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MATERIALS PROPERTIES MODELS FOR SEVERE CORE DAMAGE ANALYSIS

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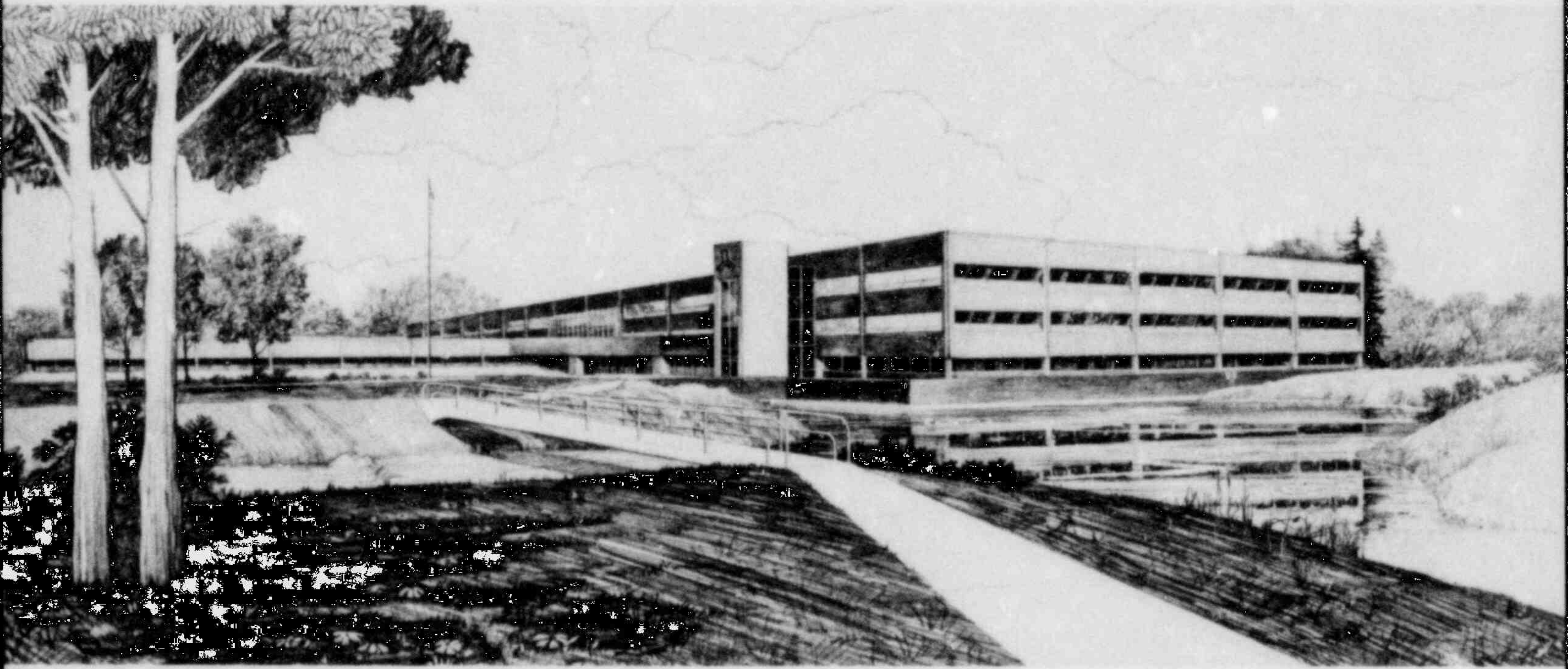
Idaho Operations Office • Idaho National Engineering Laboratory



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INTERIM REPORT

ABSTRACT

This report documents the extension of an older package of light water reactor materials properties computer subcodes to consider properties appropriate to severe core damage modeling. The work is preliminary because no effort has been made to subject the new data to the critical review given to the data used in the older package.

SUMMARY

Recent interest in analyzing severe core damage in light water reactors has created a need for properties not present in the light water reactor materials properties subcode package, MATPRO. In addition, the subcodes for properties that have been available were being used at temperatures beyond those intended. For this reason a preliminary update has been completed to extend the package to temperatures above cladding melt and to include properties of interest for modeling molten material flow.

New materials have been added to the package so that analysis may consider control rods and liquefied fuel rods. The new materials are silver-indium-cadmium alloy, boron carbide, stainless steel, Inconel 718 and zirconium-uranium-oxygen melts.

Although no effort has been made to subject the data base for the extended package to critical analysis, it is obvious that there is a critical shortage of nearly all data for zirconium-uranium-oxygen melts and liquid metal properties like viscosity, interfacial surface tension and fusion volume changes. Error estimates have been included for each model and many of the estimates are more than half the given value of the property. Data are particularly sparce for compounds rich in unoxidized zircaloy, the composition which is likely to be formed by liquefaction of uranium dioxide due to flowing cladding in the temperature range 2100 through 2600 K. There are some data for ZrO_2-UO_2 mixtures so the description of oxidized melts is fairly well founded.

ACKNOWLEDGEMENTS

The author wishes to thank E. R. Carlson for providing plot package programming.

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MATERIALS PROPERTIES MODELS FOR SEVERE CORE DAMAGE ANALYSIS

D. L. Hagrman

1. INTRODUCTION

The United States Nuclear Regulatory Commission is sponsoring development of a Severe Core Damage Analysis (SCDAP) computer code to analyze the thermal, mechanical, and chemical behavior of light water reactor fuel rod bundles during a severe reactor accident.[1] An important part of this development is the extension of the existing materials properties data base to the high temperatures and complex mixtures or compounds which may be present in a severely damaged core. This document is a preliminary extension of the MATPRO materials properties package[2-5] to include new properties required for the initial version of SCDAP, SCDAP/MODO.

The extension includes fifty subcodes and is preliminary because the data supporting the subcodes have not been subjected to the critical review that has been given to the data used in the balance of the MATPRO package. The subcodes described in this report have been prepared in a preliminary fashion so that sensitivity studies can be conducted with the SCDAP code to help determine what data are most urgently needed and the precision to which they must be measured Uncertainty estimates are included in each subcode to help guide these sensitivity studies.

Most of the new properties needs come from the fact that severe core damage scenarios include core melting and mixing.[6] Existing properties for fuel and zircaloy cladding must therefore be extended to include the liquid phases of these materials. In addition, liquid zircaloy can flow onto UO_2 and dissolve the oxide to form a uranium-zirconium-oxygen compound whos behavior must be modeled. Since the current MATPRO package includes only fuel, cladding, and gap gas property descriptions, a major new section has been added in this report to deal with these compounds. Sections for control rod neutron absorbers, their stainless steel cladding, and Inconel grid spacers have also been included because these bundle components are considered by the SCDAP/MODO computer code. Water properties are not included in this update because they are already available from the THERMO and FPROP subroutines of the TRAC-BD1 code[7] which is being adapted for use with SCDAP/MODO.

The new properties subcodes are contained in appendicies to this report. These appendicies are organized in a format which is compatable with their eventual addition to the MATPRO handbook.

2. EXTENSION OF MATPRO PROPERTIES TO INCLUDE SEVERE CORE DAMAGE ANALYSIS

Most of the fuel, cladding and gas material properties required for severe core damage analysis are contained in Appendices A, B, and C of the MATPRO handbook.[2] Minor changes to these routines to extend them to higher temperatures are described in Appendices A and B of this report. Appendices D through G are descriptions of materials properties subcodes that are new. No change has been made to the models in Appendix C of the MATPRO handbook.

Table 1 is a list of the materials properties which are available. The location of the model description is indicated by footnotes. Appendix A, Fuel Material Properties, models uranium dioxide and plutonium-uranium dioxide fuels. Appendix B, Cladding Material Properties, includes both zircaloy and zircaloy oxide properties. The gases included in Appendix C are helium, argon, krypton, xenon, hydrogen, nitrogen, oxygen carbon monoxide, carbon dioxide and water vapor. Appendix D considers both silver-indium-cadmium and boron carbide control rod absorbers. The cladding properties of Appendix E assume that the control rod cladding is 304 stainless steel. Appendix F assumes the grid spacers are made of Inconel 718 (the properties of Appendix B can be used if the grid spacers are zircaloy).

TABLE 1. PROPERTIES AVAILABLE

Property	Subcode
Fuel Material Properties (Appendix A)	
Specific heat capacity[a]	FCP, FENTHL
Thermal conductivity[a,b]	FTHCON
Emissivity[a]	FEMISS
Thermal expansion[a,c]	FTHEXP, FDEN
Elastic moduli[a]	FELMOD, FPOIR
Creep rate[a]	FCREEP
Densification[a]	FUDENS
Swelling[a]	FSWELL
Pressure sintering[a]	FHOTPS
Restructuring[a]	FRESTR
Fracture strength[a]	FFRACS
Fission gas release[a]	FGASRL
Cessium and iodine release[a]	CESIOD
Vapor pressure[a]	FVAPRS
Visocity[a]	FVISCO
Oxidation[d]	FOXY
Melting temperatures[b]	FHYPRP
Fuel Rod Cladding Material Properties (Appendix B)	
Specific heat capacity and enthalpy[a,b]	CCP, CHSCP, CENTHL, ZOCP, ZONTHL
Thermal conductivity[a,b]	CTHCON, ZOTCON
Emissivity[a]	ZOEMIS

TABLE 1. (continued)

Property	Subcode
Fuel Rod Cladding Material Properties (Appendix B)	
Thermal Expansion and Density[a,b]	CTHEXP, CDEN, ZOTEXP, ZODEN
Elastic Moduli[a,b]	CELMOD, CSHEAR, CELAST, ZOEMOD, ZOPOIR
Axial growth[a]	CAGROW
Creep rate[a]	CCSTRN, CCSTRS
Plastic deformation[a]	CSTRES, CSTRAN, CSTRNI, CANISO
Annealing[a]	CANEAL
Texture factors[a]	CTXTUR
Mechanical limits[a,b] and embrittlement[a]	CMLIMT, CBRTTL, ZORUP
Cyclic fatigue[a]	CFATIG
Collapse pressure[a]	CCLAPS
Oxidation[e]	CORROS, COBILD, COXIDE, COXWTK, COXTHK
Hydrogen uptake[a]	CHUPTK
Meyer hardness[a]	CMHARD
Melting temperatures, phase transformation temperatures[b,c]	CHYPRP, ZOPRP
Gas Material Properties (Appendix C)	
Thermal conductivity[a]	GASCON, GTHCON, GJUMP
Gas viscosity[d]	GVISCO
Neutron Absorber Properties (Appendix D)	
Specific heat capacity and enthalpy[c]	ACP, AENTHL
Thermal conductivity[c]	ATHCON

TABLE 1. (continued)

Property	Subcode
Thermal expansion and density[c]	ATHEXP, ADEN
Surface tension[c]	ASTEN
Viscosity[c]	AVISC
Melting temperature[c]	AHYPRP
Control Rod Cladding Properties (Appendix E)	
Specific heat capacity and enthalpy[c]	SCP, SENTHL
Thermal conductivity[c]	STHCON
Thermal expansion and density[c]	STHEXP, SDEN
Oxidation[c]	SOXIDE, SOXWGN, SOXTHK
Melting temperature[c]	SHYPRP
Grid Spacer Properties (Appendix F)	
Melting temperature[c]	HYPRP
Zirconium-Uranium-Oxygen Componds Properties (Appendix G)	
Specific heat capacity and enthalpy[c]	ZUCP, ZUNTHL
Thermal condictivity[c]	ZUTCON
Thermal expansion and density[c]	ZUTEXP, ZUDEN
Coefficient of friction[c]	ZUFRIC
Interfacial surface tension[c]	ZUSTEN
Viscosity[c]	ZUVISC
Rate of UO_2-zircaloy reaction[f]	PSUZ
Heat of solution of solid UO_2 by zirconium-uranium-oxygen compounds[c]	ZUSOLN
Melting temperatures and solubility[g]	PSOL, PLIQ, PSLV

TABLE 1. (continued)

Supporting Material for MATPRO (Appendix H)	
Linear interpolation[h]	POLATE
Collected heats of fusion[c]	QFUSON
Mass fraction-mole fraction conversions[c]	PMOLE, PMASS

---

a. The model is described in the MATPRO-11 document with Revisions 1 and 2 (Reference 2).

b. A revision to the existing MATPRO-11 Revision 2 model is described in this document.

c. The model is a preliminary subcode described in this document.

d. The model is described in Reference 3.

e. The models are described in Reference 5.

f. The model is described in Reference 4.

g. The model is currently described in Appendix D of the MATPRO-11 Revision 2 document but will be moved to Appendix G.

h. The model is currently described in Appendix D of the MATPRO-11 Revision 2 document but will be moved to Appendix H.

3. REFERENCES

1. C. M. Allison et al., Severe Core Damage Analysis Package (SCDAP) Code Conceptual Design Report, EGG-CDAP-5397, April 1981.

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APPENDIX A
FUEL MATERIAL PROPERTIES

APPENDIX A

FUEL MATERIAL PROPERTIES

The only changes required to extend the MATPRO-11, Revision 2 fuels materials properties to high temperatures are a revision of the fuel thermal conductivity subcode to incorporate the first data for liquid UO_2 thermal conductivity and the addition of a subcode to calculate fuel density. An additional subroutine which calculates melting temperatures has been added for consistency.

FUEL THERMAL CONDUCTIVITY (FTHCON)

The revised expression for the thermal conductivity of liquid UO_2 or UO_2 - PuO_2 mixtures is

$$K = 11.5 \qquad \text{(A-1)}$$

where

K = thermal conductivity (W/m•K).

Kim et al.(A-1) provided the data which allow a calculation of thermal conductivity. They measured the thermal diffusivity of 0.813 and 1.219 mm layers of molten UO_2, in the temperature range 3187 through 3315 K. The values obtained, 1.90×10^{-6} to 3.23×10^{-6} m^2/s, can be used with measurements of specific heat and density to calculate the thermal conductivity from the relation

$$K = C_p \rho \alpha$$

where

C_p = specific heat capacity (J/kg K)

ρ = density (kg/m^3)

α = thermal diffusivity (m^2/s).

Substitution of the MATPRO values for C_p and ρ at melting[a] into Equation (A-1) yields thermal conductivities in the range 8.5 to 14.5 W/m•K. These conductivities are an order of magnitude larger than the estimate used in MATPRO-11 Revision 2.

Kim et al., interpret this unusually high conductivity as being due to internal infrared radiation heat transfer in the liquid UO_2 which is not allowed in the solid because of the effect of scattering centers such as grain boundaries or voids. Although they caution that radiative thermal diffusivity depends on the thickness of the material as well as on the emissivity of the boundary surfaces, the variations they estimate are only 0.10 to 0.30 times the measured value. The constant used in Equation (A-1) is the average of the range of values calculated from the data of Kim et al. An uncertainty of ±0.3 times the given liquid conductivity is estimated from the range of values measured.

The revised FTHCON subcode is listed in Table A-1. Figure A-1 was generated using the subroutine with an input value of 0.95 of the theoretical density.

FUEL DENSITY (FDEN)

The FDEN function determines the theoretical density of UO_2 using room temperature data and thermal expansion strains calculated by the FTHEXP subcode. The relation used is

$$\rho = 10,980\ (1 - 3\varepsilon_{UO_2}) \qquad \text{(A-2)}$$

---

[a] $C_p = 502\ J/kg{\bullet}K$
$\rho = 10.98 \times 10^3/[1 + 3\ (0.035 + 0.045)]\ Kg/m^3$.

TABLE A-1. LISTING OF THE FTHCON SUBROUTINE

```
      SUBROUTINE FTHCON (FTEMP,FRADEN,FOTMTL,CON,DKDT)
C
C     FTHCON CALCULATES THE FUEL THERMAL CONDUCTIVITY AND ITS
C     DERIVATIVE WITH RESPECT TO TEMPERATURE AS A FUNCTION OF
C     TEMPERATURE, DENSITY, OXYGEN TO METAL RATIO, COMPOSITION
C     AND BURNUP
C
C     CON    = OUTPUT FUEL THERMAL CONDUCTIVITY (W/(M*K))
C     DKDT   = OUTPUT DERIVATIVE OF FUEL THERMAL CONDUCTIVITY
C              WITH RESPECT TO TEMPERATURE (W/M*K*K))
C
C     FTEMP  = INPUT FUEL TEMPERATURE (K)
C     FRADEN = INPUT FUEL DENSITY (RATIO OF ACTUAL DENSITY TO
C              THEORETICAL DENSITY)
C     FOTMTL = INPUT OXYGEN TO METAL RATIO OF FUEL (ATOMS OXYGEN/
C              ATOMS METAL)
C
C     THE FOLLOWING INPUTS ARE BY COMMON BLOCK
C     COMP          = INPUT PUO2 CONTENT OF FUEL (PERCENT PUO2
C                     IN TOTAL FUEL WEIGHT)
C     BU            = INPUT BURNUP (MW-S/KG-U)
C
C     THE FOLLOWING UNCERTAINTY IS COMPUTED BUT NOT RETURNED
C     UCON   = OUTPUT EXPECTED STANDARD ERROR OF THE FUEL
C              THERMAL CONDUCTIVITY (W/(M*K))
C
C     THE EQUATIONS USED IN THIS SUBROUTINE ARE BASED ON DATA FROM
C     (1)   J. A. CHRISTENSEN ET AL., URANIUM DIOXIDE THERMAL
C           CONDUCTIVITY, TRANSACTIONS OF THE AMERICAN NUCLEAR
C           SOCIETY  7 (1964) PP. 391 - 392
C     (2)   T. G. GODFREY ET AL., THERMAL CONDUCTIVITY OF
C           URANIUM DIOXIDE AND ARMCO IRON BY AN IMPROVED
C           HEAT FLOW TECHNIQUE, ORNL-3556 (1954)
C     (3)   J. L. BATES, HIGH TEMPERATURE THERMAL CONDUCTIVITY
C           OF ROUND ROBIN URANIUM DIOXIDE, BNWL-1431 (1970)
C     (4)   R. L. GIBBY, THE EFFECT OF PLUTONIUM CONTENT ON THE
C           THERMAL CONDUCTIVITY OF (U,PU)O2 SOLID SOLUTIONS,
C           JOURNAL OF NUCLEAR MATERIALS 38 (1971) PP 163 - 177
C     (5)   J. C. WEILBACHER, DIFFUSIVITE THERMIQUE DE L OXIDE
C           D URANIUM ET DE L OXIDE DE THORIUM A HAUTE TEMPERATURE,
C           HIGH TEMPERATURES - HIGH PRESSURE 4, (1972) PP 431 - 438
C     (6)   L. A. GOLDSMITH AND J. A. M. DOUGLAS, MEASUREMENTS
C           THE THERMAL CONDUCTIVITY OF URANIUM DIOXIDE AT 670 -
C           1270 K, JOURNAL OF NUCLEAR MATERIALS 47, (1973) PP 31 - 42
C     (7)   I. C. HOBSON ET AL., EFFECT OF POROSITY AND STOICHIOMETRY
C           ON THE THERMAL CONDUCTIVITY OF URANIUM DIOXIDE, JOURNAL
C           OF PHYSICS SECTION D: APPLIED PHYSICS 7 (1974)
C           PP 1003 - 1015
C     (8)   R. L. GIBBY, THE THERMAL DIFFUSIVITY AND THERMAL
```

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C          CONDUCTIVITY OF STOICHIOMETRIC (UO.8,PUO.2)O2, BNWL-704
C          (1968)
C     (9)  R. L. GIBBY, THE EFFECT OF OXYGEN STOICHIOMETRY ON THE
C          THERMAL DIFFUSIVITY AND CONDUCTIVITY OF (UO.75,PUO.25)
C          O2-X BNWL-927 (1969)
C     (10) L. A. GOLDSMITH AND J. A. M. DOUGLAS, THE THERMAL
C          CONDUCTIVITY OF PLUTIONIUM-URANIUM DIOXIDE AT
C          TEMPERATURES UP TO 1373 K, JOURNAL OF NUCLEAR MATERIALS
C          43 (1972) PP 225 - 233
C     (11) H. E. SCHMIDT, DIE WAERMELEITFAEHIGKEIT VON URAN AND
C          URAN-PLUTINIUM DIOXYD BEI HOHEN TEMPERATUREN, FORSCHUNG
C          INGENIEUR-WEISEN 38 (1976) PP 149 - 151
C     (12) D. R. OLANDER, FUNDAMENTAL ASPECTS OF NUCLEAR REACTOR
C          FUEL ELEMENTS, TID-26711-P1 (1976)
C     (13) C. S. KIM ET. AL.,MEASUREMENT OF THERMAL DIFFUSIVITY
C          OF MOLTEN UO2, PROCEEDINGS OF THE SEVENTH SYMPOSIUM ON
C          THERMOPHYSICAL PROPERTIES AT THE NATIONAL BUREAU OF
C          STANDARDS, GAITHERSBURG, MARYLAND, MAY 10-12, 1977,
C          PP. 338-343. CONF 770537-3.
C
C     FTHCON WAS ORIGIONALLY CODED BY C. S. OLSEN FEB 1975
C     MODIFIED BY D. L. HAGRMAN MARCH 1982
C
       COMMON  / PHYPRO / FTMELT,FHEFUS,CTMFLT,CHEFUS,CTRANB,
     #                    CTRANE,CTRANZ,FDELTA,BU,COMP,DELOXY
C
      DIMENSION C(2)
C
C     IF FUEL HAS MELTED SET OUTPUT AND RETURN
C
      IF(FTEMP .LT. FTMELT) GO TO 5
      CON = 11.5
      DKDT = 0.
      UCON = 3.45
      RETURN
    5 CONTINUE
C
C     FIND CONSTANTS
C
      FRPU = COMP/100.
      A = 0.339 + 12.6 * ABS( 2.0 - FOTMTL )
      IF(FRPU .GT. 0.75) FRPU = 0.75
      B = 6.867E-02 * (1.0 + 0.6238 * FRPU )
      T = FTEMP
      I = 1
C
C     FIND SPECIFIC HEAT AT CONST. VOL. AND VOLUME CHANGE
C
   10 TR = 535.265/T
      CV = 296.7 * TR * TR * EXP(TR) / (( EXP(TR) - 1.0)**2 )
      DV = 1.0 + 3.0*(1.0E-05 * T - 3.0E-03 + 4.0E-02 *
     #     EXP(-5.0E+03/T))
      IF(FRPU .LT. 0.0001) GO TO 20
```

```
C
C     USE RULE OF MIXTURES FOR MIXED OXIDES
      TR = 571.0/T
      CV = CV * (1.0 - FRPU) + ( 347.4 * TR * TR  *  EXP(TR) /
     #     (( EXP(TR) - 1.0 )**2 )) * FRPU
      DV = (DV - 1.0 ) * (1.0 - FRPU)  +  3.0 * ( 9.0E-06 * T
     #     - 2.7E-03 + 7.0E-02 * EXP(-5.072E+03/T)) * FRPU  + 1.0
C
C     FIND POROSITY CORRECTION
C
   20 BETA = 6.50 - 4.69E-03 * T
      IF(T .GE. 1364.647) BETA =  15.811308 - T*(.01833647-T*5.E-6)
      IF(T .GT. 1833.647) BETA = - 1.0
C
C     FIND ELECTRONIC CONTRIBUTION
C
      CONE = (5.2997E-03 *  T  *  EXP(-13358.0/ T )) *
     #       (1.0 + 0.169 * ((13358.0/ T + 2.0)**2 ))
      BTEMP = T
      IF(T .GE. 1800.) BTEMP = -3240. + T * (4.6 - T * 0.001)
      IF(T .GE. 2300.) BTEMP =  2050.
C
C     FIND CONDUCTIVITY
C
      C(I) = (CV * FRADEN)/(DV * (A + B * BTEMP ) *
     #       (1.0 + BETA * (1.0 - FRADEN))) + CONE
C
C
C     FIND DERIVATIVE OF FUEL CONDUCTIVITY
C
C
C
C
C
      I    = I + 1
      T    = FTEMP + ((-1.0)**I)
      IF(I .LT. 3) GO TO 10
      CON  =  C(1)
C
      DKDT = (C(2) - C(1))
C
C     FIND UNCERTAINTY
C
C
C
C
C
      UCON =(0.2 * (1.0 - FRPU) + 0.7 * FRPU ) * (1.0 + ABS(2.0 -
     #       FOTMTL) * 10.)
C
      RETURN
      END
```

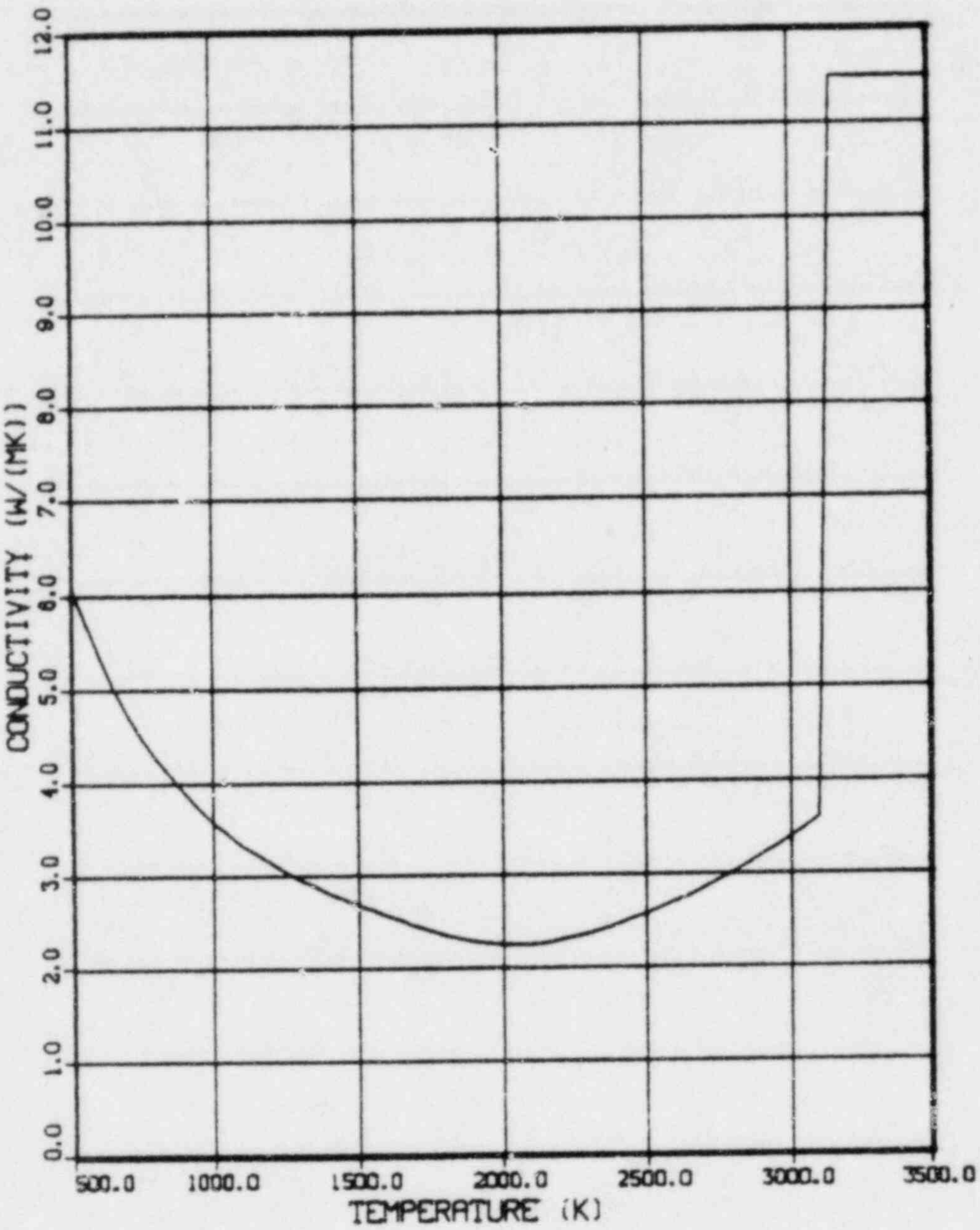

Figure A-1. Fuel thermal conductivity of uranium dioxide with a density of 0.95 times the theoretical density.

where

ρ = theoretical density of UO_2 (kg/m^3)

ϵ_{UO_2} = linear thermal expansion strain calculated for UO_2 using a reference (zero strain) temperature of 300 K (m/m).

The room temperature density, 10,980 kg/m^3, was taken from Olander$^{(A-2)}$ and is accurate to ±20 kg/m^3.

Table A-2 is a listing of the FDEN function and Figure A-2 shows the predicted theoretical density as a function of temperature.

FUEL MELTING TEMPERATURES (FHYPRP)

The subroutine FHYPRP calculates the temperature of the appearance of the first liquid phase (solidus) and the temperature of the melting of the last solid phase (liquidus) and UO_2 and (U,Pu) O_2. These temperatures are calculated as a function of burnup and plutonia content.

Equations for these temperaures are from the MATPRO-11 Revision 2 PHYPRP subroutine.

Table A-3 is a listing of the FHYPRP subroutine.

TABLE A-2. LISTING OF THE FDEN FUNCTION

```
      FUNCTION FDEN(FTEMP,FACMOT)
C
C     FDEN RETURNS THE DENSITY OF UO2 FUEL
C
C     FDEN   = OUTPUT FUEL DENSITY (KG/M**3)
C
C     FTEMP  = INPUT FUEL TEMPERATURE (K)
C     FACMOT = INPUT FUEL FRACTION WHICH IS MOLTEN (UNITLESS)
C
C     THE SUBCODE FTHEXP IS CALLED BY THIS FUNCTION
C
C     FDEN WAS CODED BY D. L. HAGRMAN 1982.
C
      EPS = FTHEXP(FTEMP,FACMOT)
      FDEN = 1.098E+04 * (1. - 3. * EPS)
      RETURN
      END
```

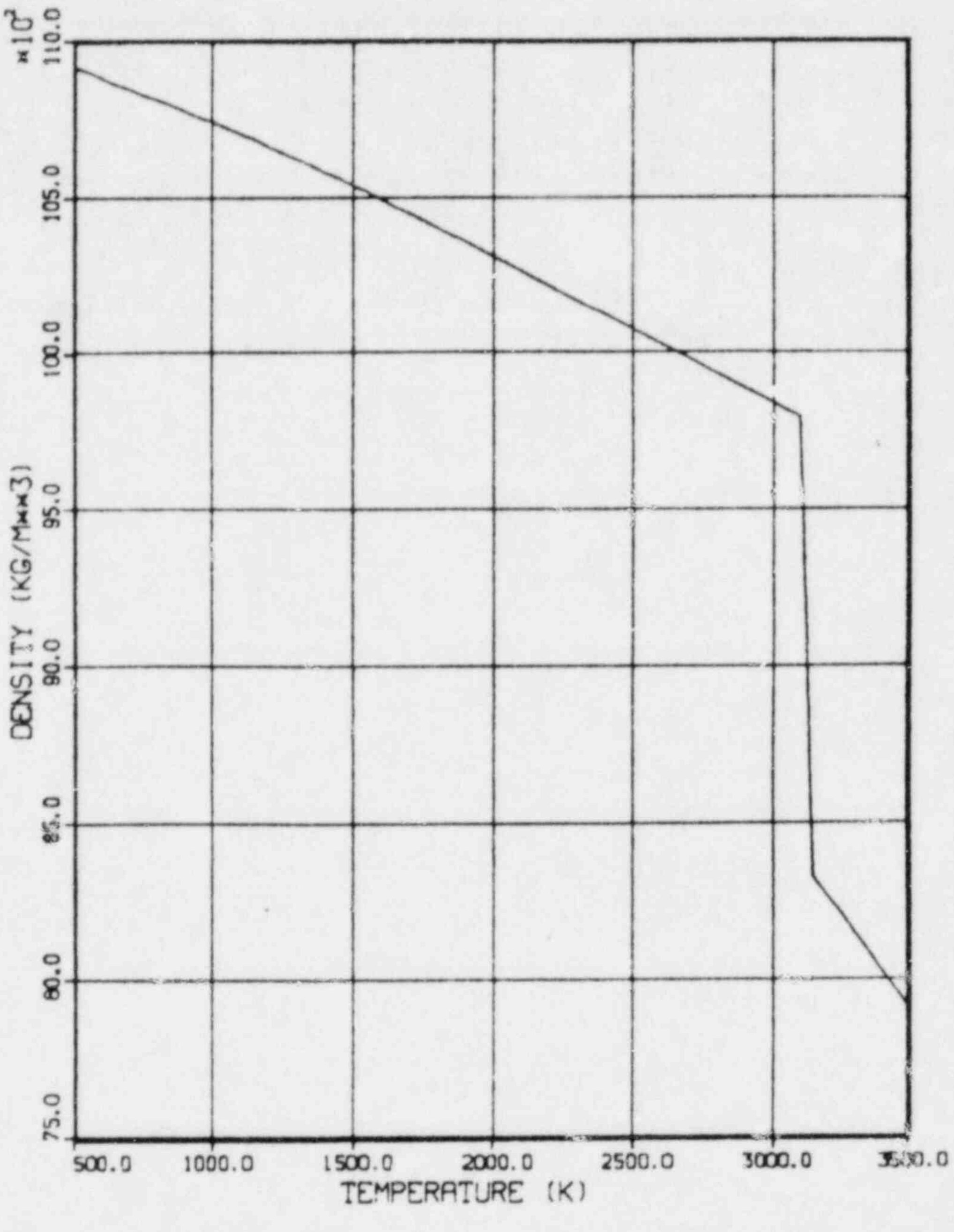

Figure A-2. Theoretical density of uranium dioxide.

TABLE A-3. LISTING OF THE FHYPRP SUBROUTINE

```
      SUBROUTINE FHYPRP(BU,COMP,TSOL,TLIQ)
C
C     FHYPRP RETURNS UO2, (U,PU)O2, MELTING POINTS.
C
C     TSOL    = OUTPUT SOLIDUS TEMPERATURE (K)
C     TLIQ    = OUTPUT LIQUIDUS TEMPERATURE (K)
C
C     BU      = INPUT BURNUP (MW-S/KG-U)
C     COMP    = INPUT PUO2 CONTENT (WT%)
C
C     FHYPRP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      FBU = BU/86.4
      IF(COMP .GT. 0.0) THEN
         TSOL = 3113.15 +COMP*(-5.41395 + COMP*7.468390E-03)
     #          -3.2E-03 * FBU
         TLIQ = 3113.15 +COMP*(-3.21660 - COMP*1.448518E-02)
     #          -3.2E-03 * FBU
      ELSE
         TSOL = 3113.15 - 3.2E-03 * FBU
         TLIQ = TSOL
      ENDIF
      RETURN
      END
```

REFERENCES

A-1. C. S. Kim et al., "Measurement of Thermal Diffusivity of Molten UO_2," Proceedings of the Seventh Symposium on Thermophysical Properties at the National Bureau of Standards Gaithersburg, Maryland, May 10-12, 1977, pp. 338-343 published by the American Society of Mechanical Engineers, CONF 770537-3.

A-2. D. R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, TID-26711-P1, 1976, p. 114.

APPENDIX B
CLADDING MATERIAL PROPERTIES

APPENDIX B

CLADDING MATERIAL PROPERTIES

Extension of the MATPRO Revision 2 cladding materials properties to high temperature requires the addition of subcodes for zircaloy enthalpy, zircaloy oxide specific heat, zircaloy oxide enthalpy, zircaloy density, zircaloy oxide thermal expansion, zircaloy oxide density, zircaloy oxide elastic moduli, and zircaloy oxide failure stress.

Some changes to existing subcodes are also required. The function for zircaloy oxide, ZOTCON, was revised to avoid a decrease in the predicted conductivity at high temperatures and to consider melting; the function for zircaloy thermal conductivity, CTHCON, was revised to estimate the change in thermal conductivity when zircaloy melts; the subroutine for zircaloy thermal expansion, CTHEXP, was modified to account for melting; and the part of the PHYPRP subroutine dealing with cladding melting or other phase changes was recoded as the CHYPRP subroutine to provide a consistent treatment of phase change temperatures.

These changes and new subcodes are described below. The material from earlier MATPRO versions which has not been changed is not included in this report.

CLADDING SPECIFIC HEAT CAPACITY AND ENTHALPY (CENTHL, ZOCP, ZONTHL)

The function CENTHL provides zircaloy enthalpy for temperatures above 300 K. ZOCP and ZONTHL return zircaloy oxide specific heat capacity and enthalpy. ZOCP requires only temperature as input while the two enthalpy subcodes require temperature and a reference temperature for which the enthalpy will be set equal to zero.

Zircaloy enthalpy is modeled by integrating the expressions used in the MATPRO-11 Revision 2 cladding specific heat subcode, CCP. Since CCP utilizes linear interpolation on the set of points reproduced in Table B-1, the CENTHL routine uses the expression

$$H(T) - H\ (300) = \sum_{j=1}^{i} \Delta H_j + C_{p_i}\ (T - T_i) + \frac{(T - T_i)^2}{2(T_{i+1} - T_i)}\ (C_{p_{i+1}} - C_{p_i}) \quad \text{(B-1)}$$

where

T_i = i-th temperature in Table A-1 (K)

C_p = specific heat capacity at T_i (J/kg•k)

ΔH_i = change in enthalpy of zircaloy between T_{i-1} and T_i

T = temperature (K)

$H(T)$ = enthalpy of zircaloy at temperature T (J/kg)

to find the enthalpy at a temperature greater than or equal to T_i, but less than T_{i+1}. Equation (B-1) can be derived by inspection of Figure B-1. The first term is the enthalpy between T_1 and T_i, that is the area under the line segments which connect C_{p_1} to C_{p_i}. The second term is the area of rectangle B and the third term is the area of traingle A. The sume of these two areas is the enthalpy between T_i and T. Table B-2 lists values of

$$\sum_{j=1}^{i} \Delta H_j$$

corresponding to the values of C_p in Table B-1. The entries for 2098 and 2099 K incorporate the heat of fusion for melting zircaloy. The melt

TABLE B-1. ZIRCALOY SPECIFIC HEAT CAPACITIES FOR CCP

Temperature (K)	Specific Heat Capacity (J/kg•K)
300	281
400	302
640	331
1090	375
1093	502
1113	590
1133	615
1153	719
1173	816
1193	770
1213	619
1233	469
1248	356
2098	356
2099	356

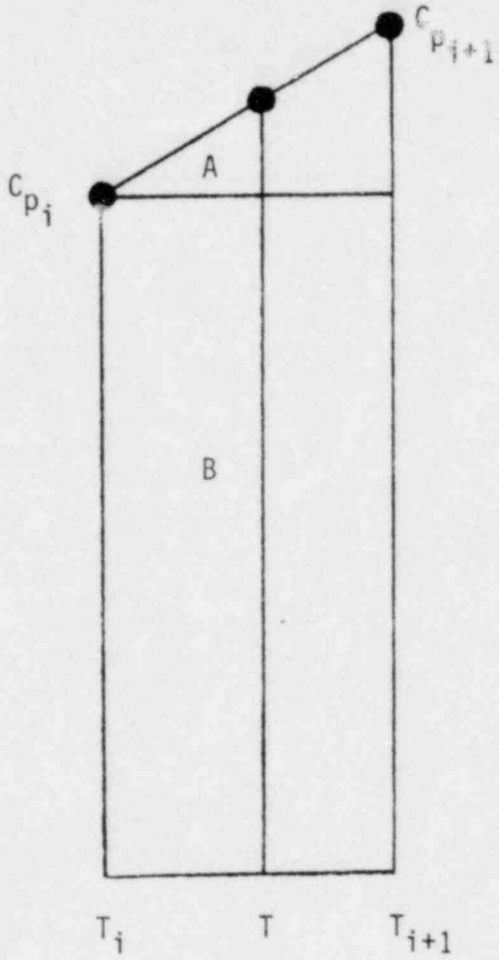

Figure B-1. Derivation of Equation (B-1).

TABLE B-2. VALUES OF $\sum_{j=1}^{i} \Delta H_j$ FOR ZIRCALOY

Temperature, T_i (K)	$\sum_{j=1}^{i-1} \Delta H_j$ (10^4 J/kg)
300	0.000
400	2.915
640	10.511
1090	26.396
1093	26.52755
1113	27.61955
1133	28.82455
1153	30.15855
1173	31.69355
1193	33.27955
1213	34.66855
1233	35.67655
1248	36.29530
2098	66.5553
2099	89.0909

temperature and heat of fusion were taken from the MATPRO-11, Revision 2 PHYPRP subcode and do not include the effect of oxidation on these quantities.

For temperatures greater than 2099 K, an enthalpy consistent with a constant specific heat capacity above 2099 K is calculated by omitting the third term on the right hand side of Equation (B-1). Table B-3 lists engineering estimates for the expected standard error of the enthalpy predicted by CENTHL with a reference temperature of 300 K.

Zircaloy oxide specific heat is modeled by the ZOCP function with the following expressions which were taken from Reference B-1:

For temperatures between 300 and 1478 K (monoclinic ZrO_2),

$$C_p^o = 565 + 6.11 \times 10^{-2}\ T - 1.14 \times 10^{+7}\ T^{-2} \tag{B-2a}$$

For temperatures in the range $1478 \leq T \leq 2000$ K (tetragonal ZrO_2),

$$C_p^o = 604.5 \quad . \tag{B-2b}$$

For temperatures between 2000 and 2973 K (tetragonal and cubic ZrO_2),

$$C_p^o = 171.7 + 0.2164\ T \quad . \tag{B-2c}$$

For temperatures above 2973 K (liquid ZrO_2),

$$C_p^o = 815\ \text{J/kg}\cdot\text{K} \quad . \tag{B-2d}$$

where

C_p^o = specific heat of zircaloy oxide (J/kg•K)

TABLE B-3. UNCERTAINTY OF ZIRCALOY ENTHALPY

Temperature Range (K)	Expected Standard Error of CNTHL (fraction of predicted value)
$300 \leq T \leq 1090$	0.03
$1090 < T < 2656.67$	$3 \times 10^{-4} (T-1090) + 0.03$
$2656.67 \leq T$	0.5

T = temperature (K).

The several equations correspond to the several phases of ZrO_2.

Zircaloy oxide enthalpy is modeled in the ZONTHL function with the integrated version of Equations (B-2a) to (B-2d), estimates of the changes of enthalpies at the phase chages[a,b], and an estimate of the heat of fusion of ZrO_2.[c]

For temperatures between 300 K and 1478 K (monoclinic ZrO_2):

$$H^o (T) - H^o (300) = 565 T + 3.055 \times 10^{-2} T^2 + 1.14 \times 10^{+7} T^{-1} - 2.102495 \times 10^5 \quad \text{(B-3a)}$$

For temperatures in the range $1478 \leq T \leq 2000$ K[a] (tetragonal ZrO_2),

$$H^o (T) - H^o (300) = 604.5 T - 1.46 \times 10^5 \ . \quad \text{(B-3b)}$$

For temperatures between 2000 and 2558 K (tetragonal and cubic ZrO_2),

$$H^o (T) - H^o (300) = 171.7 T + 0.1082 T^2 + 2.868 \times 10^5 \ . \quad \text{(B-3c)}$$

For temperatures in the range $2558 \leq T < 2973$ K[b],

$$H^o (T) - H^o (300) = 171.7 T + 0.1082 T^2 + 3.888 \times 10^5 \ . \quad \text{(B-3d)}$$

---

[a] Monalinic to Tetragonal transition ΔH = 48,200 J/kg.

[b] Tetragonal to Cubic transition ΔH = 102,000 J/kg.

[c] Heat of fusion = 706,000 J/kg.

For temperatures ≥ 2973 K (liquid ZrO_2)[a]

$$H^o (T) - H^o (300) = 815 T + 1.39 \times 10^5 \qquad \text{(B-3e)}$$

where

$H^o (T)$ = enthalpy of zircaloy oxide at temperature T (J/kg).

T = oxide temperature (K).

The principal contribution to the expected standard error of the enthalpy and specific heat capacity predictions for cladding oxide is not the uncertainty of the correlations for ZrO_2 because C_p measurements are typically accurate to several percent. It is the probability that the oxide film that appears on cladding differs significantly from the ZrO_2 used to produce the correlations. The oxide is substoichometric and has enough stress from the volume expansion during oxidation to cause significant changes of the phase transition temperatures.(B-2) Therefore, a relatively large expected standard error of ±0.2 times the given values is suggested for both the predicted specific heat capacity and enthalpy of zircaloy oxide.

Tables B-4 to B-6 are listings of the CENTHL, ZOCP, and ZONTHL functions. A code-generated plot of zircaloy enthalpy change as a function of temperature is presented in Figure B-2. The specific heat capacity predicted with the ZOCP function is shown in Figure B-3. Comparison of the predicted specific heat capacity with data reported by Gilchrest,(B-3) which are reproduced in Table B-7, suggests an expected standard error of ±150 J/kg•K. Figure B-4 is a plot of the zircaloy oxide enthalpy predicted with the ZONTHL function. The numerous steps are heats of transitions for the several phase changes of zircaloy dioxide.

---

[a] Heat of fusion = 706,000 J/kg.

TABLE B-4. LISTING OF THE CENTHL FUNCTION

```
      FUNCTION CENTHL(CTEMP,RFTEMP)
C
C     CENTHL RETURNS THE CHANGE IN ENTHALPY OF ZIRCALOY DURING
C     A CONSTANT PRESSURE CHANGE IN TEMPERATURE FROM RFTEMP TO CTEMP.
C
C     CENTHL = OUTPUT CHANGE IN CLADDING ENTHALPY (J/KG)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     CENTHL WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      DIMENSION CPDATA(30),HDATA(15)
      DATA CPDATA/   281., 300.,   302., 400.,   331., 640.,
     #  375.,1090.,  502.,1093.,   590.,1113.,   615.,1133.,
     #  719.,1153.,  816.,1173.,   770.,1193.,   619.,1213.,
     #  469.,1233.,  356.,1248.,   356.,2098.,   356.,2099./
C
      DATA HDATA/   0.00000,  2.91500, 10.51100, 26.39600,
     #   26.52755, 27.51955, 28.82455, 30.15855, 31.69355,
     #   33.27955, 34.66855, 35.67655, 36.29530, 66.55530,
     #   89.09090/
C
      T = RFTEMP
      N = -1
C     START AT LOW TEMPERATURES AND LOOK TO SEE WHERE T FITS
   10 K = 1
C
C     CHECK FOR A TEMPERATURE LOWER THAN THE TABLE RANGE
      IF(T .LE. 300.) THEN
         H = CPDATA(1) * (T - 300.)
      ELSE
C     CHECK FOR A TEMPERATURE WITHIN THE TABLE RANGE
   20    IF(T .LE. CPDATA(2*K+2)) THEN
            H = HDATA(K)*1.0E+04 + (T-CPDATA(2*K))*(CPDATA(2*K-1) +
     #          (T-CPDATA(2*K))*(CPDATA(2*K+1)-CPDATA(2*K-1))/
     #          (2. * (CPDATA(2*K+2)-CPDATA(2*K))))
         ELSE
            K = K + 1
            IF(K .LE. 14) THEN
               GO TO 20
C     THE ONLY REMAINING POSSIBILITY IS A TEMPERATURE HIGHER
C     THAN THE TABLE RANGE
            ELSE
               H = HDATA(15)*1.0E+04 + (T-CPDATA(30))*CPDATA(29)
            ENDIF
         ENDIF
      ENDIF
C
C
       IF(N .LT. 0) THEN
          N = N + 2
          HR = H
          T = CTEMP
          GO TO 10
      ELSE
          CENTHL = H - HR
      ENDIF
      RETURN
      END
```

TABLE B-5. LISTING OF THE ZOCP FUNCTION

```
      FUNCTION ZOCP(ZOTEMP)
C
C     ZOCP RETURNS THE SPECIFIC HEAT CAPACITY AT CONSTANT
C     PRESSURE FOR ZIRCALOY CLADDING OXIDE
C
C     ZOCP    = OUTPUT ZIRCALOY CLADDING OXIDE SPECIFIC HEAT
C               (J/(KG*K))
C
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C
C     ZOCP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ZOTEMP .LE. 300.) THEN
         ZOCP = 456.6633
      ELSE
         IF(ZOTEMP .LT. 1478.) THEN
            ZOCP = 656. + 6.11E-02*ZOTEMP -1.14E+07/(ZOTEMP**2)
         ELSE
            IF(ZOTEMP .LE. 2000.) THEN
               ZOCP = 604.5
            ELSE
               IF(ZOTEMP .LT. 2973.) THEN
                  ZOCP = 171.7 + 0.2164 * ZOTEMP
               ELSE
                  ZOCP = 815.
               ENDIF
            ENDIF
         ENDIF
      ENDIF
      RETURN
      END
```

TABLE B-6. LISTING OF THE ZONTHL FUNCTION

```
      FUNCTION ZONTHL(ZOTEMP,RFTEMP)
C
C     ZONTHL RETURNS THE CHANGE IN ENTHALPY OF ZIRCALOY OXIDE
C     DURING A CONSTANT PRESSURE CHANGE IN TEMPERATURE
C     FROM RFTEMP TO ZOTEMP.
C
C     ZONTHL = OUTPUT CHANGE IN OXIDE ENTHALPY (J/KG)
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     ZONTHL WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      T = RFTEMP
      N = -1
C
   10 IF(T .LE. 300.) THEN
         H = 456.6633 * (T - 300.)
      ELSE
         IF(T .LT. 1478.) THEN
            H = T*(565.+3.055E-02*T)+(1.14E+07/T)-2.102495E+05
         ELSE
            IF(T .LE. 2000.) THEN
               H = T*604.5 - 1.46E+05
            ELSE
               IF(T .LT. 2558.) THEN
                  H = T*(171.7 + 0.1082*T) + 2.868E+05
               ELSE
                  IF(T .LT. 2973.) THEN
                     H = T*(171.7 + 0.1082*T) + 3.888E+05
                  ELSE
                     H = T*815. + 1.39E+05
                  ENDIF
               ENDIF
            ENDIF
         ENDIF
      ENDIF
C
C
      IF(N .LT. 0) THEN
         N = N + 2
         HR = H
         T = ZOTEMP
         GO TO 10
      ELSE
         ZONTHL = H - HR
      ENDIF
      RETURN
      END
```

TABLE B-7. ZIRCALOY CLADDING OXIDE SPECIFIC HEAT CAPACITY DATA FROM GILCHRIST[B-3]

Temperature (K)	Specific Heat Capacity (J/kg•K)	Comment
324	462	Measured by Gilchrist
348	481	Measured by Gilchrist
377	486	Measured by Gilchrist
422	402	Measured by Gilchrist
462	510	Measured by Gilchrist
500	523	Measured by Gilchrist
598	543	Measured by Gilchrist
698	566	Measured by Gilchrist
801	569	Measured by Gilchrist
899	592	Measured by Gilchrist
945	598	Measured by Gilchrist
975	601	Measured by Gilchrist
1004	603	Measured by Gilchrist
772	563	Measured by Smithells
373	437	Measured by Washburn
774	525	Measured by Washburn
1272	631	Measured by Washburn
325	442	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"
399	486	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"

TABLE B-7. (continued)

Temperature (K)	Specific Heat Capacity (J/kg•K)	Comment
494	510	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"
598	535	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"
692	555	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"
790	576	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"
1198	606	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"
1398	612	Reported by Gilchrist as data from "Thermophysical Properties of Solid Material"

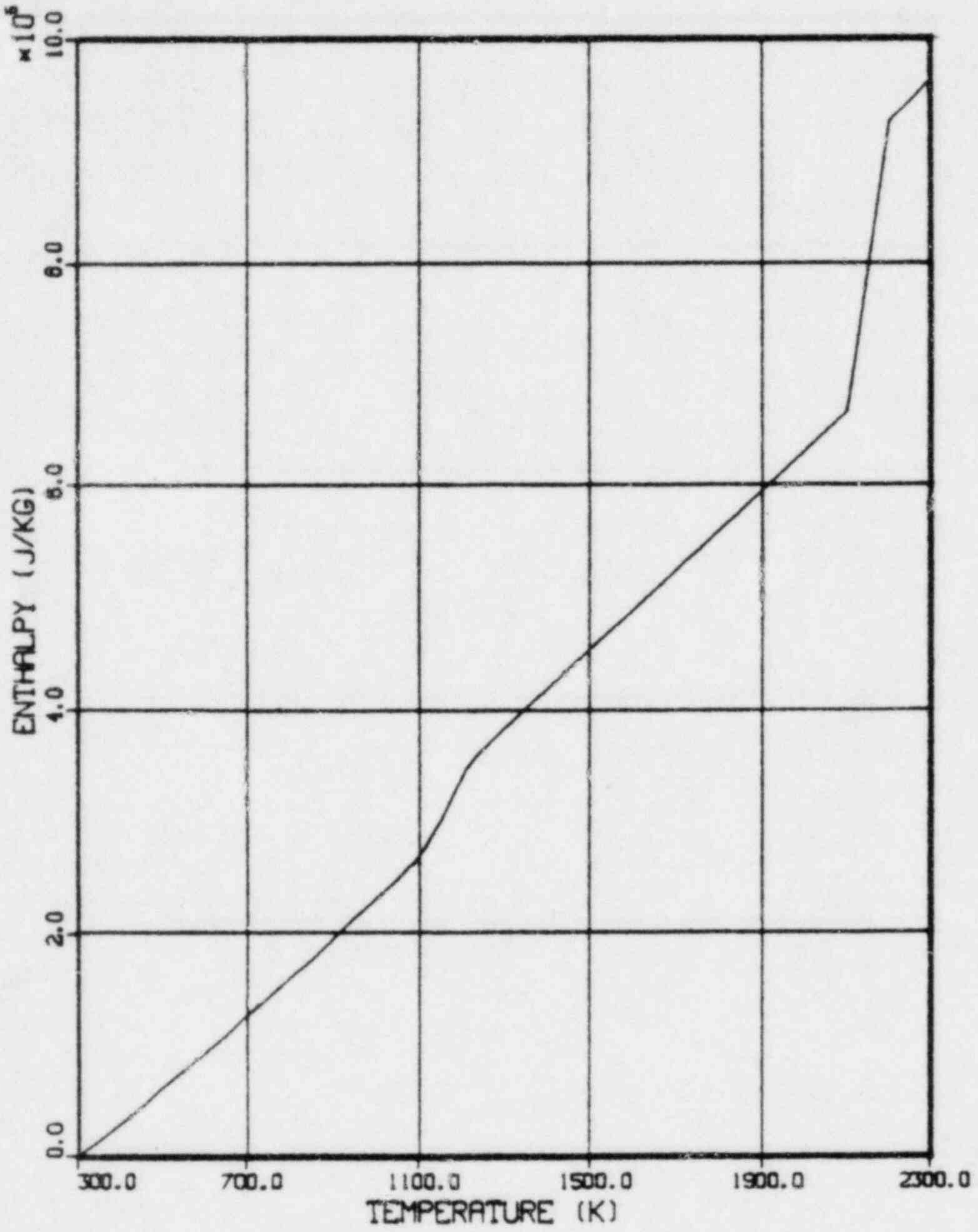

Figure B-2. Zircaloy enthalpy as a function of temperature.

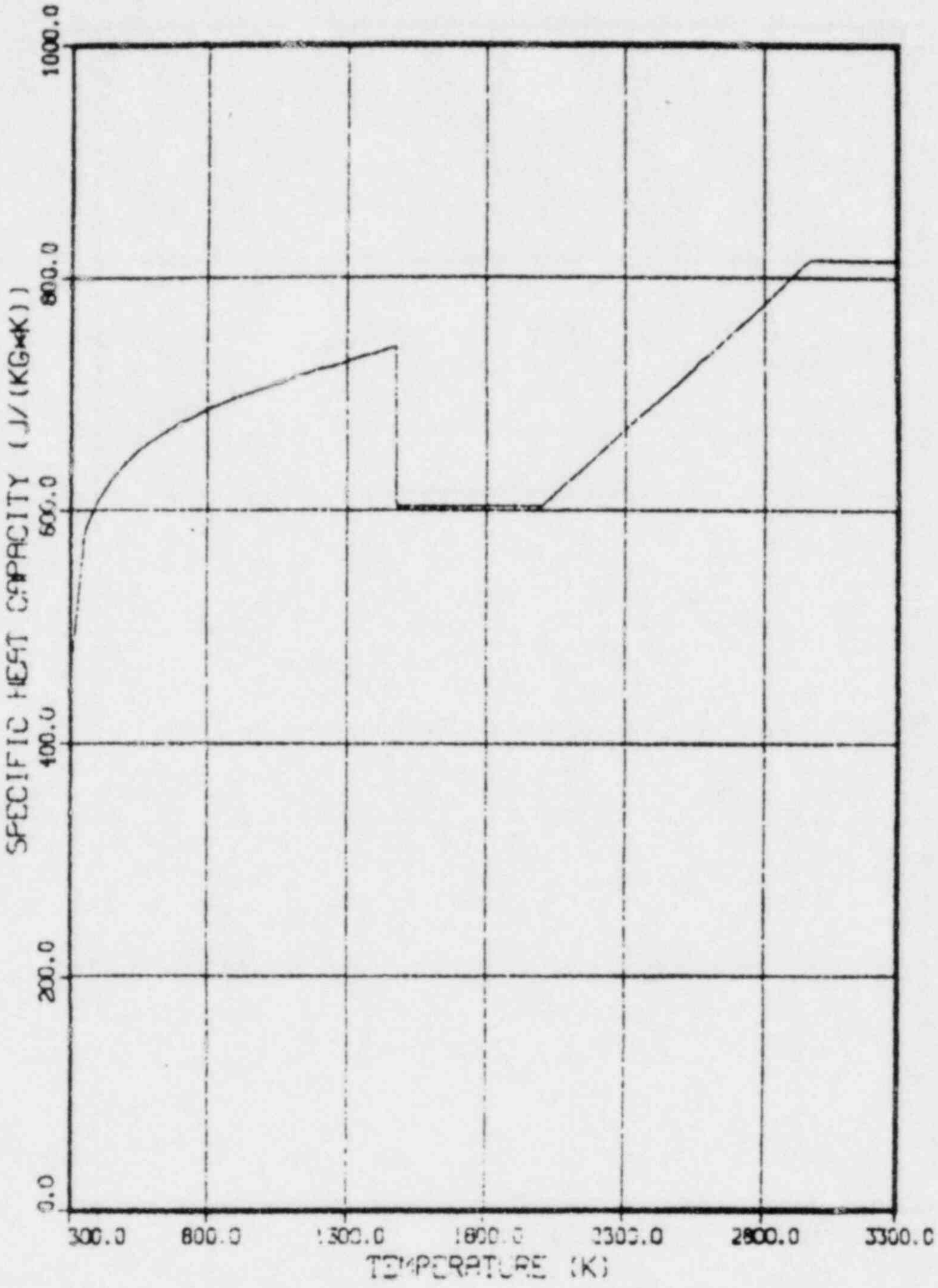

Figure B-3. Zircaloy oxide specific heat capacity as a function of temperature.

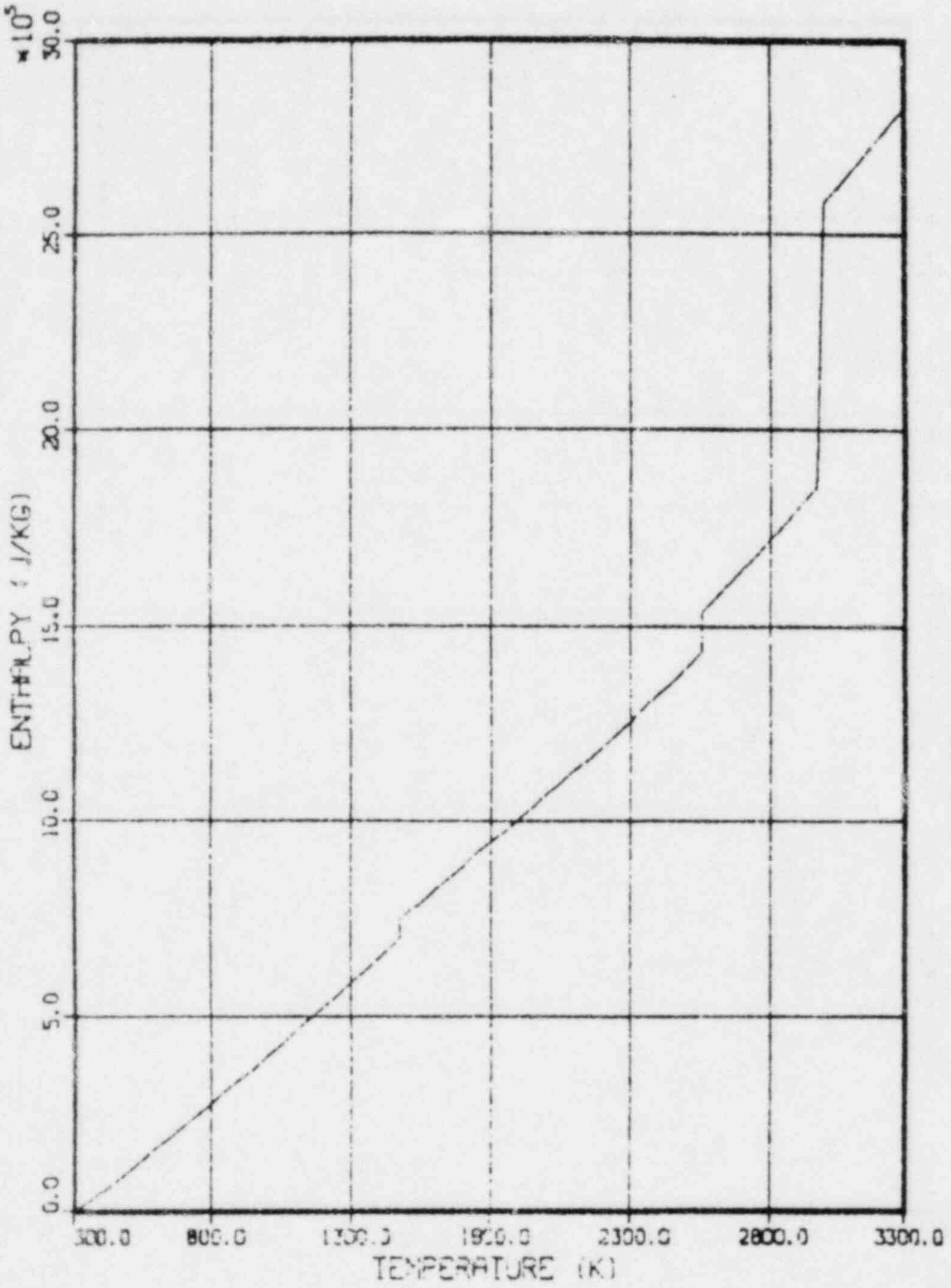

Figure B-4. Zircaloy oxide enthalpy as a function of temperature.

CLADDING THERMAL CONDUCTIVITY (CTHCON, ZOTCON)

CTHCON and ZOTCON return zircaloy and zircaloy oxide conductivity, respectively. The only input information required is the temperature of the material.

Extension of the MATPRO-11 Revision 2 correlations for zircaloy thermal conductivity to high temperatures required only consideration of the effect of melting on thermal conductivity. No data for liquid zircaloy thermal conductivity have been found but Nazare, Ondracek, and Schulz(B-4) have reported that the ratios of solid state conductivities to liquid state conductivities at the melting temperatures for metals like zircaloy with eight nearest neighbor atoms is 1.6 ± 0.2.[a] Since the solid state conductivity predicted by the CTHCON function is 58 W/m•K, the liquid state conductivity should be about 36 ± 5 W/m•K. The modified CTHCON function therefore uses

$$K = 36 \pm 5 \tag{B-4}$$

where

K = thermal conductivity of zircaloy (W/m•K).

The MATPRO-11 Revision 2 function for zircaloy oxide conductivity has been completely reformulated because:

1. The third degree polynomial used to calculate conductivity predicted a non-physical decrease in conductivity for temperatures above 1900 K.

---

[a] The body centered cubic lattice of beta phase zircaloy has eight nearest neighbors.

2. The points shown in Figure E-2.2 of the MATPRO document and used as data were not data. They were smoothed-curve predictions deduced from data of Adams.(B-5)

3. The smoothed-curve predictions corrected the data to a theoretical density of 6100 Kg/m^3, a value which is inconsistent with the MATPRO-11 Revision 2 density of 5820 kg/m^3 for oxide films.

4. The material used by Adams was "stabilized ZrO_2."(B-6) a ZrO_2 base material to which CaO, Y_2O_3, or MgO has been added to cause the material to have a cubic structure.(B-7) Since unstabilized ZrO_2 has a monoclinic structure below 1478 K and a tetragonal structure from 1478 to 2000 K, the conductivity of the stabilized ZrO_2 may be significantly different from that of the unstabilized zircaloy oxide.

5. An accurate value of oxide thermal conductivity is probably important to accurate calculations of the peak cladding temperature during the rapid heating of cladding due to oxidation that occurs at high temperature.

Data from the one sample that Adams reports are presented in Table B-8. Additional sources of data are Maki,(B-8) Lapshov and Bashkatov,(B-9) and Gilchrist.(B-3)

Data of Maki from two samples oxidized in steam are reproduced in Table B-9. The data cover a small temperature range and show a sharp increase in conductivity between 400 and 500 K. The principal recommendation for the data is that they were taken with black oxide from zircaloy tubes. Two data attributed to Waldman by Maki are also shown in the table.

TABLE B-8. STABILIZED ZIRCALOY DIOXIDE THERMAL CONDUCTIVITY DATA FROM ADAMS[B-5]

Temperature (K)	Thermal Conductivity (W/m•K)	T.C. Corrected to 5820 kg/m^3 (W/m•K)
370	1.69	1.88
460	1.69	1.88
547	1.70	1.89
641	1.78	1.98
698	1.73	1.91
743	1.74	1.93
817	1.74	1.93
882	1.74	1.93
945	1.76	1.95
993	1.79	1.98
1059	1.78	1.97
1123	1.79	1.98
1187	1.86	2.06
1245	1.89	2.09
1285	1.95	2.16
1305	1.92	2.13
1329	1.93	2.14
1338	1.94	2.15
1354	1.96	2.17
1390	1.96	2.18
1405	1.99	2.20
1427	1.98	2.19
1440	2.02	2.24
1448	2.08	2.31
1480	2.01	2.23
1485	2.03	2.25
1505	2.01	2.23
1554	2.01	2.23
1566	2.02	2.24
1583	2.01	2.23

TABLE B-9. ZIRCALOY OXIDE THERMAL CONDUCTIVITY DATA REPORTED BY MAKI[B-8]

Average of Inside and Outside Temperature (K)	Thermal Conductivity (W/m•K)	Comment
401	0.70	Sample 4
434	4.78	Sample 4
488	6.35	Sample 4
536	5.41	Sample 4
588	5.45	Sample 4
400	1.07	Sample 5
437	4.50	Sample 5
490	5.76	Sample 5
536	6.11	Sample 5
589	6.27	Sample 5
373	0.90	Data from Waldman
373	1.35	Data from Waldman

The data of Lapshov and Bashkatov are presented in Table B-10. These data are from films formed by plasma sputtering of zirconium dioxide on tungsten substrates. Since sputtered coatings are quite porous and may not be very adherent to the substrate, these data may not be representative of zircaloy cladding oxide conductivity.

Table B-11 presents the data of Gilchrest. Two types of oxide films were employed, one nodular oxide and the other a black oxide characteristic of the kinds of layers usually reported in high temperature tests with cladding. The black oxide thermal conductivities are much lower than the nodular oxide thermal conductivities and both kinds of oxide have conductivities which are significantly lower than the stabilized zircaloy dioxide conductivities reported by Adams. Considerable uncertainty is reported by Gilchrist because of difficulty in measuring oxide film thickness.

Figure B-5 is a plot of the data in Tables B-8 to B-11. The plot shows that with the exception of the anomalously high data of Maki the principal uncertainty in thermal conductivity is caused by sample-to-sample variations. Measurement inaccuracies with any one sample are much smaller than sample-to-sample variations. It is also clear from an inspection of Figure B-5 that the slopes of the measurements on individual samples are quite consistent. The difference between the various samples is essentially a displacement of a line with a constant slope.

The slope of the thermal conductivity of a given sample was determined with a least squares linear fit to the data of Adams. These data were used because they extend over a large temperature range and were made with the most accurate epxerimental technique. The equation which results from this fit is

$$K_{ZrO_2} = 1.67 + 3.62 \times 10^{-4} T \qquad (B-4)$$

TABLE B-10. ZIRCALOY DIOXIDE THERMAL CONDUCTIVITY DATA OF LAPSHOV AND BASHKATOV[B-9]

Temperature (K)	Thermal Conductivity (W/m•K)
571	0.509
618	0.636
642	0.508
654	0.627
664	0.715
684	0.474
721	0.652
739	0.448
755	0.441
771	0.558
802	0.430
817	0.512
827	0.605
855	0.456
882	0.522
929	0.477
969	0.506
984	0.509
999	0.509
1006	0.472
1050	0.509
1071	0.522
1088	0.493
1097	0.587
1104	0.527
1162	0.563
1189	0.636
1201	0.577
1220	0.555
1250	0.623
1302	0.623
1354	0.577
1366	0.661
1380	0.663
1491	0.708

TABLE B-10. (continued)

Temperature (K)	Thermal Conductivity (W/m•K)
1527	0.656
1558	0.717
1626	0.801
1638	0.776
1685	0.788
1735	0.854

TABLE B-11. ZIRCALOY OXIDE DATA OF GILCHRIST[B-3]

Temperature (K)	Thermal Conductivity (W/m•K)	Comment
297	1.354	Black oxide
668	0.955	Black oxide
712	0.958	Black oxide
806	1.048	Black oxide
854	1.060	Black oxide
916	1.090	Black oxide
983	1.163	Black oxide
1043	1.242	Black oxide
1193	1.443	Black oxide
1260	1.407	Black oxide
1327	1.393	Black oxide
1386	1.487	Black oxide
1450	1.586	Black oxide
299	0.324	Nodular oxide
659	0.137	Nodular oxide
733	0.160	Nodular oxide
806	0.192	Nodular oxide
867	0.219	Nodular oxide
944	0.271	Nodular oxide
1018	0.410	Nodular oxide
1141	0.606	Nodular oxide
1222	0.825	Nodular oxide
1246	0.864	Nodular oxide
1326	0.743	Nodular oxide
1425	0.700	Nodular oxide

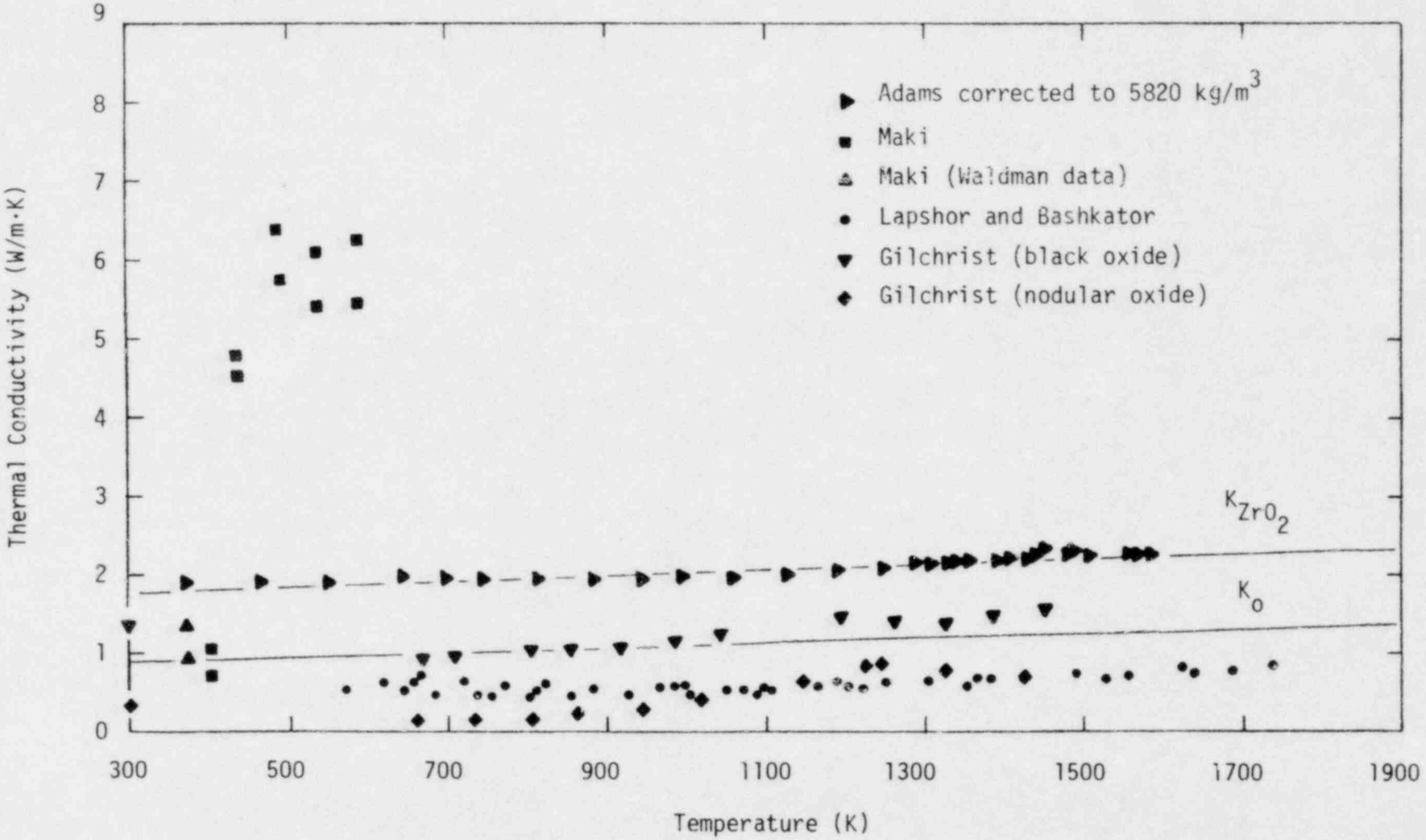

Figure B-5. Zircaloy oxide thermal conductivity data and correlations.

where

K_{ZrO2} = zircaloy dioxide thermal conductivity (W/m•K).

Since the black oxide data of Gilchrest are the most representative of the oxide found on cladding, Equation (B-4) is modified for zircaloy oxide by dividing the right hand side by two. The resultant expression is

$$K_o = 0.835 + 1.81 \times 10^{-4}\ T \tag{B-5}$$

where

K_o = zircaloy cladding oxide thermal conductivity (W/m•K).

Values of K_{ZrO_2} and K_o calculated with Equations (B-4) are shown with the data in Figure B-5. Inspection of the figure suggests an expected standard error of ±0.75 of the measured value for K_o. For material that is known to be ZrO_2, the expected standard error is much less, approximately 10% of the value of K_{ZrO_2}.

For liquid zircaloy oxide (temperature >2973 K) the conductivity is assumed to be approximately the value of K_o at the melting temperature of ZrO_2:

$$K_{o_{liquid}} = 1.4\ \text{W/m•K} \quad . \tag{B-6}$$

This number is a compromise between the decrease in conductivity at melt due to the loss of the phonon contribution and the increase in conductivity at melt due to the loss of porosity.

Tables B-12 and B-13 are listings of the CTHCON and ZOTCON functions. Figures B-6 and B-7 are plots of the conductivities predicted by the functions as a function of temperature.

TABLE B-12. LISTING OF THE CTHCON FUNCTION

```
      SUBROUTINE CTHCON(CTEMP,CCON,CDKDT)
C
C     CTHCON RETURNS ZIRCALOY THERMAL CONDUCTIVITY
C
C     CCON   = OUTPUT THERMAL CONDUCTIVITY OF ZIRCALOY (W/(M*K))
C     CDKDT  = OUTPUT DERIVATIVE OFTHERMAL CONDUCTIVITY
C              WITH RESPECT TO TEMPERATURE (W/(M*K*K))
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C
C     CTHCON WAS CODED BY R. L. MILLER DECEMBER 1975
C     LAST MODIFIED BY D. L. HAGRMAN MARCH 1982
C
      IF(CTEMP .LT. 2098.) THEN
         CCON = 7.511 + CTEMP*(2.088E-02 + CTEMP*(-1.45E-05 +
     #          CTEMP*7.668E-09))
         CDKDT = 2.088E-02 + CTEMP*(-2.9E-05 + CTEMP*2.3E-08)
      ELSE
         CCON = 36.
         CDKDT = 0.0
      ENDIF
      RETURN
      END
```

TABLE B-13. LISTING OF THE ZOTCON FUNCTION

```
      FUNCTION ZOTCON(ZOTEMP)
C
C     ZOTCON RETURNS ZIRCALOY OXIDE THERMAL CONDUCTIVITY
C
C     ZOCP   = OUTPUT THERMAL CONDUCTIVITY OF
C              ZIRCALOY OXIDE (W/(M*K))
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C
C     ZOTCON WAS CODED BY R. L. MILLER IN MARCH 1974
C     LAST MODIFIED BY D. L. HAGRMAN MARCH 1982
C
      IF(ZOTEMP .LT. 2973.) THEN
         ZOTCON = 0.835 + ZOTEMP * 1.81E-04
      ELSE
         ZOTCON = 1.4
      ENDIF
      RETURN
      END
```

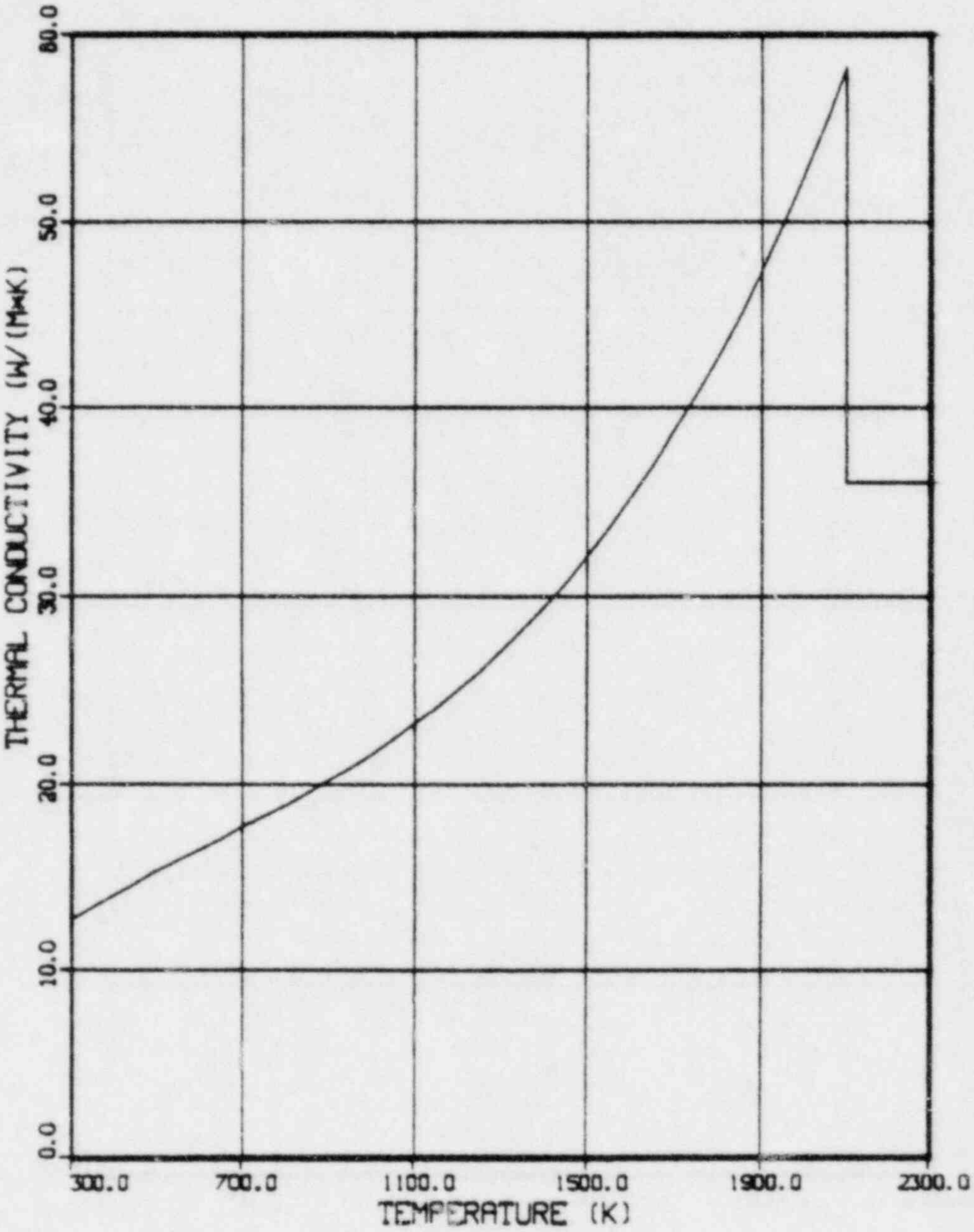

Figure B-6. Zircaloy thermal conductivity as a function of temperature.

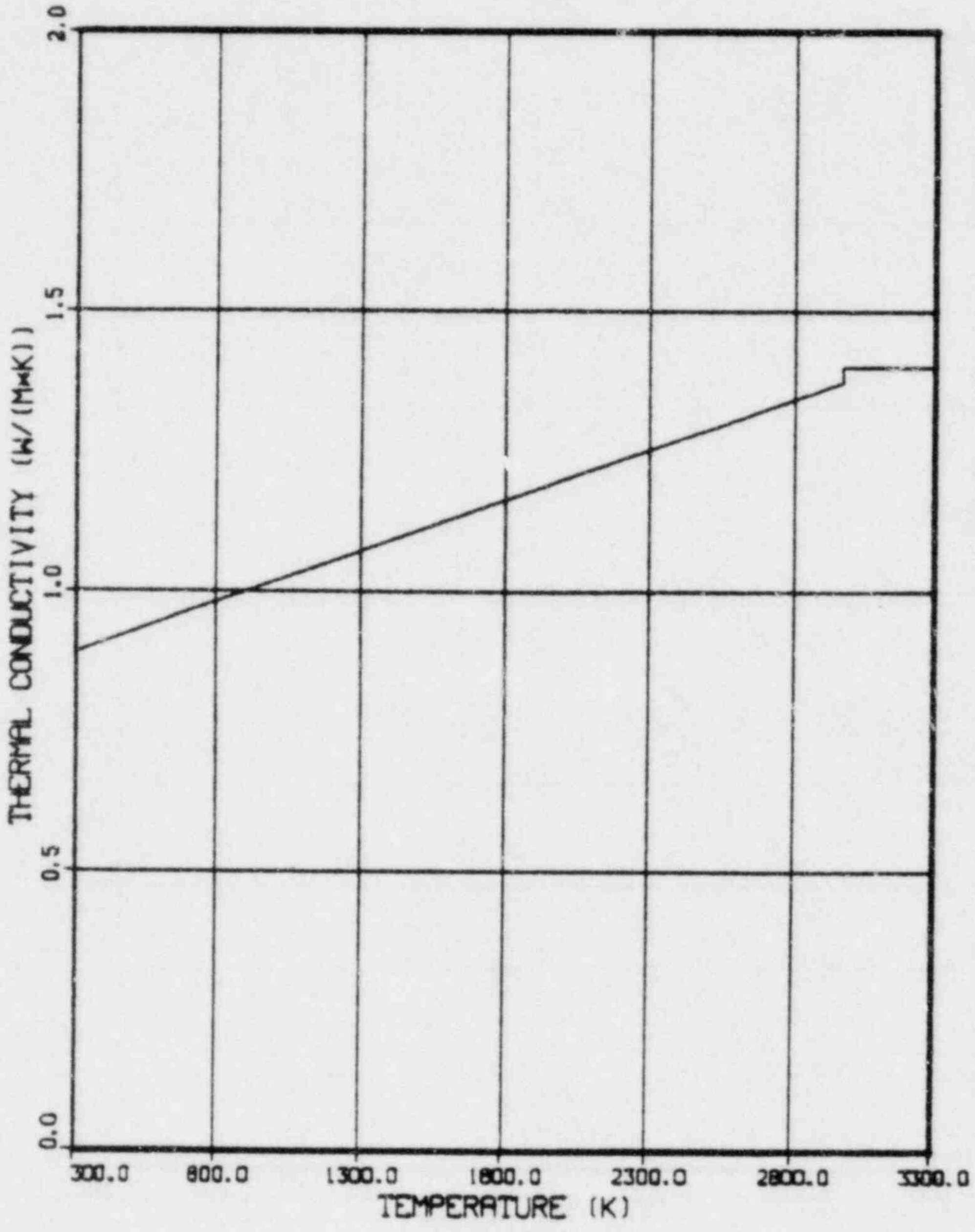

Figure B-7. Zircaloy oxide thermal conductivity as a function of temperature.

CLADDING THERMAL EXPANSION AND DENSITY
(CTHEXP, CDEN, ZOTEXP, ZODEN)

The subroutine CTHEXP calculates the three principal strains for zircaloy. CDEN returns zircaloy density. ZOTEXP and ZODEN compute zircaloy oxide thermal strains and density, respectively. The required input for CTHEXP is texture information (needed because the thermal strains are anisotropic), a reference temperature (for which the strains will be zero), and the cladding temperature. ZOTEXP requires a reference temperature and the oxide temperature. CDEN and ZODEN require only temperature.

To extend the MATPRO-11 Revision 2 CTHEXP subroutine to high temperatures, consideration of the volume change associated with melting is required. Since no data have been found, a typical 2% volume increase at melt is assumed. The expressions used for the thermal strain in liquid zirconium (temperatures $\geq$2098 K) are thus

$$\varepsilon_{\rho} = \frac{2}{3}\varepsilon_{11} + \frac{1}{3}\varepsilon_{33} + 0.0067 \qquad \text{(B-6)}$$

where

ε_{ρ} = thermal expansion strain in liquid zircaloy (m/m)

ε_{11} = circumferential thermal expansion strain of a single crystal of zircaloy at 2098 K (m/m)

ε_{33} = axial thermal expansion strain of a single crystal of zircaloy at 2098 K (m/m).

Equations (B-4.3) and (B-4.4) of the MATPRO-11 Revision 2 handbook are used to calculate ε_{11} and ε_{33}.

The CDEN function determines zirconium density from room temperature data and the thermal expansion strains calculated with the CTHEXP subroutine. By definition

$$\rho = \frac{m}{V} \quad \text{(B-7)}$$

where

ρ = density (kg/m^3)

m = mass of a sample of material (kg)

V = volume of the given mass of material (m^3).

Thermal expansion changes only the volume. The volume is related to a reference volume by

$$V = V_o \exp \varepsilon_x \exp \varepsilon_y \exp \varepsilon_z \quad \text{(B-8)}$$

where

V_o = volume of the mass m when strains are zero (m^3)

ε_x, ε_y, ε_z = true strains for any orthoginal coordinate system (m/m).

Substituion of Equation (B-8) into Equation (B-7) shows

$$\rho = \rho_o \exp(-\varepsilon_x) \exp(-\varepsilon_y) \exp(-\varepsilon_z) \quad \text{(B-9)}$$

where

ρ_o = the density at any reference temperature (kg/m^3).

Since thermal strains are always much less than one,

$$\rho \approx \rho_0 (1 - e_x - e_y - e_z) \quad . \tag{B-10}$$

The three orthoginal strains are provided by CTHEXP and the reference density used is the value of 6.55 10^3 kg/m^3 at 300 K reported by Scott$^{(B-10)}$. This value is consistent with the high temperature value of 6490 kg/m^3 often used in the MATPRO document. The predicted zircaloy thermal strains are estimated in MAPTRO-11 Revision 2 to have an expected standard error near 0.1 of their predicted valves for temperatures below 1090 K and 50% for higher temperatures.

Expressions used in ZOTEXP to calculate the thermal strains of solid zirconium oxide are taken from Reference B-1:

For temperatures between 300 and 1478 K (monoclinic ZrO_2),

$$\varepsilon_0 = 7.8 \times 10^{-6}\ T - 2.34 \times 10^{-3} \quad , \tag{B-11a}$$

and for temperatures in the range $1478 \leq T < 2973$ (tetragonal and cubic ZrO_2)

$$\varepsilon_0 = 1.302 \times 10^{-5}\ T - 3.338 \times 10^{-2} \tag{B-11b}$$

where

ε_0 = linear thermal strain of zircaloy oxide (m/m).

These expressions show a 7.7% decrease in volume at the monoclinic-tetragonal phase change (1478 K).

For liquid zirconium oxide a 5% reduction in volume is assumed when the oxide melts. This assumption corresponds to the assumption that the 5% porosity of the oxide is removed when it melts. The resultant expression is

$$\varepsilon_0 = -1.1 \times 10^{-2} \tag{B-12}$$

for temperatures greater than or equal to 2973 K.

Equations (B-11a) to (B-12) are also used in ZODEN to calculate the density of zircaloy oxide. The relation employed is

$$\rho_x = \rho_{xo} (1 - 3e_o) \tag{B-13}$$

where

ρ_x = zirconium oxide density at the given temperature (kg/m^3)

ρ_{xo} = zirconium oxide density at 300 K (kg/m^3).

The value of ρ_{xo} used is the density of black oxide reported by Gilchrist,$^{(B-3)}$ 5800 kg/m^3.

The expected standard error of Equations (B-11a) and (B-11b) is large, the greater of half the predicted value or ±5 10^{-3}, because the equations are based on zircaloy dioxide data. The cladding oxide is not only substoichiometric but is formed under large stress because of the different densities of the oxide and the zircaloy on which it is formed.

Tables B-14 to B-17 are listings of the CTHEXP, CDEN, ZOTEXP and ZODEN subcodes. Figure B-8 is a plot of the circumferential axial and radial thermal strains predicted by the CTHEXP subroutine for zircaloy for cladding with typical texture (COSTH2 = 0.71013 and COSFI2 = 0.69177) and a reference temperature of 300 K. Figure B-9 shows the zircaloy density predicted by CDEN. The zircaloy dioxide thermal strains predicted by ZOTEXP are shown in Figure B-10 and the density of the oxide predicted by ZODEN is illustrated in Figure B-11. ZrO_2 thermal expansion data by Fulkerson^{B-11} and from pages 17 and 70 of Brassfield et al.,$^{B-12}$ are listed in Tables B-18 and B-19 and included in Figure B-12 so that they may be compared with code predictions.

TABLE B-14. LISTING OF THE CTHEXP SUBROUTINE

```
      SUBROUTINE CTHEXP(COSTH2,COSFI2,CTEMP,RFTEMP,STRN11,STRN22,STRN33)
C
C       CTHEXP CALCULATES THE THERMAL EXPANSION STRAIN FOR A PIECE OF
C       ZIRCALOY CLADDING AS A FUNCTION OF TEMPERATURE AND OF CLADDING
C       TEXTURE.
C
C       STRN11 = OUTPUT THERMAL EXPANSION STRAIN IN THE CIRCUMFERENTIAL
C                DIRECTION (M/M)
C       STRN22 = OUTPUT THERMAL EXPANSION STRAIN IN THE AXIAL
C                DIRECTION (M/M)
C       STRN33 = OUTPUT THERMAL EXPANSION STRAIN IN THE THICKNESS
C                DIRECTION (M/M)
C
C       CTEMP  = INPUT CLADDING TEMPERATURE (K)
C       COSFI2 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE SQUARED
C                SINE OF PHI (UNITLESS)
C       COSTH2 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE SQUARED
C                COSINE OF THETA (UNITLESS)
C
C       VALUES FOR COSFI2 AND COSTH2 MAY BE OBTAINED THROUGH USE OF THE
C       SUBROUTINE CTXTUR
C
C       THESE CALCULATIONS ARE BASED ON DATA AND TECHNIQUES IN THE
C       FOLLOWING SOURCES
C
C       (1) L.R. BUNNELL ET AL, HIGH TEMPERATURE PROPERTIES OF ZIRCALOY-
C           OXYGEN ALLOYS, EPRI NP-524 (MARCH 1977).
C       (2) D.L. DOUGLASS, "THE PHYSICAL METALLURGY OF ZIRCONIUM", ATOMIC
C           ENERGY REVIEW,1,#4 (DECEMBER 1963).
C       (3) C. KITTEL, INTRODUCTION TO SOLID STATE PHYSICS, 3RD EDITION,
C           NEW YORK, JOHN WILEY AND SONS INC., 1966.
C       (4) G.B. SKINNER, H.L. JOHNSTON, "THERMAL EXPANSION OF ZIRCONIUM
C           BETWEEN 298 AND 1600K", JOURNAL OF CHEMICAL PHYSICS,21 (1953)
C
C       CTHEXP WAS CODED BY G. A. REYMANN JANUARY 1980.
C       LAST MODIFIED BY D. L. HAGRMAN MARCH 1982.
C
C       CALCULATE SINGLE CRYSTAL STRAINS
C            STRS11 = SINGLE CRYSTAL STRAIN PERPENDICULAR TO THE C-AXIS
C            STRE33 = SINGLE CRYSTAL STRAIN ALONG THE C-AXIS
C
      T = RFTEMP
      N = -1
    5 IF(T .GE. 2098.) GO TO 40
      IF(T .GT. 1244.0) GO TO 20
      IF(T .GT. 1083.0) GO TO 10
C
       STRS11 = 4.95E-06*T - 1.485E-03
       STRS33 = 1.26E-05*T - 3.780E-03
       GO TO 30
C
 10    STRS11 = (2.77763 + 1.09822*COS((T-1083.0)*3.141593/161.0))
       STRS11 = STRS11*1.0E-03
```

```
       STRS33 = (8.76758 + 1.09822*COS((T-1083.0)*3.141593/161.0))
       STRS33 = STRS33*1.0E-03
       GO TO 30
C
 20    STRS11 = 9.7E-06*T - 1.04E-02
       STRS33 = 9.7E-06*T - 4.40E-03
C
C      CALCULATE CLADDING STRAINS USING SINGLE CRYSTAL STRAINS
C
 30    STRN11 = (COSFI2 +COSTH2*(1.0-COSFI2))*STRS11
     #             + (1.0-COSTH2)*(1.0-COSFI2)*STRS33
C
       STRN22 = (1.0-COSFI2 + COSTH2*COSFI2)*STRS11
     #             + (1.0-COSTH2)*COSFI2*STRS33
C
       STRN33 = (1.0-COSTH2)*STRS11 + COSTH2*STRS33
C
      GO TO 50
   40 STRS11 = 9.9506E-03
      STRS33 = 1.59506E-02
      STRN11 = 0.67 * STRS11 + 0.33 * STRS33 + 0.0067
      STRN22 = STRN11
      STRN33 = STRN11
C
   50 IF(N .LT. 0) THEN
         N = N + 2
         STRN1R = STRN11
         STRN2R = STRN22
         STRN3R = STRN33
         T = CTEMP
         GO TO 5
      ELSE
         STRN11 = STRN11 - STRN1R
         STRN22 = STRN22 - STRN2R
         STRN33 = STRN33 - STRN3R
      ENDIF
C       USTRN2 = UNCERTAINTY IN THE TUBE AXIAL THERMAL STRAIN
C       USTRN1 = UNCERTAINTY IN THE TUBE CIRCUMFERENTIAL THERMAL STRAIN
C       USTRN1 = 0.12*STRN11
C       USTRN2 = 0.08*STRN22
C
       RETURN
       END
```

TABLE B-15. LISTING OF THE CDEN FUNCTION

```
      FUNCTION CDEN(CTEMP)
C
C     CDEN RETURNS THE DENSITY OF ZIRCALOY CLADDING
C
C     CDEN    = OUTPUT ZIRCALOY DENSITY (KG/M**3)
C
C     CTEMP   = INPUT CLADDING TEMPERATURE (K)
C
C     THE SUBROUTINE CTHEXP IS CALLED BY THIS FUNCTION
C
C     CDEN WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      CALL CTHEXP(0.33,0.5,CTEMP,300.,STRN11,STRN22,STRN33)
      CDEN = 6.55E+03 * (1. - STRN11 - STRN22 - STRN33)
      RETURN
      END
```

TABLE B-16. LISTING OF THE ZOTEXP FUNCTION

```
      FUNCTION ZOTEXP(ZOTEMP,RFTEMP)
C
C     ZOTEXP RETURNS THE THERMAL EXPANSION STRAIN OF
C     ZIRCALOY OXIDE
C
C     ZOTEXP = OUTPUT ZIRCALOY OXIDE THERMAL EXPANSION (M/M)
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     ZOTEXP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      T = RFTEMP
      N = -1
C
   10 IF(T .LT. 1478.) THEN
         EPS = T * 7.8E-06 - 2.34E-03
      ELSE
         IF(T .LT. 2973.) THEN
            EPS = T * 1.302E-05 - 3.338E-02
         ELSE
            EPS = -1.1E-02
         ENDIF
      ENDIF
C
      IF(N .LT. 0) THEN
         N = N + 2
         EPSR = EPS
         T = ZOTEMP
         GO TO 10
      ELSE
         ZOTEXP = EPS - EPSR
      ENDIF
      RETURN
      END
```

TABLE B-17. LISTING OF THE ZODEN FUNCTION

```
      FUNCTION ZODEN(ZOTEMP)
C
C     ZODEN RETURNS THE DENSITY OF ZIRCALOY OXIDE
C
C     ZODEN  = OUTPUT ZIRCALOY OXIDE DENSITY (KG/M**3)
C
C     ZOTEMP = INPUT OXIDE TEMPERATURE (K)
C
C     THE FUNCTION ZOTEXP IS CALLED BY THIS FUNCTION
C
C     ZODEN WAS CODED BY D. L. HAGRMAN MARCH 1982.
C
      EPS = ZOTEXP(ZOTEMP,300.)
      ZODEN = 5.8E+03 * (1. - 3. * EPS)
      RETURN
      END
```

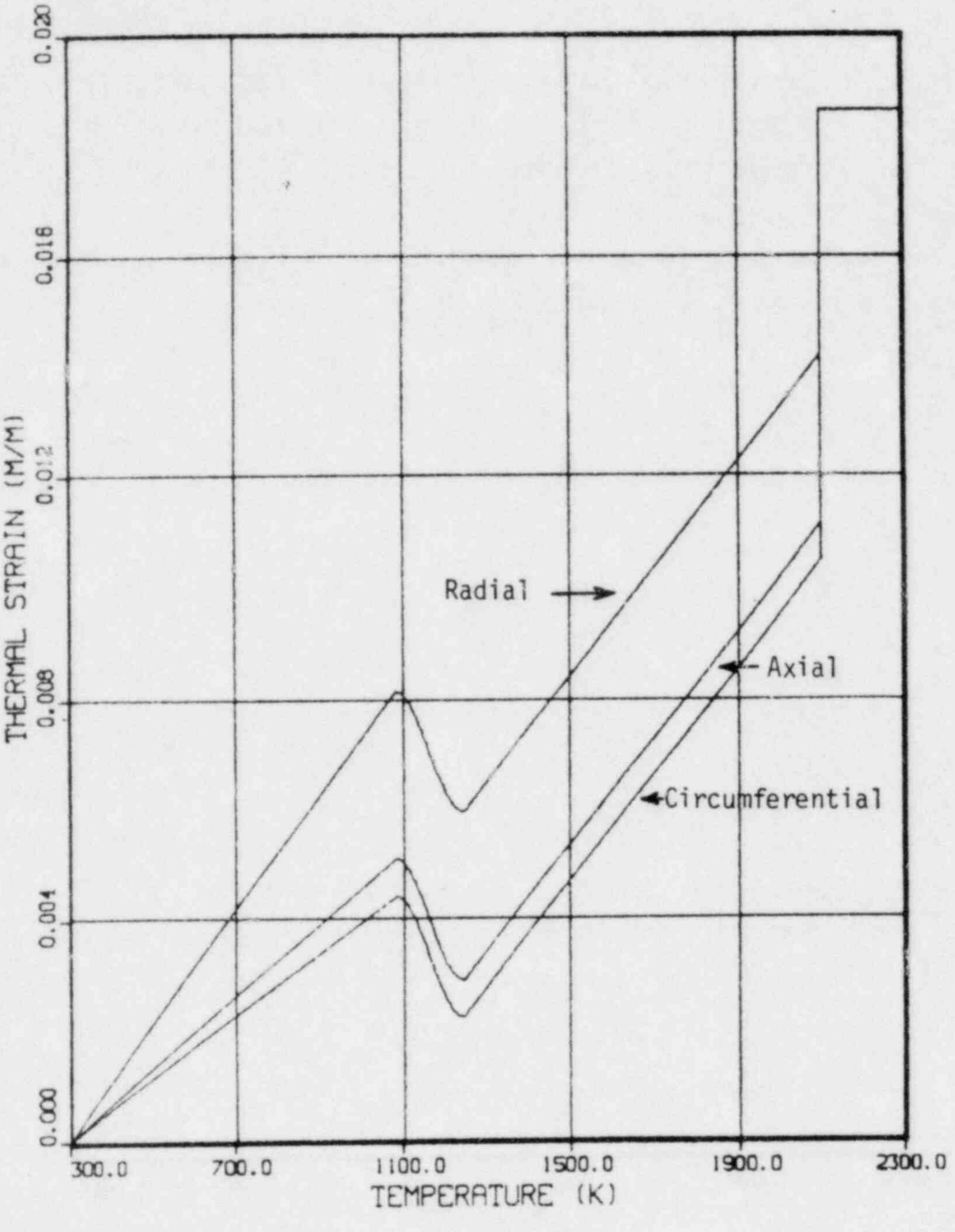

Figure B-8. Zircaloy cladding thermal strains for typical texture.

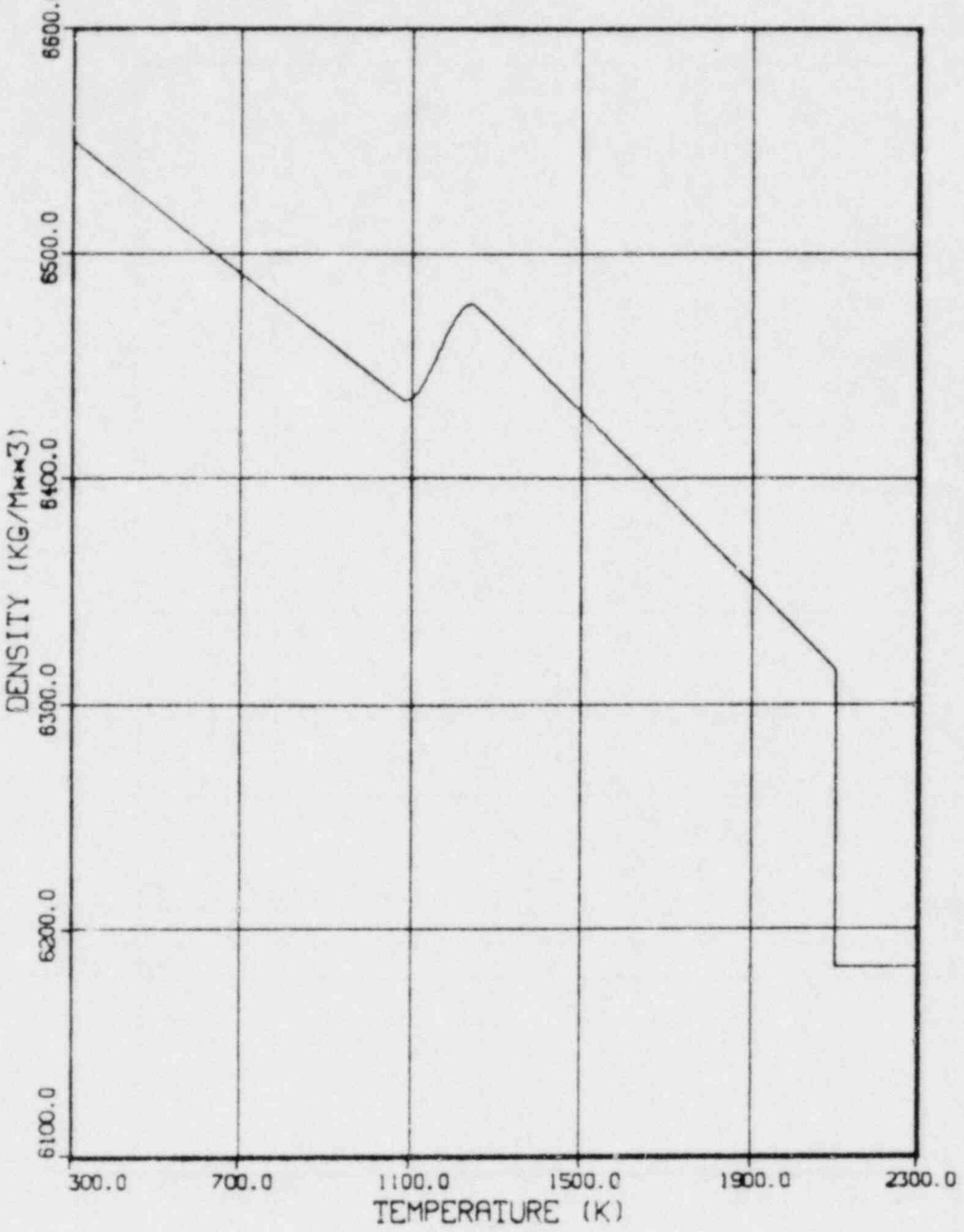

Figure B-9. Zircaloy density as a function of temperature.

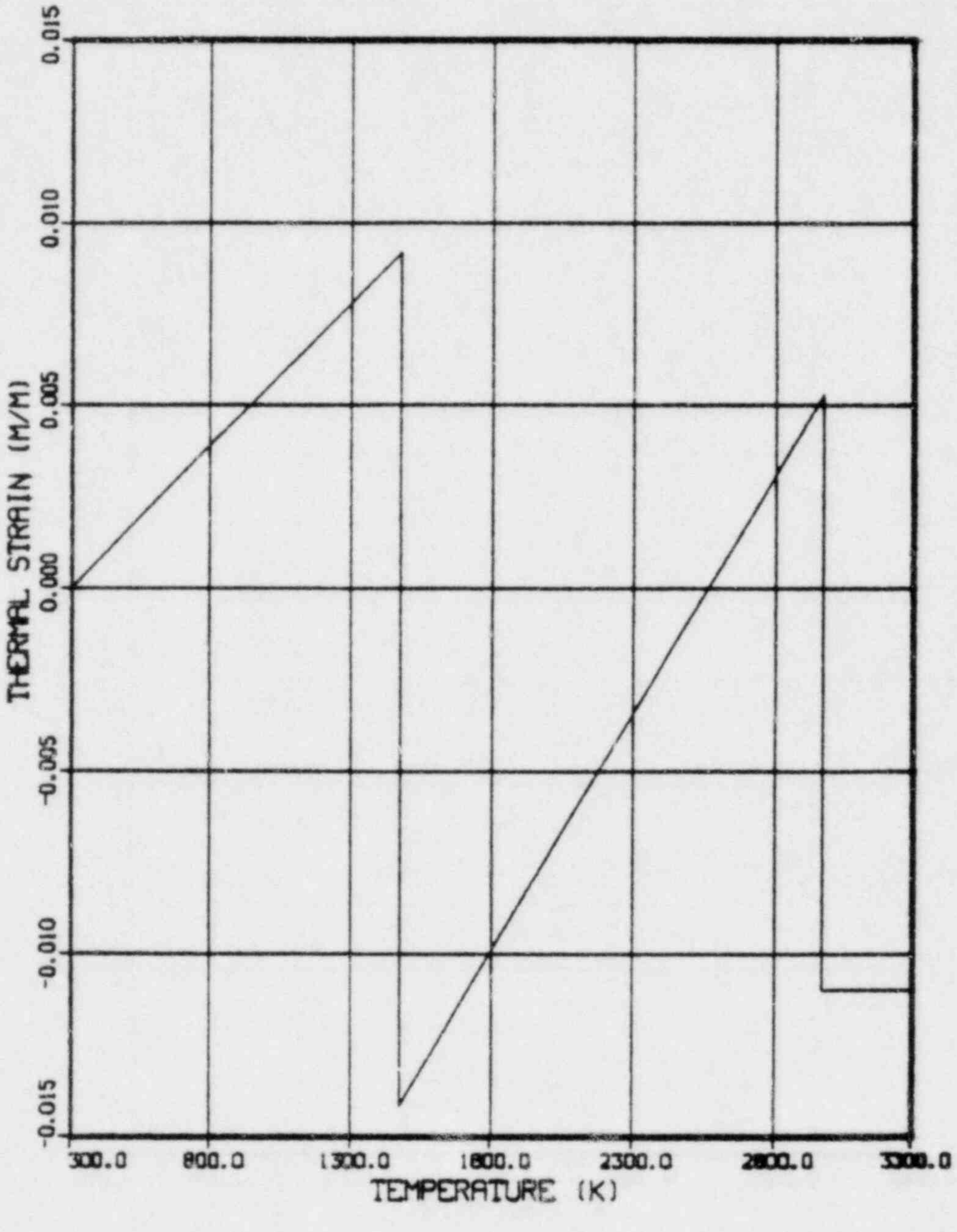

Figure B-10. Zircaloy oxide thermal strain.

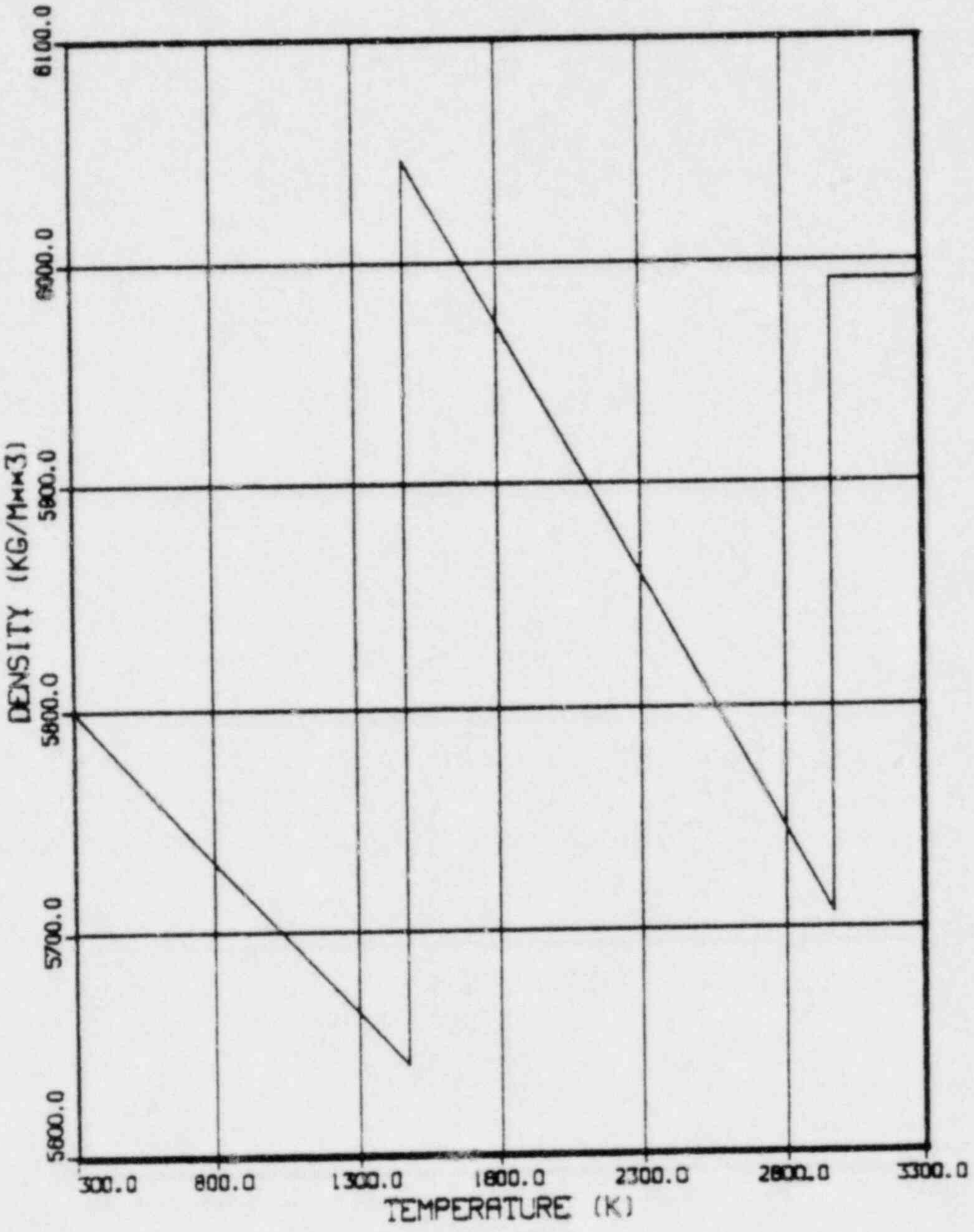

Figure B-11. Zircaloy oxide density as a function of temperature.

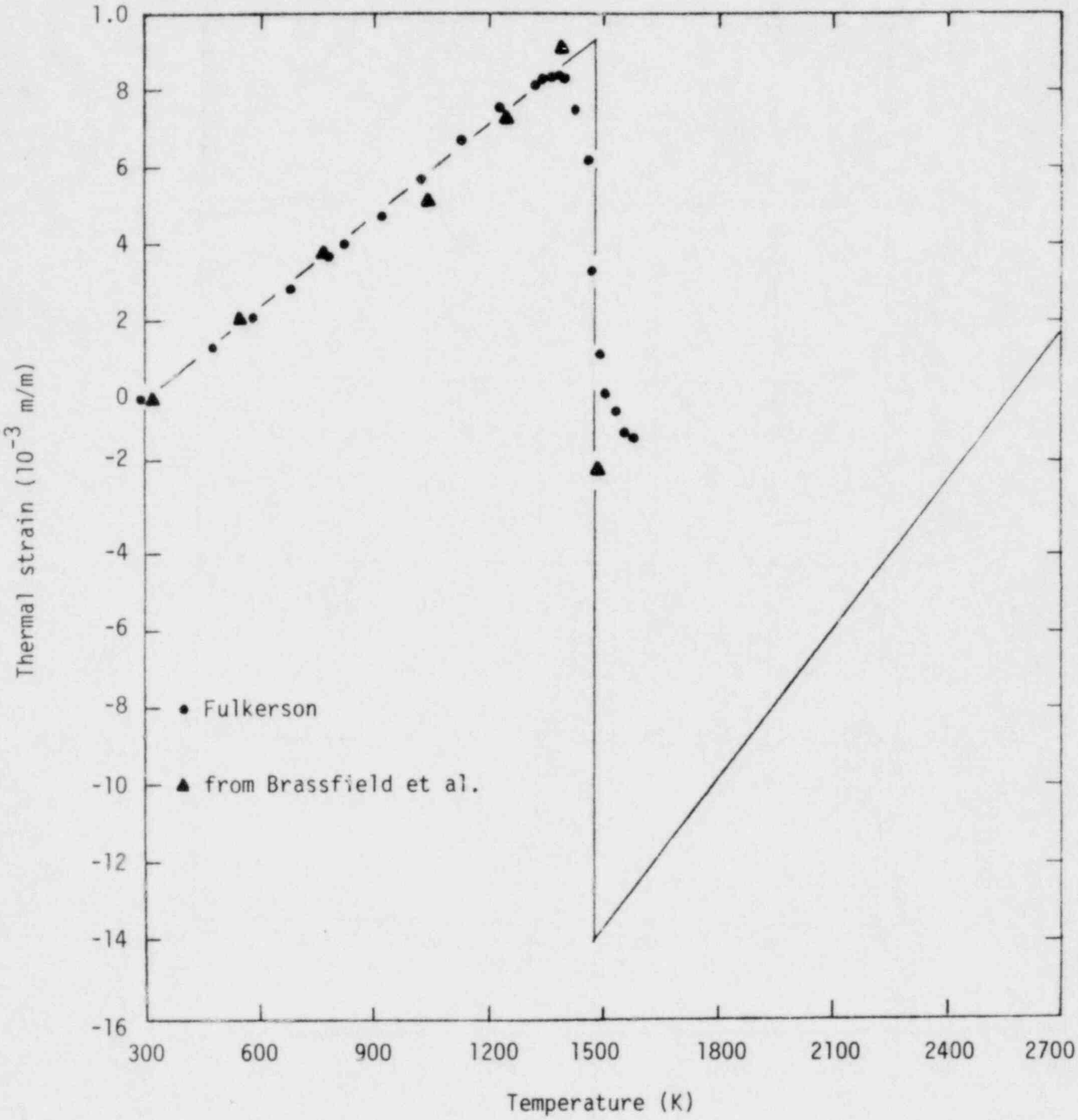

Figure B-12. Thermal strain data compared to code prediction.

TABLE B-18. ZIRCALOY DIOXIDE THERMAL EXPANSION DATA BY FULKERSON[B-11]

Temperature (K)	Thermal Strain (10^{-3} m/m)
289	0
473	1.34
571	2.05
673	2.82
773	3.64
818	4.02
922	4.78
1019	5.61
1119	6.63
1222	7.51
1308	8.06
1330	8.25
1349	8.33
1369	8.38
1390	8.34
1430	7.63
1450	6.10
1466	3.27
1487	1.16
1508	0.17
1529	-0.38
1550	-0.82
1571	-1.05

TABLE B-19. ZIRCALOY DIOXIDE THERMAL EXPANSION DATA FROM BRASSFIELD ET AL.[B-12]

Temperature (K)	Thermal Strain (10^{-3} m/m)
300	0
537	2.1
778	3.7
1031	5.05
1238	7.35
1383	9.10
1488	-1.8

CLADDING ELASTIC MODULI
(CELMOD, CSHEAR, CELAST, ZOEMOD, ZOPOIR)

The only change required to extend the MATPRO-11 Revision 2 zircaloy elastic moduli subcodes to high temperature is a logic branch that sets the moduli to zero (actually 1.0×10^{-10} is used to avoid dividing by zeros) above the melting temperature, 2098 K.

Young's modulus for zircaloy oxide is returned by the ZOEMOD function. Oxide temperature and oxide oxygen-to-metal ratio are the only required inputs. The function uses the following correlation to calculate the modulus for temperature between 300 and 1478 K (monoclinic phase):

$$Y_o = -3.77 \times 10^7 \, T + 1.637 \times 10^{11} \quad . \qquad \text{(B-14a)}$$

For temperatures in the range $1478 \leq T < T_{SOL}$ (tetragonal and cubic phase)

$$Y_o = -8.024 \times 10^7 T + 2.255 \times 10^{11} \quad . \qquad \text{(B-14b)}$$

For temperatures greater than T_{SOL}

$$Y_o = 1 \qquad \text{(B-14c)}$$

where

Y_o = zircaloy oxide Young's modulus (Pa)

T = oxide temperature (K)

T_{SOL} = zircaloy oxide solidus temperature (K). Obtained from the ZOPRP subroutine.

The equations are least squares fits to data from page 89 of Reference B-12. Table B-20 reproduces the data and Figure B-13 shows the data and values of Y_o calculated with the ZOEMOD function. The function sets Y_o = 1 Pa for temperatures above 2810 K where Equation (B-14b) would predict a negative modulus. Since so few data are available, a large expected standard error of ±0.2 times the predicted value is recommended.

ZOPOIR returns a constant value, 0.3, for the Poisson's ratio of solid zircaloy oxide and 0.5 for the ratio of liquid oxide. No data for these ratios have been found. The number 0.3 is merely typical of many solid materials and 0.5 is the constant-volume, isotropic material value of Poisson's ratio. The expected standard error is therefore large, ±0.2

Tables B-21 to B-25 are listings of the CELMOD, CSHEAR, CELAST, ZOEMOD and ZOPOIR subcodes. Figures B-14 to B-18 are plots of the quantities predicted by these subcodes. For CELAST the following typical texture coefficients were input:

COSTH2 = 0.71013
COSTH4 = 0.55578
COSFI2 = 0.69177
COSFI4 = 0.58836
CTSCF2 = 0.47126
CT2CF2 = 0.39473
CT4CF2 = 0.35503
CT4CF4 = 0.29320

CLADDING MECHANICAL LIMITS AND EMBRITTLEMENT
(ZORUP)

No modifications are required for the MATPRO-11 Revision 2 zircaloy cladding mechanical limits and embrittlement subcodes. The function ZORUP returns zircaloy oxide failure stress as a function of temperature.

The correlations used to calculate the oxide failure stress are listed below:

TABLE B-20. ZIRCALOY DIOXIDE MODULUS OF ELASTICITY DATA FROM BRASSFIELD ET AL.[B-12]

Temperature (K)	Elastic Modulus (10^{10} Pa)	Comment
1323	11.38	Monoclinic phase
1453	10.89	Monoclinic phase
1498	10.48	Tetragonal phase
1563	10.10	Tetragonal phase
1633	9.41	Tetragonal phase

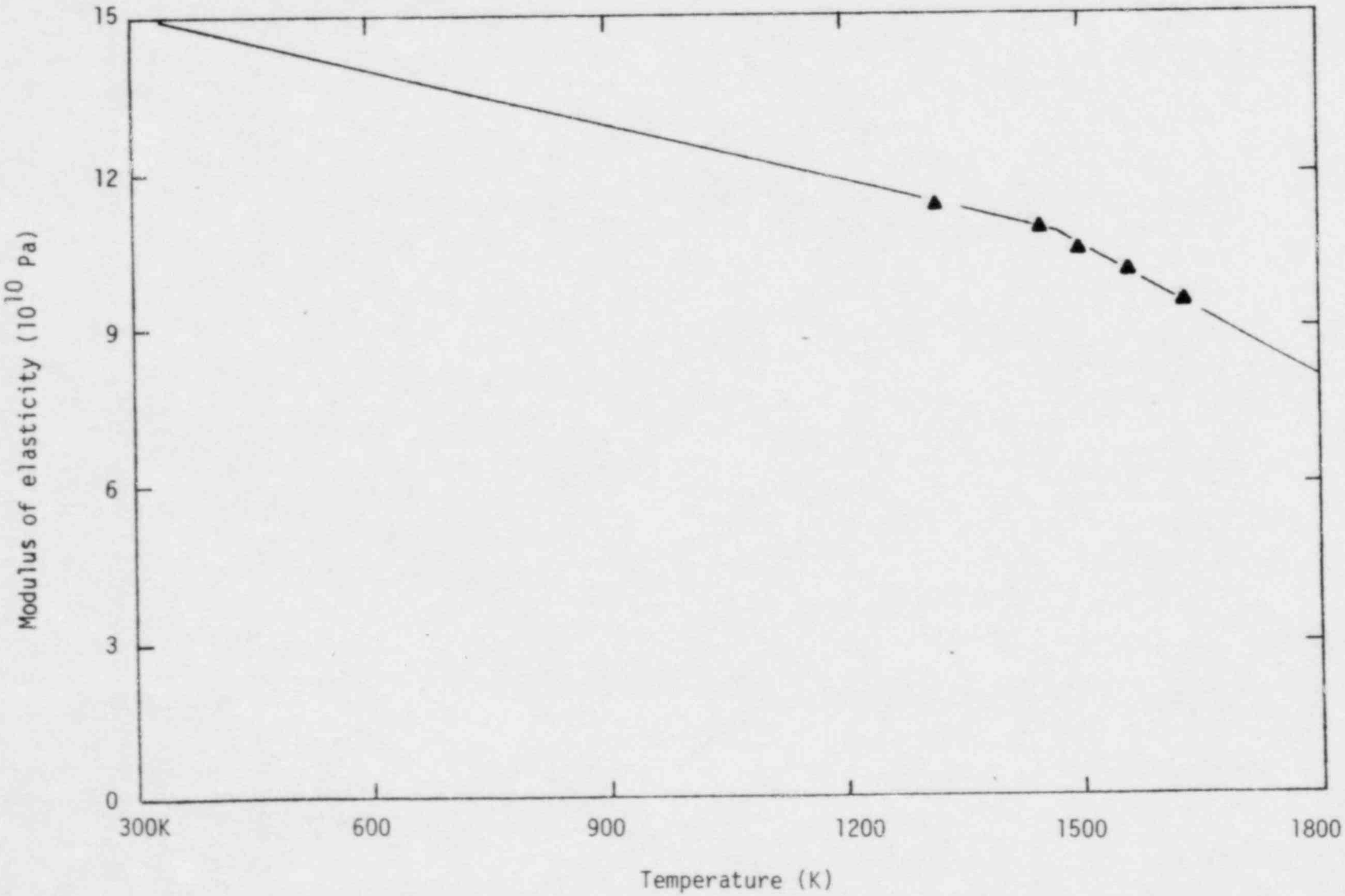

Figure B-13. Data and calculated values of Young's Modulus for Zircaloy oxide.

TABLE B-21. LISTING OF THE CELMOD FUNCTION

```
      FUNCTION CELMOD (CTEMP, FNCK, CWKF, DELOXY)
C
C     CELMOD CALCULATES CLADDING YOUNG'S MODULUS AS A FUNCTION
C     OF TEMPERATURE, FAST NEUTRON FLUENCE, COLD WORK, AND AVERAGE
C     OXYGEN CONCENTRATION.  GRAIN ORIENTATION IS ASSUMED RANDOM.
C     THE EXPECTED STANDARD ERROR IS COMPUTED BUT NOT RETURNED
C     (UCELMD).
C
C     CELMOD = OUTPUT YOUNG'S MODULUS FOR ZIRCALOY 2 AND 4
C              WITH RANDOM TEXTURE (PA)
C     UCELMD = OUTPUT STANDARD ERROR EXPECTED IN CELMOD (PA)
C                 (NOT CURRENTLY RETURNED)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C     FNCK   = INPUT EFFECTIVE FAST FLUENCE (NEUTRONS/(M**2))
C     CWKF   = INPUT EFFECTIVE COLD WORK (UNITLESS RATIO OF AREAS)
C     DELOXY = INPUT AVERAGE OXYGEN CONCENTRATION EXCLUDING
C              OXIDE LAYER - AVERAGE OXYGEN CONCENTRATION OF
C              AS-RECEIVED CLADDING  (KG OXYGEN/KG ZIRCALOY)
C
C     THE YOUNG'S MODULUS CALCULATED BY THIS FUNCTION IS BASED ON
C     DATA FROM THE FOLLOWING REFERENCES
C     (1) L. R. BUNNELL, G. B. MELLINGER  AND J. L. BATES, HIGH
C         TEMPERATURE PROPERTIES OF ZIRCALOY - OXYGEN ALLOYS, EPRI
C         REPORT NP - 524 (1977).
C     (2) E. S. FISHER AND C. J. RENKEN, PHYSICAL REVIEW 135 2A
C         (20 JULY 1964) PP A482 - 494.
C     (3) P. E. ARMSTRONG AND H. L. BROWN, TRANSACTIONS OF THE
C         METALLURGICAL SOCIETY OF AIME 230 (AUGUST 1964)
C         PP 962 - 966
C     (4) A. PADEL AND A. GROFF, JOURNAL OF NUCLEAR MATERIALS 59
C         (1976) PP 325-326
C     (5) W. R. SMALLEY, SAXTON CORE II FUEL PERFORMANCE EVALUATION.
C         PART I: MATERIALS, WCAP-3385-56 (SEPTEMBER 1971)
C
C     THE EXPECTED STANDARD ERROR WAS DERIVED USING ADDITIONAL
C     DATA FROM THE FOLLOWING REFERENCES
C     (1) C. C. BUSBY AND C.R. WOODS (EDS.) "PROPERTIES OF ZIRCALOY-4
C         TUBING", USAEC REPORT WAPD-TM-585 (DECEMBER 1966) P 65
C     (2) Z. SPASIC, M. PAVLOVIC AND G. SIMIS, CONFERENCE ON
C         THE USE OF ZIRCONIUM ALLOYS IN NUCLEAR REACTORS, MARIANSKE
C         LANZE, CZECH. CONF-681086 (1968) PP 277 - 284
C     (3) R. L. MEHAN, MODULUS OF ELASTICITY OF ZIRCALOY-2 BETWEEN
C         ROOM TEMPERATURE AND 1000 F, KAPL-M-RLM-16 (JULY 1958)
C     (4) D. O. NORTHWOOD, I. M LONDON, AND L. E. BAHEN, JOURNAL
C         OF NUCLEAR MATERIALS 55 (1975) PP 299-310
C     (5) F. R. SHOBER, J. A. VAN ECHO, L. L. MARSH JR. AND
C         J. R. KEELER, THE MECHANICAL PROPERTIES OF ZIRCONIUM  AND
C         ZIRCALOY-2, BMI-1168 (1957)
C
C     CELMOD WAS CODED BY R. L. MILLER IN MARCH 1974.
C     LAST MODIFIED BY D. L. HAGRMAN MARCH 1982
C
```

```
C
      IF(CTEMP .LT. 2098.) THEN
C
      C1 = (1.16E+11 + CTEMP*1.037E+08) * 5.7015
      C2 = 1.0
      IF(FNCK .GT. 1.0E+22) C2 = 0.88*(1.0 - EXP(-FNCK/1.0E+25))
     #                           + EXP(-FNCK/1.0E+25)
      C3 = -2.6E+10
      CELMOD = (1.088E+11 - 5.475E+07*CTEMP + C1*DELOXY + C3*CWKF)/C2
      IF(CTEMP .LT. 1090. ) GO TO 101
C
C     CALCULATE A TO A + B AND A + B TO B BOUNDARIES
      WFOX = DELOXY + 0.0012
      TAAB = 1094. + WFOX * (-1.289E+03 + WFOX * 7.914E+05)
      IF ( WFOX .LT. 0.025) GO TO 15
      TAAB = 1556.4 + 3.8281E+04 * (WFOX - 0.025)
   15 TABB = 392.46 * ((100*DELOXY + 0.1242807)**2 + 3.1417)
      IF (DELOXY .LT. 4.7308937E-03) GO TO 25
      TABB = (100 * DELOXY + 0.12) * 491.157 + 1081.7413
   25 CONTINUE
C
      IF (CTEMP .LT. TAAB) GO TO 101
      IF (CTEMP .GT. TABB) GO TO 35
      AMODL  = (1.088E+11 - 5.475E+07*TAAB + C1*DELOXY + C3*CWKF )/C2
      AMODR  = 9.21E+10 - TABB * 4.05E+07
      CELMOD = AMODL + (CTEMP - TAAB ) * (AMODR - AMODL )/(TABB - TAAB)
      GO TO 101
   35 CELMOD = 9.21E+10 - CTEMP * 4.05E+07
  101 CONTINUE
C
      ELSE
         CELMOD = 1.0E-10
      ENDIF
      UCELMD = 6.4E+09
C
      RETURN
      END
```

TABLE B-22. LISTING OF THE CSHEAR FUNCTION

```
      FUNCTION CSHEAR (CTEMP, FNCK, CWKF, DELOXY)
C
C     CSHEAR CALCULATES THE SHEAR MODULUS OF ZIRCALOY-2 AND -4
C     AS A FUNCTION OF TEMPERATURE, FAST NEUTRON FLUENCE,
C     COLD WORK, AND AVERAGE OXYGEN CONCENTRATION.  GRAIN
C     ORIENTATION IS ASSUMED RANDOM.
C     THE EXPECTED STANDARD ERROR IS COMPUTED BUT NOT RETURNED
C     (UCSHER)
C
C     CSHEAR = OUTPUT SHEAR MODULUS FOR ZIRCALOY-2 AND -4
C              WITH RANDOM TEXTURE (PA)
C     UCSHER = OUTPUT STANDARD ERROR EXPECTED IN CSHEAR (PA)
C                (NOT CURRENTLY RETURNED)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C     FNCK   = INPUT EFFECTIVE FAST FLUENCE (NEUTRONS/(M**2))
C     CWKF   = INPUT EFFECTIVE COLD WORK (UNITLESS RATIO OF AREAS)
C     DELOXY = INPUT AVERAGE OXYGEN CONCENTRATION EXCLUDING
C              OXIDE LAYER - AVERAGE OXYGEN CONCENTRATION OF
C              AS-RECEIVED CLADDING  (KG OXYGEN/KG ZIRCALOY)
C
C     THE SHEAR MODULUS CALCULATED BY THIS FUNCTION IS BASED ON
C     DATA FROM THE FOLLOWING REFERENCES
C
C     (1) L. R. BUNNELL, G. B. MELLINGER  AND J. L. BATES, HIGH
C         TEMPERATURE PROPERTIES OF ZIRCALOY - OXYGEN ALLOYS, EPRI
C         REPORT NP - 524 (1977)
C     (2) E. S. FISHER AND C. J. RENKEN, PHYSICAL REVIEW 135 2A
C         (20 JULY 1964) PP A482 - 494.
C     (3) P. E. ARMSTRONG AND H. L. BROWN, TRANSACTIONS OF THE
C         METALLURGICAL SOCIETY OF AIME 230 (AUGUST 1964)
C         PP 962 - 966
C     (4) A. PADEL AND A. GROFF, JOURNAL OF NUCLEAR MATERIALS 59
C         (1976) PP 325 - 326.
C     (5) W. R. SMALLEY, SAXTON CORE II FUEL PERFORMANCE EVALUATION.
C         PART I: MATERIALS. WCAP-3385-56 (SEPTEMBER 1971)
C
C     CSHEAR WAS CODED BY R. L. MILLER, JUNE 1974
C     MODIFIED BY D. L. HAGRMAN DECEMBER 1977
C
      C1 = 7.07E+11 - CTEMP * 2.315E+08
      C2 = 1.0
      IF(FNCK .GT. 1.0E+22) C2 = 0.88*(1.0 - EXP(-FNCK/1.0E+25))
     #                         + EXP(-FNCK/1.0E+25)
      C3 = -.867E+10
      CSHEAR = (4.04E+10-2.168E+07*CTEMP + C1*DELOXY + C3*CWKF)/C2
      IF(CTEMP .LT. 1090. ) GO TO 101
C
C     CALCULATE A TO A + B AND A + B TO B BOUNDARIES
      WFOX = DELOXY + 0.0012
      TAAB = 1094. + WFOX * (-1.289E+03 + WFOX * 7.914E+05)
      IF ( WFOX .LT. 0.025) GO TO 15
      TAAB = 1556.4 + 3.8281E+04*(WFOX - 0.025)
```

TABLE B-22. (continued)

```
   15 TABB = 392.46 * ((100*DELOXY + 0.1242807)**2 + 3.1417)
      IF (DELOXY .LT. 4.7308937E-03) GO TO 25
      TABB = (100*DELOXY + 0.12) * 491.157 + 1081.7413
   25 CONTINUE
C
      IF (CTEMP .LT. TAAB) GO TO 101
      IF (CTEMP .GT. TABB) GO TO  35
      AMODL  = (4.04E+10-2.168E+07*TAAB  + C1*DELOXY + C3*CWKF)/C2
      AMODR  = 3.49E+10 - TABB * 1.66E+07
      CSHEAR = AMODL + (CTEMP - TAAB ) * (AMODR - AMODL )/(TABB - TAAB)
      GO TO 101
   35 CSHEAR = 3.49E+10 - CTEMP*1.66E+07
  101 CONTINUE
      IF(CSHEAR .LT. 1.0 ) CSHEAR = 1.0
      UCSHER = 9.0E+09
C
      RETURN
      END
```

TABLE B-23. LISTING OF THE CELAST SUBROUTINE

```
      SUBROUTINE CELAST (COSTH2,COSTH4,COSFI2,COSFI4,CT2CF2,CT2CF4,
     #                   CT4CF2,CT4CF4,CTEMP,FNCK,CWKF,DELOXY,CRS)
C
      DIMENSION CC(12),CS(12),CRS(9)
C
C     CELAST CALCULATES ELASTIC COMPLIANCE CONSTANTS OF ZIRCALOY
C     FROM ORIENTATION PARAMETERS.
C
C     IN THE FOLLOWING, THETA IS THE ANGLE BETWEEN THE RADIAL
C     OR NORMAL DIRECTION OF THE SAMPLE AND THE BASAL POLE
C     DIRECTION. PHI IS THE ANGLE BETWEEN THE PROJECTION OF THE
C     BASAL POLE DIRECTION ONTO THE PLANE CONTAINING THE AXIAL
C     AND CIRCUMFERENTIAL DIRECTIONS AND THE CIRCUMFERENTIAL
C     DIRECTION. ALPHA IS THE COMPLEMENT OF PHI.
C
C     CRS(I) = OUTPUT ELASTIC COMPLIANCE CONSTANTS (1/PA).  S MATRIX
C              ELEMENTS ARE
C
C                ( CRS(1)  CRS(7)  CRS(9)    0       0       0     )
C
C                ( CRS(7)  CRS(2)  CRS(8)    0       0       0     )
C
C                ( CRS(9)  CRS(8)  CRS(3)    0       0       0     )
C
C                (   0       0       0     CRS(4)    0       0     )
C
C                (   0       0       0       0     CRS(5)    0     )
C
C                (   0       0       0       0       0     CRS(6)  )
C
C              WHERE DIRECTION 1 IS CIRCUMFERENTIAL OR TRANSVERSE
C                              2 IS AXIAL OR LONGITUDINAL
C                              3 IS RADIAL OR NORMAL
C
C     COSTH2 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE SQUARED
C              COSINE OF THETA (UNITLESS)
C     COSTH4 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE
C              FOURTH POWER OF THE COSINE OF THETA (UNITLESS)
C     COSFI2 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE SQUARED
C              COSINE OF ALPHA (UNITLESS RATIO)
C     COSFI4 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE
C              FOURTH POWER OF THE COSINE OF ALPHA (UNITLESS)
C     CT2CF2 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE PRODUCT
C              OF THE SQUARED COSINE OF THETA AND THE SQUARED COSINE
C              OF ALPHA (UNITLESS)
C     CT2CF4 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE PRODUCT
C              OF THE SQUARED COSINE OF THETA AND THE FOURTH POWER OF
C              THE COSINE OF ALPHA (UNITLESS)
C     CT4CF2 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE PRODUCT
C              OF THE FOURTH POWER OF THE COSINE OF THETA AND THE
C              SQUARED COSINE OF ALPHA (UNITLESS)
C     CT4CF4 = INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE PRODUCT
```

TABLE B-23. (continued)

```
C                 OF THE FOURTH POWER OF THE COSINE OF THETA AND THE
C                 FOURTH POWER OF THE COSINE OF ALPHA (UNITLESS)
C       CTEMP   = INPUT CLADDING TEMPERATURE (K)
C       FNCK    = INPUT EFFECTIVE FAST FLUENCE (NEUTRONS/(M**2))
C       CWKF    = INPUT EFFECTIVE COLD WORK (UNITLESS RATIO OF AREAS)
C       DELOXY  = INPUT AVERAGE OXYGEN CONCENTRATION EXCLUDING
C                 OXIDE LAYER - AVERAGE OXYGEN CONCENTRATION OF
C                 AS RECEIVED CLADDING  (KG OXYGEN/KG ZIRCALOY)
C
C       THE ELASTIC COMPLIANCE CONSTANTS ARE BASED ON DATA FROM
C       (1) L. R. BUNNELL, G. B. MELLINGER  AND J. L. BATES, HIGH
C           TEMPERATURE PROPERTIES OF ZIRCALOY - OXYGEN ALLOYS, EPRI
C           REPORT NP - 524 (1977)
C       (2) E. S. FISHER AND C. J. RENKEN, PHYSICAL REVIEW 135 2A
C           (20 JULY,1964)  PP A482 - 494.
C       (3) P. E. ARMSTRONG AND H. L. BROWN, TRANSACTIONS OF THE
C           METALLURGICAL SOCIETY OF AIME 230 (AUGUST 1964)
C           PP 962 - 966
C       (4) A. PADEL AND A. GROFF, JOURNAL OF NUCLEAR MATERIALS 59
C           (1976) PP 325 - 326
C       (5) W. R. SMALLEY, SAXTON CORE II FUEL PERFORMANCE EVALUATION.
C           PART I: MATERIALS, WCAP-3385-56 (SEPTEMBER 1971)
C
C       CELAST WAS CODED BY D. L. HAGRMAN IN DECEMBER 1977
C       LAST MODIFIED BY D. L. HAGRMAN MARCH 1982
C
        IF(CTEMP .LT. 2098.) THEN
C
        CC(1) = 1.562E+11- 4.464E+07*CTEMP
        CC(2) = 1.746E+11- 3.262E+07*CTEMP
        CC(3) = 3.565E+10- 1.281E+07*CTEMP
        CC(5) = 6.448E+10+ CTEMP*(3.[illegible]882E+07- CTEMP*1.2318E+04)
        CC(6) = 6.516E+10- 6.817E+06*CTEMP
        IF( CC(1)  .LT. (0.999*CC(5)).) CC(5) = 0.999*CC(1)
        CC(4) = (CC(1) - CC(5))/2.
        FACTOR= (CC(1) - CC(5))*((CC(1) + CC(5))*CC(2) - 2*((CC(6)**2)))
        CS(1) = 0.102641E-10 + CTEMP * (-0.541683E-14 + CTEMP *
     *          0.147552E-16)
        CS(2) = (CC(1) + CC(5))*(CC(1) - CC(5))/FACTOR
        CS(3) = 0.390354E-10+CTEMP * (-0.81186E-14+ CTEMP *
     *          0.211523E-16)
        CS(4) = 1.0/CC(4)
        CS(5) = ((CC(6))**2-(CC(5)*CC(2)))/FACTOR
        CS(6) = (CC(5) - CC(1))*CC(6)/FACTOR
        B     = (1.16E+11+ CTEMP*1.037E+08) * 5.7015
        BS    = (1.24E+11- CTEMP*0.406E+08) * 5.7015
        C2    = 1.0
        IF(FNCK .GT. 1.0E+22) C2 = 0.88*(1.0 - EXP(-FNCK/1.0E+25))
     *                              + EXP(-FNCK/1.0E+25)
        C3    = -2.6E+10
        CS(1) = C2/(1.0/CS(1) + B  * DELOXY + C3 * CWKF )
        CS(2) = C2/(1.0/CS(2) + B  * DELOXY + C3 * CWKF )
        CS(3) = C2/(1.0/CS(3) + BS * DELOXY )
```

```
      CS(5) = C2/(1.0/CS(5) + B  * DELOXY + C3 * CWKF )
      CS(6) = C2/(1.0/CS(6) + B  * DELOXY + C3 * CWKF )
      IF( CS(1) .LT. (0.999*CS(5))) CS(5) = 0.999*CS(1)
      CS(4) = 2*(CS(1) - CS(5))
      CRS(1)    = (COSFI4-2*CT2CF4+CT4CF4+2*CT2CF2-2*CT4CF2+COSTH4)*CS(1)
     # + (1.0 -2*COSFI2 + COSFI4 -2*COSTH2 +4*CT2CF2-2*CT2CF4
     # + COSTH4 - 2*CT4CF2 + CT4CF4) * CS(2) +  (-COSFI4 + 2*CT2CF4
     # - CT4CF4 + COSFI2 - 3*CT2CF2 +2*CT4CF2 + COSTH2 - COSTH4 )
     # * ( 2* CS(6) + CS(3) )
      CRS(2)    = (COSFI4-2*CT2CF4+CT4CF4-2*COSFI2+2*CT2CF2+1.0)*CS(1)
     # + (COSFI4 - 2*CT2CF4 + CT4CF4 )*CS(2) + (COSFI2 - COSFI4
     # + 2*CT2CF4 - CT2CF2 - CT4CF4) * (2*CS(6) + CS(3))
      CRS(3)    = (1.0 - 2*COSTH2 + COSTH4) * CS(1)
     # +(COSTH2 - COSTH4)* (2*CS(6) + CS(3)) + COSTH4 * CS(2)
      CRS(4)    =  ( 2 * (1.0 - COSTH2 - COSFI2) + 6 *  CT2CF2
     # -4 * CT4CF2 ) *CS(1) + 4 * ( CT2CF2 - CT4CF2 ) * CS(2)
     # + ( COSTH2 + COSFI2 - 5 * CT2CF2 + 4 * CT4CF2 ) * CS(3)
     # + 2 * (-1.0 + COSTH2 + COSFI2 - CT2CF2 ) * CS(5)
     # + 8 * (-CT2CF2 + CT4CF2 ) * CS(6)
      CRS(5)    = (COSTH2 - COSTH4 + 0.5*COSFI2 - 1.5*CT2CF2 + CT4CF2) *
     # CS(1) +  (COSTH2 - COSTH4 - CT2CF2 + CT4CF2 ) * CS(2)  +
     # (1.0 - 4*COSTH2 + 4*COSTH4 - COSFI2 + 5*CT2CF2 - 4*CT4CF2)*0.25*
     # CS(3) - 0.5*(COSFI2 - CT2CF2)*CS(5) - 2*(COSTH2 - COSTH4 -CT2CF2
     # +CT4CF2 )*CS(6)
      CRS(5)    =  4.0 * CRS(5)
      CRS(6)    = (0.5*COSTH2 + COSFI2 - COSFI4 - 2*CT2CF2 + 2*CT2CF4 +
     # CT4CF2 - CT4CF4) * CS(1) + (COSFI2 - COSFI4 - 2*CT2CF2 +2*CT2CF4+
     # CT4CF2 - CT4CF4) * CS(2) + (1.0 - 4*COSFI2 + 4*COSFI4 - COSTH2 +
     # 8*CT2CF2 - 8*CT2CF4 - 4*CT4CF2 + 4*CT4CF4 ) * 0.25*CS(3) -
     # 0.5*COSTH2 * CS(5) -2.0 * (COSFI2 - COSFI4 - 2*CT2CF2 +
     # 2 * CT2CF4 + CT4CF2 - CT4CF4 ) * CS(6)
      CRS(6)    =  4.0 * CRS(6)
      CRS(7)    = (COSFI2 - COSFI4 - 2*CT2CF2 + 2*CT2CF4 + CT4CF2
     # - CT4CF4) * CS(1) + (COSFI2 - COSFI4 -2*CT2CF2 + 2*CT2CF4
     # + CT4CF2 - CT4CF4) * ( CS(2) - CS(3) ) + COSTH2 * CS(5)
     # + ( 1.0 - COSTH2 - 2*COSFI2 + 2*COSFI4 + 4*CT2CF2 - 4*CT2CF4
     # - 2*CT4CF2 + 2*CT4CF4) * CS(6)
      CRS(8)    = (CT2CF2 - CT4CF2) * ( CS(1) + CS(2) - CS(3) ) +
     # (1.0 - COSTH2 - COSFI2+ CT2CF2) * CS(5) + ( COSTH2 + COSFI2
     # - 3*CT2CF2 + 2*CT4CF2 ) * CS(6)
      CRS(9)    = (COSTH2 - COSTH4 - CT2CF2 + CT4CF2) * ( CS(1) +
     # CS(2) - CS(3) ) + (COSFI2 - CT2CF2) * CS(5) + (1.0 - 2*COSTH2
     # +2*COSTH4 - COSFI2 + 3*CT2CF2 - 2*CT4CF2) * CS(6)
      IF(CTEMP .LT. 1090. ) GO TO 101
C
C     CALCULATE A TO A + B AND A + B TO B BOUNDARIES
      WFOX = DELOXY + 0.0012
      TAAB = 1094. + WFOX * (-1.289E+03 + WFOX * 7.914E+05)
      IF ( WFOX .LT. 0.025) GO TO 15
      TAAB = 1556.4 + 3.8281E+04*(WFOX - 0.025)
   15 TABB = 392.46*((100*DELOXY + 0.1242807)**2 + 3.1417)
      IF (DELOXY .LT. 4.7308937E-03) GO TO 25
      TABB = (100*DELOXY + 0.12) * 491.157 + 1081.7413
```

TABLE B-23. (continued)

```
   25 CONTINUE
C
      IF (CTEMP .LT. TAAB) GO TO 101
      IF (CTEMP .GT. TABB) GO TO 35
      CC(7) = 1.562E+11- 4.484E+07*TAAB
      CC(8) = 1.746E+11- 3.282E+07*TAAB
      CC(9) = 3.565E+10- 1.281E+07*TAAB
      CC(11)= 6.446E+10+ TAAB *(3.1882E+07- TAAB *1.2318E+04)
      CC(12)= 6.518E+10- 6.817E+06*TAAB
      IF( CC(7) .LT. (0.999*CC(11))) CC(11) = 0.999*CC(7)
      FXCTOR= (CC(7) -CC(11))*((CC(7) +CC(11))*CC(8) -2*((CC(12)**2)))
      CS(7) = 0.102841E-10 + TAAB  * (-0.541663E-14 + TAAB  *
     *        0.147552E-16 )
      CS(8) = (CC(7) +CC(11))*(CC(7) -CC(11))/FXCTOR
      CS(9) = 0.390354E-10+TAAB  * (-0.61186E-14+ TAAB  *
     *        0.211523E-16)
      CS(11)=((CC(12))**2-(CC(11)*CC(8)))/FXCTOR
      CS(12)=(CC(11) -CC(7))*CC(12)/FXCTOR
      BT     =(1.16E+11+ TAAB *1.037E+08) * 5.7015
      BST    =(1.24E+11- TAAB *0.406E+08) * 5.7015
      CS(7) = C2/(1.0/CS(7) + BT * DELOXY + C3 * CWKF )
      CS(8) = C2/(1.0/CS(8) + BT * DELOXY + C3 * CWKF )
      CS(9) = C2/(1.0/CS(9) + BST* DELOXY )
      CS(11)= C2/(1.0/CS(11)+ BT * DELOXY + C3 * CWKF )
      CS(12)= C2/(1.0/CS(12)+ BT * DELOXY + C3 * CWKF )
      IF( CS(7) .LT. (0.999*CS(11))) CS(11) = 0.999*CS(7)
      CS(10)= 2*(CS(7) - CS(11))
      CLS1      = (COSFI4-2*CT2CF4+CT4CF4+2*CT2CF2-2*CT4CF2+COSTH4)*CS(7)
     # + (1.0 -2*COSFI2 + COSFI4 -2*COSTH2 +4*CT2CF2-2*CT2CF4
     # + COSTH4 - 2*CT4CF2 + CT4CF4) * CS(8) +  (-COSFI4 + 2*CT2CF4
     # - CT4CF4 + COSFI2 - 3*CT2CF2 +2*CT4CF2 + COSTH2 - COSTH4 )
     # * ( 2* CS(12)+ CS(9) )
      CLS2      = (COSFI4-2*CT2CF4+CT4CF4-2*COSFI2+2*CT2CF2+1.0)*CS(7)
     # + (COSFI4 - 2*CT2CF4 + CT4CF4 )*CS(8) + (COSFI2 - COSFI4
     # + 2*CT2CF4 - CT2CF2 - CT4CF4) * (2*CS(12)+ CS(9))
      CLS3      = (1.0 - 2*COSTH2 + COSTH4) * CS(7)
     # +(COSTH2 - COSTH4)* (2*CS(12)+ CS(9)) + COSTH4 * CS(8)
      CLS4      =  ( 2 * (1.0 - COSTH2 - COSFI2) + 6 *  CT2CF2
     # -4 * CT4CF2 ) *CS(7) + 4 * ( CT2CF2 - CT4CF2 ) * CS(8)
     # + ( COSTH2 + COSFI2 - 5 * CT2CF2 + 4 * CT4CF2 ) * CS(9)
     # + 2 * (-1.0 + COSTH2 + COSFI2 - CT2CF2 ) * CS(11)
     # + 8 * (-CT2CF2 + CT4CF2 ) * CS(12)
      CLS5      = (COSTH2 - COSTH4 + 0.5*COSFI2 - 1.5*CT2CF2 + CT4CF2) *
     # CS(7) +  (COSTH2 - COSTH4 - CT2CF2 + CT4CF2 ) * CS(8)  +
     # (1.0 - 4*COSTH2 + 4*COSTH4 - COSFI2 + 5*CT2CF2 - 4*CT4CF2)*0.25*
     # CS(9) - 0.5*(COSFI2 - CT2CF2)*CS(11)- 2*(COSTH2 - COSTH4 -CT2CF2
     # +CT4CF2 )*CS(12)
      CLS5 = CLS5 * 4.0
      CLS6      = (0.5*COSTH2 + COSFI2 - COSFI4 - 2*CT2CF2 + 2*CT2CF4 +
     # CT4CF2 - CT4CF4) * CS(7) + (COSFI2 - COSFI4 - 2*CT2CF2 +2*CT2CF4+
     # CT4CF2 - CT4CF4) * CS(8) + (1.0 - 4*COSFI2 + 4*COSFI4 - COSTH2 +
     # 8*CT2CF2 - 8*CT2CF4 - 4*CT4CF2 + 4*CT4CF4 ) * 0.25*CS(9) -
     # 0.5*COSTH2 * CS(11)-2.0 * (COSFI2 - COSFI4 - 2*CT2CF2 +
```

TABLE B-23. (continued)

```
# 2 * CT2CF4 + CT4CF2 - CT4CF4 ) * CS(12)
  CLS6 = CLS6 * 4.0
  CLS7       = (COSFI2 - COSFI4 - 2*CT2CF2 + 2*CT2CF4 + CT4CF2
# - CT4CF4) * CS(7) + (COSFI2 - COSFI4 -2*CT2CF2 + 2*CT2CF4
# + CT4CF2 - CT4CF4) * ( CS(8) - CS(9) ) + COSTH2 * CS(11)
# + ( 1.0 - COSTH2 - 2*COSFI2 + 2*COSFI4 + 4*CT2CF2 - 4*CT2CF4
# - 2*CT4CF2 + 2*CT4CF4) * CS(12)
  CLS8       = (CT2CF2 - CT4CF2) * ( CS(7) + CS(8) - CS(9) ) +
# (1.0 - COSTH2 - COSFI2+ CT2CF2) * CS(11)+ ( COSTH2 + COSFI2
# - 3*CT2CF2 + 2*CT4CF2 ) * CS(12)
  CLS9       = (COSTH2 - COSTH4 - CT2CF2 + CT4CF2) * ( CS(7) +
# CS(8) - CS(9) ) + (COSFI2 - CT2CF2) * CS(11)+ (1.0 - 2*COSTH2
# +2*COSTH4 - COSFI2 + 3*CT2CF2 - 2*CT4CF2) * CS(12)
  CTS1 = 9.21E+10 - TABB * 4.05E+07
  CTS2 = CTS1
  CTS3 = CTS1
  CTS4 = 3.49E+10 - TABB * 1.66E+07
  CTS5 = CTS4
  CTS6 = CTS4
  CTS7 = (2*CTS4*CTS1)/(2*CTS4 - CTS1)
  CTS8 = CTS7
  CTS9 = CTS7
  CRS(1) = 1.0/((1.0/CLS1) + (CTEMP - TAAB) * (CTS1 - (1.0/CLS1))/
#          (TABB - TAAB))
  CRS(2) = 1.0/((1.0/CLS2) + (CTEMP - TAAB) * (CTS2 - (1.0/CLS2))/
#          (TABB - TAAB))
  CRS(3) = 1.0/((1.0/CLS3) + (CTEMP - TAAB) * (CTS3 - (1.0/CLS3))/
#          (TABB - TAAB))
  CRS(4) = 1.0/((1.0/CLS4) + (CTEMP - TAAB) * (CTS4 - (1.0/CLS4))/
#          (TABB - TAAB))
  CRS(5) = 1.0/((1.0/CLS5) + (CTEMP - TAAB) * (CTS5 - (1.0/CLS5))/
#          (TABB - TAAB))
  CRS(6) = 1.0/((1.0/CLS6) + (CTEMP - TAAB) * (CTS6 - (1.0/CLS6))/
#          (TABB - TAAB))
  CRS(7) = 1.0/((1.0/CLS7) + (CTEMP - TAAB) * (CTS7 - (1.0/CLS7))/
#          (TABB - TAAB))
  CRS(8) = 1.0/((1.0/CLS8) + (CTEMP - TAAB) * (CTS8 - (1.0/CLS8))/
#          (TABB - TAAB))
  CRS(9) = 1.0/((1.0/CLS9) + (CTEMP - TAAB) * (CTS9 - (1.0/CLS9))/
#          (TABB - TAAB))
  GO TO 101
C
 35 CRS(1) = 1.0/(9.21E+10 - CTEMP*4.05E+07)
    CRS(2) = CRS(1)
    CRS(3) = CRS(1)
    CRS(4) = 1.0/(3.49E+10 - CTEMP*1.66E+07)
    CRS(5) = CRS(4)
    CRS(6) = CRS(4)
    CRS(7) = CRS(1) - 0.5*CRS(4)
    CRS(8) = CRS(7)
    CRS(9) = CRS(7)
101 CONTINUE
    ELSE
       DO 50 I=1,9
 50 CRS(I) = 1.0E+10
    ENDIF
C
    RETURN
    END
```

TABLE B-24. LISTING OF THE ZOEMOD FUNCTION

```
      FUNCTION ZOEMOD(ZOTEMP,YE)
C
C     ZOEMOD RETURNS THE YOUNGS MODULUS OF ZIRCALOY OXIDE
C
C     ZOEMOD = OUTPUT ZIRCALOY OXIDE YOUNGS MODULUS (PA)
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C     YE     = INPUT OXYGEN-TO-METAL RATIO (ATOMS OXYGEN/
C              ATOMS METAL)
C
C     THE SUBROUTINE ZOPRP IS CALLED BY THIS FUNCTION
C
C     ZOEMOD WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ZOTEMP .LE. 1478.) THEN
         ZOEMOD = 1.637E+11 - ZOTEMP * 3.77E+07
      ELSE
         IF(ZOTEMP .LT. 2810.) THEN
            ZOEMOD = 2.255E+11 - ZOTEMP * 8.024E+07
         ELSE
            ZOEMOD = 1.0
         ENDIF
         CALL ZOPRP(YE,ZOSOL,ZOLIQ,ZOTC,ZOMT)
         IF(ZOTEMP .GE. ZOSOL) THEN
            ZOEMOD = 1.0
         ENDIF
      ENDIF
      RETURN
      END
```

TABLE B-25. LISTING OF THE ZOPOIR FUNCTION

```
      FUNCTION ZOPOIR(ZOTEMP,YE)
C
C     ZOPOIR RETURNS THE POISSINS RATIO OF ZIRCALOY OXIDE
C
C     ZOPOIR = OUTPUT ZIRCALOY CLADDING OXIDE POISSINS RATIO (M/M)
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C     YE     = INPUT OXYGEN-TO-METAL RATIO (ATOMS OXYGEN/
C              ATOMS METAL)
C
C     THE SUBROUTINE ZOPRP IS CALLED BY THIS FUNCTION
C
C     ZOPOIR WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      CALL ZOPRP(YE,ZOSOL,ZOLIQ,ZOTC,ZOMT)
      IF(ZOTEMP .LE. ZOSOL) THEN
         ZOPOIR = 0.3
      ELSE
         ZOPOIR = 0.5
      ENDIF
      RETURN
      END
```

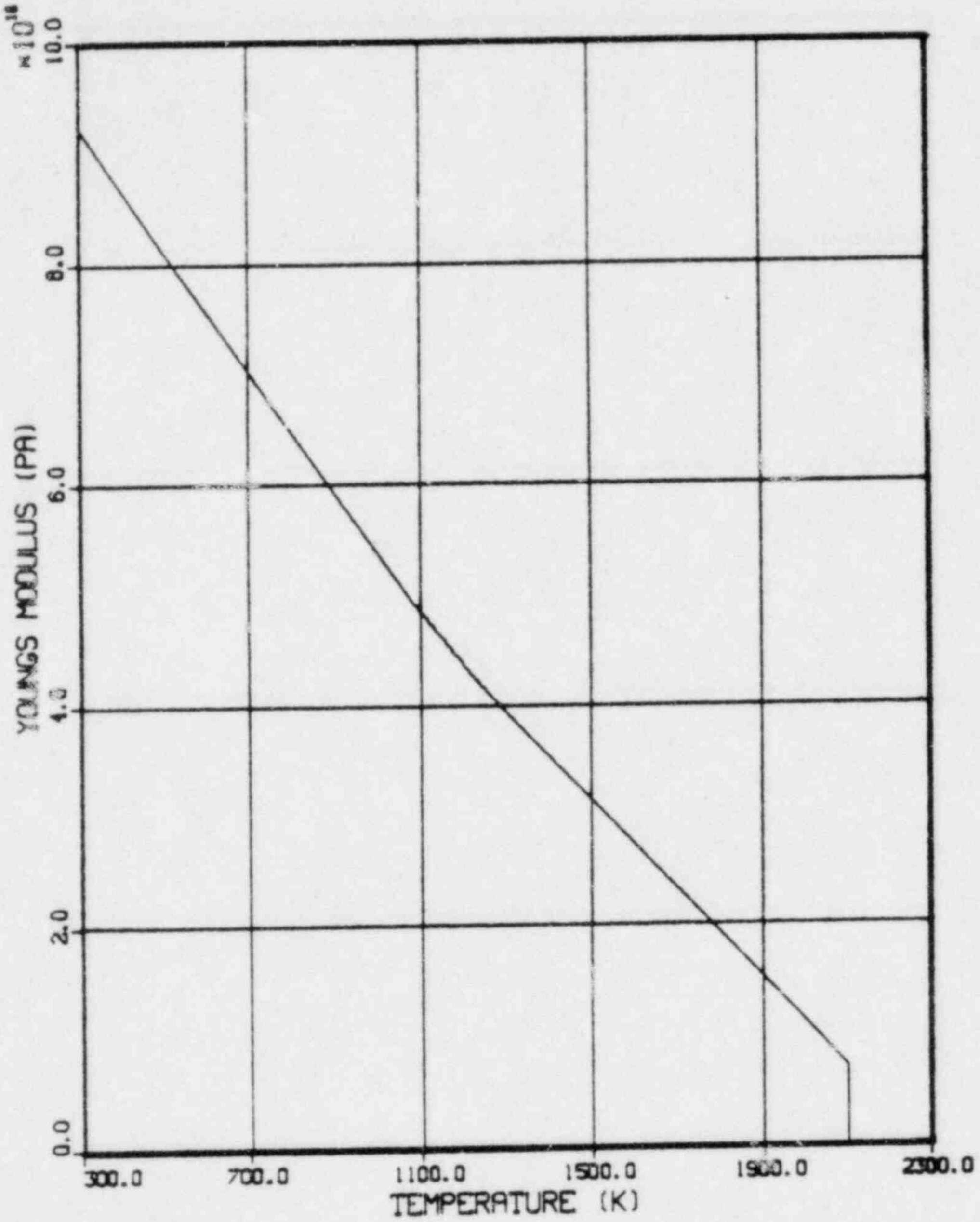

Figure B-14. Zircaloy Young's modulus for random texture.

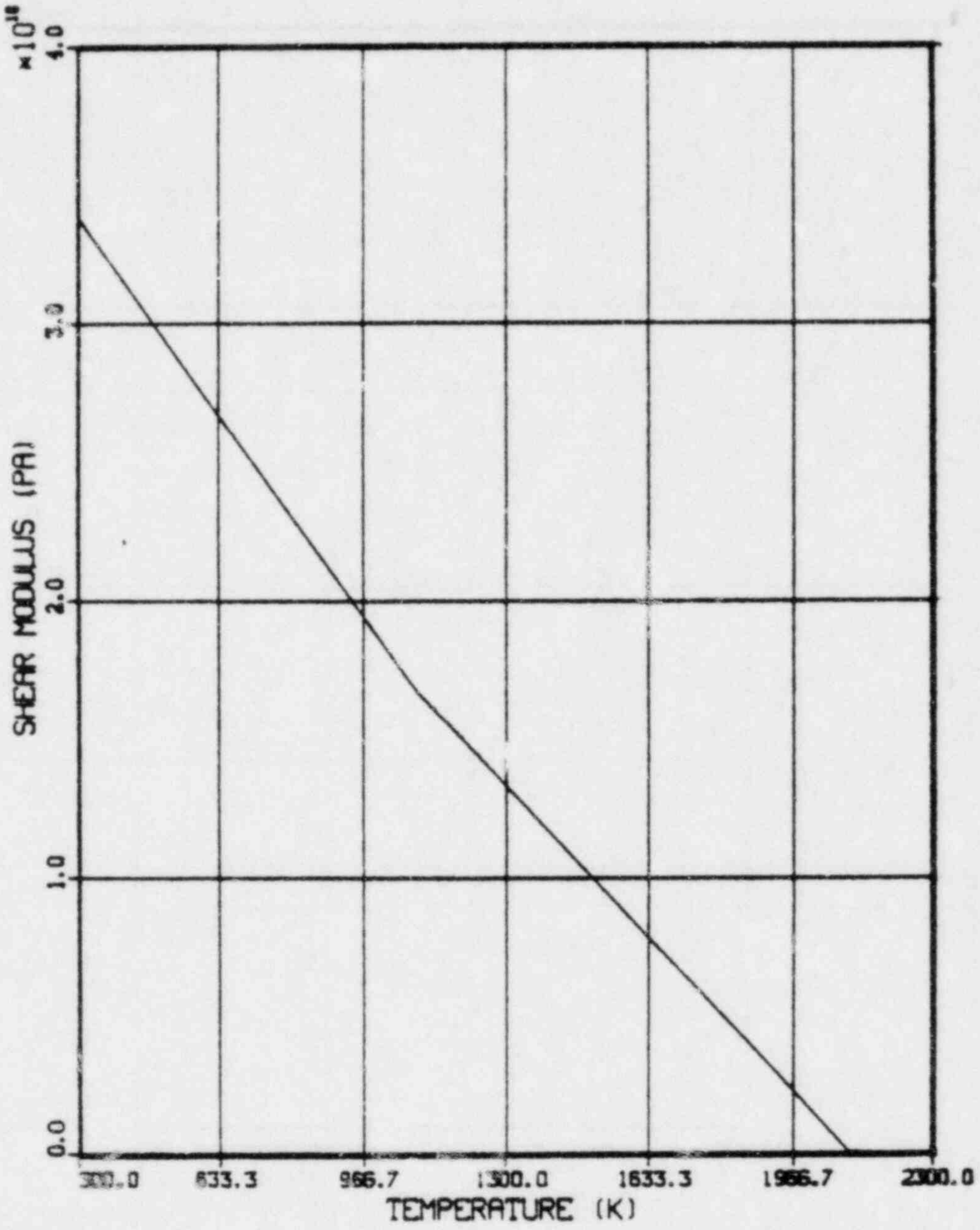

Figure B-15. Zircaloy shear modulus for random texture.

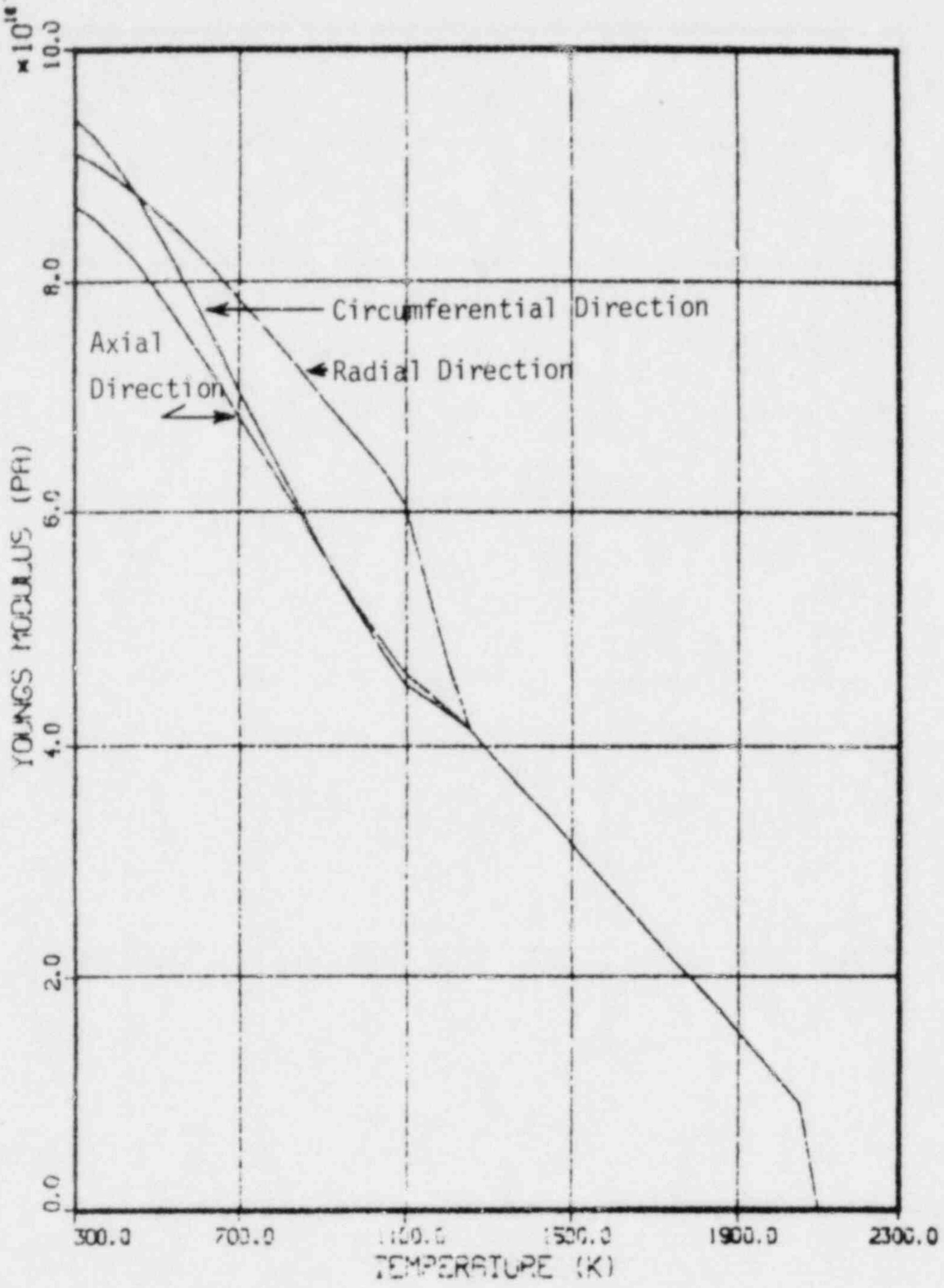

Figure B-16. Young's moduli for typical cladding texture.

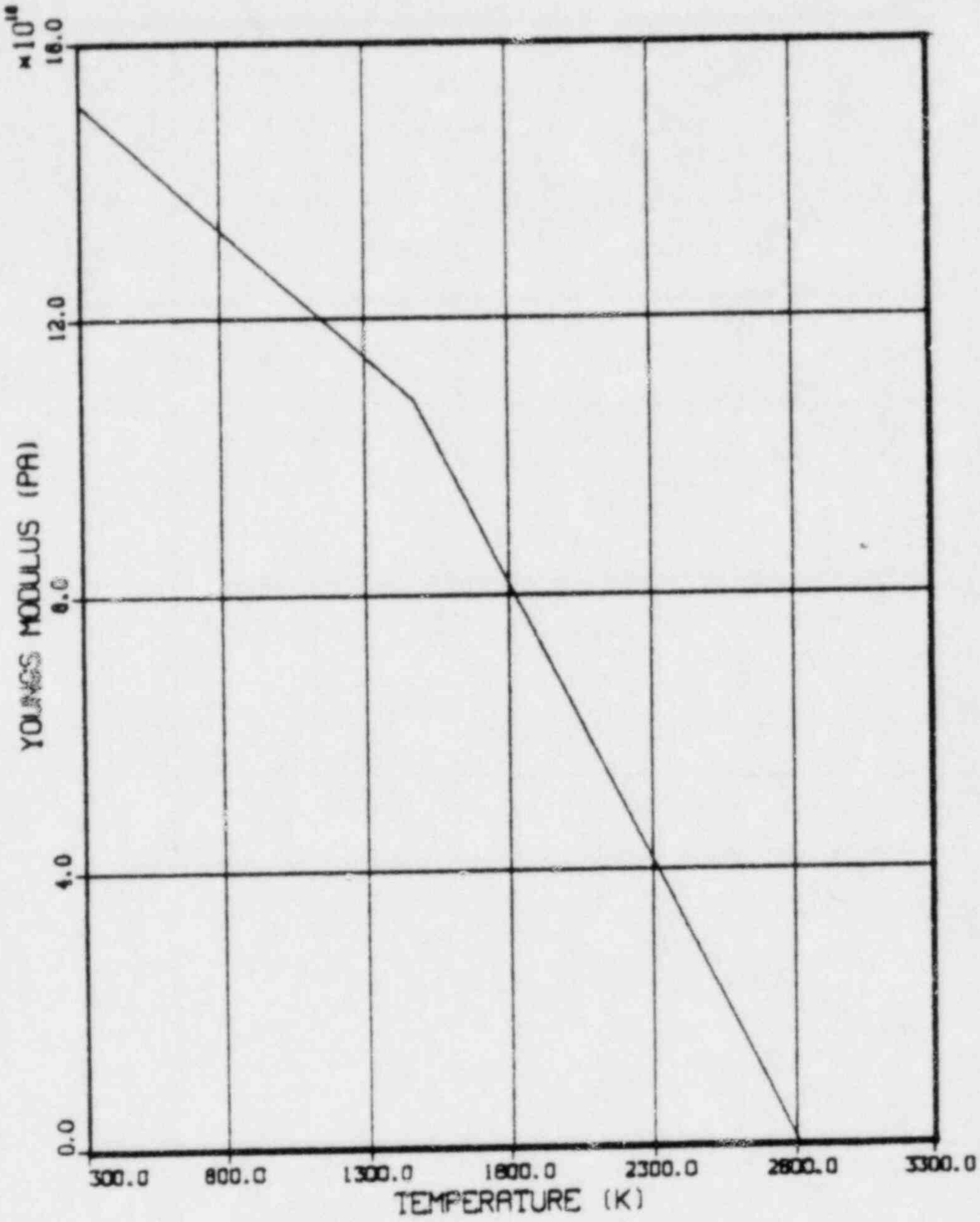

Figure B-17. Zircaloy oxide Young's modulus.

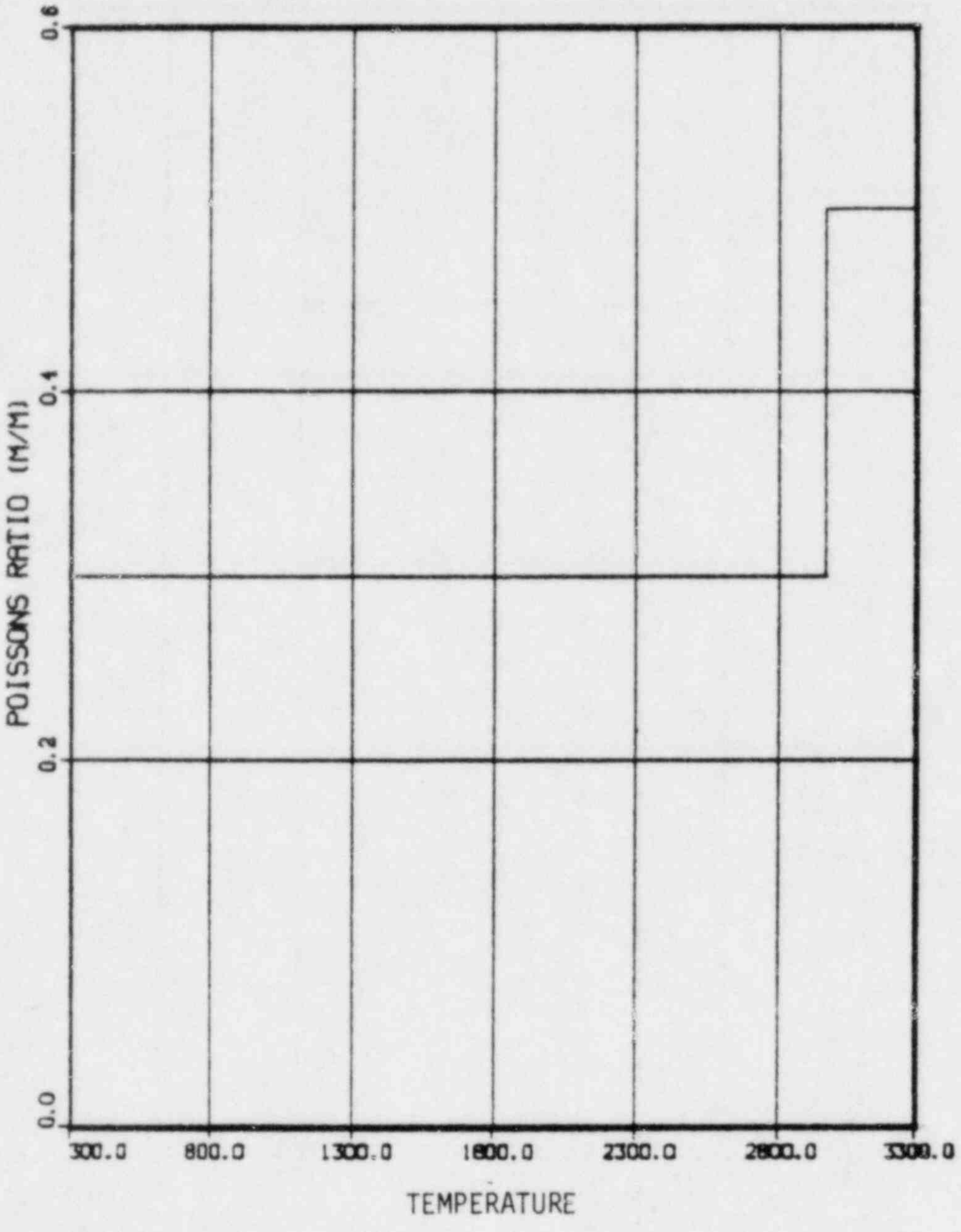

Figure B-18. Zircaloy oxide Poisson's ratio.

For temperature in the range $300 \leq T \leq 1200$ K (monoclinic phase of ZrO_2),

$$S_B = 96.28 \times 10^6 \quad . \tag{B-15a}$$

For temperature between 1200 and 1478 K (monoclinic phase of ZrO_2),

$$S_B = -5.06 \times 10^4\, T + 1.57 \times 10^8 \quad . \tag{B-15b}$$

For temperature in the range $1478 \leq T < 1869.4$ K (tetragonal and cubic phases of ZrO_2),

$$S_B = -2.075 \times 10^5\, T + 3.889 \times 10^8 \quad . \tag{B-15c}$$

For temperature in the range $1869.4 \leq T \leq T_{SOL}$,

$$S_B = 10^6 \quad . \tag{B-15d}$$

For temperature $> T_{SOL}$

$$S_B = 0 \quad . \tag{B-15e}$$

where

S_B = circumferential or axial stress on the oxide at failure (Pa)

T = oxide temperature (K)

T_{SOL} = zircaloy oxide solidus temperature (K) (Obtained from the ZOPRP subroutine).

These correlations are fits to the three ZrO_2 tensile strength data reported in Table 2 on Page 89 of Reference 12. The data are shown in Table B-26 and are compared with the correlation values in Figure B-19.

The values and shape of the curve are similar to the values and shape of the more extensive data for UO_2 failure. In the temperature range of the data the oxide failure stress is about three times the failure stress of zircaloy. In spite of these similarities, the very limited data used to construct the expressions for oxide failure stress suggest a large expected standard error for the correlation, ±0.7 times the predicted value.

Table B-27 is a listing of the ZORUP function and Figure B-20 is a plot of the failure stresses returned by the function.

CLADDING MELTING AND PHASE TRANSFORMATION TEMPERATURES
(CHYPRP, ZOPRP)

The subroutine CHYPRP calculates zircaloy phase transition temperatures of interest in light water reactor analysis. The equations used are from the MATPRO-11 Revision 2 PHYPRP, PSOL, and PLIQ subcodes. The only required input is the oxygen concentration in the zircaloy. Output temperatures are the solidus (appearance of the first liquid phase), liquidus (melting of the last solid phase), alpha to alpha + beta phase boundary, and alpha + beta to beta phase boundary.

ZOPRP returns transition temperatures between the monoclinic, tetragonal, cubic, and liquid phases of zircaloy oxide. The oxygen-to-metal ratio of the oxide is required input. The monoclinic-to-tetragonal and tetragonal-to-cubic transition temperatures are constants which have been reported by Reference B-1 for ZrO_2 (1478 and 2558 K). They are assumed to apply to zircaloy oxide in spite of the fact that the oxide is substoichiometric and may be under significant stress. The solidus and liquidus temperatures are calculted as a function of oxygen-to-metal ratio using the equations in Tables D-3.I and D-3.II of the MATPRO-11 Revision 2 handbook.

TABLE B-26. ZIRCALOY DIOXIDE TENSILE STRENGTH DATA FROM BRASSFIELD ET AL.[B-12]

Temperature (K)	Tensile Strength (10^6 Pa)
1303	91.2
1473	82.6
1813	12.7

TABLE B-27. LISTING OF THE ZORUP FUNCTION

```
      FUNCTION ZORUP(ZOTEMP,YE)
C
C     ZORUP RETURNS ZIRCALOY OXIDE FAILURE STRESS
C
C     ZORUP = OUTPUT OXIDE FAILURE STRESS (PA)
C
C     ZOTEMP = INPUT CLADDING OXIDE TEMPERATURE (K)
C     YE     = INPUT OXYGEN-TO METAL RATIO (ATOMS OXYGEN/
C              ATOMS METAL)
C
C     THE SUBROUTINE ZOPRP IS CALLED BY THIS FUNCTION
C
C     ZORUP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ZOTEMP .LT. 1478.) THEN
         ZORUP = 1.57E+08 - ZOTEMP * 5.06E+04
      ELSE
         IF(ZOTEMP .LT. 1869.4) THEN
            ZORUP = 3.889E+08 - ZOTEMP * 2.075E+05
         ELSE
            CALL ZOPRP(YE,ZOSOL,ZOLIQ,ZOTC,ZOMT)
            IF(ZOTEMP .LE. ZOSOL) THEN
               ZORUP = 1.0E+06
            ELSE
               ZORUP = 0.0
            ENDIF
         ENDIF
      ENDIF
      RETURN
      END
```

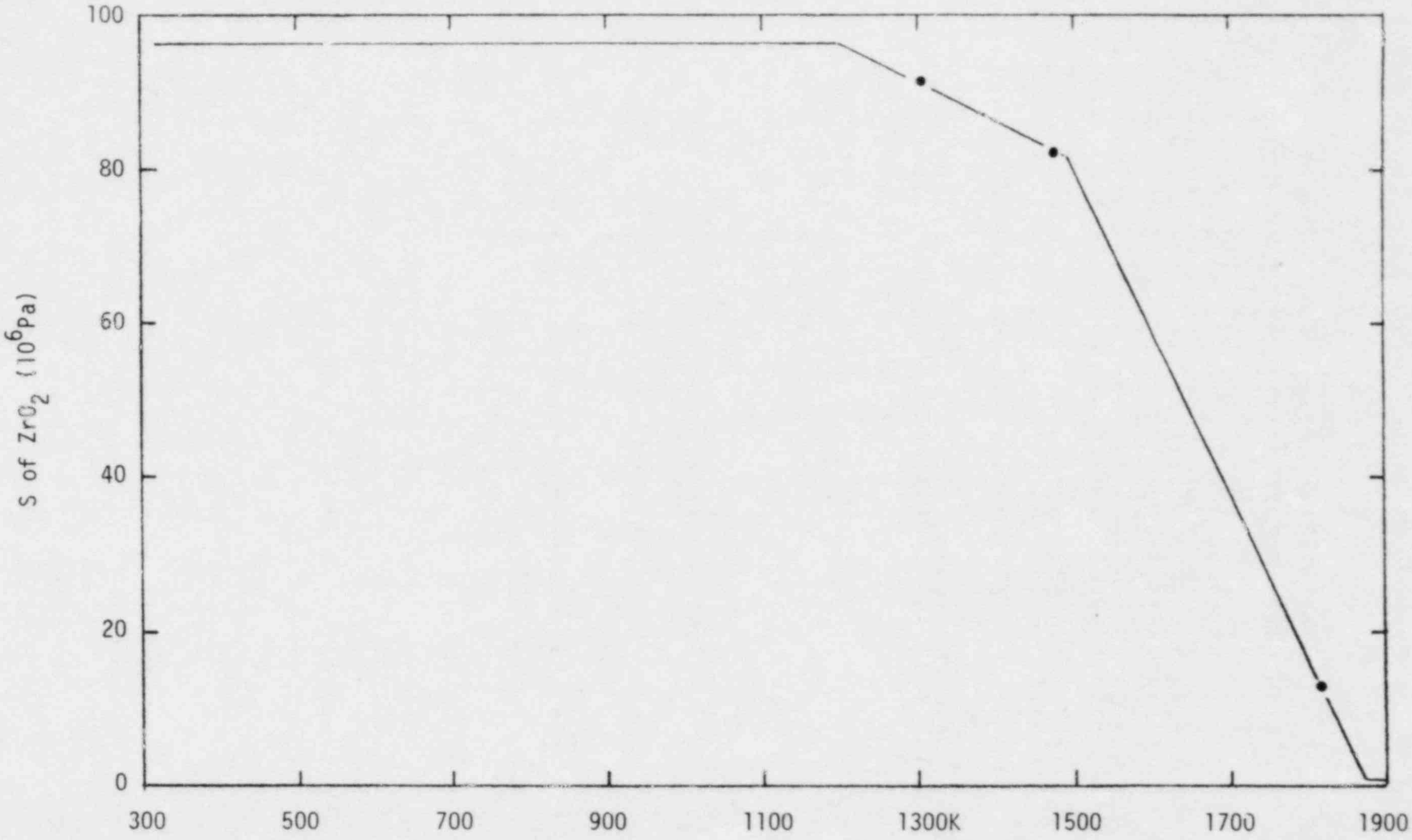

Figure B-19. Zircaloy oxide failure stress data and correlations versus temperature.

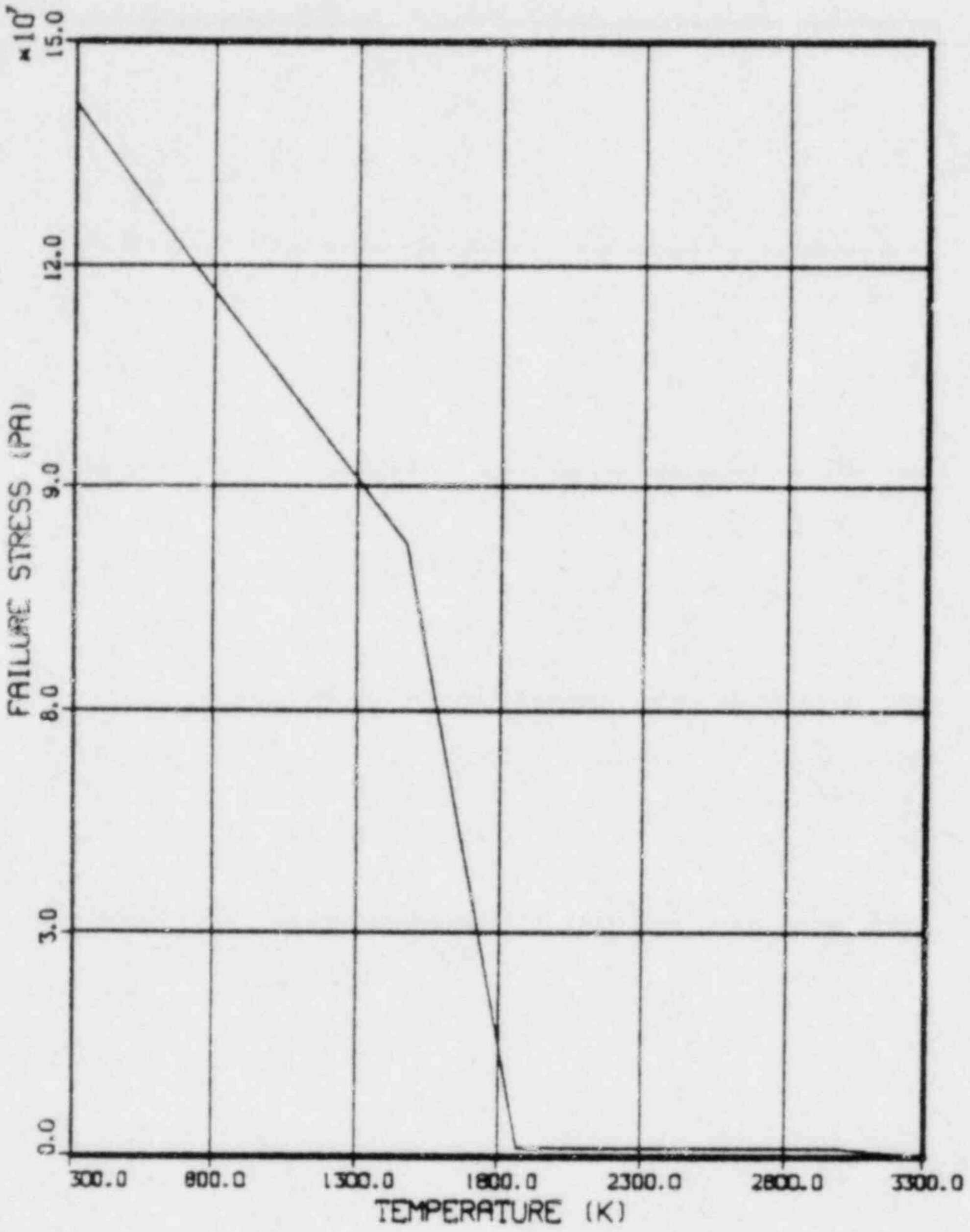

Figure B-20. Zircaloy oxide failure stress calculated with the ZORUP function.

Tables B-28 and B-29 are listings of the CHYPRP and ZOPRP subroutines. Figures B-21 and B-22 show the predicted solidus and liquidus temperatures as a function of oxygen concentration or oxygen-to-metal ratio. The alpha to alpha plus beta and alpha plus beta to beta phase boundaries are also shown in Figure B-21.

Table B-30 has been prepared to show the relation between four popular parameters used to describe the oxygen concentration in zircaloy. The first column gives the excess oxygen fraction parameter, DELOXY. The second column shows corresponding values for the total weight fraction of oxygen, assuming an as-received oxygen concentration of 0.0012 by weight. The third column presents corresponding values of the atomic fraction of oxygen in the compound which is related to the weight fraction of oxygen in zirconium oxide by the equation

$$X = \frac{WFOX}{WFOX + \frac{0.016}{0.09122}(1 - WFOX)} \qquad \text{(B-16)}$$

where

X = atomic fraction of oxygen in zircaloy oxide (atoms of O/atoms of compound)

WFOX = weight fraction of oxygen in zircaloy oxide (kg of O/kg of compound).

The fourth column gives the corresponding values of the oxygen-to-metal ratio, YE. This ratio is related to the atomic fraction of oxygen by

$$YE = \frac{X}{1 - X} \quad . \qquad \text{(B-17)}$$

The first row of numbers in Table B-24 represent as-received zircaloy cladding. The eighth row represents the solubility limit of oxygen in alpha phase zircaloy near the melting point, and the final row represents zircaloy dioxide.

TABLE B-28. LISTING OF THE CHYPRP SUBROUTINE

```
      SUBROUTINE CHYPRP(DELOXY,CSOL,CLIQ,CTRANB,CTRANE)
C
C     CHYPRP RETURNS ZIRCALOY PHASE TRANSITION TEMPERATURES
C
C     CSOL   = OUTPUT ZIRCALOY SOLIDUS TEMPERATURE (K)
C     CLIQ   = OUTPUT ZIRCALOY LIQUIDUS TEMPERATURE (K)
C     CTRANE = OUTPUT HIGH TEMPERATURE BOUNDARY OF THE
C              ALPHA-BETA PHASE REGION (K). B TO A + B BOUNDARY
C              EQUAL CSOL MEANS NO BOUNDARY AT GIVEN DELOXY
C     CTRANB = OUTPUT LOW TEMPERATURE BOUNDARY OF THE
C              ALPHA-BETA PHASE REGION (K). A + B TO A BOUNDARY
C              EQUAL CSOL MEANS NO BOUNDARY AT GIVEN DELOXY
C
C     DELOXY = INPUT OXYGEN CONCENTRATION - OXYGEN CONCENTRATION
C              OF AS RECEIVED CLADDING (KG OXYGEN/KG ZIRCALOY)
C
C     CHYPRP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
C
C     CONVERT WEIGHT FRACTION OXYGEN TO ATOMIC FRACTION OXYGEN = X
C     WFOX EQUALS TOTAL OXYGEN CONTENT IN WEIGHT FRACTION UNITS
      WFOX = DELOXY + 0.0012
      X = WFOX/(WFOX + 0.1754 *(1. - WFOX))
C
C     SOLIDUS CORRELATIONS
      IF(X .LE. 0.1) THEN
         CSOL = X * 1150. + 2098.
      ELSE
         IF(X .LE. 0.18) THEN
            CSOL = 2213.
         ELSE
            IF(X .LE. 0.29) THEN
               CSOL = 1.3695317E+03 + X*(7.6400748E+03 -
     *                X * 1.7029172E+04)
            ELSE
               IF(X .LE. 0.63) THEN
                  CSOL = 2173.
               ELSE
                  IF(X .LE. 0.667) THEN
                     CSOL = -1.1572454E+04 + X*2.1818181E+04
                  ELSE
                     CSOL = -1.1572454E+04 + (1.334 - X) *
     *                      2.1818181E+04
                  ENDIF
               ENDIF
            ENDIF
         ENDIF
      ENDIF
C
C     LIQUIDUS CORRELATIONS
      IF(X .LE. 0.19) THEN
         CLIQ = 2.125E+03 + X*(1.6321637E+03 - X*5.3216374E+03)
      ELSE
```

TABLE 28. (continued)

```
            IF(X .LE. 0.41) THEN
               CLIQ = 2.11165553E+03 + X*(1.1590909E+03 -
     *                X * 2.4621212E+03)
            ELSE
               IF(X .LE. 0.667) THEN
                  CLIQ = 8.9507792E+02 + X * 3.1168831E+03
               ELSE
                  CLIQ = 8.9507792E+02 + (1.34 - X)*3.1168831E+03
               ENDIF
            ENDIF
         ENDIF
C
C        CALCULATE ALPHA-BETA PHASE BOUNDARIES
         IF(WFOX .LT. 0.025) THEN
            CTRANB = 1094. + WFOX * (-1.289E+03 + WFOX * 7.914E+05)
         ELSE
            CTRANB = 1556.4 + 3.8281E+04 * (WFOX - 0.025)
         ENDIF
         IF(CTRANB .GT. CSOL) THEN
            CTRANB = CSOL
         ENDIF
         IF(DELOXY .LT. 4.7308937E-03) THEN
            CTRANE = 392.46 * ((100.*DELOXY + 0.1242807)**2 + 3.1417)
         ELSE
            CTRANE = (100. * DELOXY + 0.12) * 491.157 + 1081.7413
         ENDIF
         IF(CTRANE .GT. CSOL) THEN
            CTRANE = CSOL
         ENDIF
         RETURN
         END
```

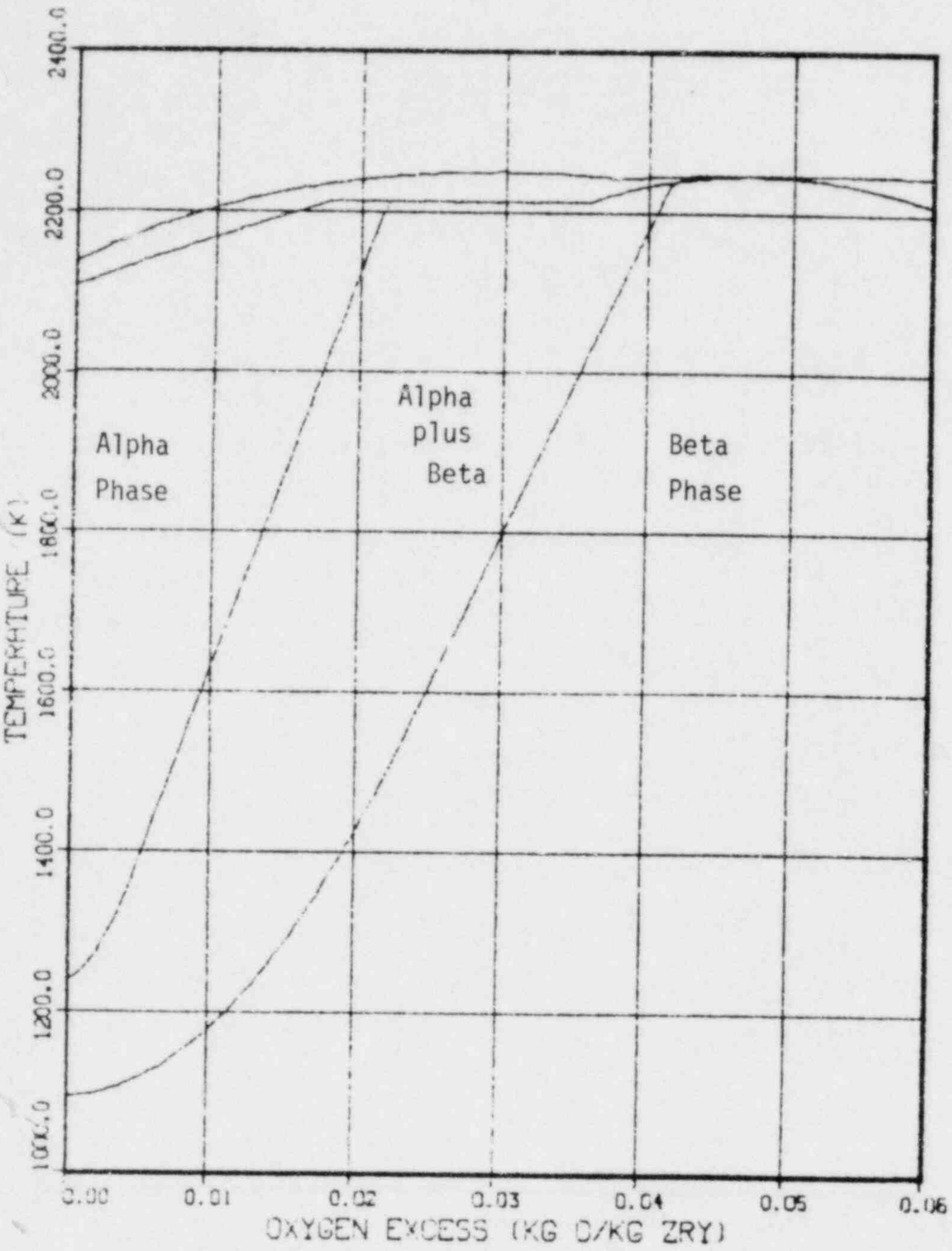

Figure B-21. Zircaloy solidus and liquidus temperatures.

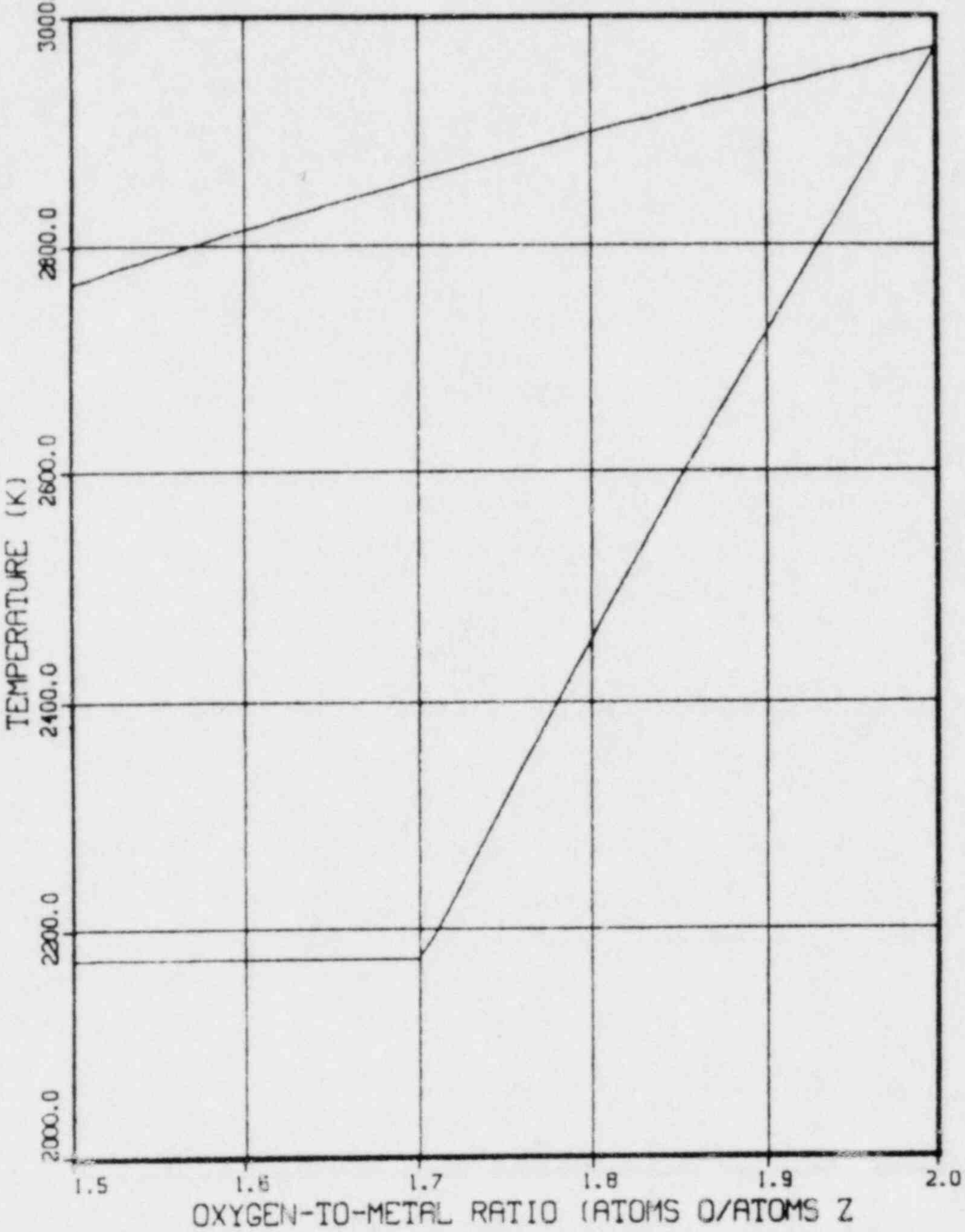

Figure B-22. Zircaloy oxide solidus and liquidus temperatures.

TABLE B-29. LISTING OF THE ZOPRP SUBROUTINE

```
      SUBROUTINE ZOPRP(YE,ZOSOL,ZOLIQ,ZOTC,ZOMT)
C
C     ZOPRP RETURNS ZIRCALOY OXIDE PHASE TRANSITION TEMPERATURES
C
C     ZOSOL  = OUTPUT ZIRCALOY OXIDE SOLIDUS TEMPERATURE (K)
C     ZOLIQ  = OUTPUT ZIRCALOY OXIDE LIQUIDUS TEMPERATURE (K)
C     ZOTC   = OUTPUT ZIRCALOY OXIDE TETRAGONAL-TO-CUBIC
C              PHASE TRANSITION TEMPERATURE (K)
C     ZOMT   = OUTPUT ZIRCALOY OXIDE MONOCLINIC-TO-TETRAGONAL
C              PHASE TRANSITION TEMPERATURE (K)
C
C     YE     = INPUT OXYGEN-TO-METAL RATIO (ATOMS OXYGEN/
C              ATOMS METAL)
C
C     ZOPRP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      ZOTC = 2558.
      ZOMT = 1478.
C
C     CONVERT OXIDE-TO-METAL RATIO TO ATOMIC FRACTION OXYGEN = X
      X = YE/(1. + YE)
C
C     SOLIDUS CORRELATIONS
      IF(X .LE. 0.1) THEN
         CSOL = X * 1150. + 2098.
      ELSE
         IF(X .LE. 0.18) THEN
            CSOL = 2213.
         ELSE
            IF(X .LE. 0.29) THEN
               CSOL = 1.3695317E+03 + X*(7.6400748E+03 -
     #                X * 1.7029172E+04)
            ELSE
               IF(X .LE. 0.63) THEN
                  CSOL = 2173.
               ELSE
                  IF(X .LE. 0.667) THEN
                     CSOL = -1.1572454E+04 + X*2.1818181E+04
                  ELSE
                     CSOL = -1.1572454E+04 + (1.334 - X) *
     #                      2.1818181E+04
                  ENDIF
               ENDIF
            ENDIF
         ENDIF
      ENDIF
C
C     LIQUIDUS CORRELATIONS
      IF(X .LE. 0.19) THEN
         CLIQ = 2.125E+03 + X*(1.6321637E+03 - X*5321.6374E+03)
      ELSE
         IF(X .LE. 0.41) THEN
            CLIQ = 2.1116553E+03 + X*(1.1590909E+03 -
     #             X * 2.4621212E+03)
         ELSE
            IF(X .LE. 0.667) THEN
               CLIQ = 8.9507792E+02 + X * 3.1168831E+03
            ELSE
               CLIQ = 8.9507792E+02 + (1.34 - X)*3.1168831E+03
            ENDIF
         ENDIF
      ENDIF
C
      ZOSOL = CSOL
      ZOLIQ = CLIQ
      RETURN
      END
```

TABLE B-30. OXYGEN CONTENT PARAMETERS FOR ZIRCALOY

DELOXY[a] [kg excess O/kg Zr(O)]	WFOX [kg O/kg Zr(O)]	X (atoms O/atoms compound)	YE (atoms O/atoms metal)
0.0000	0.0012	0.007	0.007
0.0100	0.0112	0.061	0.065
0.0200	0.0212	0.110	0.124
0.0300	0.0312	0.155	0.183
0.0400	0.0412	0.197	0.245
0.0500	0.0512	0.235	0.307
0.0600	0.0612	0.271	0.372
0.0657	0.0669	0.290	0.408
0.2585	0.2597	0.667	2.000

---

[a] As-received zircaloy is presumed to have 0.0012 wt fraction oxygen.

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APPENDIX C
GAP GAS PROPERTIES

APPENDIX C

GAP GAS PROPERTIES

No change in the MATPRO-11 Revision 2 gap gas properties models is required to extend them to high temperatures.

APPENDIX D
NEUTRON ABSORBER PROPERTIES

APPENDIX D

NEUTRON ABSORBER PROPERTIES

A set of control rod neutron absorber properties for Ag-In-Cd alloys (80% Ag, 15% In, 5% Cd by weight) and B_4C has been prepared to allow modeling of the possible flow and freezing of these materials during a severe core disruption. Properties for both substances have been included in each subcode. An input argument, ICTYPE, is used to determine which substances properties are returned.

No models have been provided for mixtures of neutron absorbers and their stainless steel cladding because it has been reported on page 4-38 of Reference D-1 that the Ag-In-Cd alloy is insoluble in stainless steel and because the very different melting temperatures of stainless steel (1700 K) and B_4C (2700 K) make it likely that the stainless steel will oxidize or melt and run away from hot regions before B_4C and stainless steel mix.

NEUTRON ABSORBER SPECIFIC HEAT CAPACITY AND ENTHALPY (ACP, AENTHL)

The function ACP provides absorber specific heat capacities as a function of temperature. AENTHL returns the absorber enthalpies as a function of temperature and a reference temperature for which the enthalpy will be zero.

The expressions used for the specific heat capacity of Ag-In-Cd are atomic fraction weighted averages of the specific heat capacities of Ag, In and Cd

$$C_p = \frac{0.808\ C_{pm_{Ag}} + 0.143\ C_{pm_{In}} + 0.049\ C_{pm_{Cd}}}{0.109\ \text{Kg/mole alloy}} \qquad \text{(D-1)}$$

where

C_p = alloy specific heat capacity (J/kg•k)

$C_{pm_{Ag}}$ = molar heat capacity of Ag (J/mole•K)

$C_{pm_{In}}$ = molar heat capacity of In (J/mole•K)

$C_{pm_{Cd}}$ = molar heat capacity of Cd (J/mole•K) .

Expressions for the Ag, In, and Cd molar heat capacities up to the beginning of melting, 1050 K, were taken from Table 2-24 of Reference D-2. All are correlations of the form

$$C_{pm} = a + b \times 10^{-3} \times T + d \times 10^{5} \times T^{-2}$$

where

C_{pm} = molar heat capacity (J/mole•K)

T = temperature (K)

and the constants a, b, and d are listed in Table D-1. For temperatures above 1050 K, C_p is assumed to be equal to its value at 1050 K.

The expressions used for the specific heat capacity of B_4C are listed below:

For temperatures less than 2700 K,

$$C_p = 563 + T\ (1.54 - T\ 2.94 \times 10^{-4}) \ . \qquad \text{(D-3a)}$$

TABLE D-1. MOLAR HEAT CAPACITY CONSTANTS FOR EQUATION (D-1) FROM REFERENCE D-2

Metal	a (J/mole•K)	b (J/mole•K^2)	d (J•K/mole)
Ag	21.3	4.27	1.51
In	24.3	10.5	0
Cd	22.2	12.3	0

for temperatures $\geq$2700 K

$$C_p = 2577.740 \quad . \tag{D-3b}$$

Equations (D-3a) and (D-3b) were developed from a curve given on page 588 of Reference D-3.

Integrals of Equation (D-2) (D-3a) or (D-3b) are used to compute enthalpy changes in the AENTHL function. The heats of fusion which are included in the AENTHL function are estimates. For Ag-In-Cd the heat of fusion, 9.56 10^4J/kg, was estimated by multiplying the molar heats of fusion of Ag, In, and Cd by the atomic fraction of each element in the alloy and dividing the sum by 0.109, the weight of a gm-mole of the alloy in kilograms. The elemental heats of fusion were obtained from Tables 2 through 24 of Reference D-2. For B_4C the heat of fusion was taken to be that of UO_2, 2.74 10^5 J/kg.

Tables D-2 and D-3 are listings of the ACP and AENTHL functions. The predicted valves of specific heat capacity and enthalpy for Ag-In-Cd and B_4C are illustrated in Figures D-1 to D-4. The predictions are expected to have a standard error near 0.1 of their value.

NEUTRON ABSORBER THERMAL CONDUCTIVITY
(ATHCON)

The only input required by ATHCON to calculate the thermal conductivity of B_4C or Ag-In-Cd is the absorber temperature.

The expressions used for Ag-In-Cd are listed below:

For temperature in the range $300 \leq T < 1050$ K,

$$K_a = 2.805 \times 10^1 + T\ (1.101 \times 10^{-1} - 4.436 \times 10^{-5}\ T) \quad . \tag{D-4a}$$

TABLE D-2. LISTING OF THE ACP FUNCTION

```
      FUNCTION ACP(ICTYPE,ATEMP)
C
C     ACP RETURNS THE SPECIFIC HEAT CAPACITY AT CONSTANT
C     PRESSURE FOR TWO TYPES OF NEUTRON ABSORBERS
C
C     ACP     = OUTPUT ABSORBER SPECIFIC HEAT CAPACITY AT
C               CONSTANT PRESSURE (J/(KG*K)
C
C     ICTYPE  = INPUT ABSORBER MATERIAL TYPE
C                  1 = SILVER-INDIUM-CADMIUM (.8,.15.05)
C                  2 = BORON CARBIDE
C     ATEMP   = INPUT ABSORBER TEMPERATURE (K)
C
C     ACP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ICTYPE .LT. 2) THEN
         IF(ATEMP .LT. 1050.) THEN
            CPAG = 21.3 + ATEMP*4.27E-03 + 1.51E+05/(ATEMP**2)
            CPIN = 24.3 + ATEMP*1.05E-02
            CPCD = 22.2 + ATEMP*1.23E-02
            ACP = 9.17 * (0.808*CPAG + 0.143*CPIN + 0.049*CPCD)
         ELSE
            ACP = 254.1542
         ENDIF
      ELSE
         IF(ATEMP .LT. 2700.) THEN
            ACP = 463. + ATEMP*(1.54 - ATEMP*2.94E-04)
         ELSE
            ACP = 2477.740
         ENDIF
      ENDIF
      RETURN
      END
```

TABLE D-3. LISTING OF THE AENTHL FUNCTION

```
      FUNCTION AENTHL(ICTYPE,ATEMP,RFTEMP)
C
C     AENTHL RETURNS THE CHANGE IN ENTHALPY OF NEUTRON ABSORBERS
C     DURING A CONSTANT PRESSURE CHANGE IN TEMPERATURE
C
C     AENTHL = OUTPUT CHANGE IN ABSORBER ENTHALPY (J/KG)
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                  1 = SILVER-INDIUM-CADMIUM (.8,.15.05)
C                  2 = BORON CARBIDE
C     ATEMP  = INPUT ABSORBER TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     AENTHL WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      T = RFTEMP
      N = -1
C
      IF(ICTYPE .LT. 2) THEN
 10      IF(ATEMP .LT. 1050.) THEN
            HAG = T * (21.3 + 2.135E-03*T) - 1.51E+05/T
     #           -6.078816E+03
            HIN = T * (24.3 + 5.250E-03*T)
     #           -7.762500E+03
            HCD = T * (22.2 + 6.150E-03*T)
     #           -7.213500E+03
            H = 9.17 * (0.808 *HAG + 0.143*HIN + 0.049*HCD)
         ELSE
            IF(T .LT. 1100.) THEN
               H = 1.946473E+04 + 2.166154E+03 * (T -1050.)
            ELSE
               H = 1.277724E+05 + 254.1542 * (T - 1100.)
            ENDIF
         ENDIF
         IF(N .LT. 0) THEN
            N = N + 2
            HR = H
            T = ATEMP
            GO TO 10
         ELSE
         AENTHL = H - HR
         ENDIF
      ELSE
 20      IF(T .LT. 2700.) THEN
            H = T*(563. + T*(0.77 - T*9.8E-05))
         ELSE
            H = 5.479E+06 + 2577.740 * (T- 2700.)
         ENDIF
         IF(N .LT. 0) THEN
            N = N + 2
            HR = H
            T = ATEMP
            GO TO 20
         ELSE
            AENTHL = H - HR
         ENDIF
      ENDIF
      RETURN
      END
```

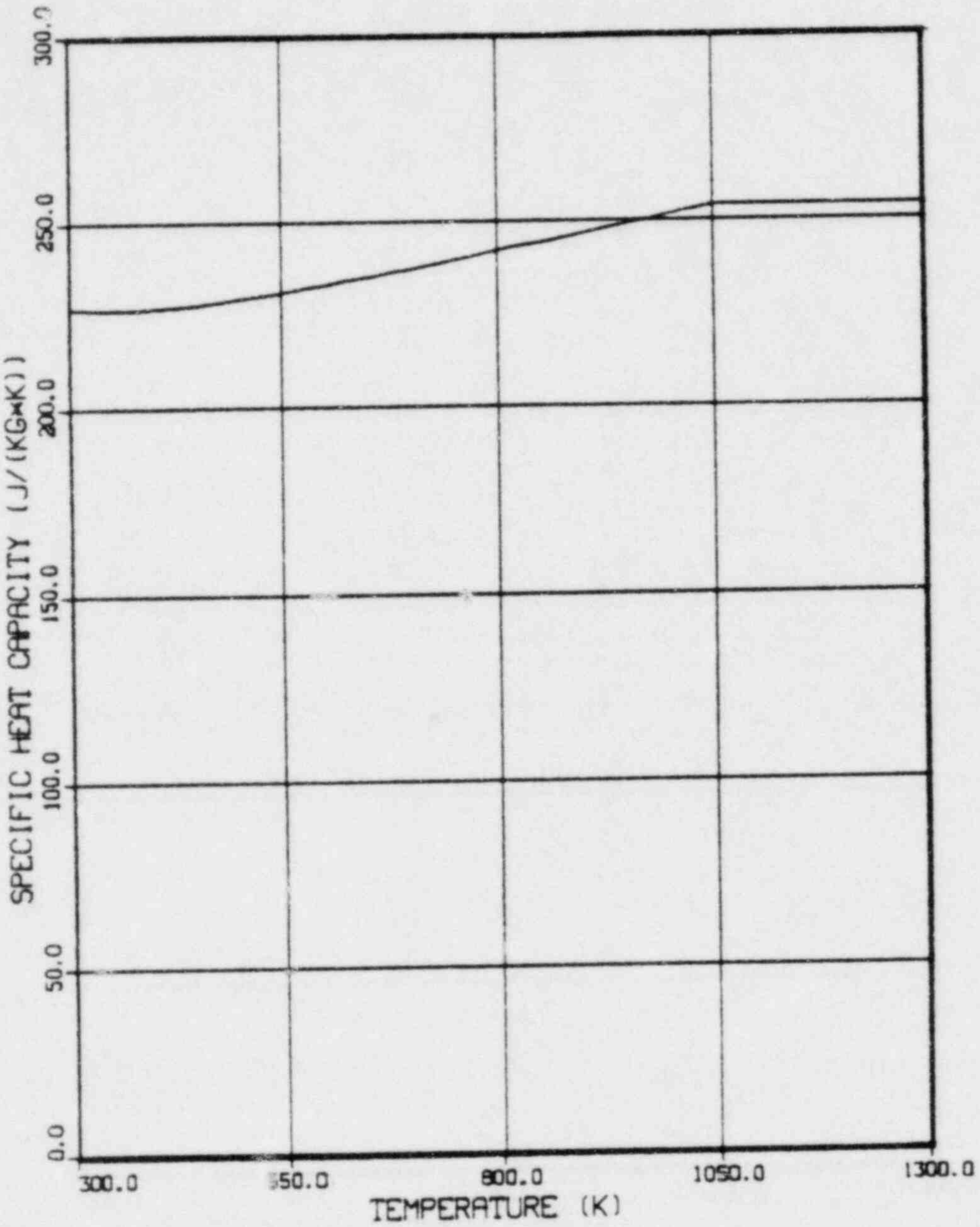

Figure D-1. Silver-Indium-Cadmium absorber heat capacity.

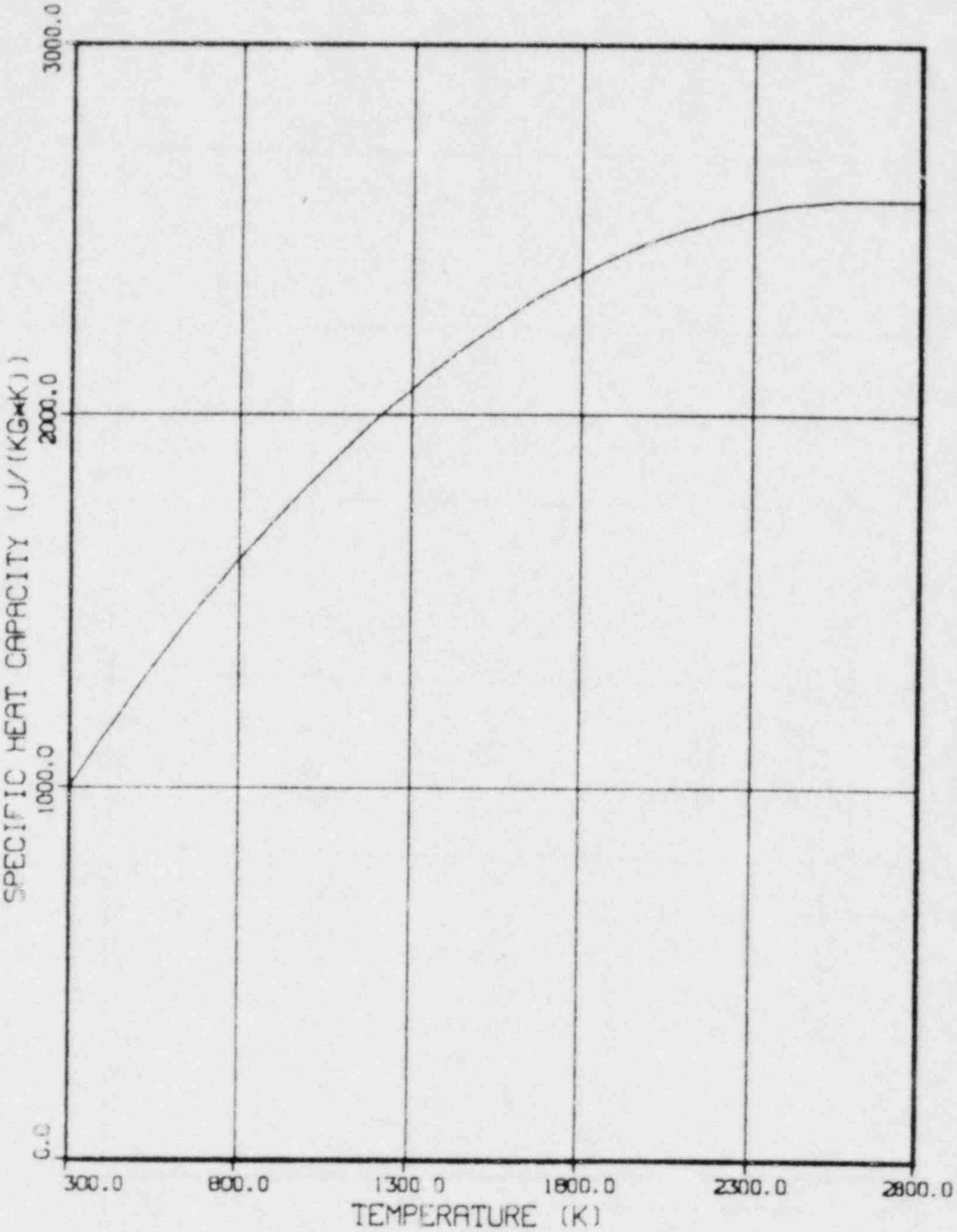

Figure D-2. Boron carbide absorber heat capacity

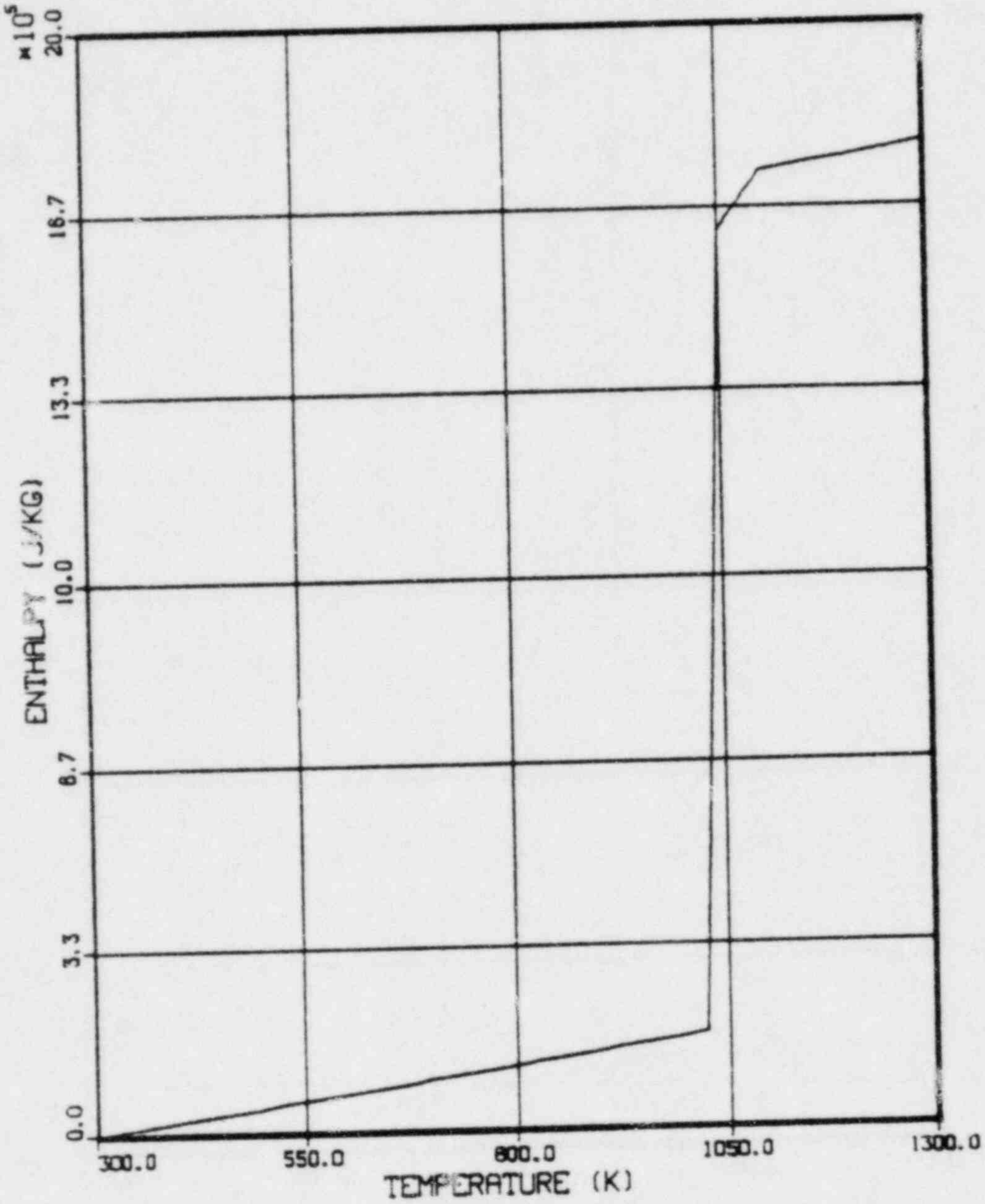

Figure D-3. Silver-Indium-Cadmium absorber enthalpy.

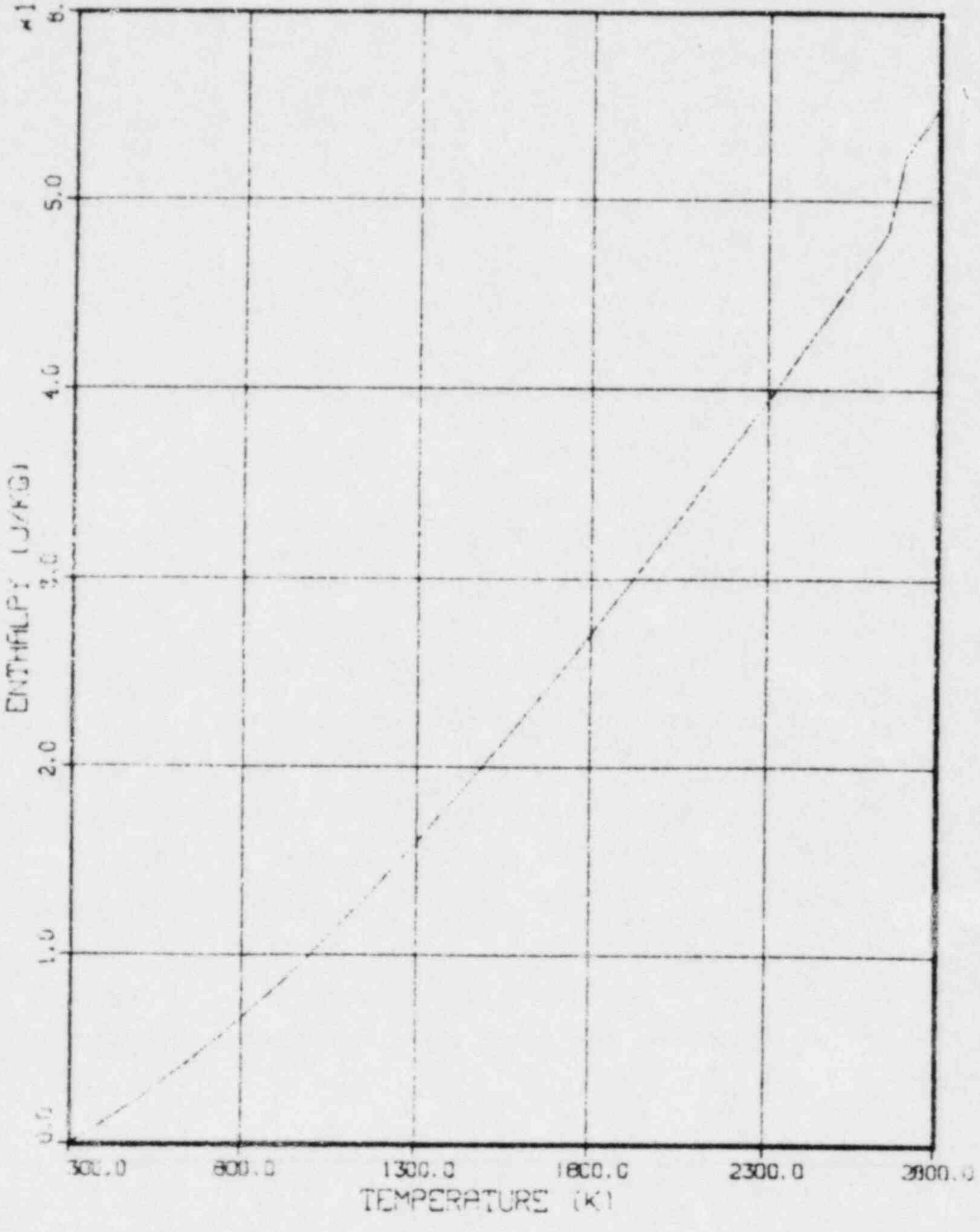

Figure D-4. Boron carbide absorber enthalpy.

For temperature in the range $1050 \leq T < 1100$ K,

$$K_a = 1.076458 \times 10^3 - 0.9349626\,T \quad . \tag{D-4b}$$

For temperatures greater than or equal to 1100 K,

$$K_a = 48 \tag{D-4c}$$

where

K_a = absorber thermal conductivity (W/m•K)

T = absorber temperature (K).

The correlation (D-4a) was derived by fitting a second degree polynomial to the first, fourth, and seventh entries of a table of properties provided by Reference D-4. The table is reproduced as Table D-4. Equation (D-4c) was derived by dividing the conductivity predicted by Equation (D-4a) for 1075 K (the middle of the melting range) by two to estimate the conductivity when this face centered cubic solid[D-4] melts. The method for estimating liquid conductivities follows recommendations by Nazare et al.[D-5] Equation (D-4b) is simply a linear interpolation between the conductivity predicted by Equation (D-4a) at the beginning of melting (1050 K) and Equation (D-4c) when melting is complete. Figure D-5 is a comparison of the predictions of Equations (D-4a) to (D-4c) with the recommended values of Table D-2. A twenty percent expected standard error is recommended.

For B_4C thermal conductivity the following expressions are used:

For temperature less than 1700 K,

$$K_a = \frac{1}{1.79 \times 10^{-2} + 4.98 \times 10^{-5}\,T} \quad . \tag{D-5a}$$

TABLE D-4. THERMAL CONDUCTIVITY VALUES FOR AG-IN-CD RECOMMENDED BY COHEN ET AL.[D-4]

Temperature (K)	Thermal Conductivity (W/m•K)
323	59.0
373	62.8
473	70.3
573	76.6
673	82.0
773	86.6
873	90.4

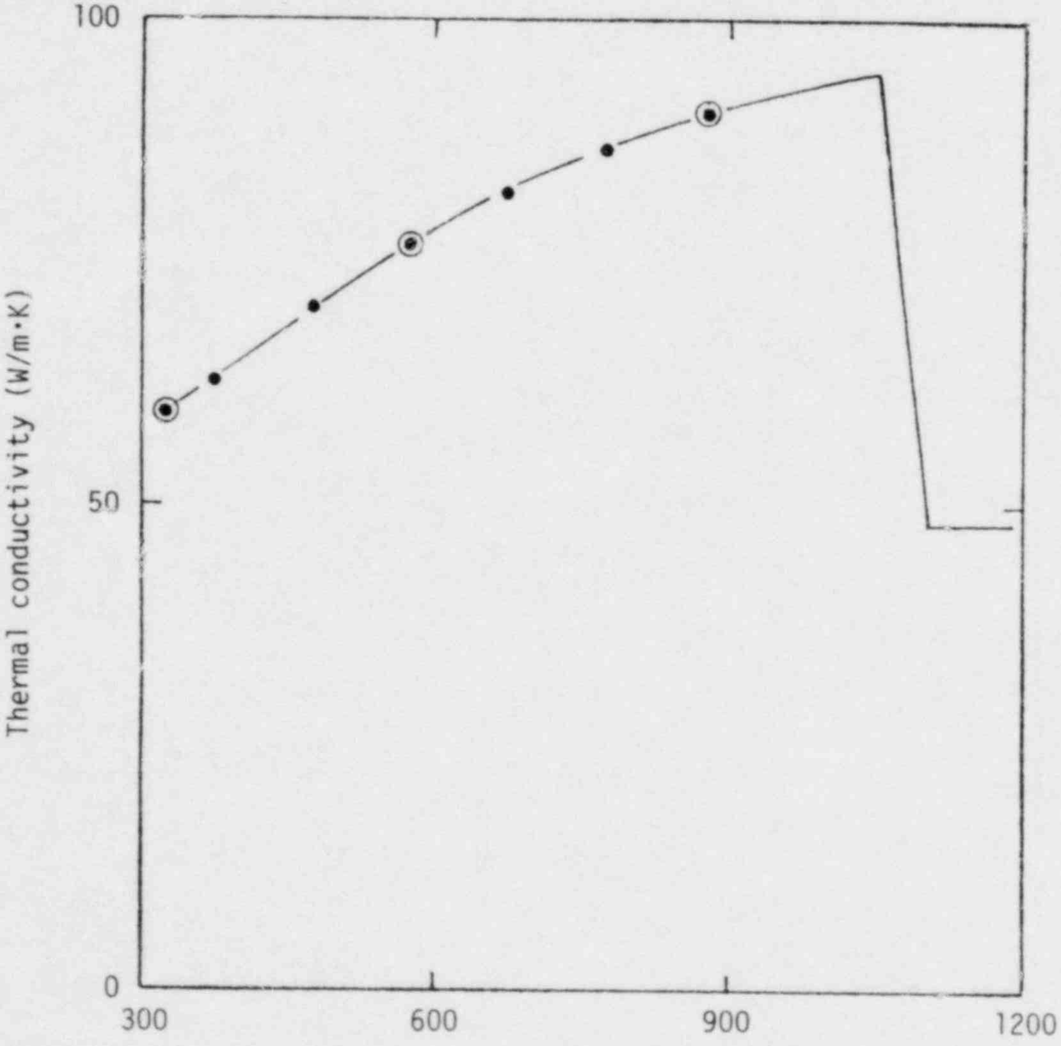

Figure D-5. Thermal conductivity of Ag-In-Cd alloy.

For temperature greater than or equal to 1700 K,

$$K_a = 9.750390 \qquad \text{(D-5b)}$$

The expression is a fit to values of 23.37 and 13.76 W/m•K at 500 and 1100 K, respectively, obtained from the 150 $\mathrm{lbm/ft^3}$ curve presented on page 947 of Reference D-6. A fifty percent expected standard deviation is recommended because of the significant effect of density of the material.

Table D-5 is a listing of the ATHCON function. The predicted valves of thermal conductivity for Ag-In-Cd and B_4C are shown in Figures D-6 and D-7.

NEUTRON ABSORBER THERMAL EXPANSION AND DENSITY
(ATHEXP, ADEN)

The function ATHEXP calculates absorber thermal expansion strain while ADEN is designed to use this information to calculate absorber densities. ATHEXP requires input values of the materials temperature and a reference temperature (for which strain will be taken as zero). ADEN requires only temperature.

The expressions used for the thermal expansion strain of Ag-In-Cd absorbers are listed below:

For temperature in the range $300 \leq T < 1050$ K,

$$\epsilon_a = 2.25 \times 10^{-5} (T - 300) \quad . \qquad \text{(D-6a)}$$

For the temperature in the range $1050 \leq T < 1100$ K,

$$\epsilon_a = -0.25875 + 2.625 \times 10^{-4} \times T \quad . \qquad \text{(D-6b)}$$

TABLE D-5. LISTING OF THE ATHCON FUNCTION

```
      FUNCTION ATHCON(ICTYPE,ATEMP)
C
C     ATHCON RETURNS ABSORBER THERMAL CONDUCTIVITIES
C
C     ATHCON = OUTPUT ABSORBER THERMAL CONDUCTIVITY (W/(M*K))
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                   1 = SILVER-INDIUM-CADMIUM (.8,.15.05)
C                   2 = BORON CARBIDE
C     ATEMP  = INPUT ABSORBER TEMPERATURE (K)
C
C     ATHCON WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ICTYPE .LT. 2) THEN
         IF(ATEMP .LT. 1050.) THEN
            ATHCON = 28.05 + ATEMP*(0.1101-ATEMP*4.436E-05)
         ELSE
            IF(ATEMP .LT. 1100.) THEN
               ATHCON = 1.076458E+03 - ATEMP*0.934962
         ELSE
            ATHCON = 48.
            ENDIF
         ENDIF
      ELSE
         IF(ATEMP .LT. 1700.) THEN
            ATHCON = 1.0/(0.0179 + ATEMP * 4.98E-05)
         ELSE
            ATHCON = 9.750390
         ENDIF
      ENDIF
      RETURN
      END
```

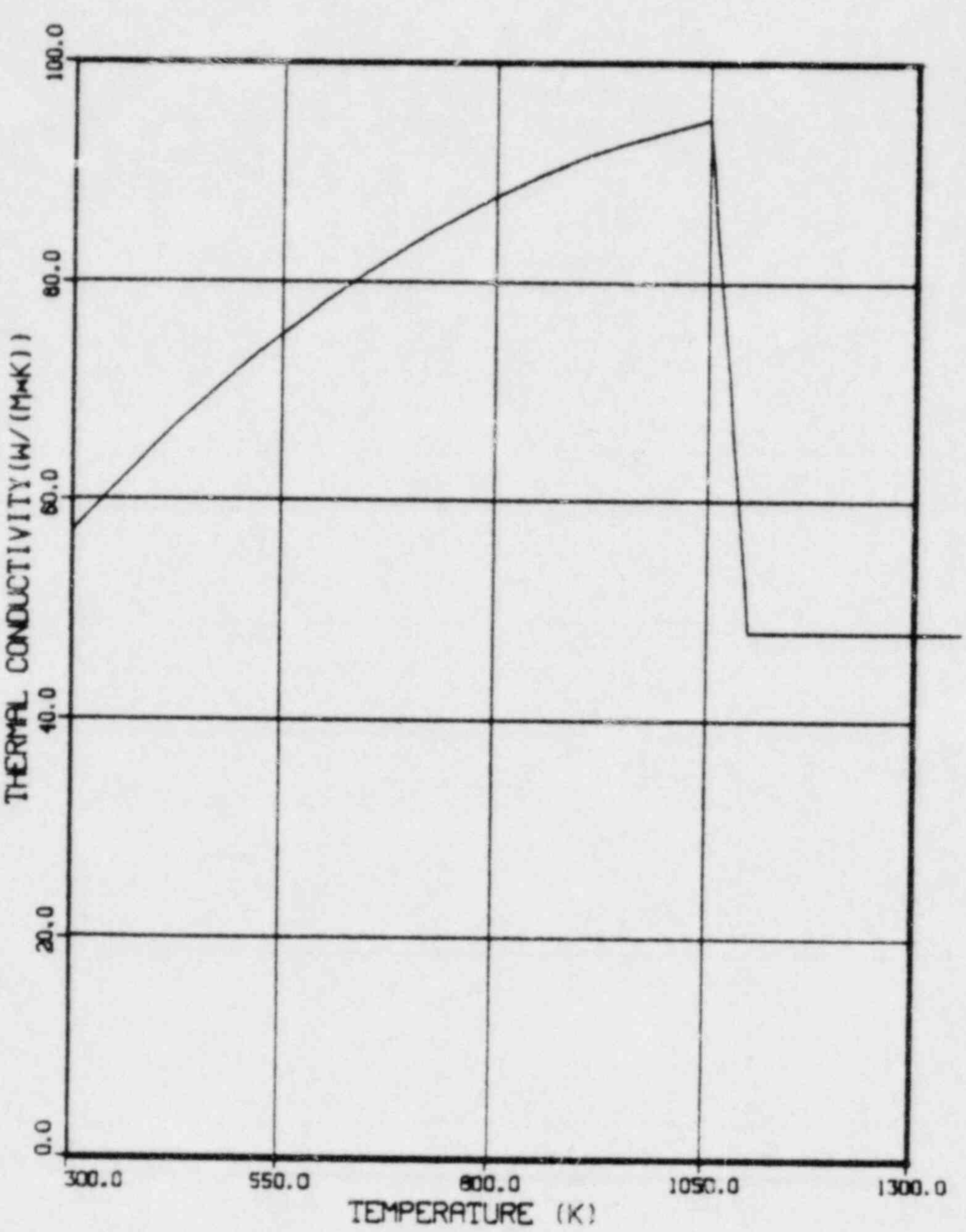

Figure D-6. Thermal conductivity of Ag-In-Cd absorber.

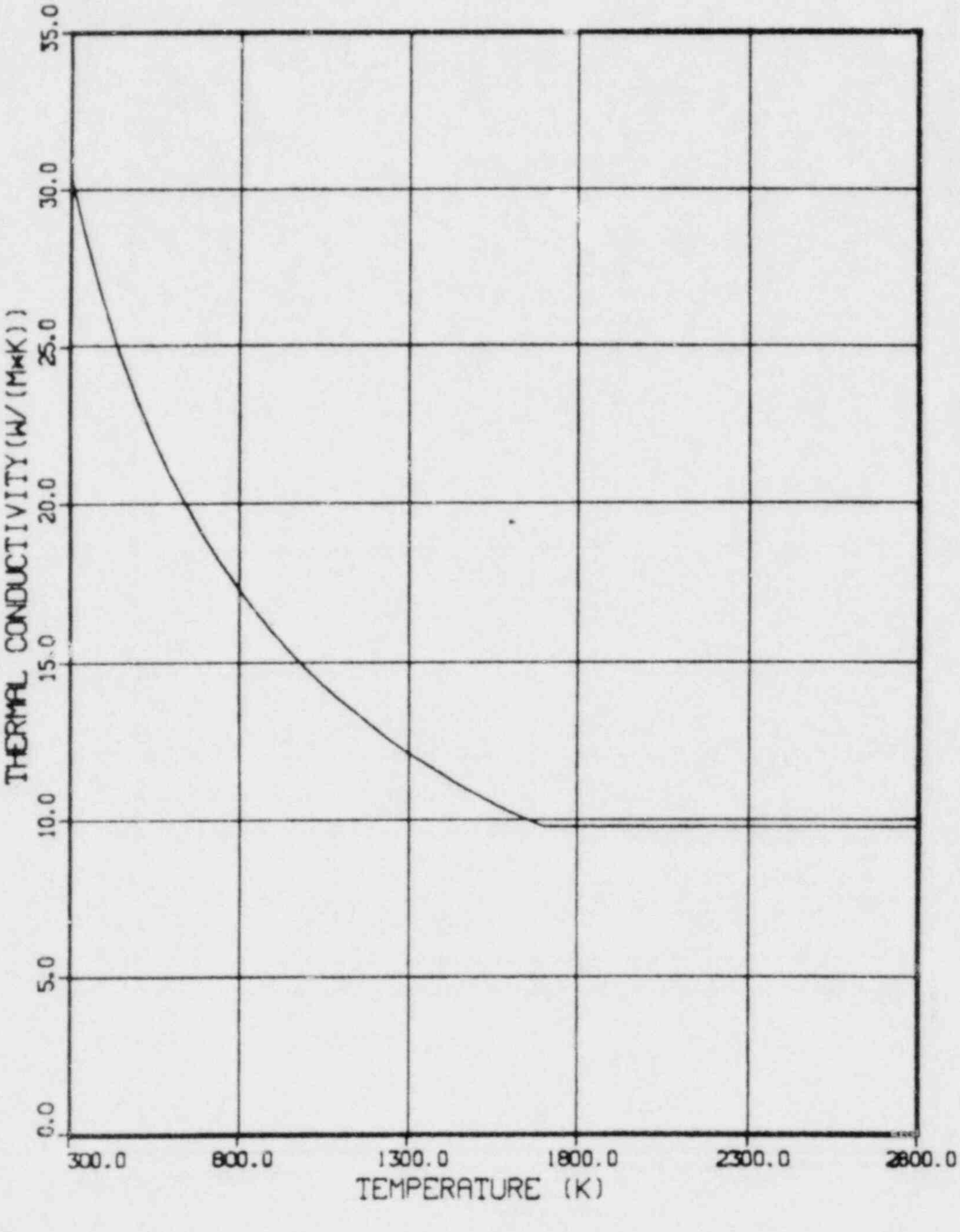

Figure D-7. Thermal conductivity of B_4C absorber.

For temperature greater than or equal to 1100 K

$$\epsilon_a = 3.0 \times 10^{-2} \qquad \text{(D-6c)}$$

where

ϵ_a = absorber thermal expansion strain (m/m)

T = absorber temperature (K).

Equation (D-6a) is taken from Table V of Reference D-4. Equation (D-6c) was obtained by modifying the prediction of Equation (D-6a) to allow for an increase of 0.038 in volume (0.013 in length) at the center of the melting range of 1050 to 1100 K because page 186 of Reference D-7 reports this value for the change in volume of Ag, the major component of the alloy, during melting. Equation (D-6b) is a linear interpolation between the predictions of Equations (D-6a) and (D-6c) for the beginning and end of the melting range. The expected standard error of Equations (D-6a) to (D-6c), 0.1 of the predicted strain, is small because the data cover most of the range of the correlations.

The expression used to calculate thermal expansion strains of B_4C is

$$\epsilon_a = -1.10 \times 10^{-3} + T\,(3.09 \times 10^{-6} + 1.88 \times 10^{-9}\,T) \quad . \qquad \text{(D-7)}$$

This correlation is a fit to values of 0, 2.58×10^{-3}, and 5.32×10^{-3} at 300, 800 and 1200 K, respectively, obtained from a curve presented on page 949 of Reference D-6. The expected standard error is ±0.2 of the predicted strain.

The function ADEN uses the general relation between density and thermal strain, Equation (B-10), together with reference densities of 10.17×10^3 Kg/m^3 at 300 K for Ag-In-Cd (Reference D-4 Table V) and

2.5×10^3 Kg/m^3 at 300 K for B_4C (page 943 of Reference D-6). For Ag-In-Cd the expected standard error is only 0.02 of the predicted density, but for B_4C it is ±0.3 of the predicted density.

Tables D-6 and D-7 are listings of the ATHEXP and ADEN functions. The predictions for Ag-In-Cd and B_4C versus temperature given by the function are reproduced in Figures D-8 to D-11.

NEUTRON ABSORBER SURFACE TENSION
(ASTEN)

The function ASTEN returns the interfacial surface tension of absorber material on stainless steel cladding. The value used is

$$ST = 0.3 \tag{D-8}$$

where

ST = interfacial surface tension (N/m).

The number used is an engineering estimate based on the relative magnitudes of zirconium and silver liquid surface tensions given by Allen[D-8] and the interfacial surface tension for zircaloy and zirconium-uranium-oxygen compounds given in the ZUSTEN function of Appendix G. The expected error of this number is

$\left(\begin{smallmatrix}+2.0\\-0.2\end{smallmatrix}\right)$.

Table D-8 is a listing of the ASTEN function.

NEUTRON ABSORBER VISCOSITY
(AVISC)

The function AVISC returns an estimate of the viscosity of Ag-In-Cd or B_4C neutron absorbers as a function of temperature.

TABLE D-6. LISTING OF THE ATHEXP FUNCTION

```
      FUNCTION ATHEXP(ICTYPE,ATEMP,RFTEMP)
C
C     ATHEXP RETURNS ABSORBER THERMAL EXPANSION STRAINS
C
C     ATHEXP = OUTPUT THERMAL EXPANSION STRAIN (M/M)
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                 1 = SILVER-INDIUM-CADMIUM (.8,.15.05)
C                 2 = BORON CARBIDE
C     ATEMP  = INPUT ABSORBER TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     ATHEXP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      T = RFTEMP
      N = -1
C
      IF(ICTYPE .LT. 2) THEN
   10    IF(T .LT. 1050.) THEN
            EPS = 2.25E-05 * (T - 300.)
         ELSE
            IF(T .LT. 1100.) THEN
               EPS = -0.25875 + 2.625E-04 * T
            ELSE
               EPS = 0.03
            ENDIF
         ENDIF
         IF(N .LT. 0) THEN
            N = N + 2
            EPSR = EPS
            T = ATEMP
            GO TO 10
         ELSE
            ATHEXP = EPS - EPSR
         ENDIF
      ELSE
   20    EPS = -1.1E-03 + T*(3.09E-06 + 1.88E-09*T)
         IF(N .LT. 0) THEN
            N = N + 2
            EPSR = EPS
            T = ATEMP
            GO TO 20
         ELSE
            ATHEXP = EPS - EPSR
         ENDIF
      ENDIF
      RETURN
      END
```

TABLE D-7. LISTING OF THE ADEN FUNCTION

```
      FUNCTION ADEN(ICTYPE,ATEMP)
C
C     ADEN RETURNS ABSORBER DENSITIES
C
C     ADEN    = OUTPUT ABSORBER DENSITY (KG/M**3)
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                1 = SILVER-INDIUM-CADMIUM (.8,.15,.05)
C                2 = BORON CARBIDE
C     ATEMP   = INPUT ABSORBER TEMPERATURE (K)
C
C     ADEN WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ICTYPE .LT. 2) THEN
         RD = 10.17E+03
      ELSE
         RD = 2.5E+03
      ENDIF
         EPS = ATHEXP(ICTYPE,ATEMP,300.)
         ADEN = RD * (1.0 - 3. * EPS)
      RETURN
      END
```

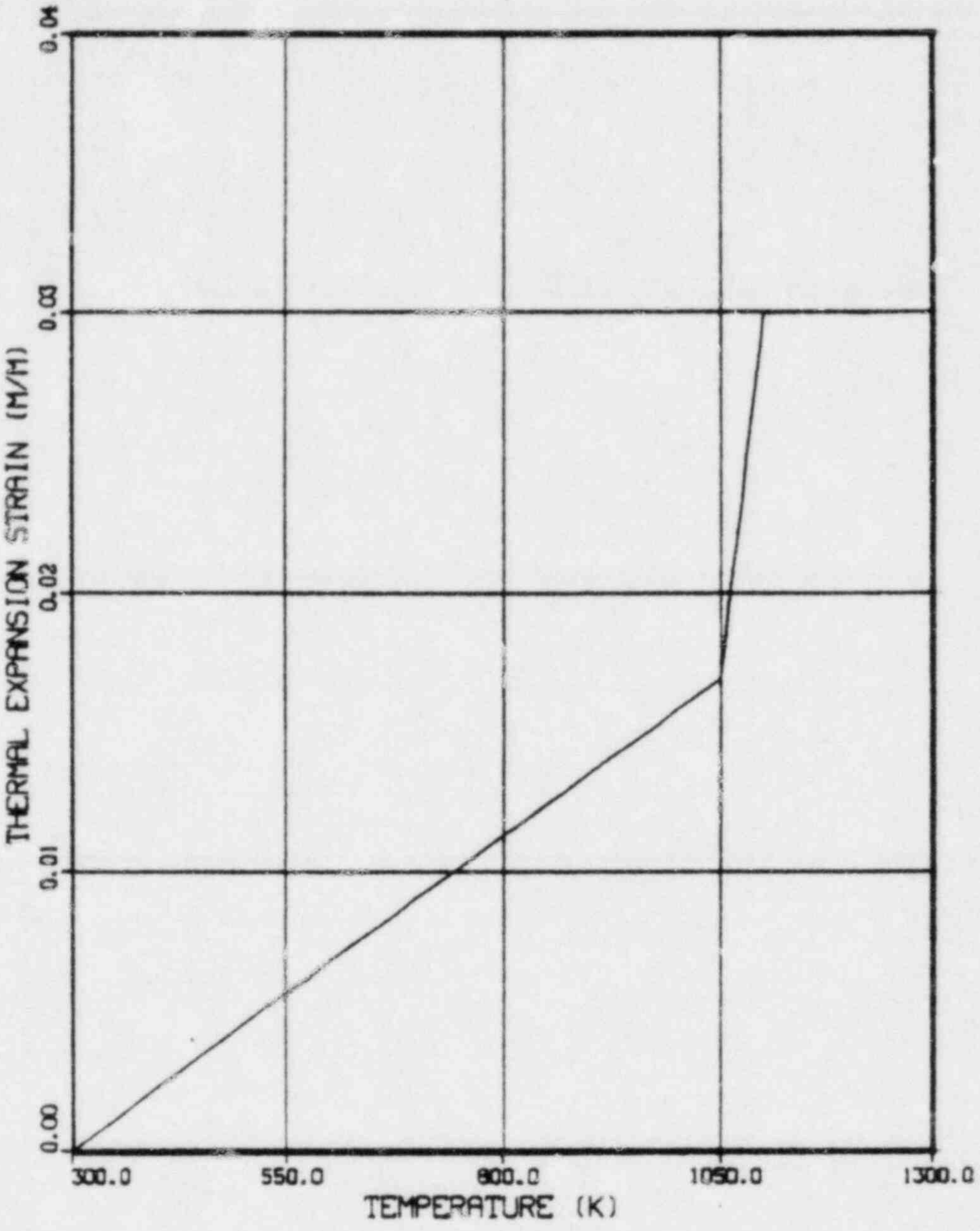

Figure D-8. Thermal expansion strain of Ag-In-Cd absorber.

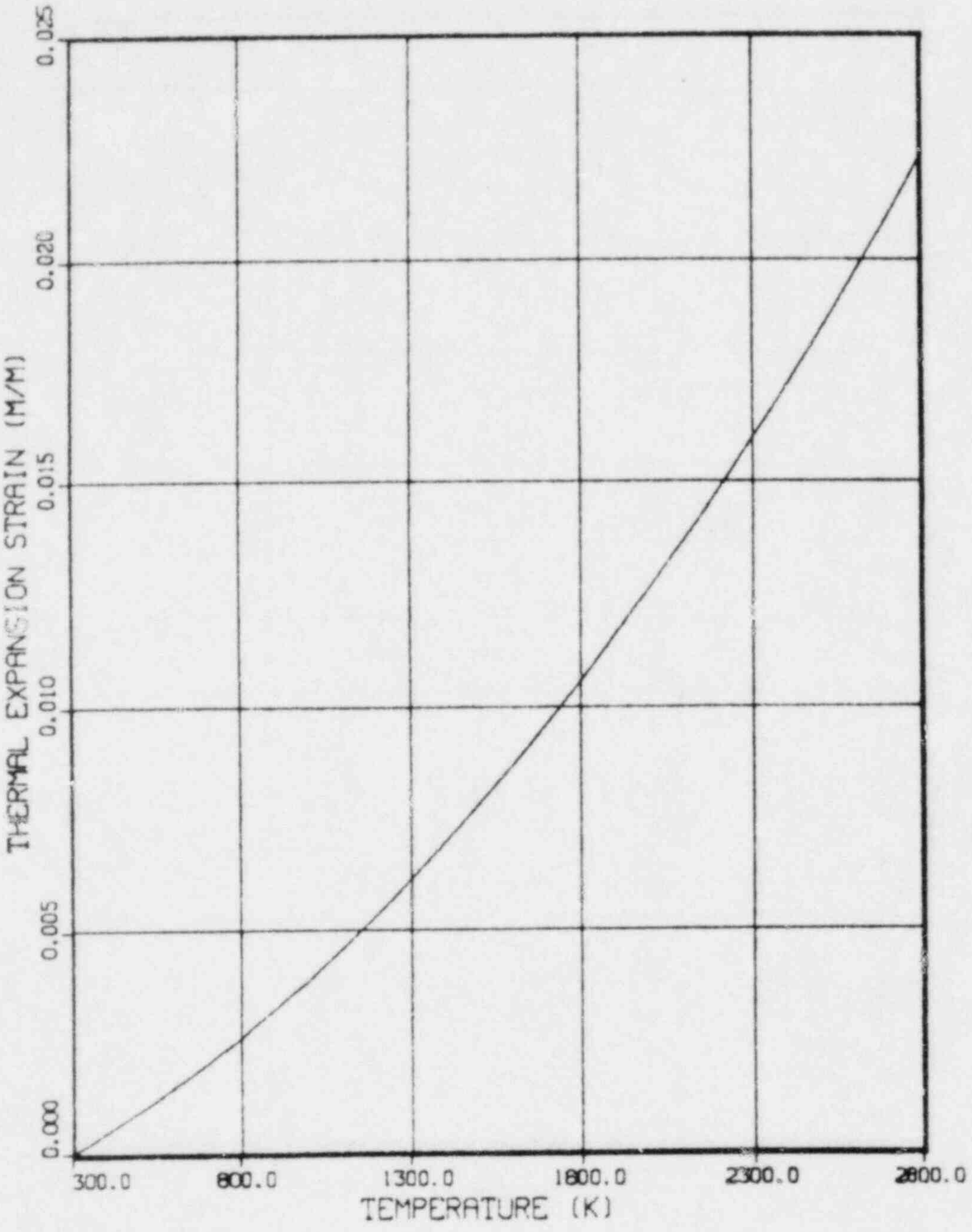

Figure D-9. Thermal expansion strain of B_4C absorber.

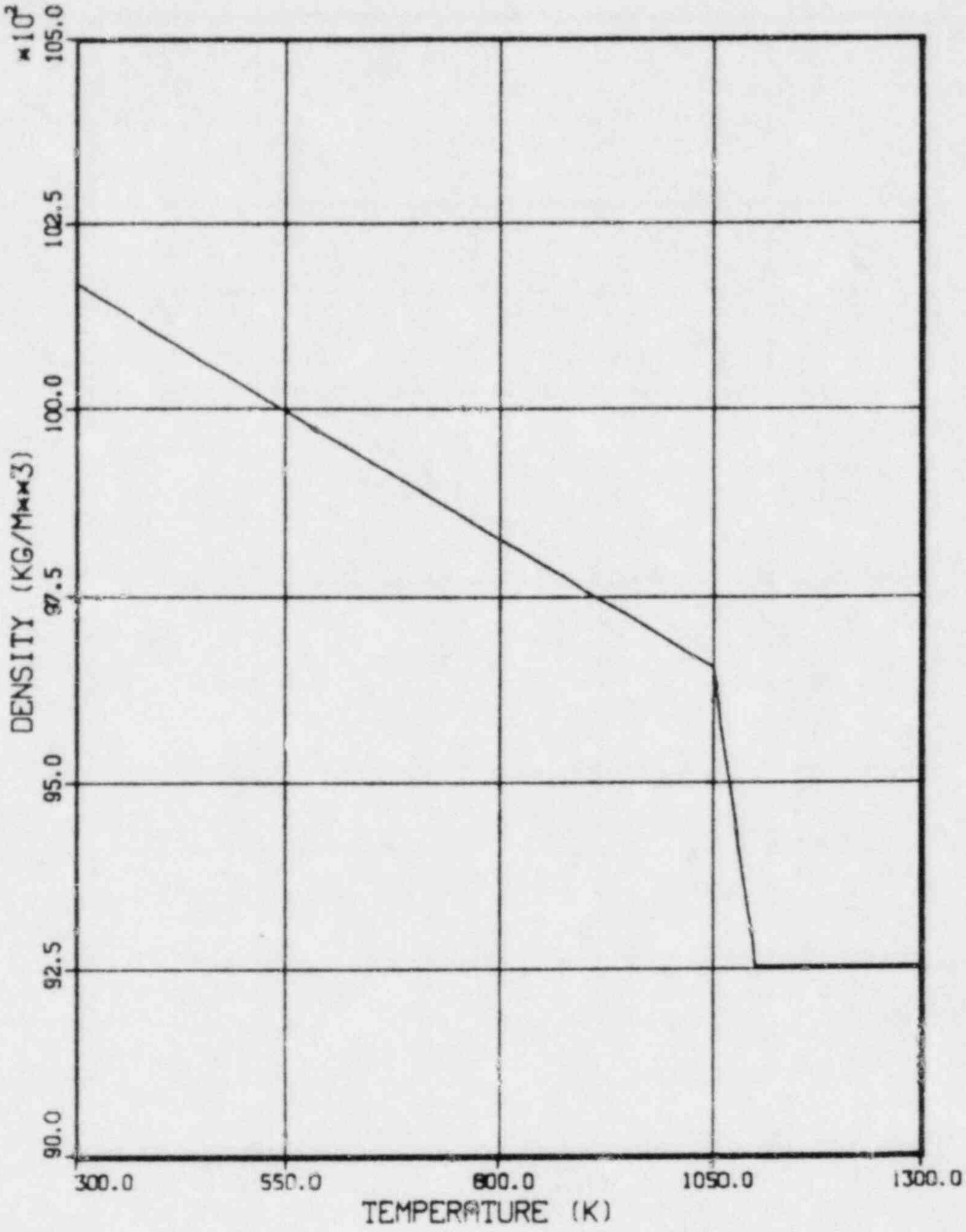

Figure D-10. Ag-In-Cd absorber density.

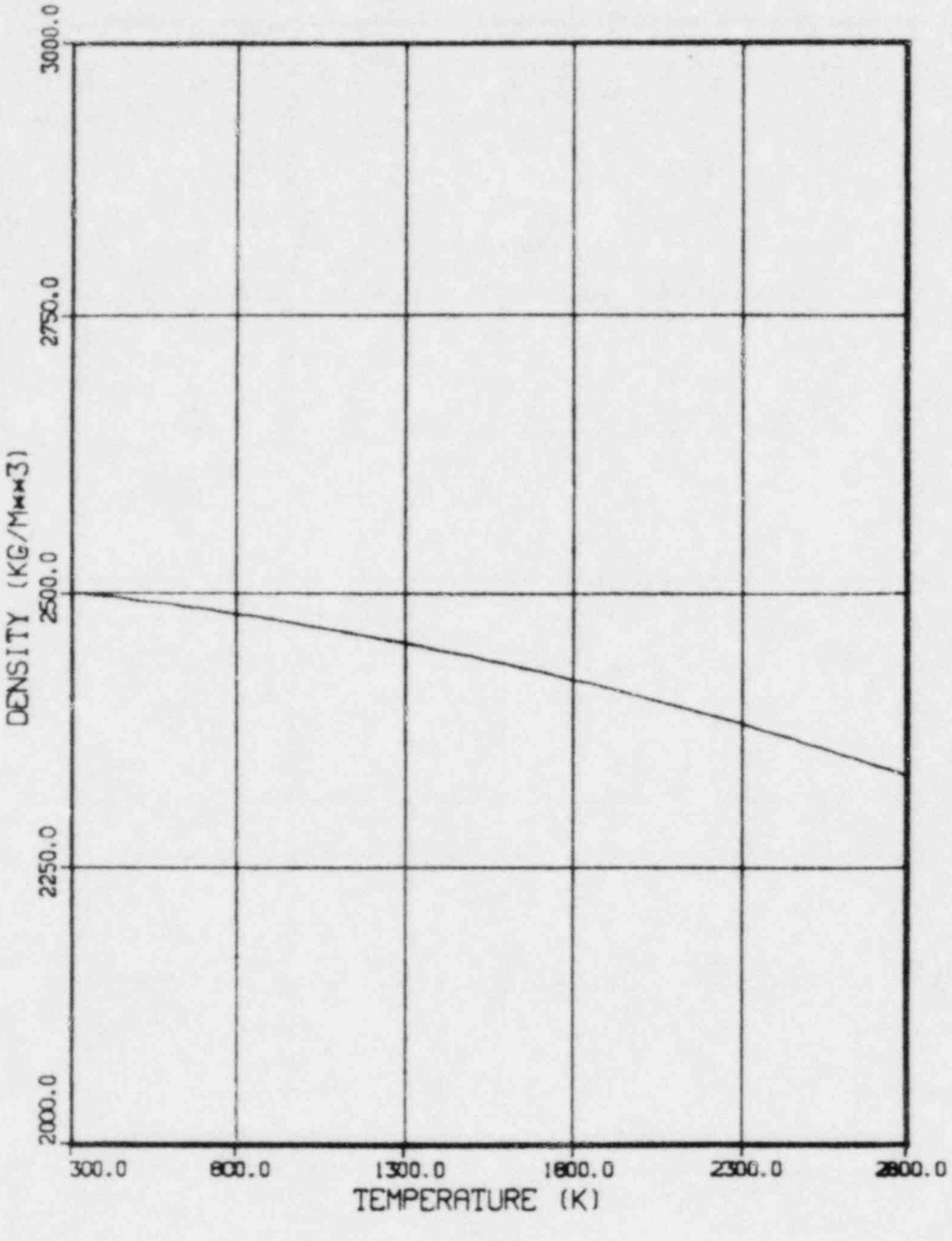

Figure D-11. B_4C absorber density.

TABLE D-8. LISTING OF THE ASTEN FUNCTION

```
      FUNCTION ASTEN(ICTYPE)
C
C     ASTEN RETURNS THE INTERFACIAL SURFACE TENSION OF MOLTEN
C     NEUTRON ABSORBERS ON ZIRCALOY SURFACES
C
C     ASTEN  = OUTPUT INTERFACIAL SURFACE TENSION (N/M)
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                  1 = SILVER-INDIUM-CADMIUM (.8,.15,.05)
C                  2 = BORON CARBIDE
C
C     ASTEN WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      ASTEN = 0.3
      RETURN
      END
```

For Ag-In-Cd a viscosity of 10^{10} Pa•s is returned for temperatures below 1050 K. When the temperature is above 1100 K, a mole fraction weighted average of the alloy component viscosities is used

$$\eta_L = f_{Ag}\,\eta_{Ag} + f_{In}\,\eta_{In} + f_{Cd}\,\eta_{Cd} \tag{D-9}$$

where

η_l = viscosity of liquid absorber (Pa•s)

f_{Ag} = mole fraction of silver in the alloy, 0.808

η_{Ag} = viscosity of silver (Pa•s)

f_{In} = mole fraction of indium in the alloy, 0.143

η_{In} = viscosity of indium (Pa•s)

f_{cd} = mole fraction of cadmium in the alloy, 0.049

η_{cd} = viscosity of cadmium (Pa•s).

The component viscosities are calculated with expressions obtained from procedures recommended by Nazare, Ondraek, and Schulz[D-5]

$$\eta_{Ag} = 2.95 \times 10^{-4} \exp\left(\frac{3187}{T}\right) \tag{D-10}$$

$$\eta_{In} = 3.18 \times 10^{-4} \exp\left(\frac{768}{T}\right) \tag{D-11}$$

$$\eta_{Cd} = 3.19 \times 10^{-4} \exp\left(\frac{1190}{T}\right) \tag{D-12}$$

where

T = absorber temperature (K).

When the temperature is between 1050 and 1100 K an interpolation scheme is used

$$\eta = \frac{\eta_l \, (T - 1050) + 10^{10} \, (1100 - T)}{50} \qquad \text{(D-13)}$$

where

η = viscosity of absorber in the two-phase temperature range, 1050 to 1100 K (Pa•s).

For B_4C absorbers, a viscosity of 10^{10} Pa•s is returned for temperatures less than 2700 K. When the temperature is at or above 2700 K, the expression used is

$$\eta_{B_4C} = 1.21 \times 10^{-4} \exp \left(\frac{9158}{T}\right)$$

where

η_{B_4C} = viscosity of liquid B_4C absorber (Pa•s).

The expected error of the viscosity models for absorbers is ±0.8 of the predicted value because there are no data in support of the model.

Table D-9 is a listing of the AVISC function. Figures D-12 and D-13 are plots showing the calculated liquid phase viscosities for Ag-In-Cd and B_4C absorbers.

TABLE D-9. LISTING OF THE AVISC FUNCTION

```
      FUNCTION AVISC(ICTYPE,ATEMP)
C
C     AVISC RETURNS ABSORBER VISCOSITIES
C
C     AVISC  = OUTPUT ABSORBER VISCOSITY (PA*S)
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                  1 = SILVER-INDIUM-CADMIUM (.8,.15.05)
C                  2 = BORON CARBIDE
C     ATEMP  = INPUT ABSORBER TEMPERATURE (K)
C
C     AVISC WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(ICTYPE .LT. 2) THEN
         IF(ATEMP .LT. 1050.) THEN
            AVISC = 1.0E+10
         ELSE
            VAG = 2.95E-04 * EXP(3187./ATEMP)
            VIN = 3.18E-04 * EXP(768./ATEMP)
            VCD = 3.91E-04 * EXP(1119./ATEMP)
            VLIQ = 0.808*VAG + 0.143*VIN + 0.049*VCD
            IF(ATEMP .LT. 1100.) THEN
               AVISC = (VLIQ*(ATEMP-1050.)+1.0E+10*(1100.-ATEMP))/
     #                 50.
            ELSE
               AVISC = VLIQ
            ENDIF
         ENDIF
      ELSE
         IF(ATEMP .LT. 2700.) THEN
            AVISC = 1.0E+10
         ELSE
            AVISC = 1.21E-04 * EXP(9158./ATEMP)
         ENDIF
      ENDIF
      RETURN
      END
```

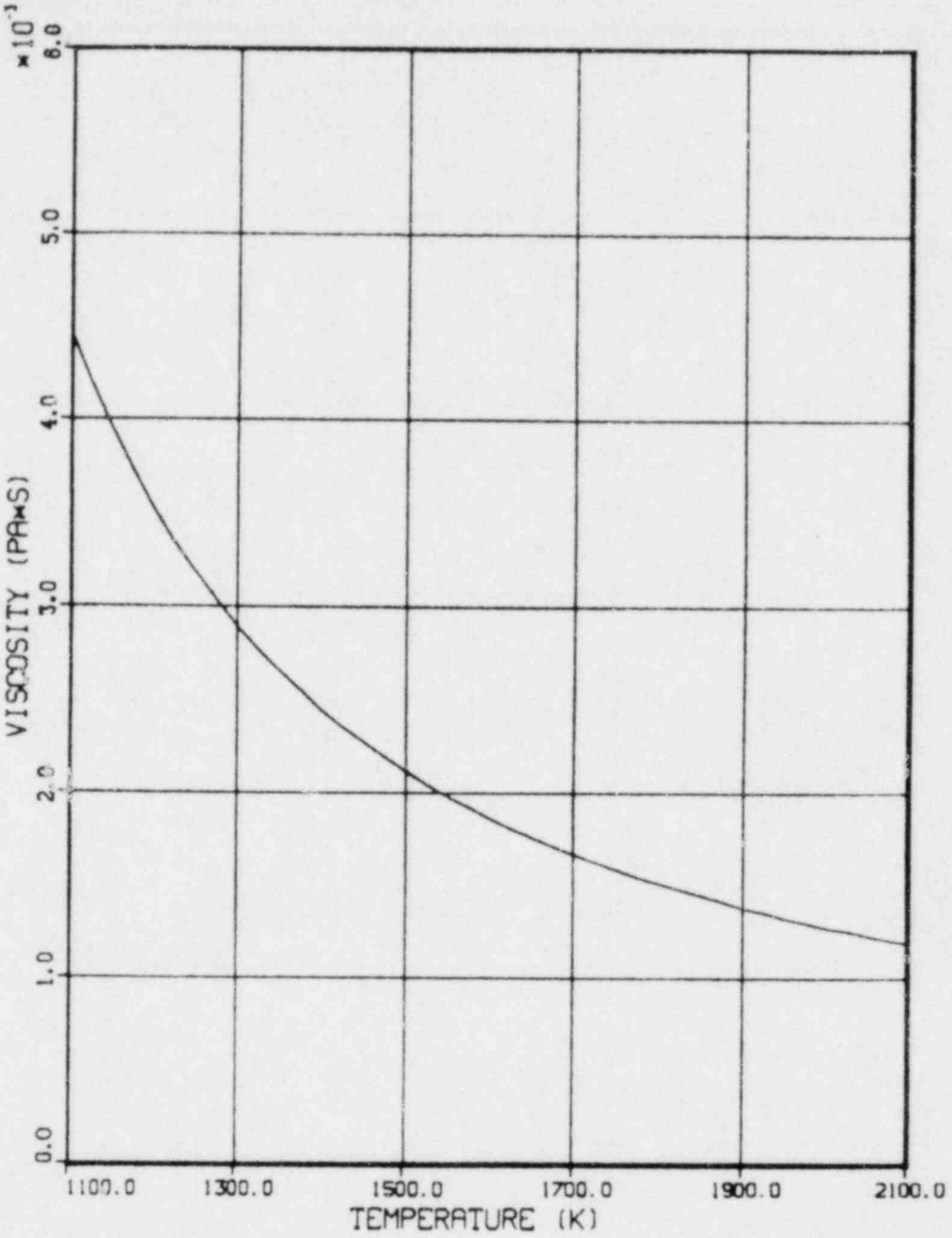

Figure D-12. Ag-In-Cd absorber viscosity.

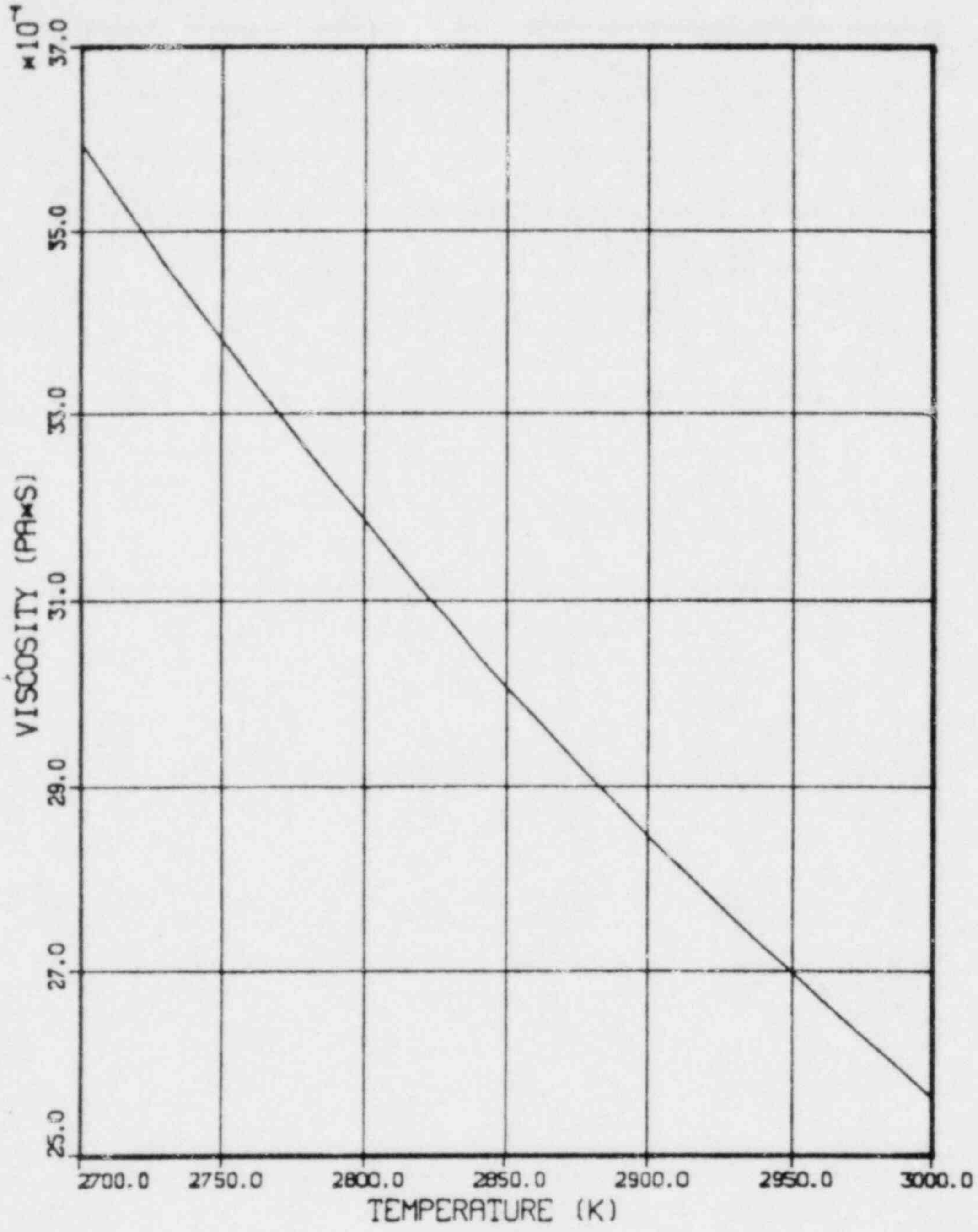

Figure D-13. B_4C absorber viscosity.

NEUTRON ABSORBER MELTING TEMPERATURES

(AHYPRP)

The subroutine AHYPRP provides absorber solidus (appearance of the first liquid phase) and liquidus (melting of the last solid phase) temperatures. There is no required input other than a parameter to identify which absorber material is used.

For the typical Ag-In-Cd alloy, Reference D-4 reports an approximate melting range of 1050 to 1100 K. These numbers are thus used for the solidus and liquidus temperatures of the alloy.

The melting temperature of 2700 K reported on page 943 of Reference D-6 is used for the solidus and liquidus temperature of B_4C.

Table D-10 is a listing of the AHYPRP subroutine.

REFERENCES

D-1. W. B. Murfin et al., Core-Meltdown Experimental Review, SAND74-0382 and NUREG-0205, 1977.

D-2. C. T. Lynch, ed, Handbook of Materials Science, Volume II: Metals, Composites and Refractory Materials, Cleveland, Ohio: CRC Press, Inc., (TA403.4 L94).

D-3. Aerojet Nuclear, Materials Properties Data Book, AGC2275, 1970.

D-4. I. Cohen, E. F. Losco and J. D. Eichenberg, "Metallurgical Design and Properties of Silver-Indium-Cadmium Alloys for PWR Control Rods," Bettis Technical Review, 1958, WAPD-BT-6.

D-5. S. Nazare, G. Ondracek, and B. Schulz, "Properties of Light Water Reactor Core Melts," Nuclear Technology, 32, 1977, pp. 239-246.

D-6. A. Goldsmith, T. E. Waterman, and H. J. Hirschhorn, Handbook of Thermophysical Properties of Solid Materials. Revised Edition Volume III: Ceramics, New York: The MacMillan Company, 1961, (TA 407 A73 V.3).

D-7. C. J. Smithells and E. A. Brandes (eds.) Metals Reference Book, London and Boston: Butterworths (TN 671 S55 1956).

D-8. B. C. Allen, "The Surface Tension of Liquid Transition Metals at Their Melting Points," Transactions of the Metallurgical Society of AIME, 227, 1963, pp. 1175-1183.

TABLE D-10. LISTING OF THE AHYPRP SUBROUTINE

```
      SUBROUTINE AHYPRP(ICTYPE,ASOL,ALIQ)
C
C     AHYPRP RETURNS ABSORBER PHASE TRANSITION TEMPERATURES
C
C     ASOL   = OUTPUT ABSORBER SOLIDUS TEMPERATURE (K)
C
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C              1 = SILVER-INDIUM-CADMIUM (.8,.15.05)
C              2 = BORON CARBIDE
C
C     AHYPRP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
C
      IF(ICTYPE .LT. 2) THEN
         ASOL = 1050.
         ALIQ = 1100.
      ELSE
         ASOL = 2700.
         ALIQ = 2700.
      ENDIF
      RETURN
      END
```

APPENDIX E
CONTROL ROD CLADDING PROPERTIES

APPENDIX E

CONTROL ROD CLADDING PROPERTIES

A collection of 304 stainless steel properties has been prepared to allow modeling of the temperature and possible failure by melting or oxidation of stainless steel control rod cladding. Properties included are specific heat capacity, enthalpy, thermal conductivity, thermal expansion, density, and oxygen uptake rate.

CONTROL ROD CLADDING SPECIFIC HEAT CAPACITY AND ENTHALPY

(SCP, SENTHL)

The function SCP returns the specific heat capacity of 304 stainless steel as a function of temperature. SENTHL calculates the enthalpy change as a function of temperature and a reference temperature (for which enthalpy change will be zero).

For specific heat capacity the expressions used are

$$C_{ps} = 326 + T\ (0.298 - 9.56 \times 10^{-5} \times T)\quad ,\ 300 \leq T < 1558\ K \qquad \text{(E-1a)}$$

$$C_{ps} = 558.228\quad ,\ T > 1558\ K \qquad \text{(E-1b)}$$

where

C_{ps} = control rod cladding specific heat capacity (J/kg•k)

T = cladding temperature (K).

Equation (E-1a) is a fit to values of 398, 488, and 540 J/kg•K at 263, 700, and 1119 K, respectively, obtained from a curve on page 19-26 of Reference E-1. Since the curve reaches a maximum between 1558 and 1559 K, Equation (E-1a) is replaced with a value equal to the maximum for temperatures greater than or equal to 1558 K.

SENTHL uses the following expressions for 304 stainless steel enthalpy:

$$h_s = 326 \times T + 0.149 \times T^2 - 3.187 \times 10^{-5} \times T^3 \text{ , } 300 \leq T < 1558 \text{ K} \qquad \text{(E-2a)}$$

$$h_s = -1.206610 \times 10^5 + 558.228 \times T \text{ , } 1558 \leq T < 1671 \text{ K} \qquad \text{(E-2b)}$$

$$h_s = -8.475661 \times 10^6 + 5558.228 \times T \text{ , } 1671 \leq T \leq 1727 \text{ K} \qquad \text{(E-2c)}$$

$$h_s = 1.593390 \times 10^5 + 558.228 \times T \text{ , } 1727 \text{ K} < T \qquad \text{(E-2d)}$$

where

h_s = control rod cladding enthalpy (J/kg)

T = control rod cladding temperature (K).

Equations (E-2a) and (E-2b) are integrals of Equations (E-1a) and (E-1b). Equation (E-2c) includes not only the specific heat but also a heat of fusion of 2.8×10^5 J/kg which is added linearly over the stainless steel melting range. This heat of fusion was calculated from heats of fusion for Cr, Fe and Ni given on page 87 of Reference E-2 and the composition of 304 stainless steel given on page 4-8 of Reference E-3. The heat of fusion was assumed to be the atomic fraction of each element times the elemental heat of fusion.

The expected standard error of Equations (E-1a) to (E-2d) is 0.1 times the predicted values.

Tables E-1 and E-2 are listings of the SCP and SENTHL functions while Figures E-1 and E-2 illustrate the calculated values of specific heat capacity and enthalpy change relative to a reference temperature of 300 K.

TABLE E-1. LISTING OF THE SCP FUNCTION

```
      FUNCTION SCP(CTEMP)
C
C     SCP RETURNS THE SPECIFIC HEAT CAPACITY AT CONSTANT
C     PRESSURE FOR 304 STAINLESS STEEL CLADDING
C
C     SCP     = OUTPUT STEEL CLADDING SPECIFIC HEAT
C               CAPACITY (J/(KG*M))
C
C     CTEMP   = INPUT CLADDING TEMPERATURE (K)
C
C     SCP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      IF(CTEMP .LT. 1558.) THEN
         SCP = 326. + CTEMP*(0.298 - CTEMP*9.56E-05)
      ELSE
         SCP = 558.228
      ENDIF
      RETURN
      END
```

TABLE E-2. LISTING OF THE SENTHL FUNCTION

```
      FUNCTION SENTHL(CTEMP,RFTEMP)
C
C     SENTHL RETURNS THE CHANGE IN ENTHALPY OF 304 STAINLESS
C     STEEL DURING A CONSTANT PRESSURE CHANGE IN TEMPERATURE
C
C     SENTHL = OUTPUT CHANGE IN STEEL ENTHALPY (J/KG)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     SENTHL WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      T = RFTEMP
      N = -1
C
   10 IF(T .LT. 1558.) THEN
         H = T*(326. + T*(0.149 - T*3.167E-05))
      ELSE
         IF(T .LT. 1671.) THEN
            H = -1.23661E+05 + T*558.226
         ELSE
            IF(T .LE. 1727.) THEN
               H = -8.475661E+06 + T*5558.228
            ELSE
               H = 1.59339E+05 + T * 558.28
            ENDIF
         ENDIF
      ENDIF
      IF(N .LT. 0) THEN
         N = N + 2
         HR = H
         T = CTEMP
         GO TO 10
      ELSE
         SENTHL = H - HR
      ENDIF
      RETURN
      END
```

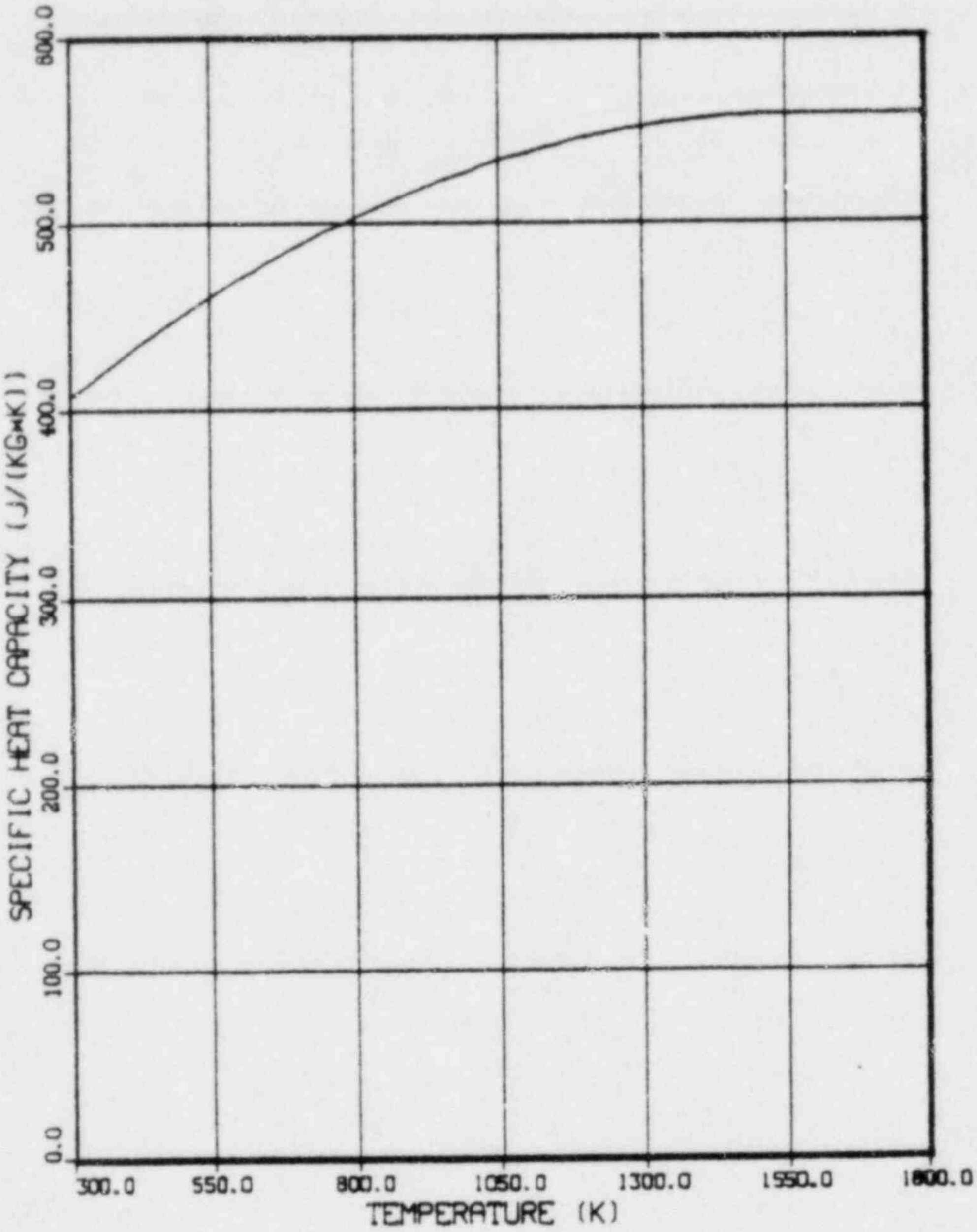

Figure E-1. Stainless steel specific heat capacity at constant pressure.

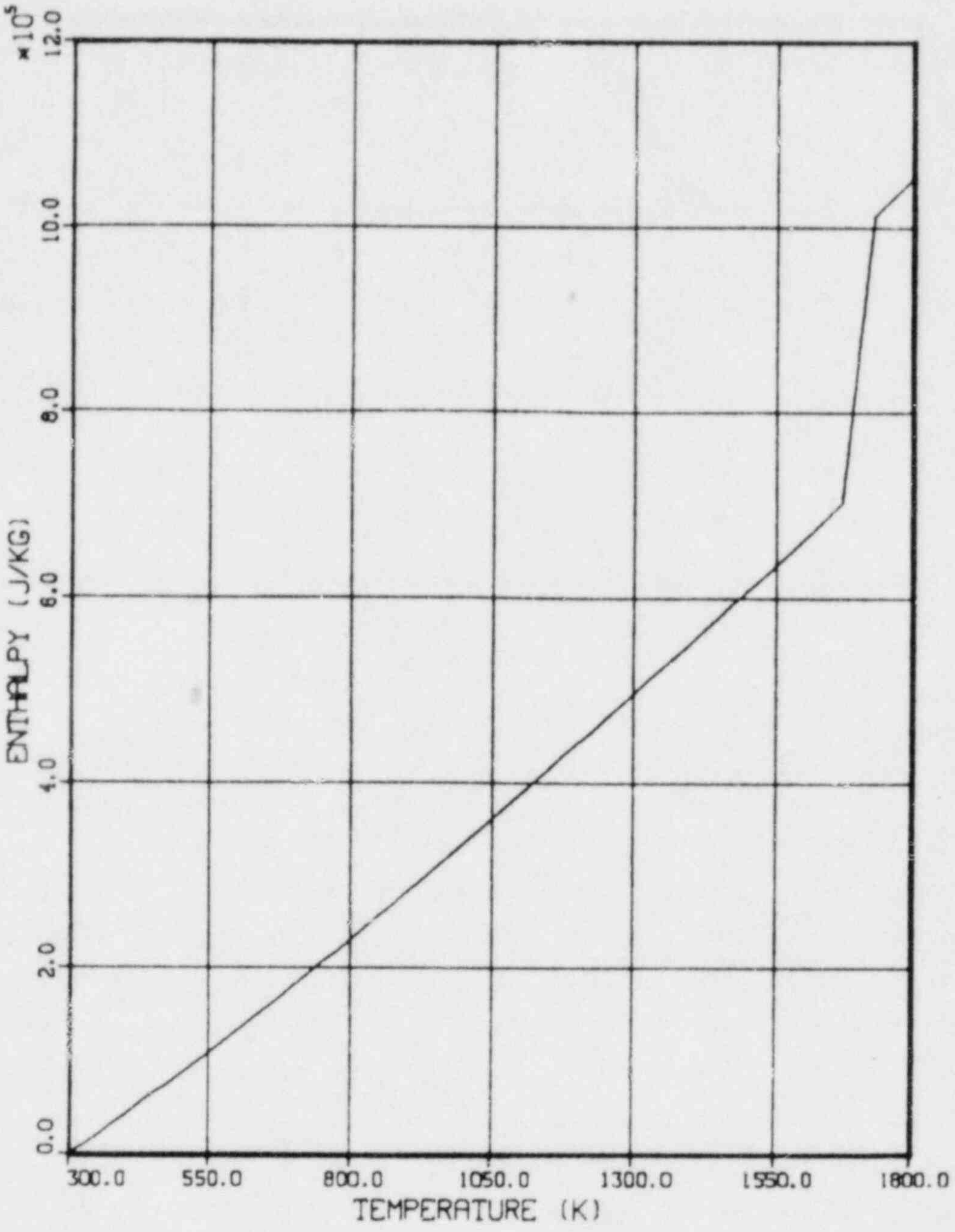

Figure E-2. Stainless steel enthalpy change at constant pressure.

CONTROL ROD CLADDING THERMAL CONDUCTIVITY
(STHCON)

The thermal conductivity of 304 stainless steel as a function of temperature is calculated in the function STCHON with the following correlation:

$$K_s = 7.58 + 0.0189\ T \quad , \ 300 \le T < 1671\ \mathrm{K} \qquad \text{(E-3a)}$$

$$K_s = 610.9393 - 0.3421767\ T \quad , \ 1671 \le T < 1727\ \mathrm{K} \qquad \text{(E-3b)}$$

$$K_s = 20 \quad , \ T \ge 1727\ \mathrm{K} \qquad \text{(E-3c)}$$

where

K_s = control rod cladding thermal conductivity (W/m•K)

T = control rod cladding temperature (K).

Equation (E-3a) is a fit to values of 14.65 and 25.83 W/m•K at 374 and 965 K obtained from a curve on page 19-18 of Reference E-1. Equation (E-3c) is an approximation of the conductivity at the lowest temperature for which the steel is completely melted. The approximation was obtained by evaluating Equation (E-3a) for the solid stainless steel at the melting temperature and noting that metals with twelve nearest neighbors like 304 stainless steel (which has a face centered cubic lattice) suffer a 50% reduction in thermal conductivity when they melt.[E-4] Equation (E-3b) interpolates between the value predicted by Equation (E-3a) at 1671 K and the value predicted by Equation (E-3c). The expected standard error of the predicted conductivities is ±0.2 times the predicted conductivity.

Table E-3 is a listing of the STHCON function and the thermal conductivity predicted by the function is illustrated as a function of temperature in Figure E-3.

CONTROL ROD CLADDING THERMAL EXPANSION AND DENSITY
(STHEXP, SDEN)

The function STHEXP calculates 304 stainless steel thermal expansion strain and SDEN computes the density of this material. STHEXP requires the control rod cladding temperature and a reference temperature (for which thermal strain will be zero) while SDEN requires only the temperature.

The expressions used to calculate thermal expansion strains are

$$\epsilon_S = 1.57 \times 10^{-5} \times T + 1.69 \times 10^{-9} \times T^2 \quad , 300 \leq T < 1671 \text{ K} \qquad \text{(E-4a)}$$

$$\epsilon_S = -2.986634 \times 10^{-1} + 1.972573 \times 10^{-4} \times T \quad , 1671 \leq T < 1727 \text{ K} \qquad \text{(E-4b)}$$

$$\epsilon_S = 4.2 \times 10^{-2} \quad , T \geq 1727 \text{ K} \qquad \text{(E-4c)}$$

where

ϵ_S = control rod cladding thermal strain (m/m)

T = control rod cladding temperature (K).

Equation (E-4a) is derived from thermal expansion rates of 17.2×10^{-6} and 18.9×10^{-6} m/m•K at 455 and 959 K. These values were taken from a curve on page 197 of Reference E-1. A linear fit to the thermal expansion rates yields an expression which can be integrated to produce Equation (E-4a). The constant of integration is ignored because the quanity returned by STHEXP is the strain predicted by Equations (E-4a) to (E-4c) at the given temperature minus the strain predicted at the reference temperature. Equation (E-4c) is the strain predicted by Equation (E-4a) at

TABLE E-3. LISTING OF THE STHCON FUNCTION

```
      FUNCTION STHCON(CTEMP)
C
C     STHCON RETURNS 304 SS STAINLESS STEEL CONDUCTIVITY
C
C     STHCON = OUTPUT STEEL THERMAL CONDUCTIVITY (W/(M*K))
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C
C     STHCON WAS CODED BY D. L. HAGRMAN MARCH 1982
      IF(CTEMP .LT. 1671.) THEN
         STHCON = 7.58 + CTEMP * 0.0189
      ELSE
         IF(CTEMP .LT. 1727.) THEN
            STHCON = 610.9393 - CTEMP * 0.3421767
         ELSE
            STHCON = 20.
         ENDIF
      ENDIF
      RETURN
      END
```

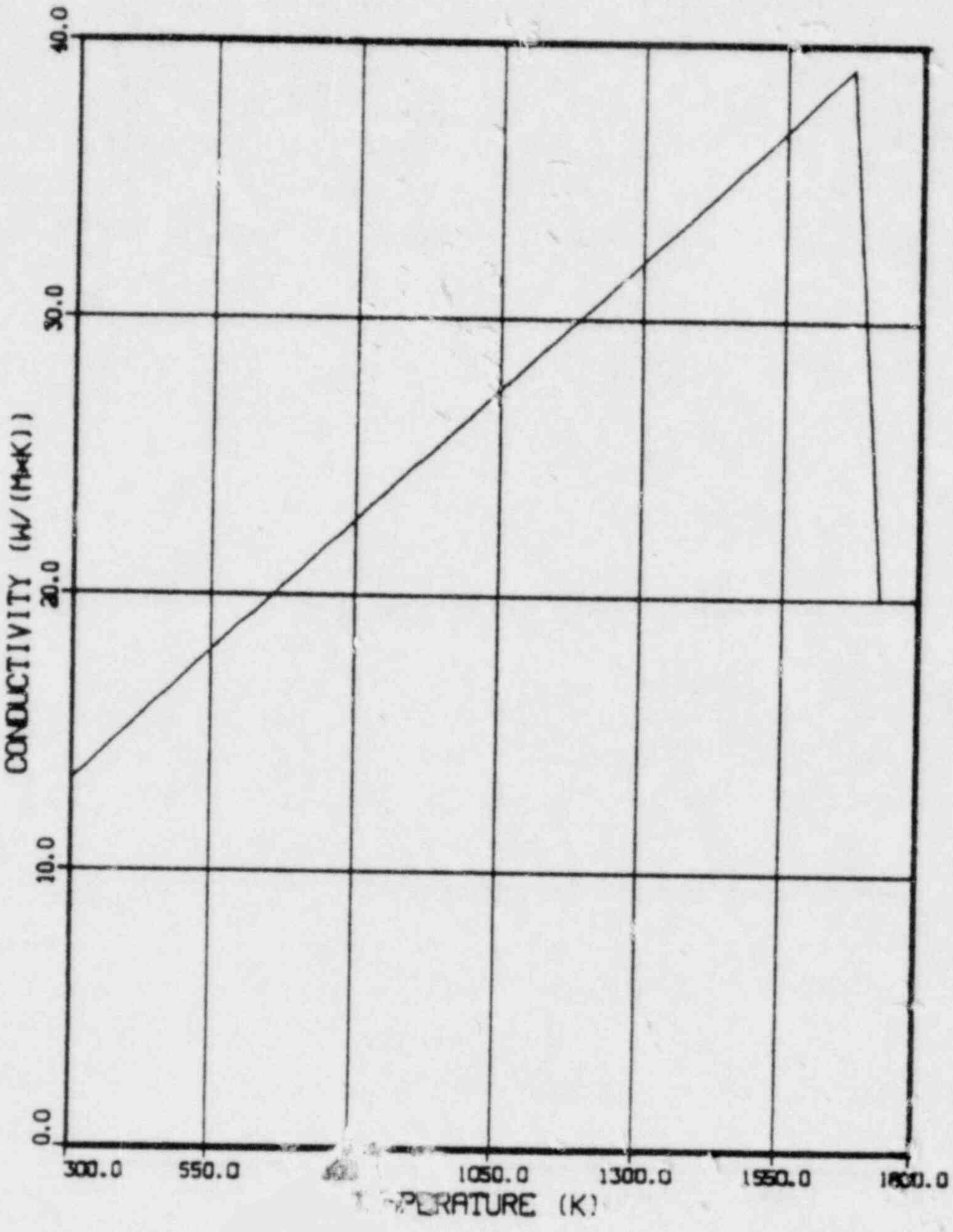

Figure E-3. Stainless steel thermal conductivity.

the lowest temperature for which the steel is completely melted, 1727 K, plus an assumed additional expansion of 1% (3% volume increase) because of the melting. Equation (E-4b) is a linear interpolation of the values predicted by Equation (E-4a) at 1671 K and Equation (E-4c) at 1727 K. The expected standard error of these expressions is about 0.1 times the predicted value.

The function SDEN uses the general relation between density and thermal strain, Equation (B-10), together with a reference density of 7.9×10^3 Kg/m^2 at 300 K obtained from page 87 of Reference E-2. The expected standard error of this density is the uncertainty of reference density, ±50 Kg/m^3.

Tables E-4 and E-5 are listings of the STHEXP and SDEN functions. The thermal expansion strain returned by STHEXP for a reference temperature of 300 K is illustrated in Figure E-4 and the density calculated with the SDEN function is shown in Figure E-5.

CONTROL ROD CLADDING OXYGEN UPTAKE
(SOXIDE, SOXWGN, SOXTHK)

Three subcodes are employed to describe the oxygen uptake of 304 stainless steel. The SOXIDE subroutine returns the linear power generated by the oxidation of stainless steel, the oxidation weight gain at the end of a time step, and an estimate of the oxide layer thickness at the end of a time step. Required input information is the cladding temperature, the time step duration, the outside diameter of the as-fabricated cladding, the initial weight gain, and the initial oxide layer thickness. SOXWGN is a function which returns the parabolic rate constant for the oxidation weight gain of stainless steel as a function of temperature. The parabolic rate constant for the oxide layer thickness is calculated by SOXTHK as a function of temperature.

TABLE E-4. LISTING OF THE STHEXP FUNCTION

```
      FUNCTION STHEXP(CTEMP,RFTEMP)
C
C     STHEXP RETURNS 304 SS THERMAL EXPANSION STRAINS
C
C     STHCON = OUTPUT STEEL THERMAL STRAIN (M/M)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C     RFTEMP = INPUT REFERENCE TEMPERATURE (K)
C
C     STHEXP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      T = RFTEMP
      N = -1
C
   10 IF(T .LT. 1671.) THEN
         EPS = T * (1.57E-05 + T * 1.69E-09)
      ELSE
         IF(T .LT. 1727.) THEN
            EPS = -0.2986634 + T*1.972573E-04
         ELSE
            EPS = 4.2E-02
         ENDIF
      ENDIF
      IF(N .LT. 0) THEN
         N = N + 2
         EPSR = EPS
         T = CTEMP
         GO TO 10
      ELSE
         STHEXP = EPS - EPSR
      ENDIF
      RETURN
      END
```

TABLE E-5. LISTING OF THE SDEN FUNCTION

```
      FUNCTION SDEN(CTEMP)
C
C     SDEN RETURNS 304 STAINLESS STEEL DENSITY
C
C     SDEN   = OUTPUT STEEL DENSITY (KG/M**3)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C
C     THE FUNCTION STHEXP IS CALLED BY THIS FUNCTION
C
C     SDEN WAS CODED BY D. L. HAGRMAN MARCH 1982
C
C
      EPS = STHEXP(CTEMP,300.)
      SDEN = 7.8E+03 * (1. - 3.0 * EPS)
      RETURN
      END
```

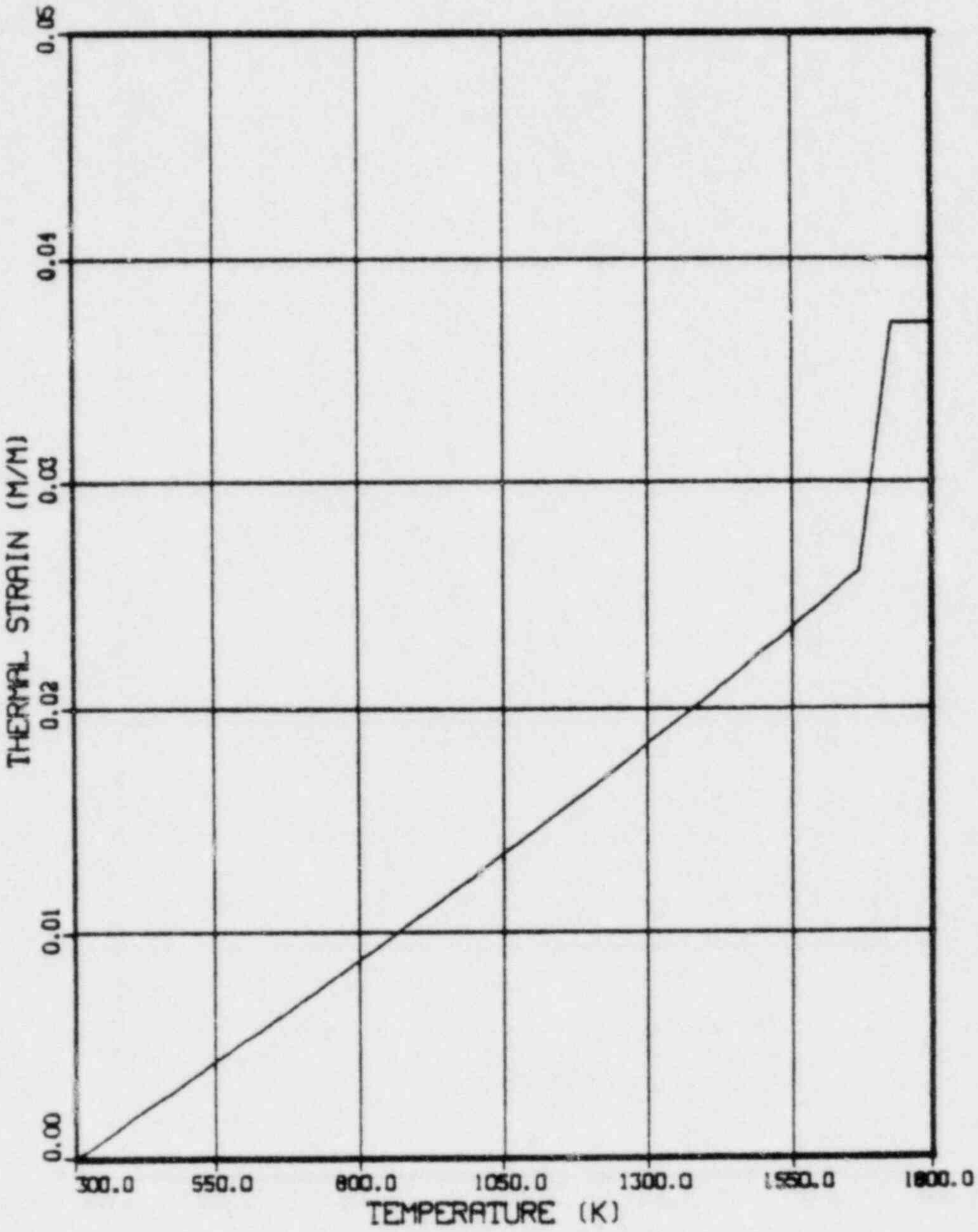

Figure E-4. Stainless steel thermal expansion strain.

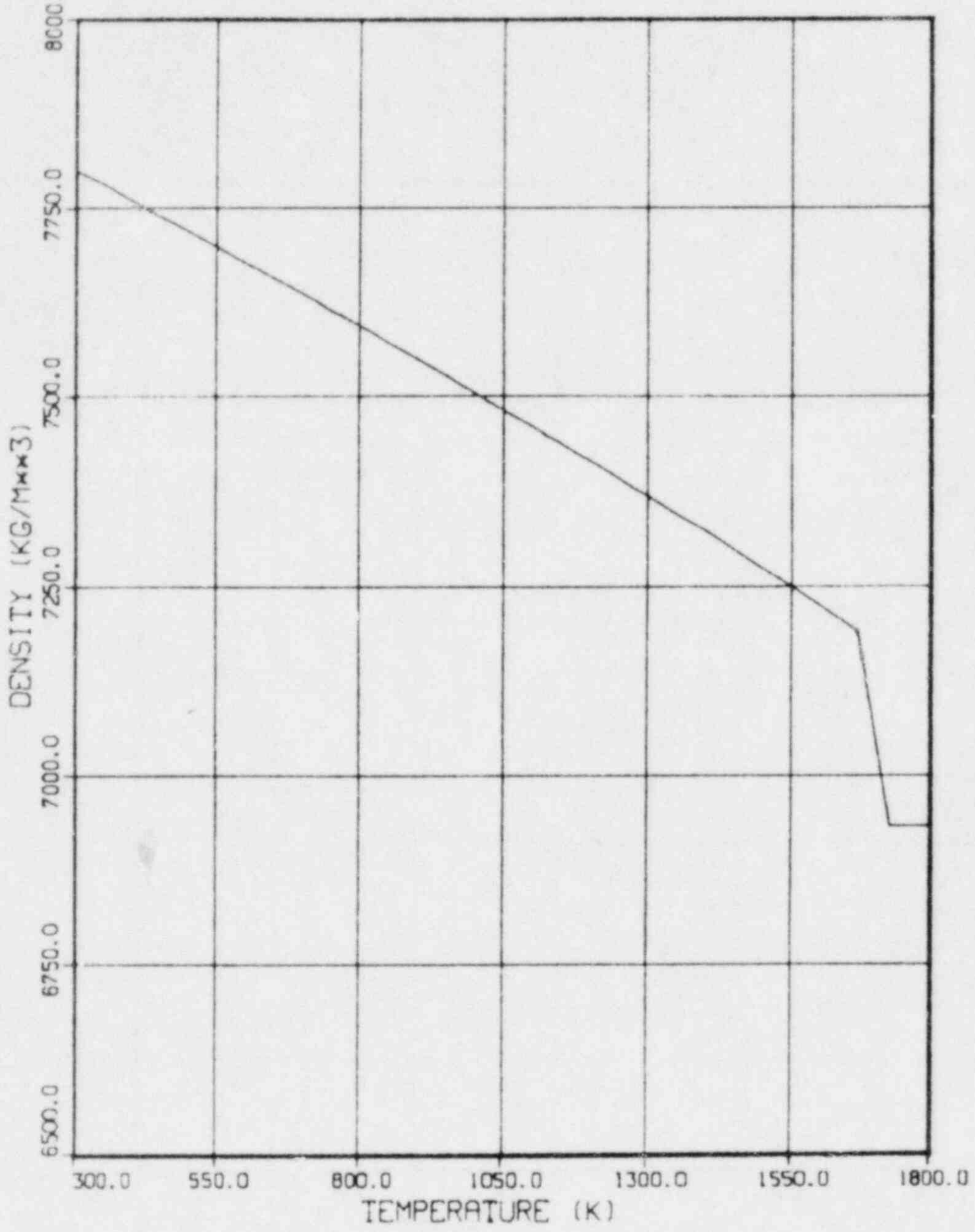

Figure E-5. Stainless steel density.

The equation used to model the oxidation parameters are both of the form

$$Z_f = \left(Z_i + 2A \exp(-B/T)\, \Delta t\right)^{\frac{1}{2}} \tag{E-5}$$

where

Z_f = value of the oxidation parameter (oxide layer thickness or cladding weight gain per unit surface area due to oxidation) at the end of a time span of Δt

Z_i = value of the oxidation parameter at the start of the time span

T = temperature of the oxide layer (K)

Δt = time span (s)

A, B = rate constants.

Table E-6 lists the rate constants the rate constants used with Equation (E-5) to model weight gain or oxide layer thickness. The parabolic rate constants calculated by SOXWGN and SOXTHK are the quantities

$$R = 2A \exp(-B/T) \tag{E-6}$$

where

R = parabolic rate constant for oxidation parameter described by rate constants A and B.

TABLE E-6. RATE CONSTANTS FOR USE WITH EQUATION (E-5) TO PREDICT OXIDATION

Oxidation Parameter	A	B
Cladding weight gain (kg/m^2 surface)	1.2×10^6 $kg^2/m^4 \cdot s$	42 428 K
Oxide thickness	300 m^2/s	42 428 K

The expression used to model the linear power generated by the oxidation of stainless steel is

$$P = 4.85 \times 10^6 \, D_o \frac{(M_f - M_i)}{\Delta t} \qquad \text{(E-7)}$$

where

P = rate of heat generation per unit length of 304 stainless steel cladding (W/m)

D_o = cladding outside diameter without oxidation (m)

M_f = mass gain per unit surface area due to oxidation at end of time step (kg/m^2)

M_i = mass gain per unit surface area due to oxidation at start of time step (kg/m^2).

The power represented by this equation is about one tenth the power represented by the corresponding equation for zircaloy oxidation when the mass gains are similar.

Equation (E-5) with oxidation rate constants for weight gain was taken from page 50 of Reference E-2. If the composition and density of the oxide are known, the rate constant for the oxide layer thickness can be determined from the rate constant for oxidation weight gain:

$$A = \frac{B}{WFOX^2 \rho^2} \qquad \text{(E-8)}$$

where

A = rate constant for oxide layer thickness (m^2/s)

B = rate constant for oxidation weight gain ($kg^2/m^4 \cdot s$)

WFOX = mass fraction oxide in the oxide (kg oxygen/kg oxide)

ρ = density of the oxide film (kg/m^3).

However, determination of a rate constant for the oxide layer thickness is complicated by uncertainty about the oxide density because of considerable foaming of the stainless steel during oxidation.[E-2,E-5]. Moreover, page 53 of Reference E-2 reports very complex oxide structures. The oxide is expected to contain some FeO, Fe_3O_4, Fe_2O_3, CrO_3, Cr_2O_3, NiO, and mixed spinels. The rate constant in Table E-6 was calculated by assuming the composition of FeO and a density of 3000 kg/m^3 (about half the density of nonporous FeO).

Equation (E-7) for the linear power generated by oxidation is derived by subtracting the heat required to dissociate H_2O, 2.4182×10^5 J/mole,[E-6] from the heat of reaction of iron and oxygen to form FeO, 2.67×10^5 J/mole.[E-7] The resultant heat of formation for one mole of FeO from one mole of H_2O is multiplied by the rate of oxygen uptake in moles and the circumference of the cladding to obtain Equation (E-7).

The expected standard deviation of the oxide layer thickness is ±0.5 times the predicted thickness. The expected standard deviation of the oxidation weight gain and oxidation power is somewhat less, ±0.25 times the predicted value, because the oxide composition and density do not affect the prediction of these quantities.

Tables E-7 to E-9 are listings of the SOXIDE, SOXWGN, and SOXTHK subcodes. Figures E-6 and E-7 illustrate the parabolic constants calculated with the SOXWGN and SOXTHK functions. The time-step-averaged power per meter of rod calculated with SOXIDE for a 1.25×10^{-2} meter diameter rod with no initial oxide layer and a one second time step is shown

TABLE E-7. LISTING OF THE SOXIDE SUBROUTINE

```
      SUBROUTINE SOXIDE(CTEMP,DT,DROD,SOWTI,SOTKI,SOWTF,SOTKF,PAVE)
C
C     SOXIDE RETURNS 304 STAINLESS STEEL OXIDATION MEASURES --
C     AVERAGE LINEAR POWER GENERATED BY THE OXIDATION REACTION,
C     OXYKGEN WEIGHT GAIN AND ESTIMATED OSIDE LAYER THICKNESS.
C
C     PAVE   = OUTPUT TIME-STEP-AVERAGED LINEAR POWER GENERATED
C              BY THE OXIDATION REACTION (W/M)
C     SOWTF  = OUTPUT OXYGEN WEIGHT GAIN AT END OF TIME STEP (KG/M**2)
C     SOTKF  = OUTPUT OXIDE LAYER THICKNESS AT END OF TIME STEP (M)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C     DT     = INPUT TIME STEP SIZE (S)
C     DROD   = INPUT DIAMETER OF AS-FABRICATED ROD (M)
C     SOWTI  = INPUT OXYGEN WEIGHT GAIN AT START OF TIME STEP (KG/M**2)
C     SOTKI  = INPUT OXIDE LAYER THICKNESS AT START OF TIME STEP (M)
C
C     THE FUNCTIONS SOXWGN AND SOXTHK ARE CALLED BY THIS SUBROUTINE
C
C     SOXIDE WAS CODED BY D. L. HAGRMAN MARCH 1982
C

      RWGN = SOXWGN(CTEMP)
      RTHK = SOXTHK(CTEMP)
C
      SOWTF = SQRT(SOWTI**2 + RWGN*DT)
      SOTKF = SQRT(SOTKI**2 + RTHK*DT)
      PAVE = 4.85E+06 * DROD * (SOWTF - SOWTI)/DT
      RETURN
      END
```

TABLE E-8. LISTING OF THE SOXWGN FUNCTION

```
      FUNCTION SOXWGN(CTEMP)
C
C     SOXWGN RETURNS THE PARABOLIC OXIDATION RATE CONSTANT,C,
C     FOR 304 SS AND FOR THE EQUATION
C
C        FINAL WEIGHT GAIN**2 = INITIAL WEIGHT GAIN**2 + C * TIME STEP
C
C     SOXWGN = OUTPUT PARABOLIC OXIDEATION RATE CONSTANT FOR
C              OXIDATION WEIGHT GAIN (KG**2/((M**4*S))
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C
C     SOXWGN WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      SOXWGN = 2. * 1.2E+08 * EXP(-42428./CTEMP)
      RETURN
      END
```

TABLE E-9. LISTING OF THE SOXTHK FUNCTION

```
      FUNCTION SOXTHK(CTEMP)
C
C     SOXTHK RETURNS THE PARABOLIC OXIDATION RATE CONSTANT,C,
C     FOR 304 SS AND FOR THE EQUATION
C
C        FINAL THICKNESS**2 = INITIAL THICKNESS**2 + C * TIME STEP
C
C     SOXWGN = OUTPUT PARABOLIC OXIDEATION RATE CONSTANT FOR
C              OXIDATION THICKNESS (M**2/S)
C
C     CTEMP  = INPUT CLADDING TEMPERATURE (K)
C
C     SOXTHK WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      SOXTHK = 2. * 300. * EXP(-42428./CTEMP)
      RETURN
      END
```

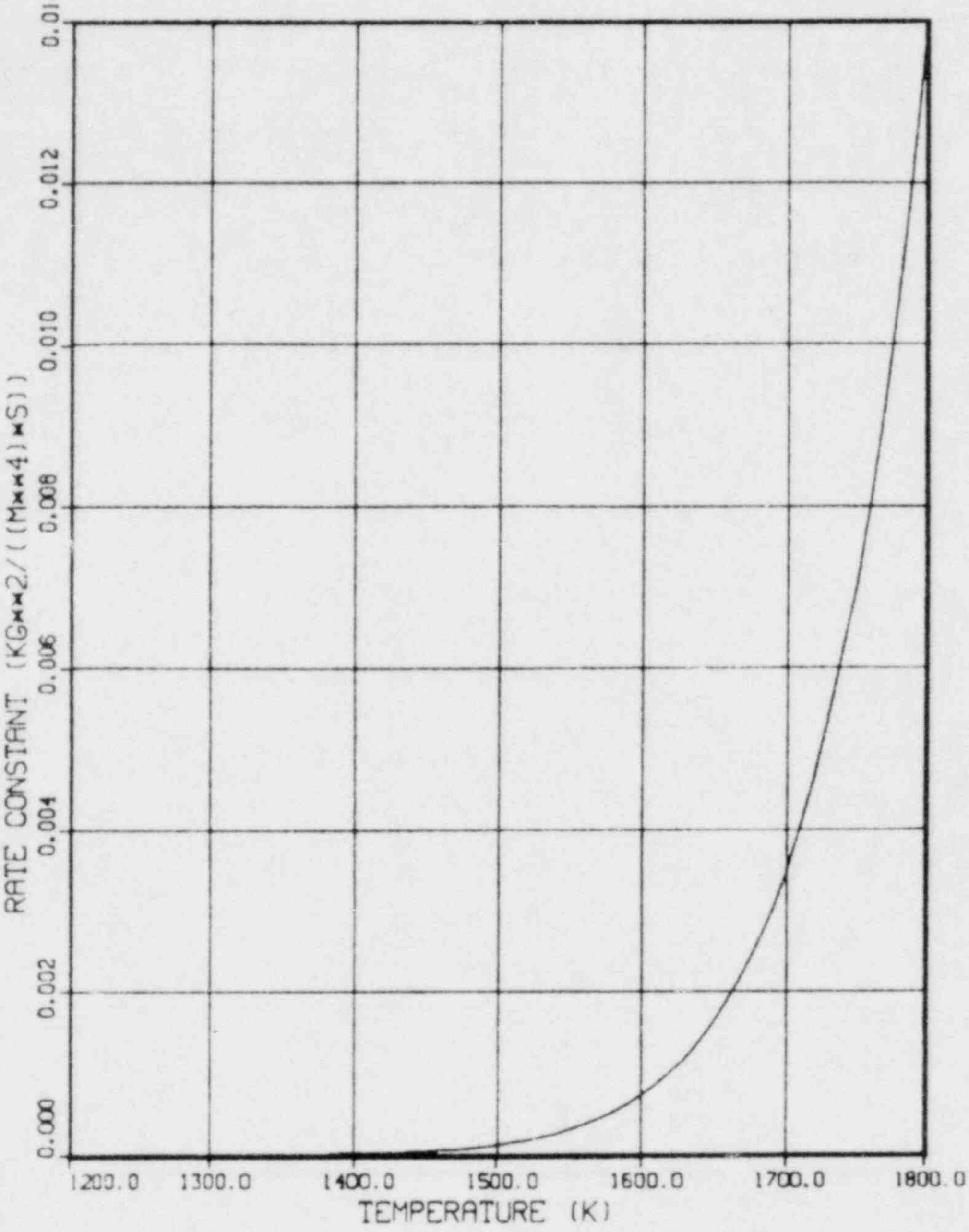

Figure E-6. Parabolic constant for oxygen weight gain calculated with SOXWGN.

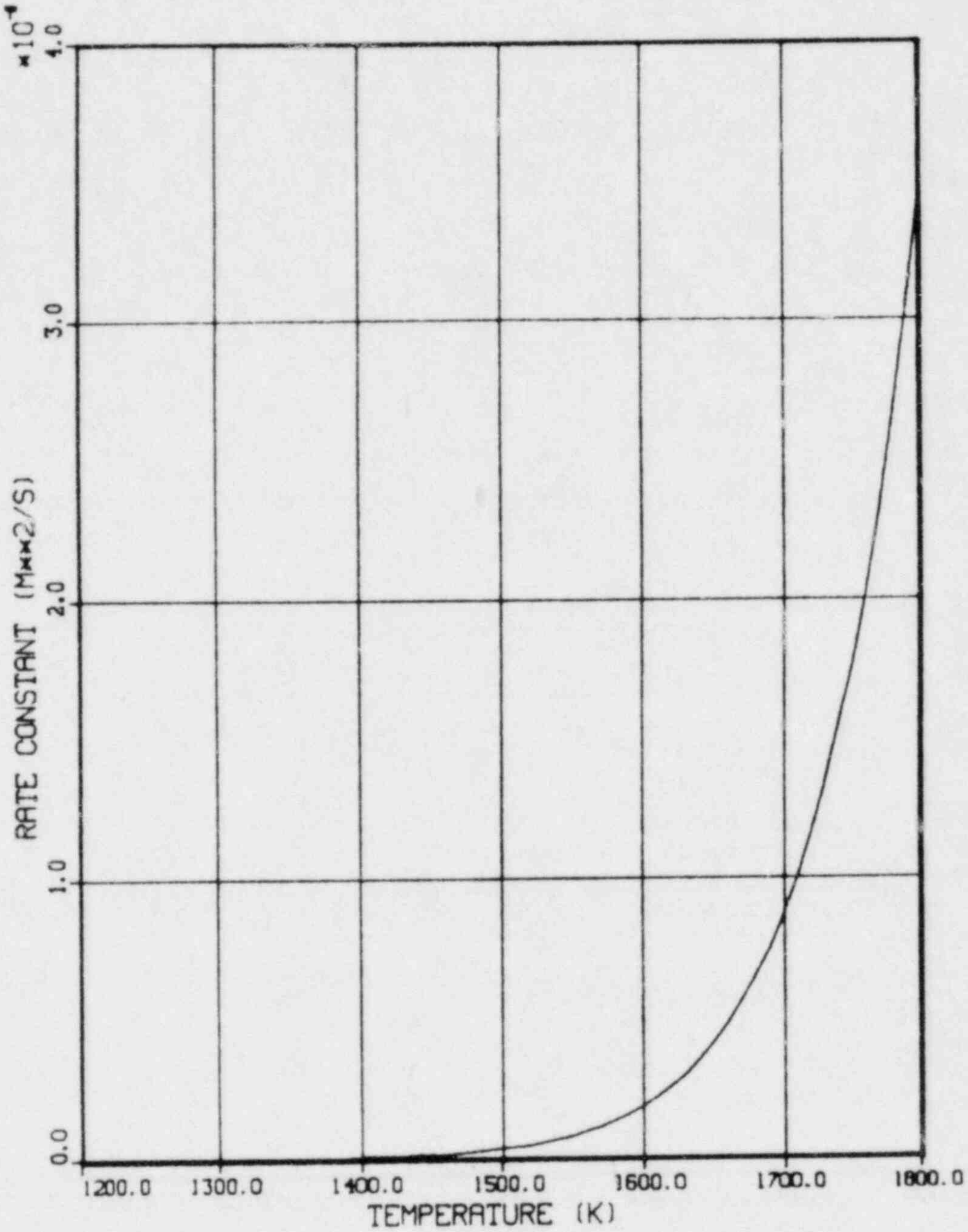

Figure E-7. Parabolic constant for oxide layer thickness calculated with SOXTHK.

in Figure E-8. Figures E-9 and E-10 illustrate oxygen uptake and the oxide layer thickness expected after a one second time step with no initial oxidation.

CONTROL ROD CLADDING MELTING TEMPERATURES
(SHYPRP)

The subroutine SPROP provides 304 stainless steel melting temperatures. There is no required input.

For this alloy, page 19-3 of Reference E-1 reports a melting range of 1671 to 1727 K. These numbers are used for the solidus (first liquid phase appears) and liquidus (last solid phase melts) temperatures of control rod cladding. Table D-8 is a listing of the SPROP subroutine.

REFERENCES

E-1. D. Peckner and I. M. Bernstein, (eds) , Handbook of Stainless Steel, New York: McGraw-Hill Book Company, 1977.

E-2. H. C. Brassfield, J. F. White, L. Sjodahl, and J. T. Bittel, Recommended Property and Reaction Kinetics Data for Use in Evaluating a Light-water-Cooled Reactor Loss-of-Coolant Incident Involving Zircaloy-4 of 304 SS Clad UO_2, GEMP 482, 1968.

E-3. W. B. Murfin et al., Core-Meltdown Experimental Review, SAND74-0382 and NUREG-0205, 1977.

E-4. S. Nazare, G. Ondracek, and B. Schulz, "Properties of Light Water Reactor Core Melts," Nuclear Technology, 32, 1977, pp. 239-246.

E-5. J. C. Hesson et al., Laboratory Simulations of Cladding--Steam Reactions Following Loss-of-Coolant Accidents in Water-Cooled Power Reactors, ANL-7609, 1970, pp. 12-18.

E-6. J. A. Dean (ed), Lange's Handbook of Chemistry, (twelfth edition), New York: McGraw-Hill Book Company, 1979, (TP 151 H25).

E-7. F. D. Rossini et al., Selected Values of Chemical Thermodynamic Properties, Circular of the National Bureau of Standards 500, Washington, D.C.: United States Government Printing Office, 1952, (QC100 U555).

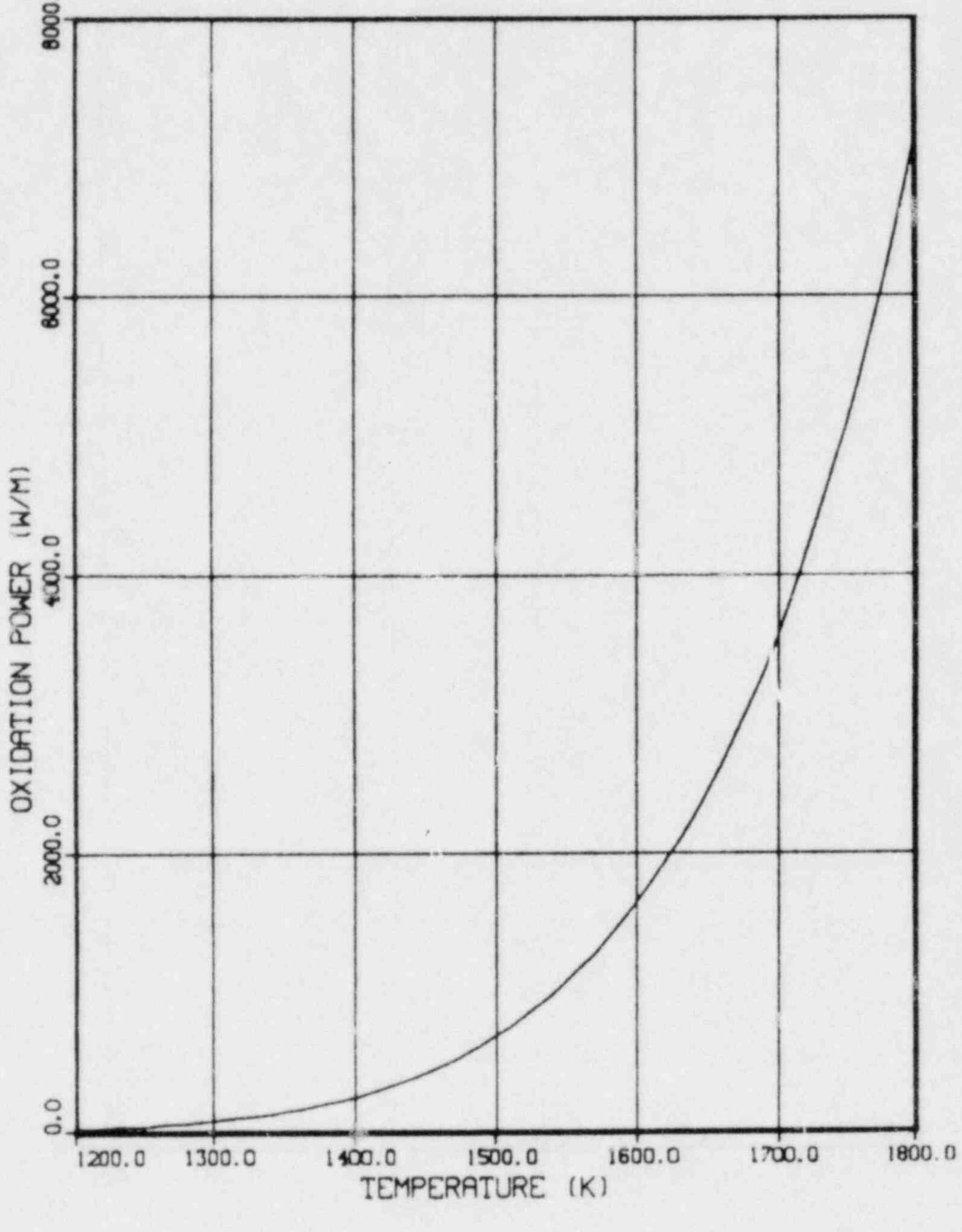

Figure E-8. Average power per meter during one second for a 1.25 10^{-2} meter stainless steel rod with no initial oxide layer.

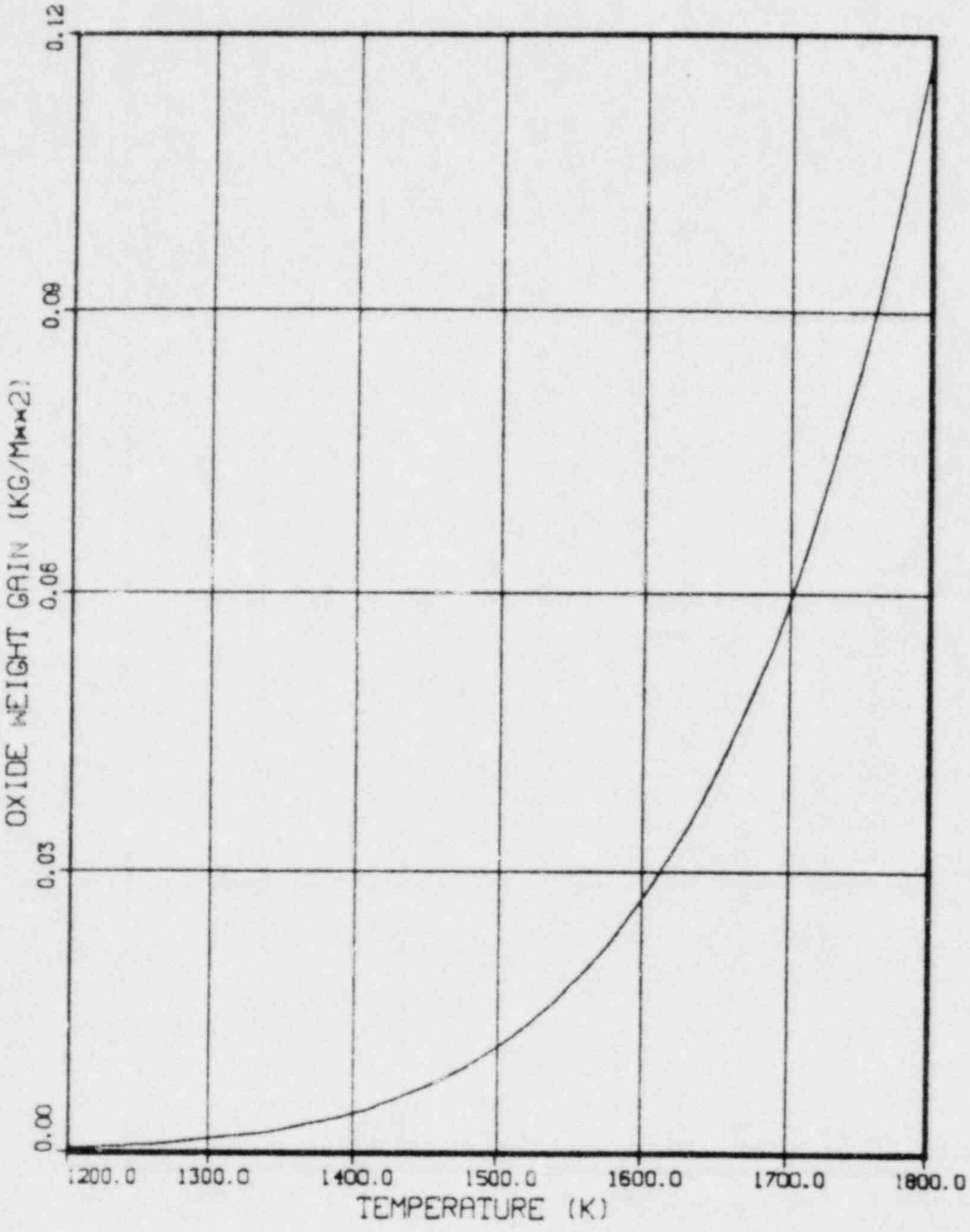

Figure E-9. Oxygen uptake after one second with no initial oxidation.

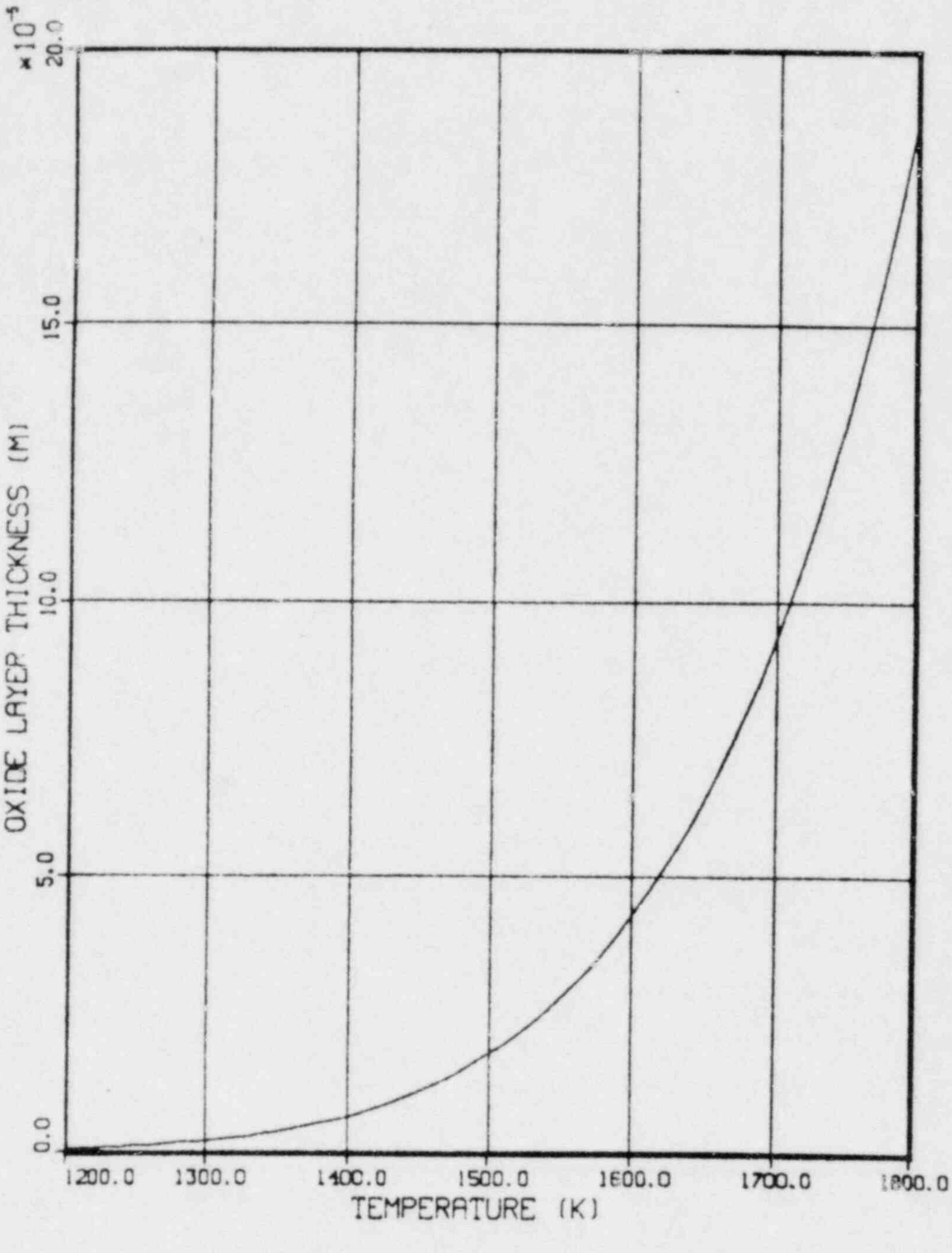

Figure E-10. Oxide layer thickness after one second with no initial oxidation.

TABLE E-10. LISTING OF THE SHYPRP SUBROUTINE

```
      SUBROUTINE SHYPRP(SSOL,SLIQ)
C
C     SHYPRP RETURNS 304 STAINLESS STEEL PHASE TRANSITION TEMPERATURES
C
C     SSOL    = OUTPUT SOLIDUS TEMPERATURE (K)
C     SLIQ    = OUTPUT LIQUIDUS TEMPERATURE (K)
C
C     SHYPRP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      SSOL = 1671.
      SLIQ = 1727.
      RETURN
      END
```

APPENDIX F
GRID SPACER MATERIAL PROPERTIES

APPENDIX F

GRID SPACER MATERIAL PROPERTIES

The only grid spacer material property required for the SCDAP/MOD0 code is the melting temperature. This information is discussed below. Readers who desire additional grid spacer material properties will find a summary in Appendix B of Reference F-1.

GRID SPACER MELTING TEMPERATURES

(HPROP)

The subroutine HPROP provides Inconel 718 melting temperatures. No input information is required.

For Inconel 718, page 267 of Reference F-2 reports a melting range of 1533 through 1609 K. These numbers are used for the solidus and liquidus temperatures of Inconel grid spacers.

Table F-1 is a listing of the HPROP subroutine.

REFERENCES

F-1. J. W. Spore et al., TRAC-BD1: An Advanced Best Estimate Computer Program for Boiling Water Reactor Loss-of-Coolant Accident Analysis, Volume I: Model Description, NUREG/CR-2178 and EGG-2109, October 1981.

F-2. C. T. Lynch (ed.), Handbook of Materials Science, Volume II: Metals, Composites, and Refractory Materials, Cleveland, Ohio: CRC Press, Inc., (TA 403.4 L94).

TABLE F-1. LISTING OF THE HPROP SUBROUTINE

```
      SUBROUTINE HPROP(HSOL,HLIQ)
C
C     HPROP RETURNS INCONEL 718 PHASE TRANSITION TEMPERATURES
C
C     HSOL   = OUTPUT SOLIDUS TEMPERATURE (K)
C     HLIQ   = OUTPUT LIQUIDUS TEMPERATURE (K)
C
C     HPROP WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      HSOL = 1533.
      HLIQ = 1609.
      RETURN
      END
```

APPENDIX G

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS MATERIAL PROPERTIES

APPENDIX G

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS MATERIAL PROPERTIES

Extension of the MATPRO-11 Revision 2 materials properties package to high temperatures requires consideration of mixtures and compounds which were not previously included in the package because they are not formed until zircaloy cladding melts. One approach to providing the properties of molten mixtures of core material has been to define standard compounds of core materials--Corium A, Corium E, Corium AX1, Corium EX1, Corium EX2, Corium EX3, etc.[G-1] This approach has been avoided here because deciding when to switch from properties of one kind of melt to another would needlessly complicate serious efforts to model severe core damage. The six different types of corium listed above are replaced with a single class of material whose properties vary with zirconium, uranium, and oxygen concentration. For the present, concentrations of iron, chrome, nickel, silver, indium, cadmium and other low melting components are ignored because compounds rich in these components will probably migrate to cooler regions of the core before the melting temperature of zircaloy is attained.

Data for all the properties modeled in this appendix are very scarce so most of the subcodes use interpolations of materials properties that are available--the properties of UO_2, ZrO_2, and Zr. These materials are used as a basis for interpolation rather than the properties of elemental U, Zr and O because UO_2, ZrO_2 and Zr more closely approximate the compositions of interest.

A Gibbs triangle plot[G-2] of the compositions of Zr-U-O compounds is shown in Figure G-1 to illustrate this point. It can be shown that the composition of a mixture of any two ternary alloys will lie on a straight line joining the points representing the original compositions on a Gibbs plot. Severe core damage will melt zircaloy (represented here as mostly zirconium) which has been previously oxidized to some state between oxygen stabilized zircaloy, Zr(O), and ZrO_2. This melt will dissolve and mix

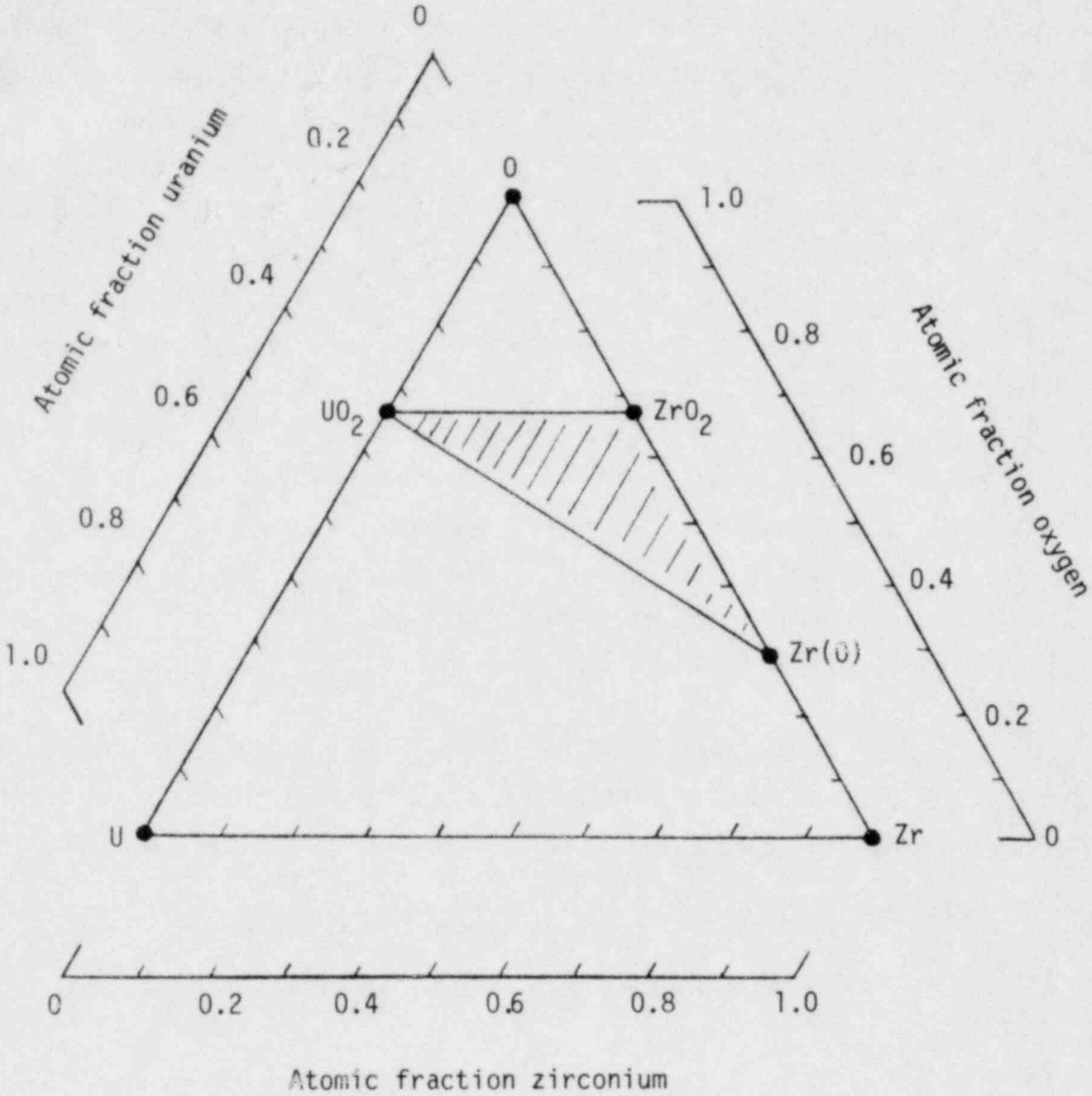

Figure G-1. Compositions of Zr-U-O compounds on a Gibbs triangle plot.

with UO_2. The gross compositions of interest are thus most likely to lie in the shaded region of the plot (some uranium rich phases which could melt and flow out of the hot region are the only known exception to this general observation).

When interpolated properties are used, input values of the atomic fractions of zircaloy, uranium, and oxygen are converted to mole fractions of UO_2, ZrO_2, and Zr with the following relations

$$f_{UO_2} = \frac{U}{U + Z} \tag{G-1a}$$

$$f_{ZrO_2} = \frac{\frac{X}{2} - U}{U + Z} \tag{G-1b}$$

$$f_{Zr} = \frac{Z - \frac{X}{2} + U}{U + Z} \tag{G-1c}$$

where

f_{UO_2} = mole fraction UO_2 in the compound

f_{ZrO_2} = mole fraction ZrO_2 in the compound

f_{Zr} = mole fraction Zr in the compound

X = atomic fraction oxygen in the compound

U = atomic fraction urainum in the compound

Z = atomic fraction zirconium in the compound.

Inspection of Equations (G-1a) to (G-1c) reveals several limitations:

First

$$X + U + Z = 1 \qquad \text{(G-2)}$$

and thus, only two of the three atomic fractions need be input. Also, the atomic fraction of oxygen must lie in the range

$$U \leq \frac{X}{2} \leq U + Z \qquad \text{(G-3)}$$

if Equations (G-1a) and (G-1c) are to return physically meaningful positive fractions. The right hand inequality means that the compound must not be oxidized beyond a metal dioxide and the left hand inequlity requires that at least enough oxygen be present to oxidize the uranium to UO_2. Inspection of Figure G-1 shows that the right hand inequlity requires the compound to lie below the line drawn between the points labeled UO_2 and ZrO_2 while the left-hand inequality requires that the compound lie above a line from the point labeled UO_2 to the point labeled Zr. All of the shaded traingle lies within this region so all compounds formed out of UO_2 and zircaloy oxidized as far as ZrO_2 will be in the acceptable range.

All subcodes which use Equations (G-1a) to (G-1c) check for acceptable ranges of oxygen concentration and raise or lower the presumed oxygen content to force it to fall within the range given by Equation (G-3). An error message is printed when the range is exceeded.

For input values of U and Z which imply X/2 is greater than U + Z, the input values of U and Z are replaced by

$$U' = \frac{U}{3(U + Z)} \qquad \text{(G-4a)}$$

$$Z' = \frac{Z}{3(U + Z)} \qquad \text{(G-4b)}$$

where

U' = revised atomic fraction of uranium in the compound

Z' = revised atomic fraction of zirconium in the compound.

Inspection of Equations (G-4a), (G-4b), and (G-2) shows that the transformation preserves the uranium-to-zircaloy ratio but decreases $X'/2$ to $U' + Z'$.

For input values of U and Z which imply $X/2$ is less than U, input values of U and Z are replaced by

$$U' = \frac{U}{3U + Z} \tag{G-5a}$$

$$Z' = \frac{Z}{3U + Z} \tag{G-5b}$$

Inspection of Equations (G-5a), (G-5b), and (G-2) shows that this transformation presurves the urainum-to-zircaloy ratio but increases $X'/2$ to U'.

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS SPECIFIC HEAT CAPACITIES AND ENTHALPIES

(ZUCP, ZUNTHL)

The function ZUCP provides the specific heat capacity of Zr-U-O compounds as a function of component concentrations and the compounds temperature. ZUENTHL returns the Zr-U-O compound enthalpy as a function of component concentrations, the compound temperature, and a reference temperature for which the enthalpy will be zero.

The expression used to calculate the specific heat capacity is an atomic-fraction-weighted average of the molar heat capacities of UO_2, ZrO_2, and Zr

$$C_{p_c} = \frac{C_{p_{UO_2}}\ 0.270\ f_{UO_2} + C_{p_{ZrO_2}}\ 0.123\ f_{ZrO_2} + C_{p_{Zr}}\ 0.091\ f_{Zr}}{0.270\ f_{UO_2} + 0.123\ f_{ZrO_2} + 0.091\ f_{Zr}} \qquad \text{(G-6)}$$

where

C_{p_c} = specific heat capacity of the compound (J/kg•K)

$C_{p_{UO_2}}$ = specific heat capacity of UO_2 obtained from the FCP subcode (J/kg•K)

$C_{p_{ZrO_2}}$ = specific heat capacity of UO_2 obtained from the ZOCP subcode (J/kg•K)

$C_{p_{Zr}}$ = specific heat capacity of zircaloy obtained from the CCP subcode (J/kg•K).

An analogous weighted average is used in ZUNTHL to calculate compound enthalpies. This technique has the advantage that the proper enthalpies are obtained for the limiting cases of UO_2, ZrO_2, or Zr but the disadvantage that the heats of fusion are not constrained to appear between the solidus and liquidus temperatures of the compound.

Tables G-1 and G-2 are listings of the ZUCP and ZUNTHL functions. Plots of the calculated specific heat capacity and enthalpy of a compound made up of 0.2 weight fraction UO_2 and 0.8 weight fraction ZrO_2 are shown in Figures G-2 and G-3.

Calculations with ZUNTHL are compared with enthalpies observed by Deem^{G-3} for several UO_2 - ZrO_2 compounds in Tables G-3 to G-6. (Deem's data are presented in Tables 14 to 17 of Reference G-3). The

TABLE G-1. LISTING OF THE ZUCP FUNCTION

```
      FUNCTION ZUCP(U,Z,ZUTEMP)
C
C     ZUCP RETURNS THE SPECIFIC HEAT CAPACITY AT CONSTANT
C     PRESSURE FOR ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS
C
C     ZUCP   = OUTPUT COMPOUND SPECIFIC HEAT CAPACITY (J/(KG*K))
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C              (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C              (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ZUTEMP = COMPOUND TEMPERATURE (K)
C
C     THE FUNCTIONS CCP, FCP, AND ZOCP ARE CALLED BY THIS FUNCTION
C
C     ZUCP WAS CODED BY D. L. HAGRMAN MARCH 1982.
C
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FUO2 = U/(U+Z)
      FZO2 = (0.5 * X - U)/(U + Z)
      FZR  = 1. - FUO2 - FZO2
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUCP HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      CZR = CCP(ZUTEMP)
      CUO2 = FCP(ZUTEMP,0.0,2.0,0.95)
      CZO2 = ZOCP(ZUTEMP)
C
      ZUCP = (CUO2*0.27*FUO2 + CZO2*0.123*FZO2 + CZR*0.091*FZR)/
     *        (0.270*FUO2 + 0.123*FZO2 + 0.091*FZR)
C
      RETURN
      END
```

TABLE G-2. LISTING OF THE ZUNTHL FUNCTION

```
      FUNCTION ZUNTHL(U,Z,ZUTEMP,RFTEMP)
C
C     ZUNTHL RETURNS THE CHANGE IN ENTHALPY OF ZIRCONIUM-URANIUM
C     OXYGEN COMPOUNDS DURING A CONSTANT PRESSURE CHANGE IN
C     TEMPERATURE
C
C     ZUNTHL = OUTPUT CHANGE IN COMPOUND ENTHALPY (J/KG)
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C                (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C                (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ZUTEMP = COMPOUND TEMPERATURE (K)
C     RFTEMP = REFERENCE TEMPERATURE (K)
C
C     THE SUBCODES CENTHL,FENTHL, AND ZONTHL ARE CALLED
C     BY THIS FUNCTION
C
C     ZUNTHL WAS CODED BY D. L. HAGRMAN MARCH 1982.
C
C
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UU = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UU + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UU = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UU + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FUO2 = U/(U+Z)
      FZO2 = (0.5 * X - U)/(U + Z)
      FZR  = 1. - FUO2 - FZO2
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUNTHL HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      HZR = CENTHL(ZUTEMP,RFTEMP)
      HUO2R = FENTHL(RFTEMP,0.0,2.0,3113.,0.0)
      HUO2 = FENTHL(ZUTEMP,0.0,2.0,3113.,0.0)
      HUO2 = HUO2 - HUO2R
      HZO2 = ZONTHL(ZUTEMP,RFTEMP)
C
      ZUNTHL = (HUO2*0.27*FUO2 + HZO2*0.123*FZO2 + HZR*0.091*FZR)/
     #         (0.270*FUO2 + 0.123*FZO2 + 0.091*FZR)
C
      RETURN
      END
```

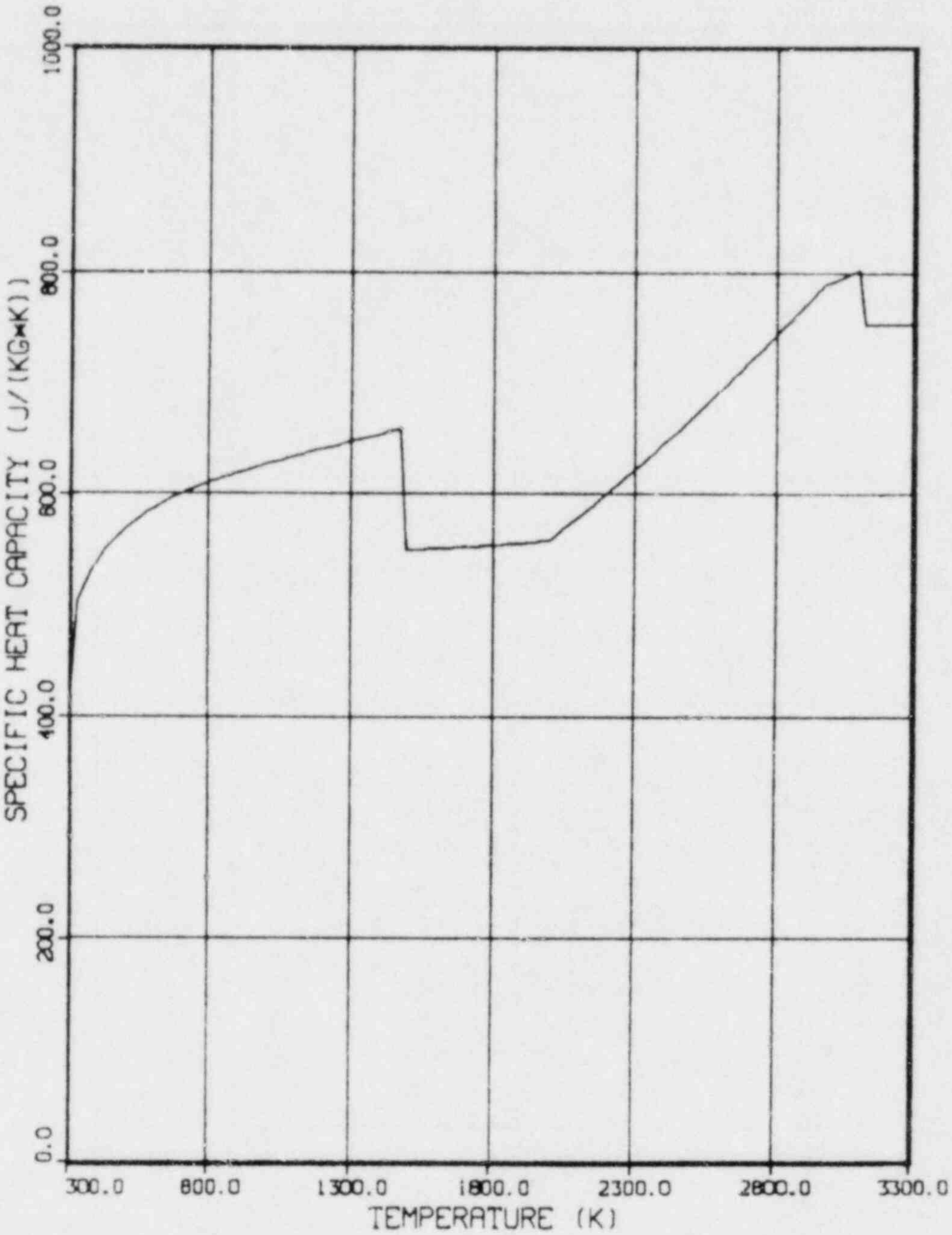

Figure G-2. Specific heat capacity calculated for a $0.2\ UO_2$ - $0.8\ ZrO_2$ weight fraction compound.

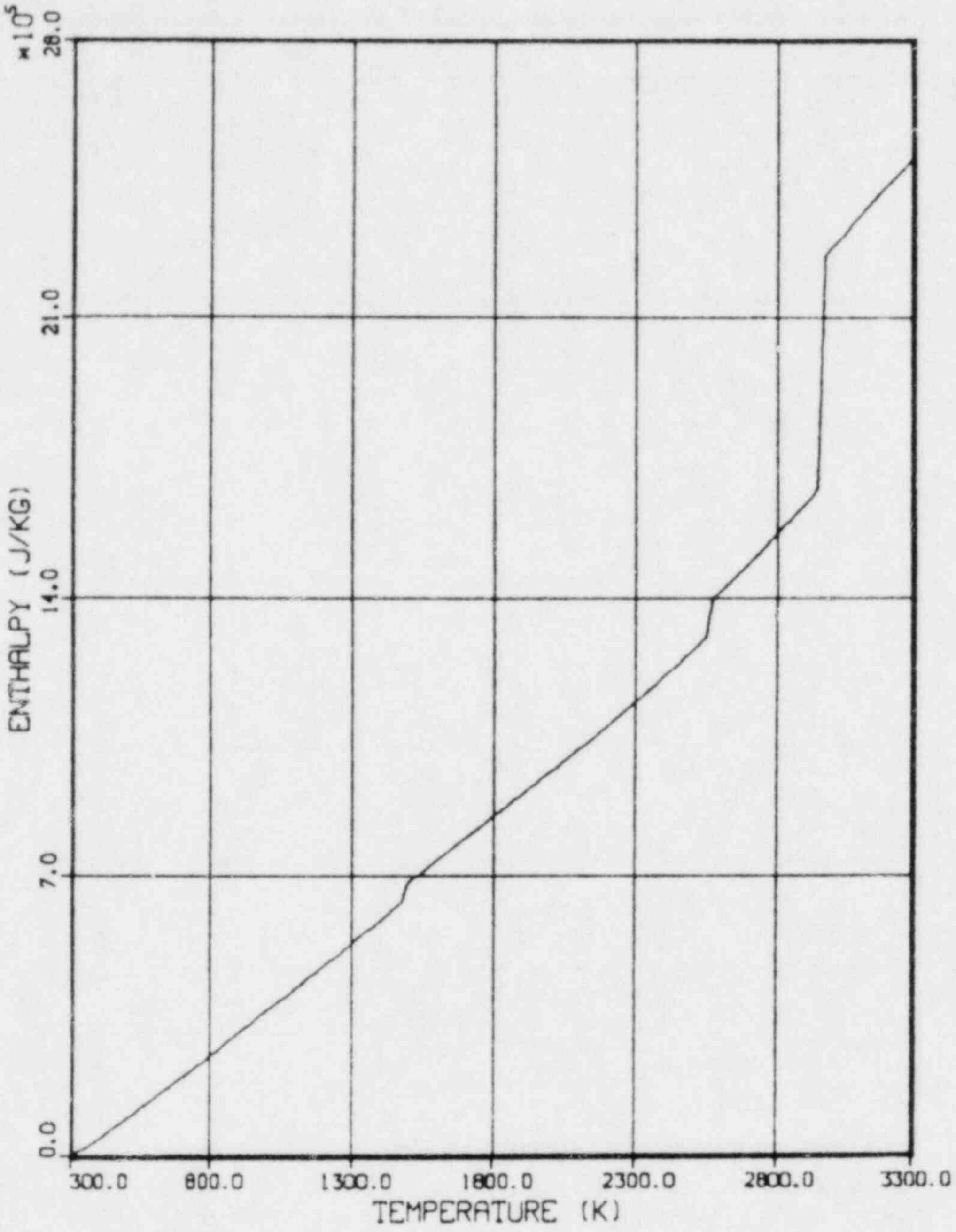

Figure G-3. Enthalpy calculated for a 0.2 UO_2 - 0.8 ZrO_2 weight fraction compound.

TABLE G-3. ZUNTHL CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.2 UO_2-0.8 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Enthalpy (10^4 J/kg)	Calculated Enthalpy (10^4 J/kg)
273	0.00	0.00
370	4.23	4.16
370	4.31	4.16
378	4.64	4.53
469	9.16	8.85
596	15.69	15.24
596	15.56	15.24
727	23.05	22.08
868	30.92	29.66
870	31.00	29.77
1095	42.59	42.22
1257	52.05	51.40
1479	63.97	68.11
1750	79.50	83.05
2108	101.0	103.10
2256	112.0	111.92

TABLE G-4. ZUNTHL CALCULATIONS AND DEEM'S DATA[G-3] FOR A $0.32\ UO_2$-$0.68\ ZrO_2$ WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Enthalpy (10^4 J/kg)	Calculated Enthalpy (10^4 J/kg)
273	0.00	0.00
348	2.93	2.97
349	2.96	3.01
371	3.95	3.93
372	3.96	3.98
390	4.74	4.75
390	4.77	4.75
408	5.57	5.54
408	5.61	5.54
541	11.97	11.63
543	11.95	11.72
690	19.20	18.82
691	19.36	18.87
829	26.21	25.76
829	26.22	25.76
947	32.30	31.78
951	32.56	31.99
1069	37.24	38.11
1292	49.71	49.94
1480	60.84	63.41
1678	70.54	73.68
1797	75.94	79.89
1878	81.17	84.14
1919	82.26	86.30
1976	86.06	89.32
2096	93.55	95.78
2175	100.96	100.19
2276	107.19	106.02
2385	119.50	112.57
2487	125.98	118.96

TABLE G-5. ZUNTHL CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.5 UO_2-0.5 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Enthalpy (10^4 J/kg)	Calculated Enthalpy (10^4 J/kg)
273	0.00	0.00
339	2.33	2.32
339	2.37	2.32
367	3.41	3.37
367	3.44	3.37
383	4.02	3.99
385	3.97	4.06
401	4.76	4.69
543	10.63	10.50
547	10.83	10.67
702	17.60	17.40
702	17.62	17.40
877	25.81	25.27
878	25.66	25.31
978	30.44	29.91
979	29.96	29.96
1102	34.98	35.70
1243	42.05	42.38
1273	43.43	43.82
1484	53.39	56.46
1521	63.64	58.19
1796	67.66	71.20
1889	72.17	75.66
1995	77.74	80.82
2086	84.60	85.34
2188	89.66	90.60
2297	99.33	96.47
2430	105.94	104.01

TABLE G-6. ZUNTHL CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.94 UO_2-0.06 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Enthalpy (10^4 J/kg)	Calculated Enthalpy (10^4 J/kg)
273	0	0
372	2.36	2.55
372	2.55	2.55
474	5.58	5.46
596	9.25	9.15
597	9.26	9.18
728	13.41	13.29
729	13.44	13.32
870	17.96	17.87
872	18.02	17.94
1030	23.32	23.15
1108	25.15	25.76
1314	32.72	32.77
1492	37.11	39.24
1816	48.45	50.81
2071	59.66	60.56
2265	68.58	68.68

standard error of these predictions, 2×10^4 J/kg or about 0.1 of the predicted value, is the expected standard error of the ZUNTHL function.

A similar expected standard error, 0.1 of the predicted specific heat capacity, is adopted for ZUCP.

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS THERMAL CONDUCTIVITIES (ZUTCON)

Required inputs to ZUTCON to calculate compound thermal conductivities are the component concentrations and compound temperature. The expression used for the compound conductivity is the smaller of K_{Zr} and

$$k_c = f_{UO_2} k_{UO_2} + f_{ZrO_2} k_{ZrO_2} + f_{Zr} k_{Zr} - 0.4 f_{UO_2} f_{ZrO_2}$$

$$+ 7.8 f_{UO_2} f_{Zr} + 7.8 f_{ZrO_2} f_{Zr} \qquad \text{(G-7)}$$

where

k_c = compound thermal conductivity (W/m•K)

k_{UO_2} = UO_2 thermal conductivity obtained from the FTHCON subcode (W/m•K)

k_{ZrO_2} = ZrO_2 thermal conductivity obtained from the ZOTCON subcode (W/m•K)

k_{Zr} = zircaloy thermal conductivity obtained from the CTHCON subcode (W/m•K).

Expression (G-7) is an atomic-fraction-weighted average of the thermal conductivities of UO_2, ZrO_2, and Zr modified to include cross-products. The modification was added to reproduce the parabolic shape typically seen in plots of conduction versus composition in binary mixtures.[G-2,G-4]

The coefficient of the UO_2 - ZrO_2 cross-product was obtained by requiring Equation (G-7) to reproduce a thermal conductivity of 1.44 W/m•K at 2073 K for a composition of 0.315 mole fraction UO_2 and 0.685 mole fraction ZrO_2 (0.5 UO_2 - 0.5 ZrO_2 by weight). The thermal conductivity was obtained from a curve published as Figure 56 in Reference G-3. A similar approach was used to determine the coefficient of the Zr-UO_2 cross product. A measurement from Rauch,$^{G-5}$ 11.09 W/m•K at 343 K for a composition of 0.80 weight fraction UO_2 and 0.20 weight fraction Zr was employed. No data were found to evaluate the Zr-ZrO_2 cross product coefficient so the Zr-UO_2 cross-product coefficient was used as an estimate.

Table G-7 is a listing of the ZUTCON function. A plot of the calculated thermal conductivity of a compound made up of 0.2 weight fraction UO_2 and 0.8 weight fraction ZrO_2 is shown in Figure G-4.

Model predictions are compared to thermal conductivities calculated by Deem (Table 26 of Reference G-3) from his data for several UO_2 - ZrO_2 compounds in Tables G-8 through G-12. The standard error of the ZUTCON calculations is ±1 W/m, most of which is caused by serious overprediction at low temperature and high UO_2 content.

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS THERMAL EXPANSIONS AND DENSITIES (ZUTEXP, ZUDEN)

The function ZUTHEXP calculates the thermal expansion strain of Zr-U-O compounds as a function of composition, temperature, and a reference temperature for which the thermal expansion strain will be zero. ZUDEN returns the compound density as a function of composition and density.

The expression used to calculate thermal expansion strains in ZUTEXP is

$$\epsilon_C = \frac{2.46\ f_{UO_2}\ \epsilon_{UO_2} + 2.12\ f_{ZrO_2}\ \epsilon_{ZrO_2} + 1.39\ f_{Zr}\ \epsilon_{Zr}}{2.46\ f_{UO_2} + 2.12\ f_{ZrO_2} + 1.39\ f_{Zr}} \qquad \text{(G-8)}$$

TABLE G-7. LISTING OF THE ZUTCON FUNCTION

```
      FUNCTION ZUTCON(U,Z,ZUTEMP)
C
C     ZUTCON RETURNS ZIRCONIUM-URANIUM-OXYGEN COMPOUND
C     CONDUCTIVITY
C
C     ZUTCON = OUTPUT COMPOUND CONDUCTIVITY (W/(M*K))
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C              (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C              (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ZUTEMP = COMPOUND TEMPERATURE (K)
C
C     THE SUBCODES CTHCON, FTHCON, AND ZOTCON ARE CALLED BY THIS
C     FUNCTION
C
C     ZUTCON WAS CODED BY D. L. HAGRMAN MARCH 1982.
C

      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FUO2 = U/(U+Z)
      FZO2 = (0.5 * X - U)/(U + Z)
      FZR  = 1. - FUO2 - FZO2
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUTCON HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      CALL CTHCON(ZUTEMP,CCON,CDKDT)
      CZR = CCON
      CALL FTHCON(ZUTEMP,1.00,2.0,CON,DKDT)
      CUO2 = CON
      CZO2 = ZOTCON(ZUTEMP)
C
      ZUTCON = FUO2*CUO2 + FZO2*CZO2 + FZR*CZR - 0.4*FUO2*FZO2
     #         +7.8*FUO2*FZR + 7.8*FZO2*FZR
      IF(ZUTCON .GT. CZR) THEN
         ZUTCON = CZR
      ENDIF
C
      RETURN
      END
```

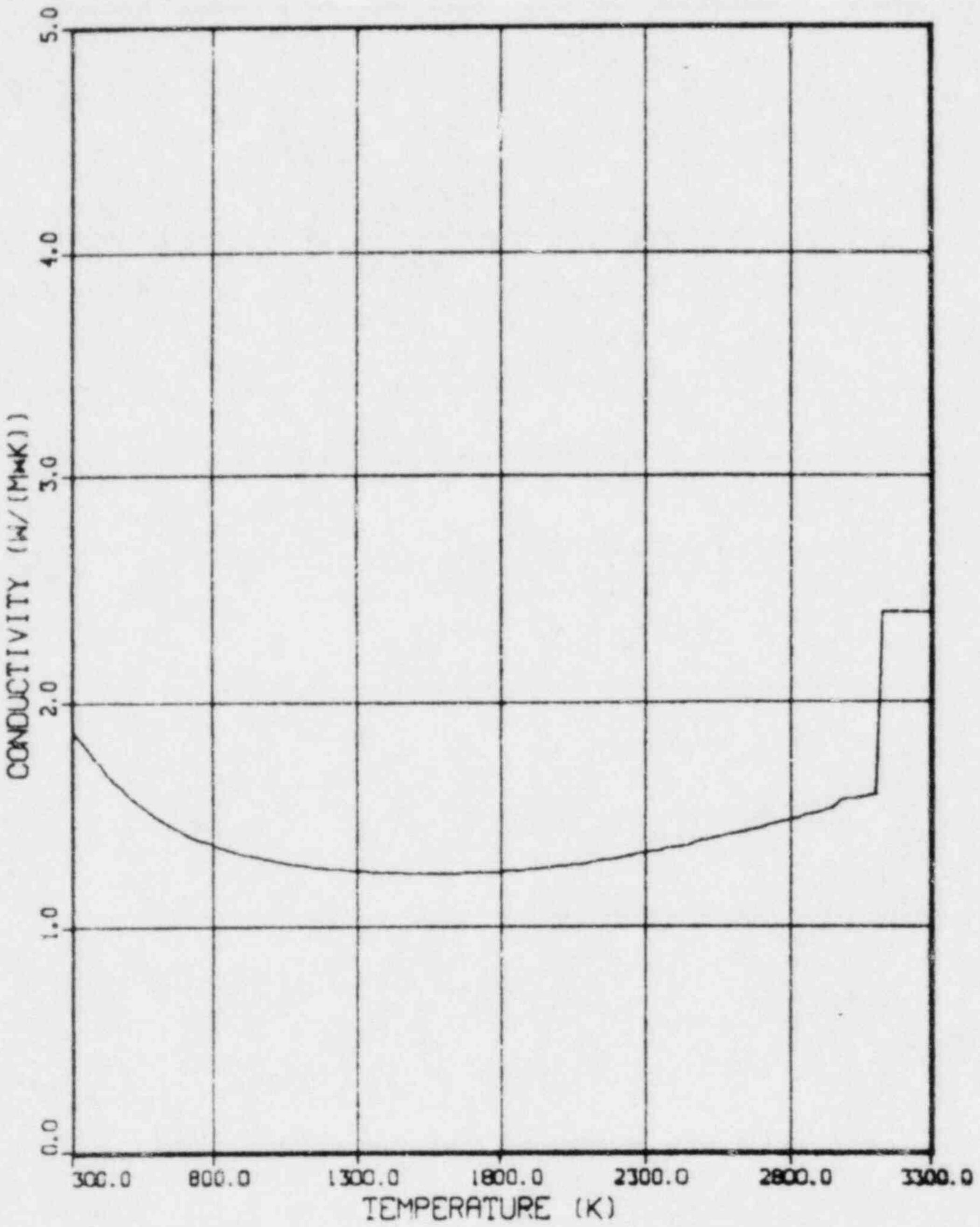

Figure G-4. Thermal conductivity calculated for a 0.2 UO_2 - 0.8 ZrO_2 weight fraction compound.

TABLE G-8. ZUTCON CALCULATIONS AND DEEM'S RESULTS[G-3] FOR A 0.2 UO_2-0.8 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Deem's Conductivity (W/m•K)	Calculated Conductivity (W/m•K)
423	2.8	1.7
473	2.6	1.6
573	2.30	1.51
673	2.42	1.43
873	2.12	1.33
1073	1.94	1.28
1273	1.82	1.25
1473	1.78	1.24
1673	1.77	1.24
1873	1.78	1.25
2073	1.72	1.28
2173	1.66	1.30
2273	1.62	1.32

TABLE G-9. ZUTCON CALCULATIONS AND DEEM'S RESULTS[G-3] FOR A 0.32 UO_2-0.68 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Deem's Conductivity (W/m•K)	Calculated Conductivity (W/m•K)
423	2.5	2.2
473	2.3	2.1
573	2.1	1.9
673	2.04	1.79
873	2.00	1.59
1073	2.00	1.47
1285	1.97	1.39
1480	1.46	1.34
1673	1.59	1.32
1873	1.73	1.31
1943	1.58	1.32
2073	1.76	1.33
2273	1.87	1.38

TABLE G-10. ZUTCON CALCULATIONS AND DEEM'S RESULTS[G-3] FOR A 0.5 UO_2-0.5 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Deem's Conductivity (W/m•K)	Calculated Conductivity (W/m•K)
423	2.2	3.3
473	2.0	3.1
573	1.8	2.7
673	1.75	2.44
873	1.71	2.06
1073	1.69	1.82
1273	1.67	1.66
1473	1.64	1.55
1673	1.60	1.48
1873	1.54	1.44
2073	1.44	1.45
2183	1.41	1.47
2293	1.79	1.51
2373	1.77	1.54

TABLE G-11. ZUTCON CALCULATIONS AND DEEM'S RESULTS[G-3] FOR A LOW DENSITY 0.32 UO_2-0.68 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Deem's Conductivity (W/m•K)	Calculated Conductivity (W/m•K)
423	2.2	2.2
473	2.1	2.1
573	1.8	1.9
673	1.55	1.79
873	1.53	1.59
1073	1.53	1.47
1273	1.53	1.39
1473	1.17	1.34
1673	1.28	1.32
1873	1.36	1.31
2073	1.40	1.33
2173	1.30	1.35

TABLE G-12. ZUTCON CALCULATIONS AND DEEM'S RESULTS[G-3] FOR A 0.94 UO_2-0.06 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Deem's Conductivity (W/m•K)	Calculated Conductivity (W/m•K)
423	3.8	7.8
473	3.6	7.2
573	2.8	6.1
673	2.41	5.32
873	2.32	4.19
1073	2.19	3.45
1273	2.05	2.93
1473	1.99	2.55
1673	1.93	2.28
1873	1.87	2.11
2073	1.84	2.07
2173	1.82	2.10

where

ϵ_C = compound thermal strain (m/m)

ϵ_{UO_2} = UO_2 thermal strain obtained from the FTHEXP subcode (m/m)

ϵ_{ZrO_2} = ZrO_2 thermal strain obtained from the ZOTEXP subcode (m/m)

ϵ_{Zr} = isotropic Zr thermal strain obtained from the CTHEXP subcode with COSTH2 = 1/3 and COSFI2 = 1/2 (m/m).

This expression is a component-volume-fraction weighted average of the component strains. The volume fraction of each component is

$$f_{V_i} = \frac{\frac{f_i m_i}{\rho_i}}{\sum_{j=1}^{3} \frac{f_j m_j}{\rho_j}} \tag{G-9}$$

where

f_{V_i} = volume fraction of i-th component (m^3/m^3)

m_i = mole weight of i-th component (kg/gm mole) (0.270 for UO_2, 0.123 for ZrO_2, and 0.091 for Zr)

ρ_i = density of i-th component (kg/m^3) (10,980 for UO_2, 5,800 for ZrO_2, and 6550 for Zr).

Expression (G-8) is derived by assuming that the compound is made up of components which produce independent thermal strains. The initial volume is thus

$$V_o = V_{UO_{2_o}} + V_{ZrO_{2_o}} + V_{Zr_o} \tag{G-10a}$$

$$= f_{V_{UO_2}} V_o + f_{V_{ZrO_2}} V_o + f_{V_{Zr}} V_o \qquad \text{(G-10b)}$$

where

$V_{UO_{2_o}}$, $V_{ZrO_{2_o}}$, and V_{Zr_o} = initial component volumes (m^3)

$f_{V_{UO_2}}$, $f_{V_{ZrO_2}}$, and $f_{V_{Zr}}$ = component volume fractions (m^3/m^3) .

The component volume after some thermal strain is, according to Equation (B-8) which relates linear strains to volume strains,

$$V = V_{UO_{2_o}} \exp(3\epsilon_{UO_2}) + V_{ZrO_{2_o}} \exp(3\epsilon_{ZrO_2}) + V_{Zr_o} \exp(3\epsilon_{Zr}) \qquad \text{(G-11a)}$$

$$V_{UO_{2_o}} (1 + 3\epsilon_{UO_2}) + V_{ZrO_{2_o}} (1 + 3\epsilon_{ZrO_2}) + V_{Zr_o} (1 + 3\epsilon_{Zr}) \qquad \text{(G-11b)}$$

The compound volume strain, ϵ_{c_V}, is

$$\epsilon_{c_V} = \frac{V - V_o}{V_o} \qquad \text{(G-12a)}$$

$$\approx \frac{V_{UO_{2_o}} 3\epsilon_{UO_2} + V_{ZrO_{2_o}} 3\epsilon_{ZrO_2} + V_{Zr_o} 3\epsilon_{Zr}}{V_{UO_{2_o}} + V_{ZrO_{2_o}} + V_{Zr_o}} \qquad \text{(G-12b)}$$

$$= f_{V_{UO_2}} 3\epsilon_{UO_2} + f_{V_{ZrO_2}} 3\epsilon_{ZrO_2} + f_{V_{Zr}} 3\epsilon_{Zr} \ . \qquad \text{(G-12c)}$$

Replacement of the compound volume strain by three times the compound linear strain and substitution using Equation (G-9) completes the derivation of Equation (G-8).

The expression used in ZUDEN to calculate compound densities is

$$\rho_c = \frac{0.270\ f_{UO_2} + 0.123\ f_{ZrO_2} + 0.091\ f_{Zr}}{\dfrac{0.270\ f_{UO_2}}{\rho_{UO_2}} + \dfrac{0.123\ f_{ZrO_2}}{\rho_{ZrO_2}} + \dfrac{0.091\ f_{Zr}}{\rho_{Zr}}} \tag{G-13}$$

where

ρ_c = compound density (kg/m^3)

ρ_{UO_2} = UO_2 density obtained from the FDEN subcode (kg/m^3)

ρ_{ZrO_2} = ZrO_2 density obtained from the ZODEN subcode (kg/m^3)

ρ_{Zr} = zircaloy density obtained from the CDEN subcode (kg/m^3) .

Equation (G-13) is derived by assuming that each compound component contributes a volume equal to the volume the component would have as a free substance. The compound density is thus the total mass divided by the total volume

$$\rho_c = \frac{\sum_{i=1}^{3} N\ f_i\ m_i}{\sum_{i=1}^{3} \dfrac{N\ f_i\ m_i}{\rho_i}} \tag{G-14}$$

where

N = number of moles present in the compound.

Cancelation of the common factor N and substitution of the component mole weights in Equation (G-14) yield Equation (G-13).

Table G-13 is a listing of the ZUTEXP function and Table G-14 presents the ZUDEN function listing. Plots of the calculated thermal expansion strain and density of a compound made up of 0.2 weight fraction UO_2 and 0.8 weight fraction ZrO_2 are shown in Figures G-5 and G-6.

Model predictions are compared with thermal expansion strains and densities measured at 293 K by Deem (Table 12 of Reference G-3) for several UO_2 - ZrO_2 compounds in Tables G-15 to G-19. The standard error of the ZUTEXP function calculations is $\pm 1.0 \times 10^{-2}$ and the standard error of the ZUDEN function calculations is $\pm 3 \times 10^{2}$. These standard errors are recommended as the expected standard errors of the ZUTEXP and ZUDEN function calculations.

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS COEFFICIENTS OF FRICTION (ZUFRIC)

The function ZURRIC returns the coefficient of friction of flowing Zr-U-O compounds. The correlations used for this coefficient are

$$F = 0.0791\ R_e^{(-0.25)} \quad , R_e > 7539.42 \qquad \text{(G-15a)}$$

$$F = \frac{64}{Re} \quad , 7539.42 \geq R_e > 10^{-6} \qquad \text{(G-15b)}$$

$$F = 6.4 \times 10^{7} \quad , Re < 10^{-6} \qquad \text{(G-15c)}$$

TABLE G-13. LISTING OF THE ZUTEXP FUNCTION

```
      FUNCTION ZUTEXP(U,Z,ZUTEMP,RFTEMP)
C
C     ZUTEXP RETURNS ZIRCONIUM-URANIUM-OXYGEN COMPOUND
C     THERMAL EXPANSION STRAINS
C
C     ZUTEXP = OUTPUT THERMAL EXPANSION STRAIN (M/M)
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C              (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C              (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ZUTEMP = COMPOUND TEMPERATURE (K)
C     RFTEMP = REFERENCE TEMPERATURE (K)
C
C     THE SUBCODES CTHEXP, FTHEXP, AND ZOTEXP ARE CALLED
C     BY THIS FUNCTION
C
C     ZUTEXP WAS CODED BY D. L. HAGRMAN MARCH 1982.
C
C
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FUO2 = U/(U+Z)
      FZO2 = (0.5 * X - U)/(U + Z)
      FZR  = 1. - FUO2 - FZO2
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUTEXP HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      CALL CTHEXP(0.33,0.5,ZUTEMP,RFTEMP,STRN11,STRN22,STRN33)
      EZR = STRN11
      EUO2R = FTHEXP(RFTEMP,0.0)
      EUO2 = FTHEXP(ZUTEMP,0.0)
      EUO2 = EUO2 - EUO2R
      EZO2 = ZOTEXP(ZUTEMP,RFTEMP)
C
      ZUTEXP = (2.46*FUO2*EUO2 + 2.12*FZO2*EZO2 + 1.39*FZR*EZR)/
     #         (2.46*FUO2 + 2.12*FZO2 + 1.39*FZR)
C
      RETURN
      END
```

TABLE G-14. LISTING OF THE ZUDEN FUNCTION

```
      FUNCTION ZUDEN(U,Z,ZUTEMP)
C
C     ZUDEN RETURNS ZIRCONIUM-URANIUM-OXYGEN COMPOUND
C     DENSITY
C
C     ZUDEN  = OUTPUT COMPOUND DENSITY (KG/M**3)
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C              (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C              (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ZUTEMP = COMPOUND TEMPERATURE (K)
C
C     THE SUBCODES CTHEXP, FTHEXP, ZOTEXP, CDEN, FDEN,
C     AND ZUDEN ARE CALLED BY THIS FUNCTION
C
C     ZUDEN WAS CODED BY D. L. HAGRMAN MARCH 1982.
C
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FUO2 = U/(U+Z)
      FZO2 = (0.5 * X - U)/(U + Z)
      FZR  = 1. - FUO2 - FZO2
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUDEN HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      RZR = CDEN(ZUTEMP)
      RUO2 = FDEN(ZUTEMP)
      RZO2 = ZUDEN(ZUTEMP)
C
      ZUDEN = (0.270*FUO2 + 0.123*FZO2 + 0.091*FZR)/
     *  (0.270*FUO2/RUO2 + 0.123*FZO2/RZO2 +  0.091*FZR/RZR)
C
      RETURN
      END
```

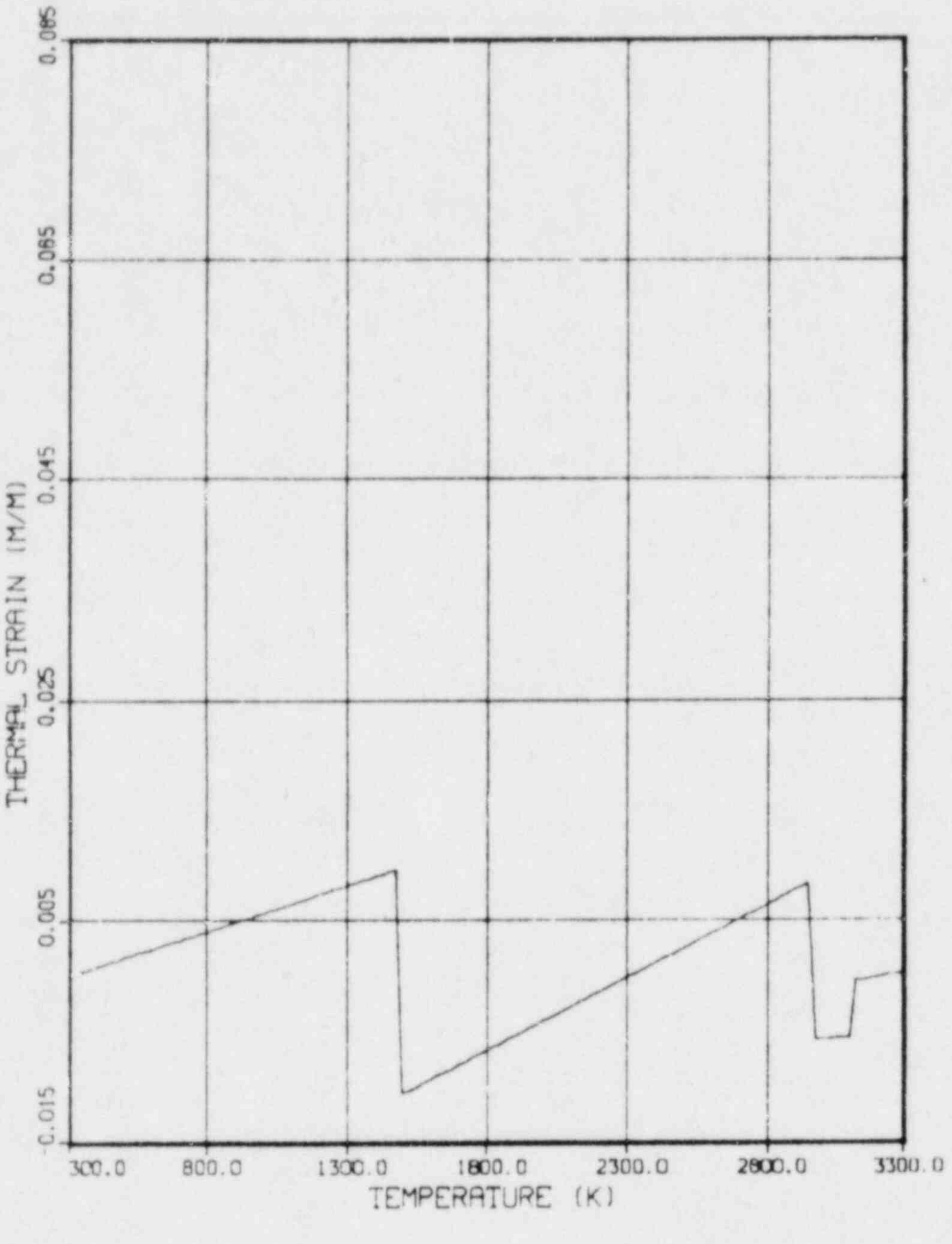

Figure G-5. Thermal strain calculated for a 0.2 UO_2 - 0.8 ZrO_2 weight fraction compound.

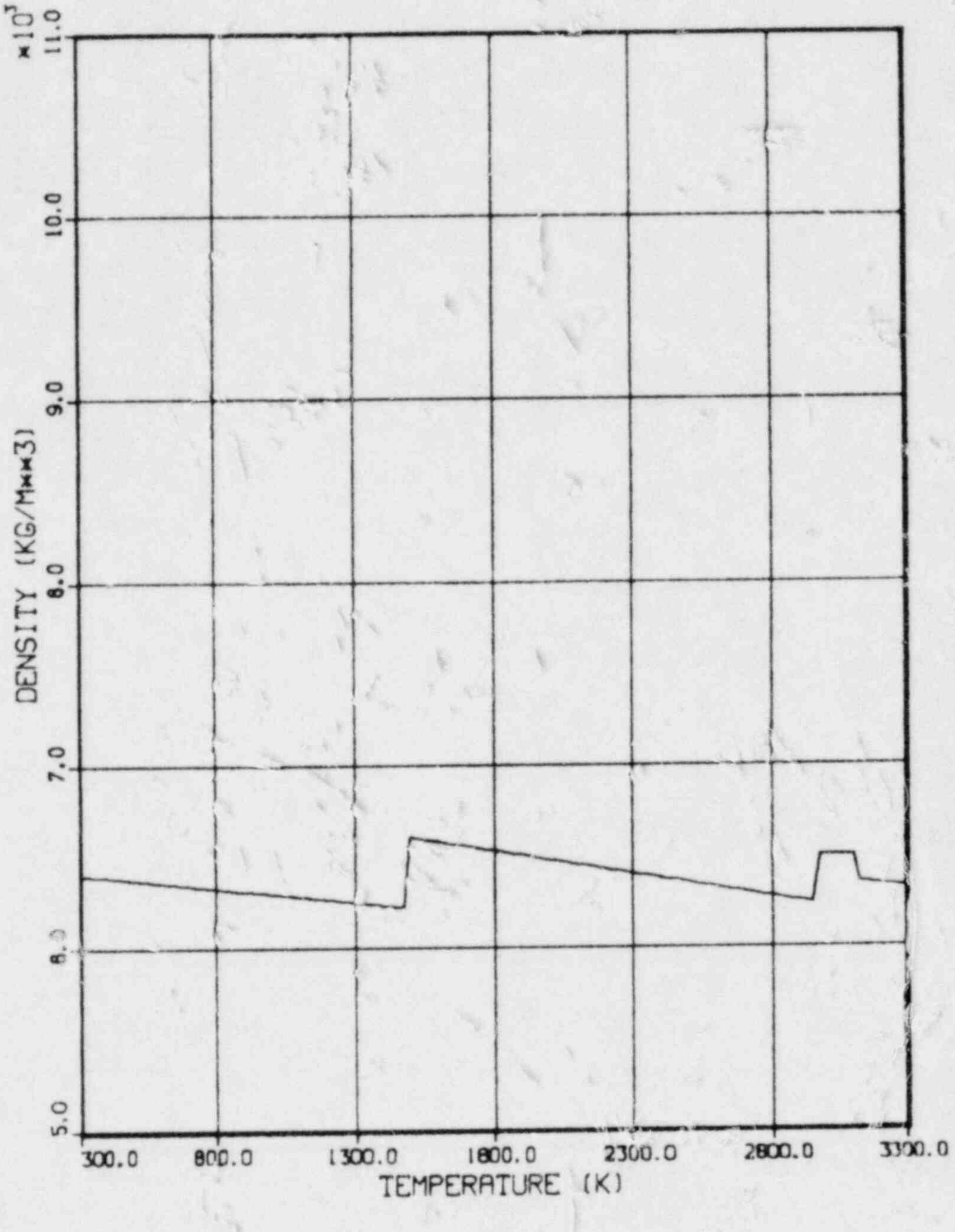

Figure G-6. Density calculated for a 0.2 UO_2 - 0.8 ZrO_2 weight fraction compound.

TABLE G-15. ZUTEXP CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.2 UO_2-0.8 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Strain (10^{-2} m/m)	Calculated Strain (10^{-2} m/m)
293	0	0
373	0.03	0.06
473	0.09	0.15
573	0.18	0.23
598	0.20	0.24
636	0.00	0.27
673	-0.33	0.31
873	-0.08	0.47
1073	0.15	0.63
1273	0.38	0.80
1473	0.59	0.97
1673	0.81	-0.84
1873	1.04	-0.57
2073	1.28	-0.31
2273	1.58	-0.05

TABLE G-16. ZUTEXP CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.32 UO_2-0.68 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Strain (10^{-2} m/m)	Calculated Strain (10^{-2} m/m)
293	0	0
473	0.17	0.07
673	0.40	0.31
873	0.65	0.48
1073	0.88	0.65
1273	1.11	0.82
1473	1.35	1.00
1673	1.57	-0.61
1873	1.81	-0.35
2073	2.05	-0.08
2273	2.33	0.18

TABLE G-17. ZUTEXP CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.5 UO_2-0.5 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Strain (10^{-2} m/m)	Calculated Strain (10^{-2} m/m)
293	0	0
473	0.16	0.15
673	0.37	0.32
873	0.61	0.50
1073	0.84	0.68
1273	1.08	0.87
1473	1.32	1.06
1673	1.56	-0.21
1873	1.80	0.05
2073	2.08	0.33
2273	2.46	0.59

TABLE G-18. ZUTEXP CALCULATIONS AND DEEM'S DATA[G-3] FOR A 0.94 UO_2-0.06 ZrO_2 WEIGHT FRACTION COMPOUND

Temperature (K)	Observed Strain (10^{-2} m/m)	Calculated Strain (10^{-2} m/m)
293	0	0
473	0.17	0.18
673	0.39	0.37
873	0.63	0.58
1073	0.87	0.80
1273	1.13	1.03
1473	1.41	1.27
1673	1.67	1.29
1873	1.94	1.56
2073	2.22	1.84
2273	2.54	2.12

TABLE G-19. ZUDEN CALCULATIONS AND DEEM'S COMPOUND DENSITY DATA[G-3]

Composition (weight fractions)	Observed Density (10^3 kg/m)	Calculated Density (10^3 kg/m)
0.2 UO_2-0.06 ZrO_2	6.26	6.40
0.32 UO_2-0.8 ZrO_2	6.81	6.83
0.5 UO_2-0.5 ZrO_2	7.62	7.59
Low density 0.32 UO_2-0.68 ZrO_2	6.46	6.83
0.94 UO_2-0.06 ZrO_2	9.92	10.04

where

F = compound coefficient of friction (Pa/Pa)

Re = Reynold's number (unitless).

The correlations are an engineering estimate and have an expected standard error of 0.90 of their calculated value.

Table G-20 is a listing of the ZUFRIC function and Figure G-7 illustrates the coefficient of friction calculated with the ZUFRIC function.

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS INTERFACIAL SURFACE TENSION (ZUSTEN)

The function ZUSTEN returns the interfacial surface tension of molten Zr-U-O compounds on zircaloy cladding. The value used is

$$T = 0.45 \qquad \text{(G-16)}$$

where

T = interfacial surface tension (N/m).

The value is an engineering estimate[G-6] and has an expected standard error of

$$^{+1.0}_{-0.4} .$$

Table G-21 is a listing of the ZUSTEN function.

ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS VISCOSITY (ZUVISC)

The function ZUVISC returns an estimate of the viscosity of both solid and liquid Zr-U-O compounds as a function the composition and temperature

TABLE G-20. LISTING OF THE ZUFRIC FUNCTION

```
      FUNCTION ZUFRIC(RE)
C
C     ZUFRIC RETURNS THE COEFFICIENT OF FRICTION OF
C     FLOWING ZIRCALOY-URANIUM-OXYGEN COMPOUNDS
C
C     ZUFRIC = OUTPUT COEFFICIENT OF FRICTION (PA/PA)
C
C     RE     = INPUT REYNOLDS NUMBER (UNITLESS)
C
C     ZUFRIC WAS CODED BY D. L. HAGRMAN MARCH 1982
C
C
      IF(RE .GT. 7539.42) THEN
         ZUFRIC = 0.0791 * (RE**(-0.25))
      ELSE
         IF(RE .GT. 1.0E-06) THEN
            ZUFRIC = 64./RE
         ELSE
            ZUFRIC = 6.4E+07
         ENDIF
      ENDIF
      RETURN
      END
```

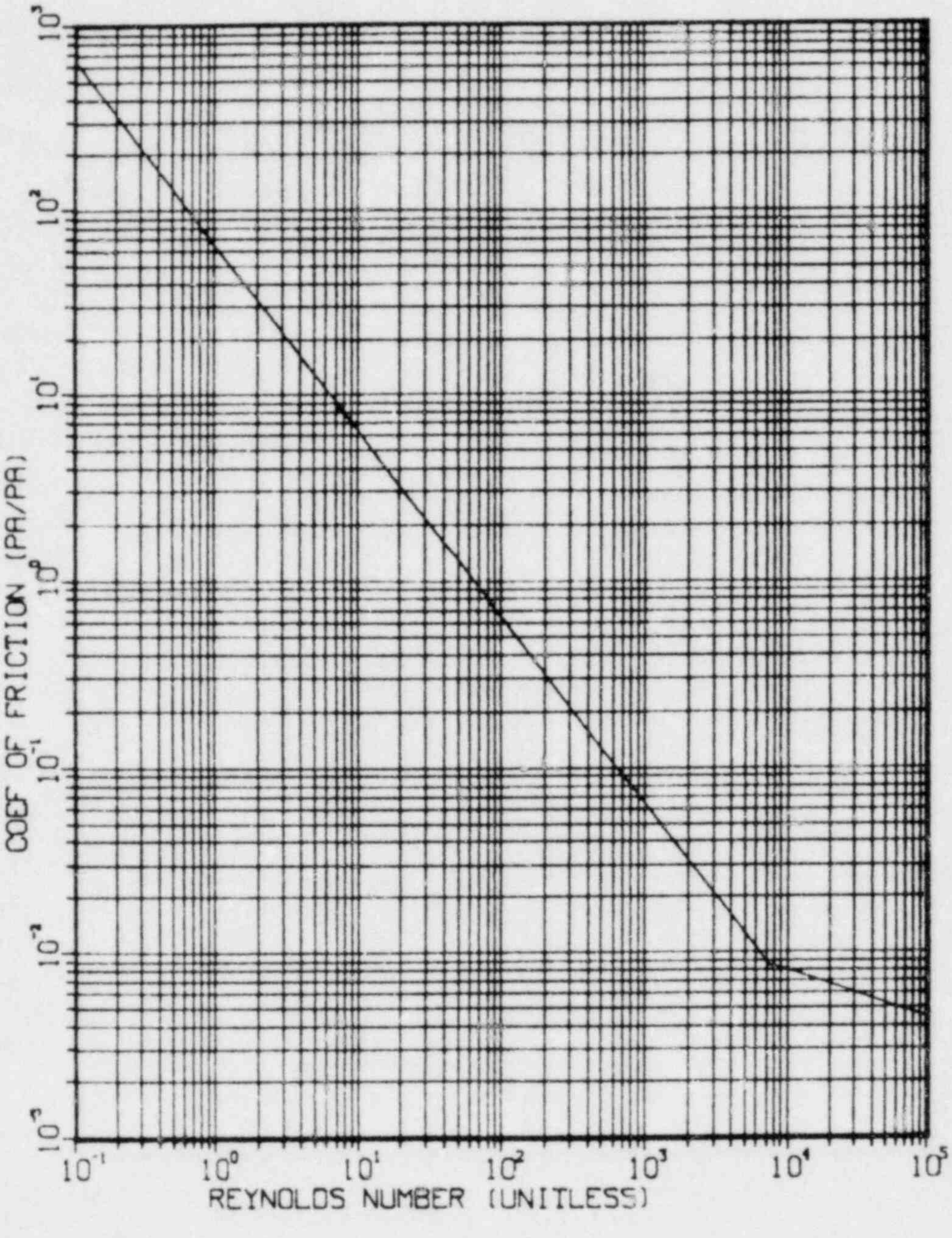

Figure G-7. Coefficient of friction calculated with the ZUFRIC function.

TABLE G-21. LISTING OF THE ZUSTEN FUNCTION

```
      FUNCTION ZUSTEN(ZUTEMP)
C
C     ZUSTEN RETURNS THE INTERFACIAL SURFACE TENSION OF MOLTEN
C     ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS ON ZIRCALOY RODS
C
C     ZUSTEN = OUTPUT INTERFACIAL SURFACE TENSION (N/M)
C
C     ZUTEMP = INPUT COMPOUND TEMPERATURE (K)
C
C     ZUSTEN WAS CODED BY D. L. HAGRMAN MARCH 1982
C
      ZUSTEN = 0.45
      RETURN
      END
```

of the compound. The expression used to calculate viscosity for temperature below the solidus temperature (which is provided by the PSOL function) is

$$\eta_s = 1.38 \exp\left(\frac{4.942 \times 10^4}{T}\right) \tag{G-17}$$

where

η_s = viscosity of solid Zr-U-O compounds (Pa s).

This correlation is the expression used for solid UO_2 viscosity in the FVISCO subcode of MATPRO-11 Revision 2. For temperatures above the liquidus temperature a mole fraction average of the component viscosities is used

$$\eta_l = f_{UO_2} \eta_{UO_2} + f_{ZrO_2} \eta_{ZrO_2} + f_{Zr} \eta_{Zr} \tag{G-18}$$

where

η_l = viscosity of liquid Zr-U-O compounds (Pa•s)

η_{UO_2} = viscosity of liquid UO_2 (Pa•s)

η_{ZrO_2} = viscosity of liquid ZrO_2 (Pa•s)

η_{Zr} = viscosity of liquid Zr (Pa•s).

η_{UO_2} is calculated with the appropriate expression from the FVISCO subcode:

$$\eta_{UO_2} = 1.23 \times 10^{-2} - 2.09 \times 10^{-6}\ T \ . \tag{G-19}$$

η_{ZrO_2} and η_{Zr} are calculated with correlations recommended by Nazare, Ondraek, and Schulz[G-1]

$$\eta_{ZrO_2} = 1.22 \times 10^{-4} \exp\left(\frac{10,500}{T}\right) \qquad \text{(G-20)}$$

$$\eta_{Zr} = 1.90 \times 10^{-4} \exp\left(\frac{6,500}{T}\right) \quad . \qquad \text{(G-21)}$$

For temperatures between the solidus and liquidus temperatures of the compound, an interpolation scheme is used

$$\eta = \frac{\eta_l\,(T - T_{Sol}) + \eta_s\,(T_{liq} - T)}{T_{liq} - T_{sol}} \qquad \text{(G-22)}$$

where

T_{Sol} = solidus temperature (K)

T_{liq} = liquidus temperature (K)

η = Viscosity of Zr-U-O compounds (Pa•s).

Table G-22 is a listing of the ZUVISC function. Figure G-8 illustrates the effect of temperature on the viscosity of a compound composed of two-thirds mole fraction zircaloy and one-third mole fraction UO_2.

The expected standard error of viscosities is ±0.8 of the predicted value because there are no data in support of the model.

TABLE G-22. LISTING OF THE ZUVISC FUNCTION

```
      FUNCTION ZUVISC(U,Z,ZUTEMP)
C
C     ZUVISC RETURNS ZIRCONIUM-URANIUM-OXYGEN COMPOUND
C     VISCOSITIES
C
C     ZUVISC = OUTPUT COMPOUND VISCOSITY (PA*S)
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C              (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C              (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ZUTEMP = COMPOUND TEMPERATURE (K)
C
C     THE SUBCODES PSOL AND PLIQ ARE CALLED BY THIS FUNCTION
C
C     ZUVISC WAS CODED BY D. L. HAGRMAN MARCH 1982.
C
C
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUVISC HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      TLIQ = PLIQ(X,U,Z)
      TSOL = PSOL(X,U,Z)
C
      IF(ZUTEMP .LE. TSOL) THEN
         ZUVISC = 1.38 * EXP(4.942E+04/ZUTEMP)
      ELSE
         FUO2 = U/(U+Z)
         FZO2 = (0.5 * X - U)/(U + Z)
         FZR  = 1. - FUO2 - FZO2
```

TABLE G-22. (continued)

```
         VUO2 = 1.23E-02 - ZUTEMP*2.09E-06
         VZO2 = 1.22E-04 * EXP(10500./ZUTEMP)
         VZR = 1.90E-04 * EXP(6500./ZUTEMP)
         VLIQ = FUO2*VUO2 + FZO2*VZO2 + FZR*VZR
         IF(ZUTEMP .LT. TLIQ) THEN
            VSOL = 1.38 * EXP(4.942E+04/ZUTEMP)
            ZUVISC = (VLIQ*(ZUTEMP-TSOL)+VSOL*(TLIQ-ZUTEMP))/
     #               (TLIQ - TSOL)
         ELSE
            ZUVISC = VLIQ
         ENDIF
      ENDIF
C
      RETURN
      END
```

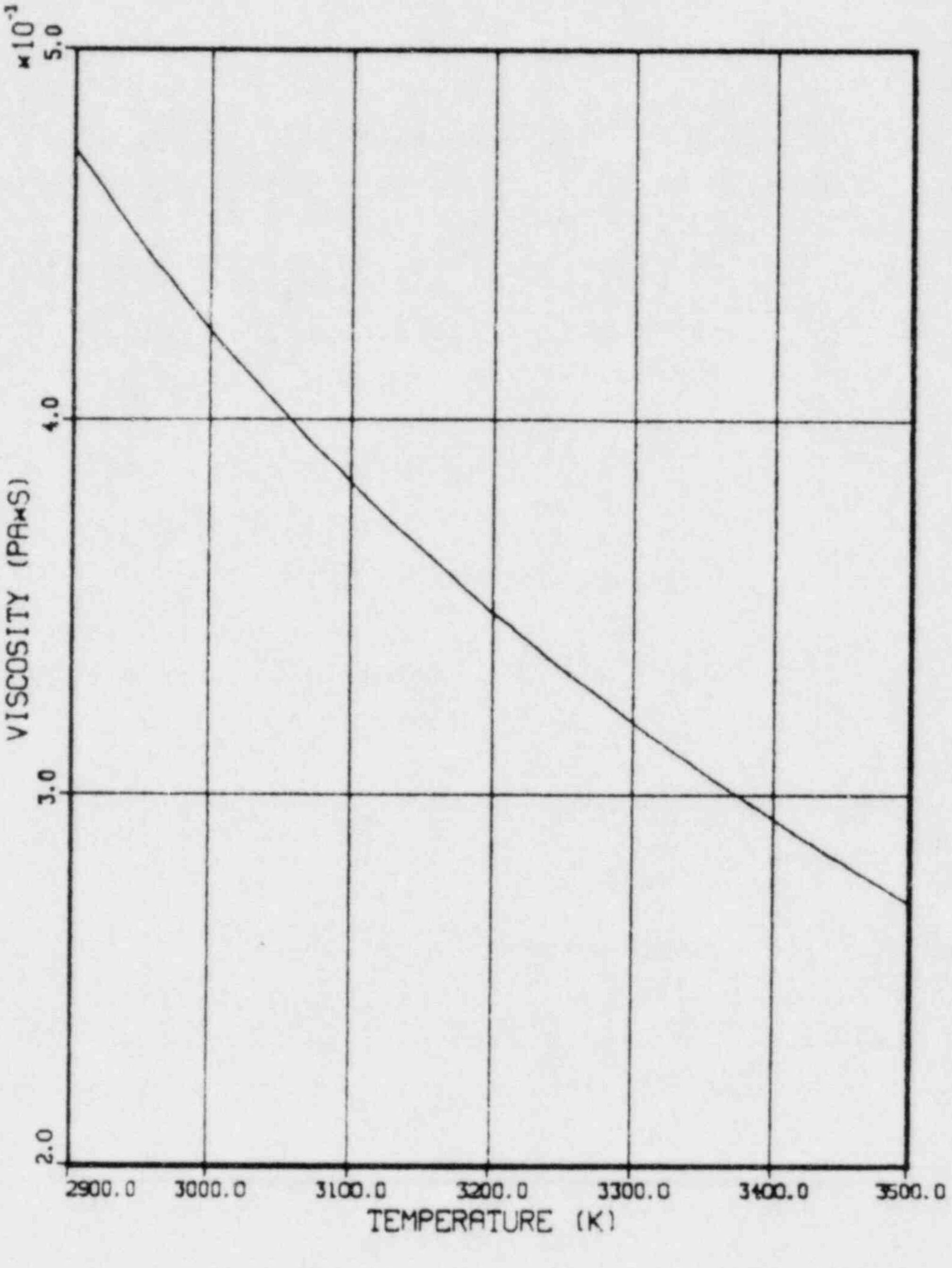

Figure G-8. Viscosity of a compound composed of 0.33 mole fraction Zr and 0.67 mole fraction UO_2.

HEAT OF SOLUTION OF UO_2 BY ZIRCONIUM-URANIUM-OXYGEN COMPOUNDS

(ZUSOLN)

ZUSOLN returns an estimate of the heat required to liquify UO_2 in a zircaloy-uranium-oxygen compound as a function of the compound composition. The expression used to calculate this heat is

$$Q = \left(\frac{1.5Z + 1.5U - 0.5}{1.5Z + 2.5U - 0.5}\right) 2.69 \times 10^5 + \left(\frac{U}{1.5Z + 2.5U - 0.5}\right) 2.74 \times 10^5 \qquad \text{(G-23)}$$

where

Q = heat required to dissolve a unit mass of UO_2 in a zircaloy-uranium-oxygen compound (J/kg)

U = atomic fraction uranium in solvent (atoms uranium/atoms solvent)

Z = atomic fraction zirconium in solvent (atoms zirconium/atoms solvent).

Equation (G-23) is an interpolation between the heat of fusion for UO_2, 2.74×10^5 J/kg,[a] and the heat of fusion for UO_2 minus the difference in the heats of formation of ZrO_2 and UO_2 given on page 208 of Reference G-7. The coefficient of the UO_2 heat of fusion is the ratio of the molecular fraction of UO_2 to the sum of fractions of UO_2 and Zr in the solvent (these fractions were derived at the beginning of this appendix). Thus, when this fraction is one, UO_2 is being melted in a mixture of UO_2 and ZrO_2 so the appropriate heat is the energy necessary to melt the UO_2.

The coefficient of the first term in Equation (G-23) is the ratio of the molecular fraction of Zr to the sum of the fractions of UO_2 and Zr in

---

[a] This number is taken from the PHYPRP subroutine.

the solvent. When this fraction is one, UO_2 is being dissolved in zirconium. There are no data for the heat required to do this so it was estimated by approximating the dissolution as a fusion of UO_2, followed by removal of the O_2 from the uranium and addition of the O_2 to a zirconium atom. The resultant number is very similar to the heat of fusion of UO_2.

With the current numbers, 2.69×10^5 and 2.74×10^5, use of Equation (G-23) to interpolate is not necessary. However, the large uncertainty, $\pm 3 \times 10^5$, suggests that it is prudent to maintain the equation until measurements confirm that the actual number for the heat of solution of UO_2 by zirconium is near the heat of fusion of UO_2.

Table G-23 is a listing of the ZUSOLN function and Figure G-9 illustrates the small effect of solvent composition on the heat required to dissolve UO_2.

REFERENCES

G-1. S. Nazare, G. Ondracek, and B. Schulz, "Properties of Light Water Reactor Core Melts," Nuclear Technology, 32, 1977, pp. 239-246.

G-2. F. Rhines, Phase Diagrams in Metallurgy and Their Development and Application, New York: McGraw-Hill Book Company, 1956, pp. 110-113.

G-3. H. W. Deem, Fabrication, Characterization, and Thermal-Property Measurements of ZrO_2--Base Fuels, BMI-1775, June 1966.

G-4. B. Abeles, "Lattice Thermal Conductivity of Disordered Semiconductor Alloys at High Temperatures," Physical Review, 131, 1963, pp. 1906-1911.

G-5. W. G. Rauch, Uranium-Zirconium Cermets, ANL 5268, 1954.

G-6. L. J. Siefken, private communication, EG&G Idaho, Inc., October 15, 1982.

G-7. C. J. Smithells and E. A. Brandes (eds.), Metals Reference Book, London and Boston: Butterworths (TN671 S55 1956).

TABLE G-23. LISTING OF THE ZUSOLN FUNCTION

```
      FUNCTION ZUSOLN(Z,U)
C
C     ZSOLN RETURNS THE HEAT REQUIRED TO LIQUEFY UO2 IN A
C     ZIRCALOY-URANIUM-OXYGEN COMPOUND
C
C     ZUSOLN = OUTPUT HEAT REQUIRED TO DISOLVE A UNIT MASS
C              OF UO2 IN A ZIRCALOY-URANIUM-OXYGEN COMPOUND (J/KG)
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN SOLVENT
C              (ATOMS URANIUM/ATOMS IN SOLVENT)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN SOLVENT
C              (ATOMS ZIRCONIUM/ATOMS IN SOLVENT)
C
C     ZUSOLN WAS CODED BY D. L. HAGRMAN APRIL 1982.
C
C
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FBUO2 = U/(1.5*Z + 2.5*U - 0.5)
      FBZR = (1.5*Z + 1.5*U - 0.5)/(1.5*Z + 2.5*U - 0.5)
  901 FORMAT(1H0,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1H0,"MATPRO FUNCTION ZUSOLN HAS REDEFINED THE COMPOUND")
  903 FORMAT(1H0," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1H0,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
C
      ZUSOLN = FBZR*2.692E+05 + FBUO2*2.74E+05
C
      RETURN
      END
```

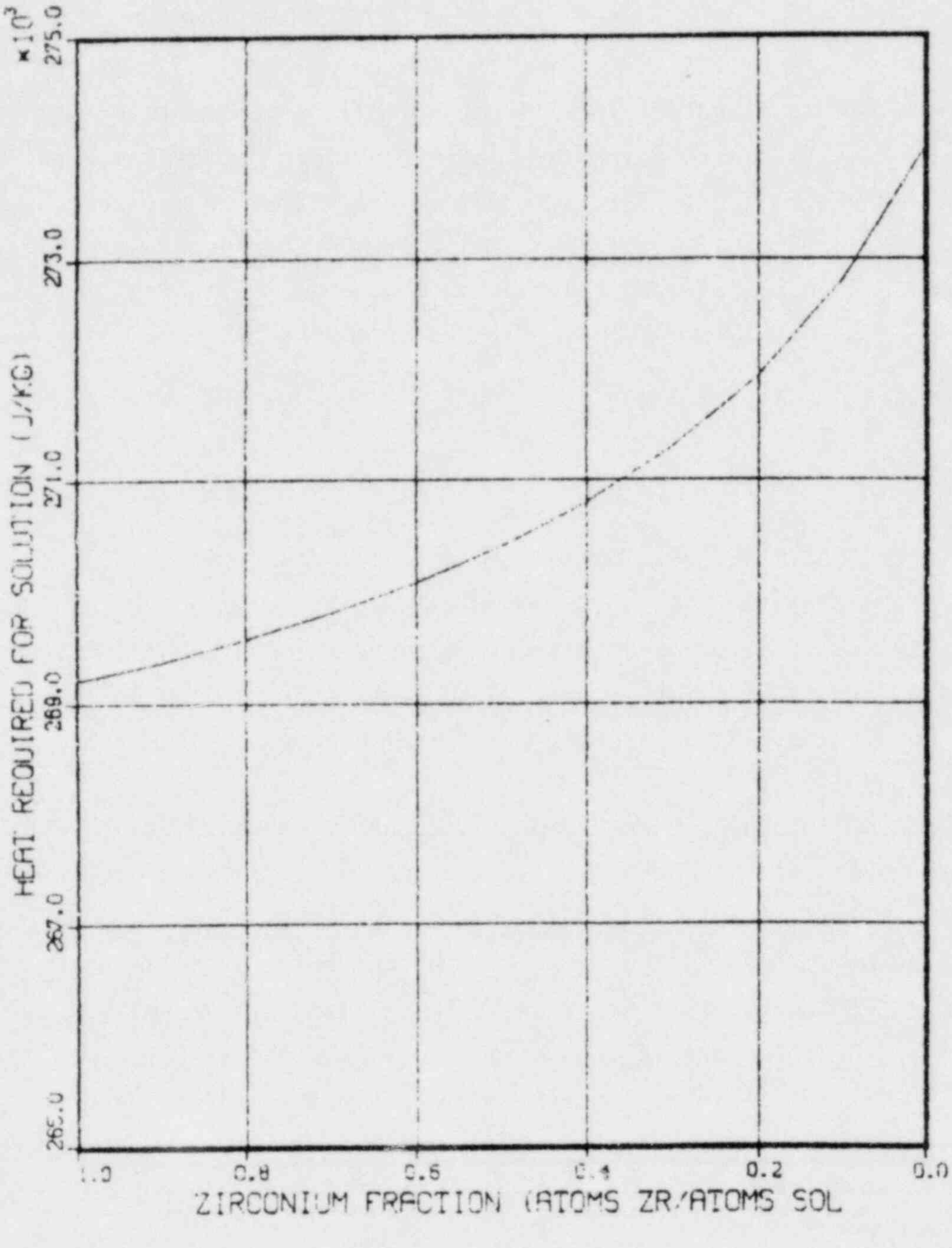

Figure G-9. Effect of solvent composition of heat required to dissolve a kilogram of UO_2.

APPENDIX H
SUPPORTING MATERIAL FOR MATPRO

APPENDIX H

SUPPORTING MATERIAL FOR MATPRO

This appendix describes functions which are not logically part of a materials properties package but are closely associated with the package. Three new functions are described here. The first simply collects heats of fusion which have been previously discussed as part of enthalpy subcodes into a single common block. The second two convert mass fractions to atomic fractions and vice-versa for zirconium-uranium-oxygen compounds.

COLLECTED HEATS OF FUSION

(QFUSON)

QFUSON calculates the heat of fusion of uranium dioxide, zircaloy, silver-indium-cadmium or boron carbide absorber material, 304 stainless steel, Inconel 718, and zirconium-uranium-oxygen compounds. The required input data are an indicator specifying which kind of neutron absorber is to be considered and the composition of the zirconium-uranium-oxygen compound.

The values of the heat of fusion used in QFUSON are given in Table H-1. All but the last two entries of the table have been discussed in conjunction with enthalpy subcodes. For Inconel 718, the heat of fusion was estimated by multiplying the molar heats of fusion of Ni and Cr, the main components of Inconel 718, by the atomic fraction of these elements in the alloy[a] and dividing the sum by 0.111, the weight of a gram-mole of the alloy in kilograms. The elemental heats of fusion were obtained from pages 186-188 of Reference H-1. For Zr-U-O compounds, a similar mole fraction weighted average of the molar heats of fusion of UO_2, ZrO_2, and Zr is employed.

Table H-2 is a listing of the QFUSON subroutine.

---

[a] A composition of 0.769 atomic fraction Ni and 0.231 atomic fraction Cr was assumed.

TABLE H-1. HEATS OF FUSION CALCULATED IN QFUSON

Material	Heat of Fusion (J/kg)
Uranium dioxide	2.74×10^5
Zircaloy	2.25×10^5
Zircaloy oxide	7.06×10^5
Silver-indium-cadmium	9.56×10^4
Boron carbide	2.74×10^5
304 stainless steel	2.5×10^5
Inconel 718	3.2×10^5
Zr-U-O compound	$\frac{2.74 \times 10^5 \times 0.27\, f_{UO_2} + 7.06 \times 10^5 \times 0.123\, f_{ZrO_2}}{0.27\, f_{UO_2} + 0.123\, f_{ZrO_2}}$ $\frac{+ 2.25 \times 10^5 \times 0.091\, f_{Zr}}{+ 0.091\, f_{Zr}}$

TABLE H-2. LISTING OF THE QFUSON SUBROUTINE

```
      SUBROUTINE QFUSON
C
C     QFUSION STORES HEATS OF FUSION IN THE COMMON BLOCK HFUSON
C
C     FHEFUS = OUTPUT UO2 HEAT OF FUSION (J/KG)
C     CHEFUS = OUTPUT ZIRCALOY HEAT OF FUSION (J/KG)
C     ZOHFUS = OUTPUT ZRO2 HEAT OF FUSION (J/KG)
C     AHEFUS = OUTPUT NEUTRON ABSORBER HEAT OF FUSION (J/KG)
C     SHEFUS = OUTPUT 304 STAINLESS STEEL HEAT OF FUSION (J/KG)
C     HHEFUS = OUTPUT INCONEL 718 HEAT OF FUSION (J/KG)
C     ZUHFUS = OUTPUT ZR-U-O COMPOUND HEAT OF FUSION (J/KG)
C
C     U      = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C              (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z      = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C              (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     ICTYPE = INPUT ABSORBER MATERIAL TYPE
C                 1 = SILVER-INDIUM-CADMIUM (.8,.15,.05)
C                 2 = BORON CARBIDE
C
C     QFUSON WAS CODED BY D. L. HAGRMAN APRIL 1982.
C
      COMMON / HFUSON / Z      ,U      ,ICTYPE,FHEFUS,CHEFUS,ZOHFUS,
     #                 AHEFUS,SHEFUS,HHEFUS,ZUHFUS
      X = 1. - U - Z
      IF((U + Z) .LT. (0.5 * X)) THEN
         UO = U
         U = U/(3. * (U + Z))
         Z = Z/(3. * (UO + Z))
         X = 1. - U - Z
         WRITE(6,901)
         WRITE(6,902)
         WRITE(6,903) U,Z
      ELSE
         IF((0.5 * X) .LT. U) THEN
            UO = U
            U = U/(3. * U + Z)
            Z = Z/(3. * UO + Z)
            X = 1. - U - Z
            WRITE(6,904)
            WRITE(6,902)
            WRITE(6,903) U,Z
         ENDIF
      ENDIF
C
      FUO2 = U/(U+Z)
      FZO2 = (0.5 * X - U)/(U + Z)
      FZR = 1. - FUO2 - FZO2
  901 FORMAT(1HO,"COMPOUND OXIDIZED BEYOND METAL DIOXIDE")
  902 FORMAT(1HO,"MATPRO FUNCTION QFUSON HAS REDEFINED THE COMPOUND")
  903 FORMAT(1HO," U = ",E15.5," Z = ",E15.5)
  904 FORMAT(1HO,"COMPOUND HAS TOO LITTLE OXYGEN TO FORM UO2 FROM U")
```

TABLE H-2. (continued)

```
C
      FHEFUS = 2.74E+05
      CHEFUS = 2.25E+05
      ZOHFUS = 7.06E+05
      IF(ICTYPE .LT. 2) THEN
         AHEFUS = 9.56E+04
      ELSE
         AHEFUS = 2.74E+05
      ENDIF
      SHEFUS = 2.5E+05
      HHEFUS = 3.2E+05
      ZUHFUS = (FHEFUS*0.27*FUO2 + ZOHFUS*0.123*FZO2 +
     * CHEFUS*0.091*FZR)/(0.270*FUO2 + 0.123*FZO2 + 0.091*FZR)
      RETURN
      END
```

MASS FRACTION-MOLE FRACTION CONVERSIONS
(PMOLE, PMASS)

PMOLE is a subroutine which calculates the atomic fraction of uranium, zirconium, and oxygen in a uranium-zirconium-oxygen compound given the mass fractions of uranium and zirconium. The inverse conversion is performed by PMASS.

The expressions used to find atomic fractions from mass fractions are:

$$U = \frac{\frac{WU}{0.238}}{\frac{WU}{0.238} + \frac{WZ}{0.091} + \frac{WX}{0.016}} \qquad \text{(H-1)}$$

$$Z = \frac{\frac{WZ}{0.091}}{\frac{WU}{0.238} + \frac{WZ}{0.091} + \frac{WX}{0.016}} \qquad \text{(H-2)}$$

$$X = 1 - U - Z \qquad \text{(H-3)}$$

where

U = atomic fraction of uranium in compound (atoms uranium/atoms compound)

Z = atomic fraction of zirconium in compound (atoms zirconium/atoms compound)

X = atomic fraction of oxygen in compound (atoms oxygen/atoms compound)

WU = mass fraction of uranium in compound (kg uranium/kg compound)

WZ = mass fraction of zirconium in compound (kg zirconium/kg compound)

WX = mass fraction of oxygen in compound (kg oxygen/kg compound).

In order to find mass fractions from atomic fractions, the following expressions are used:

$$WU = \frac{0.238U}{0.238U + 0.091Z + 0.016X} \qquad (H-4)$$

$$WZ = \frac{0.091Z}{0.238U + 0.091Z + 0.016X} \qquad (H-5)$$

$$WX = 1 - WU - WZ \quad . \qquad (H-6)$$

All of these equations can be deduced by regarding the atomic weights of uranium, zirconium and oxygen (0.238 kg/gm-mole, 0.091 kg/gm-mole and 0.016 kg/gm-mole, respectively) as factors which convert fractions of a kilogram of compound to moles or fractions of a mole of compound to kilograms. Equations (H-3) and (H-6) are simplified forms which use the constraint that all fractions of a compound must sum to one.

Tables H-3 and H-4 are listings of the PMOLE and PMASS subroutines.

REFERENCE

H-1. C. J. Smithells and E. A. Brandes (eds.) Metals Reference Book, London and Boston: Butterworths (TN671 S55 1956).

TABLE H-3. LISTING OF THE PMOLE SUBROUTINE

```
      SUBROUTINE PMOLE(WU,WZ,U,Z,X)
C
C     PMOLE CONVERTS INPUT MASS FRACTIONS OF URANIUM AND
C     ZIRCONIUM IN A ZIRCONIUM-URANIUM-OXYGEN COMPOUND TO
C     CORRESPONDING ATOMIC FRACTIONS.
C
C     U       = OUTPUT ATOMIC FRACTION URANIUM IN COMPOUND
C               (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z       = OUTPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C               (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C     X       = OUTPUT ATOMIC FRACTION OXYGEN IN COMPOUND
C               (ATOMS OXYGEN/ATOMS IN COMPOUND)
C
C     WU      = INPUT MASS FRACTION OF URANIUM IN COMPOUND
C               (KG URANIUM/KG COMPOUND)
C     WZ      = INPUT MASS FRACTION OF ZIRCONIUM IN COMPOUND
C               (KG ZIRCONIUM/KG COMPOUND)
C
C     PMOLE WAS CODED BY D. L. HAGRMAN APRIL 1982.
C
C
C
      WX = 1. - WU - WZ
      APKG = (WU/0.238) + (WZ/0.091) + (WX/0.016)
      U = WU/(0.238*APKG)
      Z = WZ/(0.091*APKG)
      X = 1. - U - Z
      RETURN
      END
```

TABLE H-4. LISTING OF THE PMASS SUBROUTINE

```
      SUBROUTINE PMASS(U,Z,WU,WZ,WX)
C
C     PMASS CONVERTS INPUT ATOMIC FRACTIONS OF URANIUM AND
C     ZIRCONIUM IN A ZIRCONIUM-URANIUM-OXYGEN COMPOUND TO
C     CORRESPONDING MASS FRACTIONS.
C
C     WU      = OUTPUT MASS FRACTION OF URANIUM IN COMPOUND
C               (KG URANIUM/KG COMPOUND)
C     WZ      = OUTPUT MASS FRACTION OF ZIRCONIUM IN COMPOUND
C               (KG ZIRCONIUM/KG COMPOUND)
C     WX      = OUTPUT MASS FRACTION OF OXYGEN IN COMPOUND
C               (KG OXYGEN/KG COMPOUND)
C
C     U       = INPUT ATOMIC FRACTION URANIUM IN COMPOUND
C               (ATOMS URANIUM/ATOMS IN COMPOUND)
C     Z       = INPUT ATOMIC FRACTION ZIRCONIUM IN COMPOUND
C               (ATOMS ZIRCONIUM/ATOMS IN COMPOUND)
C
C     PMASS WAS CODED BY D. L. HAGRMAN APRIL 1982.
C
C
      X = 1. - U - Z
      WGPM = U*0.238 + Z*0.091 +X*0.016
      WU = U*0.238/WGPM
      WZ = Z*0.091/WGPM
      WX = 1. - WU - WZ
      RETURN
      END
```