2/
6-29-77

SAND-76 0742
Unlimited Release

3151

TEMPERATURE CAPABILITY FOR DTF-IV (DTF-71 VERSION)

D. W. Varela and J. S. Philbin

Prepared by Sandia Laboratories, Albuquerque, New Mexico 87115
and Livermore, California 94550 for the United States Energy Research
and Development Administration under Contract AT (29-1)-789

May 1977

Sandia Laboratories

SF 2900 Q(7-73)

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Issued by Sandia Laboratories, operated for the United States Energy Research and Development Administration by Sandia Laboratories.

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Printed in the United States of America

Available from:

National Technical Information Service
U. S. Department of Commerce
5258 Port Royal Road
Springfield, VA 22151

Price: Printed Copy \$3.50; Microfiche \$3.00

SAND-76 0742

TEMPERATURE CAPABILITY FOR DTF-IV (DTF-71 VERSION)*

David W. Varela
Reactor Studies Division 5422

and

Jeffrey S. Philbin
Reactor Design and Development Division 5452
Sandia Laboratories
Albuquerque, New Mexico 87115

May 1977

ABSTRACT

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

A subroutine has been developed for calculating adiabatic temperature distributions as part of the activity edit in the DTF-IV S_N neutron transport code.

The specific heat input is simple and versatile. The subroutine integrates the specific heat functions and solves for the temperatures which match the energy deposition supplied by the activity edit. There is no heat transfer modeling in the subroutine. The temperatures are only valid for cases where the energy deposition time is short compared to the thermal relaxation time of the media. The code can be used, for example, to calculate the initial temperature distributions in certain pulsed reactors or pulsed reactor experiments.

*This work was supported by the United States Energy Research and Development Administration.

MASTER

See

CONTENTS

	<u>Page</u>
I. INTRODUCTION	1
II. DESCRIPTION OF CODE	1
A. Theory	1
B. Input Data	3
1. Integer Parameters	3
2. Specific Heat Functions	3
3. Bounding Temperatures	6
4. Specific Heat Intervals	7
5. Input Specifications	7
C. Code Diagnostics	9
III. SAMPLE PROBLEM	10
A. Description of Problem	10
B. Input Data	11
C. Results	16
IV. SUMMARY	18
V. REFERENCES	19

TEMPERATURE CAPABILITY FOR DTF-IV (DTF-71 VERSION)

I. Introduction

A set of update cards has been developed to provide the DTF-71 transport code^{*1} with the capability of calculating temperature values from existing energy deposition values. The incentive for this work has been to make possible direct comparisons between DTF-71 calculations and temperature-related data from experiments.

II. Description of Code

A version of DTF-71 updated with the temperature subroutine has been stored on magnetic tape. Information on how to access this update file may be obtained from the authors.

It is assumed in this report that the reader is familiar with the DTF-IV transport code; most of the discussion is, therefore, limited to the description of the temperature subroutine.

A. Theory

Temperature solutions are calculated using the following relation:

$$\Delta Q = \int_{T_0}^T C_p dT , \quad (II-1)$$

^{*}DTF-71 is a 1971 version of the DTF-IV code.

where:

Q = adiabatic energy deposition per gram of material,
 T_0 = initial temperature*,
 T = temperature solution, and
 C_p = specific heat as a function of temperature.

Previous modifications² to DTF-71 allow the user to calculate energy depositions at every mesh point for each material zone specified in the input data. In order to obtain temperature values at these mesh points, the specific heat as a function of temperature must be known.

When the specific heat function is linear, quadratic, or exponential, Eq. II-1 is integrated analytically. This results in an equation in temperature. The roots of this equation are then analyzed to obtain the appropriate temperature solution.

All other specific heat functions are integrated numerically using QNC7³, which is one of the integrating subroutines available in Sandia's Mathematical Subroutine Library. For a given mesh, the upper limit of the integral is varied until the value of the integration is within specified limits of the energy deposition calculated in DTF. The final value of the upper limit is then selected as the temperature solution for that mesh.

Tabulated specific heat data must be fitted with a curve before it can be used in the temperature subroutine. Due to the nonlinear behavior of most specific heat functions, it is suggested that the curve be subdivided into several segments fitting each segment with a quadratic, linear, or exponential function in temperature. This will, in general, result in a much better curve fit than if a single function were fitted to the entire range. Also, as mentioned earlier, these types of functions are integrated analytically and are, therefore, likely to result in reduced computer execution times.

* Enthalpy calculations assume that $H = 0$ at the lowest bounding temperature (T_0).

Utility mathematical subroutines are readily available for deriving polynomial or exponential coefficients for specific heat functions from raw enthalpy or specific heat data (see Ref. 3 for example). FORTRAN programs utilizing these routines may be obtained from the authors upon request.

B. Input Data

1. Integer Parameters

There are two input integer parameters required for the use of the updated version of DTF-71: ITEM specifies if temperature solutions are desired (0/1 = no/yes); NUMF specifies the total number of specific heat functions. These two parameters should be read in format 2I5 on a separate card following the input integer parameter FILM. (NOTE: In the present version, the number of spatial meshes, IM, normally unrestricted in DTF input is limited to 135 due to dimension statements in the new subroutines.)

2. Specific Heat Functions

The input of specific heat functions requiring numerical integration is different from those which may be integrated analytically. In order to differentiate these types of functions, a set of five parameters is associated with every specific heat function to be read in. Different values and arrangements of these parameters are used by DTF to separate quadratic, linear, and exponential functions from other empirical relations. The array of parameters should be read in after the material zone numbers in the usual 6(I1, I2, E9.4) or 6(I1, I2, I9) generalized DTF floating point format (see Ref. 1 for description of the I1, I2, control parameter fields).

The order in which specific heat functions are read in is very important. It must correspond exactly to the order in which the material numbers were specified for the activity and energy deposition edits. If a specific heat

function corresponding to a given material zone has been divided into intervals (quadratic, linear, or exponential), then each one of these intervals will be considered as an individual specific heat function. The order of these intervals must correspond to increasing temperature values.

When quadratic, linear, or exponential functions are read in, the five parameters associated with each of these functions are just the coefficients of the following equation:

$$A(1) + A(2)T + A(3)T^2 + A(4) e^{A(5)T} \quad . \quad (II-2)$$

Quadratic, linear, or constant specific heat functions are defined when the last two parameters (A(4) and A(5)) are set equal to zero. Exponential specific heat functions are defined when the first three parameters are set equal to zero.

Any other empirical functions must be external to the DTF code. A set of ten external function subroutines is provided and may be accessed through the use of update cards. The following dummy statements (page 5) may be deleted and replaced by an external function. (NOTE: These functions must have the name associated with each of these statements.)

Statement Identification	Function Name
MØD03.47	FUNT1
MØD03.51	FUNT2
MØD03.55	FUNT3
MØD03.59	FUNT4
MØD03.63	FUNT5
MØD03.67	FUNT6
MØD03.71	FUNT7
MØD03.75	FUNT8
MØD03.79	FUNT9
MØD03.83	FUNT10

As previously mentioned, a set of five parameters for each of these functions is required as part of the input data. The parameters for this case are of the following form:

$$A(1) = A(2) = A(3) = A(4) = A(5) = X ,$$

$$X = 1.0, 2.0, 3.0, \dots , 10.0 .$$

The variable X specifies the location of the external specific heat function of interest in relation to the other external specific heat functions. The energy deposition values, as calculated in DTF-71, are in units of cal/g. The temperatures to be calculated may have different units ($^{\circ}\text{C}$, K, $^{\circ}\text{F}$, etc.) for different materials, but there must be a consistency between the mass and energy units of the energy depositions and the specific heat functions used. If the specific heat functions have units other than $\text{cal/g}^{\circ}\text{X}$, where $^{\circ}\text{X}$ is any unit of temperature, then a conversion factor, CF, can be used

to modify the energy deposition array, T5(I,J). The following update cards may be used:

```
*I, M0D01.2
CF = X.XX (defined by the user)
D0 150 I = 1, ID3
D0 150 J = 1, IM
150 T5(I,J) = T5(I,J) * CF
```

This operation is done after the deposition table is printed in units of cal/g, not before. Alternatively, the specific heat functions can be modified to make the units compatible with the energy deposition array.

3. Bounding Temperatures

These values define the valid temperature range of the specific heat functions. However, the lowest bounding temperature for each material should be set equal to the ambient temperature of that material, even though the expression used is valid below that temperature. The reason is that a zero enthalpy value is assumed for the lowest bounding temperature. The bounding temperatures are read in after the specific heat functions in 6(I1, I2, E9.4) format.

A set of bounding temperatures is required for each of the ID3 materials specified in the normal DTF-IV activity edit. The set will consist of two bounding temperatures (upper and lower limits) whenever a single specific heat function defines the entire temperature range of interest. For a material in which more than one specific heat function has been specified, the number of bounding temperatures in the set will be one more than the number of functions. In other words, there should be a bounding temperature at every division between specific heat functions in addition to the two bounding temperatures

defining the upper and lower limits. The output temperatures for each material will be in the temperature units used in the specific heat functions and bounding temperatures supplied by the user for that material.

4. Specific Heat Intervals

These values specify the number of specific heat functions, or intervals, for each of the ID3 materials specified in the normal DTF-IV activity edit. They should be read in after the bounding temperatures in 6(I1, I2, I9) format.

5. Input Specifications

Card 1 -- 2I5 Format -- Follows the third integer parameter card of the normal DTF data deck.

<u>Number Word on Card</u>	<u>Name of Variable</u>	<u>Comments:</u>
1	ITEM	(0/1 = no/yes) temperature solutions required.
2	NUMF	Total number of specific heat functions. Each interval defined by a separate set of coefficients, or an empirical expression counts as one function.

Card 2 -- 6(I1, I2, E9.4) Format -- Follows the material numbers, MZ block, of the normal DTF data deck.

<u>Block Name</u>	<u>Number of Entries</u>	<u>Comments:</u>
PAR	5*NUMF	Coefficients for quadratic, linear, or exponential specific heat functions, as per Eq. II-2 or location keys for empirical functions as described in Sect. B.2, page 5.

Card 2 (Cont'd)

Comments:

The sets must be input in the same order as the material numbers, block MK3, of the activity edit. There may be more than one set for each material ordered by increasing temperature intervals.

Repeat Card 2 until the total number of entries is accommodated.

Card 3 -- 6(I1, I2, E9.4) Format

<u>Block Name</u>	<u>Number of Entries</u>	<u>Comments:</u>
BOUTE	NUMF+ID3*	Bounding temperatures associated with each of the specific heat functions whose coefficients were read on Card 2.

Repeat Card 3 until the total number of entries is accommodated.

Card 4 -- 6(I1, I2, I9) Format

<u>Block Name</u>	<u>Number of Entries</u>	<u>Comments:</u>
NHCI	ID3*	Specifies the number of specific heat functions, or intervals, for each material in the DTF-IV activity edit.

Repeat Card 4 until the total number of entries is accommodated.

* ID3 is a DTF-IV control integer (input parameter). It indicates the number of activities that are requested in the activity edit.

C. Code Diagnostics

The code may print one of three diagnostic signals (-1.0, -2.0, and -3.0) in place of a temperature at any given mesh point (or points) indicating the following conditions:

- 1.0 -- Occurs for two conditions--but only if the specific heat function is of a linear, quadratic, or exponential form.
 - (a) The solution root is more than two degrees outside of the appropriate bounding temperature range.
 - (b) There are two real roots between two of the bounding temperatures.
- 2.0 -- Temperature out-of-range. The specific heat function is undefined at the enthalpy value specified in the energy deposition table. This would occur if Eq. II-1 (evaluated at the highest bounding temperature) is less than the energy deposition value calculated by DTF.
- 3.0 -- This value is printed whenever the energy deposition value is 0.0. This situation may arise if the material of interest exists in only one (or only a few) region(s) of a multiregion problem, or if there really was no energy deposition in the material at a particular mesh. In the second case, the correct temperature would be the ambient temperature of the material (i.e., the lowest bounding temperature of the material).

III. Sample Problem

A sample problem has been included to illustrate the use of this code. All of the required input data is reproduced and discussed. Also, the results are analyzed to give an indication of the accuracy which can be obtained.

A. Description of Problem

It is desired in this problem to obtain the temperature solutions for a DTF-IV case in which energy deposition calculations have been specified for two material zones containing UO_2 . There are 132 radial mesh points in each material zone.

In the first material zone, temperature solutions are obtained using the following specific heat function⁴:

$$C_p(T) = \frac{K_1 \Theta^2 \exp(\Theta/T)}{T^2 [\exp(\Theta/T) - 1]^2} + 2K_2 T$$

(III-1)

$$+ \frac{K_3 E_D}{RT^2} \exp(-E_D/RT)$$

where:

$$\begin{aligned}\Theta &= 535.3 \text{ K}, \\ E_D &= 37.69 \text{ kcal/mole}, \\ K_1 &= 19.15 \text{ cal/mole} \cdot \text{K}, \\ K_2 &= 7.85 \times 10^{-4} \text{ cal/mole} \cdot \text{K}^2, \\ K_3 &= 5.64 \times 10^6 \text{ cal/mole}, \text{ and} \\ R &= 1.987 \times 10^{-3} \text{ kcal/mole} \cdot \text{K}.\end{aligned}$$

In the second material zone, the specific heat of UO_2 was divided into nine intervals and fitted with linear, quadratic, and exponential curves. The temperature range considered was from 298 to 3118 K. Figure 1 shows the specific heat of UO_2 as a function of temperature. The interval subdivision and corresponding bounding temperatures are also included in this figure.

In order to specify new functions for each interval shown in Fig. 1, a data bank of specific heat values as a function of temperature was obtained by evaluating Eq. (III-1). This data was then fitted with subroutine CURVEFIT, which uses a least squares fitting procedure described in detail in Ref. 5. The error differences between the actual and fitted curves were always less than 2 percent.

B. Input Data

The fifth data card (title card included) should have the input integer parameters ITEM and NUMF. A value of 1 in column 5 of this card will specify that temperature calculations are desired and a value of 10 starting in column 9 of this same card will specify that there are 10 specific heat functions (1 external function and 9 specific heat intervals). No other variables should appear on this card.

The input parameters of the specific heat functions should be read in after the material numbers. The array of parameters for this problem is given in Table 1. There are 5 parameters for each specific heat function or interval. It is noted that the first row of parameters is all set equal to 1.0. This means that an external specific heat function will be used in the first material zone. Therefore, the following update cards were used:

Interval	Bounding Temperature (K)
1	298*
2	793
3	998
4	1203
5	1598
6	1998
7	2398
8	2598
9	2803
	3118**

* Lower bound of Interval 1.

** Upper bound of Interval 9.

Figure 1. Specific Heat of UO_2 as a Function of Temperature

TABLE 1
ARRAY OF SPECIFIC HEAT PARAMETERS

FUNCTION	TYPE	PARAMETERS				
		1	2	3	4	5
1	External	1.0	1.0	1.0	1.0	1.0
2	Quadratic	8.971E+0	2.715E-2	-1.751E-5	0.0	0.0
3	Linear	1.746E+1	1.816E-3	0.0	0.0	0.0
4	Linear	1.798E+1	2.288E-3	0.0	0.0	0.0
5	Linear	2.066E+1	3.785E-4	0.0	0.0	0.0
6	Exponential	0.0	0.0	0.0	1.419E+1	2.63E-4
7	Quadratic	5.261E+1	-3.744E-2	1.162E-5	0.0	0.0
8	Linear	-2.064E+1	2.094E-2	0.0	0.0	0.0
9	Linear	-3.362E+1	2.594E-2	0.0	0.0	0.0
10	Linear	-4.944E+1	3.155E-02	0.0	0.0	0.0

*D,MØD03.47

TH = 535.3

ED = 37.69

RK1 = 19.15

RK2 = 7.85×10^{-4}

RK3 = 6.64×10^6

R = 1.987×10^{-3}

$$\text{FUNT1} = \frac{(\text{RK1})(\text{TH}^2) \text{EXP}(\text{TH}/\text{T})}{\text{T}^2 [\text{EXP}(\text{TH}/\text{T}) - 1]^2}$$

$$+ 2(\text{RK2})\text{T} + \frac{\text{RK3}(\text{ED})}{\text{R}(\text{T}^2)} \text{EXP} \frac{-\text{ED}}{\text{R}(\text{T})}$$

It is also noted that the units of the specific heat function are cal/mole K. In order to have consistent units, a conversion factor was applied to the energy deposition array, T5, using update cards (see Sect. II-B-2):

*I,MØD01.2

CF = 270

CF = MOLES PER GRAM CONSTANT ... COMMENT CARD

DO 150 I = 1, ID3

DO 150 J = 1, IM

150 T5(I,J) = T5(I,J)*CF

Alternatively, the specific heat functions can be modified to make the units compatible with the energy deposition array.

The array of boundary temperatures is shown in Table 2. There is a total of 12 boundary temperatures (2 for the external specific heat function and 10 for the specific heat intervals).

TABLE 2
ARRAY OF BOUNDARY TEMPERATURES

BOUNDARY NUMBER	MATERIAL ZONE	BOUNDARY TEMPERATURE, K
1	1	298.0
2	1	3118.0
3	2	298.0
4	2	793.0
5	2	998.0
6	2	1203.0
7	2	1598.0
8	2	1998.0
9	2	2398.0
10	2	2598.0
11	2	2803.0
12	2	3118.0

This array should be read in after the specific heat parameter array in 6(I1, I2, E9.4) format.

Finally, the array of specific heat intervals should be read in after the boundary temperature array. In this case, a data card having the values 1 and 9 in columns 12 and 24, respectively, will specify that there is 1 function for the first material zone and 9 intervals for the second material zone. A "3" in column 13 ends the array.

C. Results

The results of this problem are given in Table 3. All mesh points above 15 have zero energy deposition and are therefore omitted in this table for neatness of presentation.

The first column represents the energy deposition values calculated in DTF-71 (units of cal/mole) for both material zones. The last column represents the temperature values calculated in the updated version of DTF-71.

For purposes of comparison, Eq. III-1 was integrated to obtain the following expression of enthalpy as a function of temperature:

$$H = K_1 \Theta \left\{ [\exp(\Theta/T) - 1]^{-1} - [\exp(\Theta/298) - 1]^{-1} \right\} + K_2 (T^2 - 298)^2 + K_3 \exp(-E_D/RT) \quad (III-2)$$

as given in Ref. 4, where the constants Θ , E_D , K_1 , K_2 , and K_3 are the same as in Eq. III-1.

A data bank of enthalpy values as a function of temperature was obtained by evaluating the above expression. The energy deposition values given in columns 2 were compared against this data bank to obtain the temperature values given in the middle section of Table 3.

TABLE 3
TEMPERATURE AS A FUNCTION OF ENERGY DEPOSITION FOR UO_2 - SAMPLE PROBLEM

MESH	Energy Deposition (cal/mole)		Temperature Eq. III-2 (K)		Temperature DTF-71 (K)	
	MATERIAL 1	MATERIAL 2	MATERIAL 1	MATERIAL 2	MATERIAL 1	MATERIAL 2
1	18767	0.0	1272.8	-- **	1272.5	-3.0*
3	20194	0.0	1341.0	----	1340.7	-3.0
5	23961	0.0	1518.0	----	1518.3	-3.0
7	0.0	12610	----	973.2	-3.0	973.2
9	0.0	15352	----	1107.8	-3.0	1107.9
11	0.0	18461	----	1258.2	-3.0	1257.3
13	0.0	22773	----	1462.8	-3.0	1460.9
15	0.0	29784	----	1782.8	-3.0	1783.1

* -3.0 is a signal indicating that the energy deposition for this material was 0.0 at this particular mesh point.

** Material i (i = 1 or 2) does not exist at this mesh point in the specification of the problem.

Analysis of the results will, at this time, be limited to the observation that the temperature values calculated in the updated version of DTF-71 are in close agreement with those calculated using Eq. III-2.

IV. Summary

The temperature capability presented here provides adiabatic temperature distributions for selected materials used in DTF-71 problems. The user must specify the materials in the DTF-71 activity edit and convert the activity into energy deposition units. Versions operating at Sandia already have the energy deposition capability for several different neutron reactions, including fission. In addition, the user must supply a specific heat function for each material. The code allows the user a great deal of flexibility in describing the specific heat functions. The code does not include any heat transfer modeling. The temperatures are instantaneous (or initial) temperatures and are only valid for cases where the energy is deposited in a short time compared to the thermal relaxation times of the media where the energy is deposited.

REFERENCES

1. K. D. Lathrop, DTF-IV, A FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering, LA-3373, Los Alamos Scientific Laboratory Report, Los Alamos, New Mexico, July 1965.
2. J. S. Philbin, Modifications to DTF-IV for Calculating Energy Depositions Due to Fission and (n,α) Reactions, unpublished Sandia Laboratories Memorandum, 1974.
3. R. E. Jones and C. O. Bailey, Brief Instructions for Using MATHLIB (Version 6), SAND-75 0545, Sandia Laboratories Report, Albuquerque, New Mexico, February 1976; original version of QNC7 was by D. L. Kahaner, Los Alamos Scientific Laboratory, Los Alamos, New Mexico.
4. J. F. Kerrisk and G. D. Clifton, "Smoothed Values of the Enthalpy and Heat Capacity of UO_2 ", Nucl. Tech. 16, 531 (1972).
5. P. R. Bevington, Data Reduction and Error Analysis for the Physical Sciences, McGraw-Hill Publishers, Inc., 1969.

DISTRIBUTION:

J. C. Vigil, R-6
Los Alamos Scientific Laboratory
P. O. Box 1663
Los Alamos, NM 87544

R. D. O'Dell, T-1
Los Alamos Scientific Laboratory
P. O. Box 1663
Los Alamos, NM 87544

5231 J. H. Renken
5231 S. A. Dupree
5410 D. J. McCloskey
5411 D. A. Dahlgren
5420 J. V. Walker
5422 R. L. Coats
5422 K. O. Reil
5422 J. B. Rivard
5422 D. W. Varela (5)
5423 J. E. Powell

5423 L. M. Choate
5423 D. A. McArthur
5423 S. A. Wright
5425 W. J. Camp
5425 D. C. Williams
5425 M. F. Young
5430 R. M. Jefferson
5432 L. L. Bonzon
5450 J. A. Reuscher
5451 T. R. Schmidt
5451 B. F. Estes
5451 K. D. Boldt
5452 L. D. Posey
5452 A. C. Marshall
5452 F. M. Morris
5452 J. S. Philbin (15)
5452 P. S. Pickard
8666 E. A. Aas (2)
3141 C. A. Pepmuelier (5)
3151 W. L. Garner (3)
For ERDA/TIC
Unlimited Release