)
	PRINT 9261,(LCOUNT(J,LL),J=1,NA)
3031	CONTINUE
	DTIME=(ICLOCKF(DUMMY)-INTIME)*1.0/60.0
	PRINT 9281, DTIME
	GO TO 301
4001	CALL EXIT
	END

	SUBROUTINE THERMY(X,Y,W,A,B,C,N DIMENSION A(LD),B(LD),C(LD),W(L	T,NTEMP,X0,Y0,ID) D),X(ID),Y(ID)
	IE(Y0)101.101.301	
101	$1 1 \in (X_0 - X_1 + 1) = 1 = 1 = 1 = 1 = 1 = 1 = 1 = 1 = 1 $	
121	I PRINT 701	
161		
าวเ	$1 \times 0 = Y(1)$	
1) 1		
141		
151	1 I = I + 1	
1)1	I = I + I I = (I = NT) 171.171.161	
161	1 PRINT 711	
101	60 TO 901	
171	$1 TF(x_0-x(T)) 191 \cdot 181 \cdot 151$	
181	$1 Y_0 = Y(1)$	
101	60 TO 301	
191	1 [E(I=NT)201.211.211	
201	1 .11=1-1	
201	12=1	
	13=[+]	
•	GO TO 221	
211	1 11=1-2	
211	12=1-1	
221	T = T = X(J2) + X(J3) + X(J3) - X(J3)	3)*X(J2)*X(J2)
~~ 1	T = T = X(J = X(J = X = X = X = X = X = X = X = X = X =	3) * X (J1) * X (J1)
	T = RM3 = X(J = 1) * X(J = 2) * X(J = 2) - X(J = 2) +	2) *X (J1) *X (J1)
	DEL TA=TER M1-TER M2+TER M3	
	$C \Lambda = (Y (11) * TERM1 - Y (12) * TERM2$	+Y(J3)*TERM3)/DELTA
	CB = (Y(12) * X(13) * X(13) - Y(13))	*X(J2)*X(J2)
	1 - Y(J1) + X(J3) + X(J3) + Y(J3)	*X(J1)*X(J1)
	2 $-Y(J1) * X(J2) * X(J2) - Y(J2)$	*X(J1)*X(J1))/DELTA
	CC = (Y(J3) * X(J2) - Y(J2) * X(J3)	-Y(J3)*X(J1)+Y(J1)*X(J3)
	$+Y(J_2) + X(J_1) - Y(J_1) + X(J_2)$)/DELTA
	$Y_0 = C_0 + X_0 \neq (C_0 + X_0 \neq C_0)$	
301	01 00 311 (=1.NT	
201	W(L) = Y(L) / Y0	
311	1 CONTINUE	
	DO 401 J=1.NTEMP	
	IF(J-NTEMP)331,341,341	
331	1 I 1=J	
	I = J + 1	
	I 3= J+ 2	
	GO TO 351	
341	1 I I = J - 1	
	[2=J	
	I 3= J+1	
351	51 TERM1=X(I2)*X(I3)*X(I3)-X([3)*X([2)*X([2)
	TERM2=X{I1}*X(I3)*X(I3)-X(I3)*X(I1)*X(I1)
	TERM3=X(I1)*X(I2)*X(I2)-X([2)*X(I1)*X(I1)
	DELTA=TERM1-TERM2+TERM3	
	A(J)=(W(I1)*TERM1-W(I2)*TE	RM2+W(I3)*TERM3)/DELTA
	B(J)=(W(I2)*X(I3)*X(I3)-W([3]*X([2)*X([2)
	1 - W(11) * X(13) * X(13) + W(.)	I3)*X(I1)*X(I1)
	2 +W([1)*X([2)*X([2)-W([2)*X([1)*X([1))/DELTA
	C(J) = (W(I3) * X(I2) - W(I2) * X(I))	[3)-W(I3)*X(I1)
	1 +W(I1)*X(I3)+W(I2)*X(I1)-W(I1)*X(I2))/DELTA
401	D1 CONTINUE	
701	01 FORMAT(49H1 TO HAS BEEN SET TO	O LOW FOR THE PRESENT PROGRAM)
711	LI FORMAT(50H1 TO HAS BEEN SET TO	D HIGH FOR THE PRESENT PROGRAM)

RETURN 901 CALL EXIT END

```
FUNCTION XINT (Y,L,H)
   DIMENSION Y(200)
   K=L
   KP=K/2*2
   NDIFF=KP-K
   IF(NDIFF)1,2
 2 K=K-1
 1 \text{ ODD} = 0.0
   EVEN=0.0
   KM2=K-2
   D060I=3,KM2,2
60 0DD=0DD+Y(1)
   KM1 = K - 1
   D062I=2,KM1,2
62 EVEN=EVEN+Y(I)
   XINT=H/3.0*(Y(1)+Y(K)+4.0*EVEN+2.0*00D)
   IF(NDIFF)3,4
 4 XINT=XINT+ H *(Y(K)+Y(K+1))/2.0
 3 RETURN
```

FUNCTION BIZERO(X) CALCULATES MODIFIED BESSEL FUNCTION OF THE FIRST KIND, IO(X), FOR (-3.75,X,IN CALCULATES BY SERIES 9.8.1 AND 9.8.2 OF N.B.S. HOBK OF MATH FUNCHS (1964) TYPE DOUBLE S,T,X,Y,BIZERO Y=X IF(Y+3.75)99,3,3 3 IF(3.75-Y)8,4,4 C***4 -3.75.LE.X.LE.3.75 4 T=Y/3.75 T=T#T BIZER0=(((((T*.0045813+.0360768)*T+.2659732)*T+1.2067492)*T +3.0899424)*T+3.5156229)*T+1. 1 RETURN C***8 3.75.LT.X 8 T=3.75/Y S=(((((((T*.00392377-.01647633)*T+.02635537)*T-.02057706)*T 1 +.00916281)*T-.00157565)*T+.00225319)*T+.01328592)*T+.39894228 BIZERO=DEXP(Y)*S/DSQRT(Y) RETURN C**99 ARGUMENT OUT OF RANGE. RETURN ZERO. 99 BIZERD=0 RETURN END

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